

THESIS FOR THE DEGREE OF DOCTOR OF PHILOSOPHY

The Dirac Equation: Numerical and Asymptotic Analysis

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Chalmers University of Technology and University of Gothenburg
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Abstract

The thesis consists of three parts, although each part belongs to a specific subject area in mathematics, they are considered as subfields of the perturbation theory. The main objective of the presented work is the study of the Dirac operator; the first part concerns the treatment of the spurious eigenvalues in the computation of the discrete spectrum. The second part considers G-convergence theory for projected parts of a family of Dirac operators and general positive definite self-adjoint operators. The third part discusses the convergence of wave operators for some families of Dirac operators and for general self-adjoint operators.

In the first part, a stable computational scheme, using finite element and Galerkin-based hp -cloud methods, is developed to remove the spurious eigenvalues from the numerical solution of the Dirac eigenvalue problem. The scheme is based on applying a Petrov-Galerkin formulation to introduce artificial diffusivity to stabilize the solution. The added diffusion terms are controlled by a stability parameter which is derived for the particular problem. The derivation of the stability parameter is the main part of the scheme, it is obtained for specific basis functions in the finite element method and then generalized for any set of admissible basis functions in the hp -cloud method.

In the second part, G-convergence theory is applied to positive definite parts of the Dirac operator perturbed by h -dependent abstract potentials, where h is a parameter which is allowed to grow to infinity. After shifting the perturbed Dirac operator so that the point spectrum is positive definite, the spectral measure is used to obtain projected positive definite parts of the operator, in particular the part that is restricted to the point spectrum. Using the general definition of G-convergence, G-limits, as h approaches infinity, are proved for these projected parts under suitable conditions on the perturbations. Moreover, G-convergence theory is also discussed for some positive definite self-adjoint h -dependent operators. The purpose of applying G-convergence is to study the asymptotic behavior of the corresponding eigenvalue problems. In this regard,

the eigenvalue problems for the considered operators are shown to converge, as h approaches infinity, to the eigenvalue problems of their associated G-limits.

In the third part, scattering theory is studied for the Dirac operator and general self-adjoint operators with classes of h -dependent perturbations. For the Dirac operator with different power-like decay h -dependent potentials, the wave operators exist and are complete. In our study, strong convergence, as h approaches infinity, of these wave operators is proved and their strong limits are characterized for specific potentials. For general self-adjoint operators, the stationary approach of scattering theory is employed to study the existence and convergence of the stationary and time-dependent h -dependent wave operators.

Keywords: Dirac operator, eigenvalue problem, finite element method, spurious eigenvalues, Petrov-Galerkin, cubic Hermite basis functions, stability parameter, meshfree method, hp -cloud, intrinsic enrichment, G-convergence, Γ -convergence, spectral measure, scattering theory, identification, wave operator, stationary approach.

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Hasan Almanasreh
Gothenburg, November 2012

To
May and Adam

List of appended papers

The thesis is based on the following appended papers:

- I **Hasan Almasreh**, Sten Salomonson, and Nils Svanstedt, *Stabilized finite element method for the radial Dirac equation*. (Submitted)
- II **Hasan Almasreh**, *hp-Cloud approximation of the Dirac eigenvalue problem: The way of stability*. (To be submitted)
- III **Hasan Almasreh** and Nils Svanstedt, *G-convergence of Dirac operators*. (Published in Journal of Function Spaces and Applications)
- IV **Hasan Almasreh**, *On G-convergence of positive self-adjoint operators*. (Submitted)
- V **Hasan Almasreh**, *Strong convergence of wave operators for a family of Dirac operators*. (Submitted)
- VI **Hasan Almasreh**, *Existence and asymptotics of wave operators for self-adjoint operators*. (To be submitted)

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1 Introduction

In quantum mechanics the Dirac equation is a wave equation that provides a description of the relativistic motion of the electrons as well the positrons, while the corresponding eigenvalue problem determines their energies (eigenvalues). The computation of the Dirac operator eigenvalues for single-electron systems is thoughtfully considered in the last decades in order to obtain stable solution that can be used as a basis in approximating the eigenvalues of the electron in some simple many-electron systems. The difficulty in computing the Dirac operator eigenvalues for a single-electron system is the presence of unphysical (spurious) eigenvalues among the genuine ones. Also, another challenging task is the study of the asymptotic behavior of the spectrum, in particular the eigenvalues, of families of perturbed Dirac operators.

The need for stable numerical approximation for the Dirac operator eigenvalues with Coulomb interaction for single-electron systems makes the construction of a stable computational scheme the main concern of this thesis. Here, we classify the spuriousity in two categories; the so-called instilled spurious eigenvalues and the spuriousity caused by the unphysical coincidence phenomenon. We provide a stable scheme to compute the Dirac operator eigenvalues implementing two different numerical methods; the finite element method (FEM) and the Galerkin-based hp -cloud method. The scheme relies on appropriate choices of the computational space that meets the properties of the Dirac wave function. On the other hand, it mainly relies on adding artificial stability terms controlled by a stability parameter. The stability parameter is derived for particular finite element basis functions in the FEM, and generalized to arbitrary basis functions in the hp -cloud approximation method. The stability scheme is computationally unexpensive, simple to apply, and guarantees complete removal of the spurious eigenvalues of both categories.

We also study the asymptotic behavior, as $h \rightarrow \infty$, of the eigenvalues of a family of perturbed Dirac operators by h -dependent potentials using the theory of G-convergence. We prove the G-limit operators of positive definite parts of this family under suitable assumptions on the perturbations. In particular we prove that the corresponding eigenvalues and the eigenvalue problem of the operator restricted to the point spectrum of the perturbed Dirac operators converge respectively to the eigenvalues and eigenvalue problem of the G-limit operator. Apart from this, we start employing Γ -convergence together with G-convergence to study the G-limits of some positive definite self-adjoint operators, and discuss the convergence of their corresponding eigenvalue problems.

Regarding the absolutely continuous part of the spectrum, we study scattering theory for a family of Dirac operators and general self-adjoint operators. For the Dirac operator with different power-like decay h -dependent potentials, the strong time-dependent wave operator (WO) exists and is complete. We prove the strong convergence, as $h \rightarrow \infty$, of this WO under suitable conditions on the assumed potential. If the added potentials are of short-range type, the convergence study of the WOs is equivalent to the convergence study of the perturbed Dirac operator in the strong resolvent sense. For the Dirac operator with long-range potentials, we consider two simplified WOs for which the study of the asymptotic behavior is easier. Depending on the power of decay of the assumed potentials, the simplified WOs are obtained by considering two particular identifications. One of these identifications is an h -free operator, thus the study of the asymptotic behavior of the WOs is also reduced to the study of the convergence of the perturbed Dirac operator in the strong resolvent sense. The other identification still has the h -dependency, but the convergence of the WOs with this identification becomes easier to study. For general h -dependent self-adjoint operators, the existence and convergence, as $h \rightarrow \infty$, of the weak and strong time-dependent WOs and of the stationary WO are studied more comprehensively.

An outline of this work is as follows: In §2, we give preliminaries and introduce some elementary properties of the Dirac operator. In §3, we explain the occurrence of the spurious eigenvalues caused by using the projection method in the numerical approximation of general eigenvalue problems. Also we discuss the causes of the spuriousity of both categories in the computation of the Dirac eigenvalue problem. We continue with the discussion on the stability scheme and the stability parameters, where we also provide numerical examples using the FEM and hp -cloud method. In §4 we give basic preliminaries on G-convergence including a general overview, a one dimensional example, and some definitions. Likewise, Γ -convergence and its connection to G-convergence are stated. We also discuss G-convergence of elliptic and positive definite self-adjoint operators. Further, we apply G-convergence theory to positive definite parts of a family of Dirac operators. In §5 we provide a general overview of scattering theory and state the definitions of the time-dependent and stationary WOs and their properties. We also study the strong convergence of the WOs for a family of Dirac operators, and discuss the simplified WOs. Finally, we discuss and prove the existence and convergence of the time-dependent and stationary WOs for the general h -dependent self-adjoint operators.

2 The Dirac equation

The free Dirac equation describes the free motion of an electron (or a positron) with no external fields or presence of other particles. It is derived from the relativistic relation between energy and momentum

$$\lambda^2 = \mathbf{p}^2 c^2 + m^2 c^4, \quad (1)$$

where λ is the total electron energy, \mathbf{p} is the electron kinetic momentum, c is the speed of light, and m is the electron rest mass. The corresponding wave equation of quantum mechanics is obtained from the classical equation of motion (1) by replacing the energy λ and the momentum \mathbf{p} by their quanta

$$\lambda = i\hbar \frac{\partial}{\partial t} \quad \text{and} \quad \mathbf{p} = -i\hbar \nabla, \quad (2)$$

where t denotes the time, \hbar is the Planck constant divided by 2π , and $\nabla = (\frac{\partial}{\partial x_1}, \frac{\partial}{\partial x_2}, \frac{\partial}{\partial x_3})$. Using (2), equation (1) can be written in the form

$$i\hbar \frac{\partial}{\partial t} u(x, t) = \sqrt{-c^2 \hbar^2 \Delta + m^2 c^4} u(x, t). \quad (3)$$

The problem with the existence of the Laplace operator under the square root was solved by Paul Dirac who derived the well-known Dirac equation that provides a description of the electron motion consistent with both the principles of quantum mechanics and the theory of special relativity. The free Dirac space-time equation (see [23] for more details) has the form

$$i\hbar \frac{\partial}{\partial t} u(x, t) = \mathbf{H}_0 u(x, t), \quad (4)$$

where $\mathbf{H}_0 : H^1(\mathbb{R}^3; \mathbb{C}^4) \rightarrow L^2(\mathbb{R}^3; \mathbb{C}^4)$ is the free Dirac operator given as

$$\mathbf{H}_0 = -i\hbar c \boldsymbol{\alpha} \cdot \nabla + mc^2 \beta, \quad (5)$$

the symbols $\boldsymbol{\alpha} = (\alpha_1, \alpha_2, \alpha_3)$ and β are the 4×4 Dirac matrices given by

$$\alpha_j = \begin{pmatrix} 0 & \sigma_j \\ \sigma_j & 0 \end{pmatrix} \quad \text{and} \quad \beta = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}.$$

Here I and 0 are the 2×2 unity and zero matrices respectively, and σ_j 's are the 2×2 Pauli matrices

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \text{and} \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

In the sequel we shall use the following notations; \mathbf{D} , \mathbf{R} , and \mathbf{N} to denote respectively the domain, range, and null spaces of a given operator. The notations σ , σ_p , σ_{ac} , and σ_{ess} will denote respectively to the spectrum, point spectrum,

absolutely continuous spectrum, and essential spectrum of operators. For simplicity, we define $X = H^1(\mathbb{R}^3, \mathbb{C}^4)$ and $Y = L^2(\mathbb{R}^3, \mathbb{C}^4)$. Separation of variables in (4) yields the free Dirac eigenvalue problem

$$\mathbf{H}_0 u(x) = \lambda u(x). \quad (6)$$

The free operator \mathbf{H}_0 is essentially self-adjoint on $C_0^\infty(\mathbb{R}^3; \mathbb{C}^4)$ and self-adjoint on X , moreover $\sigma(\mathbf{H}_0) = (-\infty, -mc^2] \cup [mc^2, +\infty)$. The free Dirac operator with an additional field V is given by

$$\mathbf{H} = \mathbf{H}_0 + V. \quad (7)$$

where V is a 4×4 matrix-valued function acting as a multiplication operator in Y . The operator \mathbf{H} is essentially self-adjoint on $C_0^\infty(\mathbb{R}^3; \mathbb{C}^4)$ and self-adjoint on X provided that the function V is Hermitian and for all $x \in \mathbb{R}^3 \setminus \{0\}$ and $i, j = 1, 2, 3, 4$, satisfies $|V_{ij}(x)| \leq a \frac{c}{2|x|} + b$, where c is the speed of light, $a < 1$, and $b > 0$, see e.g. [50]. From now on, the function V will be considered as the Coulomb potential which has the form $V(x) = \frac{-Z}{|x|} I$, here I is the 4×4 identity matrix (I will be dropped from the definition of the Coulomb potential for simplicity), and $Z \in \{1, 2, \dots, 137\}$ is the electric charge number. The spectrum of the Dirac operator with Coulomb potential is $(-\infty, -mc^2] \cup \{\lambda^k\}_{k \in \mathbb{N}} \cup [mc^2, +\infty)$, where $\{\lambda^k\}_{k \in \mathbb{N}}$ is a discrete sequence of eigenvalues.

For simple computations, to obtain the eigenvalues of the Dirac operator with Coulomb potential, the radial part of the operator is considered. Before proceeding, from now on, for simplicity, by the radial Dirac operator (eigenvalue problem) we shall mean the radial Dirac operator (eigenvalue problem) with Coulomb potential. The radial Dirac eigenvalue problem is obtained by separation of variables of the radial and angular parts, i.e., by assuming $u(x) = \frac{1}{r} \begin{pmatrix} f(r) \mathcal{L}_{\kappa, m}(\varpi, \theta) \\ i g(r) \mathcal{L}_{-\kappa, m}(\varpi, \theta) \end{pmatrix}$, where r represents the radial variable, f and g are the Dirac radial functions referred to as the large and small components respectively, and $\mathcal{L}_{\cdot, m}$ is the angular part of the wave function u . The radial Dirac eigenvalue problem is then given by

$$H_\kappa \varphi(r) = \lambda \varphi(r), \quad \text{where} \quad (8)$$

$$H_\kappa = \begin{pmatrix} mc^2 + V(r) & c \left(-\frac{d}{dr} + \frac{\kappa}{r} \right) \\ c \left(\frac{d}{dr} + \frac{\kappa}{r} \right) & -mc^2 + V(r) \end{pmatrix} \quad \text{and} \quad \varphi(r) = \begin{pmatrix} f(r) \\ g(r) \end{pmatrix}. \quad (9)$$

As defined before, λ is the relativistic energy, $V(r) = -Z/r$ is the radial Coulomb potential, and κ is the spin-orbit coupling parameter defined as $\kappa = (-1)^{j+\ell+\frac{1}{2}}(j + \frac{1}{2})$, where j and ℓ are the total and orbital angular momentum numbers respectively.

3 Computation of the eigenvalues of the Dirac operator

Accurate and stable computation of the electron energies (eigenvalues) in single-electron systems (Hydrogen-like ions) is of vital interest in many applications. Approximation of electron eigenvalues in many-electron systems, as in Helium-like ions, is based on studying quantum electrodynamic effects (QED-effects). QED-effects are known as a perturbation procedure which mainly concerns the interactions between the existing electrons in the system where these interactions are used to measure the electron correlation. An approach for calculating QED-effects, see [31, 40], is based on a basis set of eigenstates of Hydrogen-like ions (the radial Dirac operator). The main difficulty in computing the eigenvalues of the radial Dirac operator is the presence of unphysical values (eigenvalues that do not match the physical observations) among the genuine eigenvalues. These values are considered as a pollution to the spectrum and known as spurious eigenvalues. The spurious eigenvalues result in oscillations in the wave functions and the emergence of states that originally do not exist. In many cases, this will substantially reduce the computation reliability of the basis set (partially or may be completely) in the practical atomic calculations.

The spuriousity problem in the computation of the radial Dirac operator eigenvalues is a challenging issue which makes obtaining accurate and stable computation for these eigenvalues a field of study by itself. Spurious eigenvalues are reported in most computational methods of eigenvalue problems, whether it is the finite element method (FEM), the finite difference method (FDM), the spectral domain approach (SDA), the boundary element method (BEM), the point matching method (PMM), or, further, the meshfree methods (MMs). Thus, spuriousity is an effect of the numerical methods and is found in the computational solution of many problems, rather than the Dirac eigenvalue problem [1, 38, 43], such as electromagnetic problems [34, 42] and general eigenvalue problems [60].

Below we present a classification of the spuriousity in the computation of the radial Dirac operator eigenvalues and its causes, we also explain the occurrence of spuriousity in the computation of general eigenvalue problems. We present some stable approaches for accurate computations with complete removal of spurious eigenvalues.

3.1 Spurious eigenvalues in the computation

We classify the spuriousity in the computation of the eigenvalues of the radial Dirac operator in two categories

- (i) The instilled spuriousity.

(ii) The unphysical coincidence phenomenon.

The first category consists of those spurious eigenvalues that may occur within the genuine eigenvalues (they occur between the true energy levels). This type of spuriousity occurs for all values of the quantum number κ . The second type is the unphysical assigning of almost the same first eigenvalue (or almost the same entire set of eigenvalues) for $2s_{1/2}(\kappa = -1)$ and $2p_{1/2}(\kappa = 1)$, $3p_{3/2}(\kappa = -2)$ and $3d_{3/2}(\kappa = 2)$, $4d_{5/2}(\kappa = -3)$ and $4f_{5/2}(\kappa = 3)$, and so on. To clarify, consider the computation of the electron eigenvalues in the Hydrogen atom using the FEM with linear basis functions (hat functions) given in Table 1, see Paper I in the appendix.

Table 1: The first computed eigenvalues, given in atomic unit, of the electron in the Hydrogen atom for point nucleus.

Level	$\kappa = 1$	$\kappa = -1$	Exact, $\kappa = -1$
1	-0.50000665661	-0.50000665659	-0.50000665659
2	-0.12500208841	-0.12500208839	-0.12500208018
3	-0.05555631532	-0.05555631532	-0.05555629517
\Rightarrow	-0.03141172061	-0.03141172060	Spurious Eigenvalue
4	-0.03118772526	-0.03118772524	-0.03125033803
5	-0.01974434510	-0.01974434508	-0.02000018105

The shaded value in the first level of Table 1 is what meant by the unphysical coincidence phenomenon, and the other two shaded values are the so-called instilled spuriousity. The right column contains the exact eigenvalues for $\kappa = -1$ obtained using the relativistic formula.

3.1.1 Spuriousity in general eigenvalue problems

The numerical computation of the eigenvalue problems that is based on the projection method onto finite dimensional subspaces is often polluted by the presence of spurious eigenvalues [7]. The spurious eigenvalues appear particularly in the computation for those problems with eigenvalues in gaps of their essential spectrum. To understand why the projection method generates spurious eigenvalues, consider a self-adjoint operator T defined on a Hilbert space \mathcal{H} , and consider an orthogonal projection $\Pi : \mathcal{H} \rightarrow \mathcal{L}$, where \mathcal{L} is a finite dimensional subspace of $\mathbf{D}(T)$. Let $z \in \mathbb{C}$ and define

$$\Theta(z) = \min_{\substack{f \in \mathcal{L} \\ f \neq 0}} \frac{\|\Pi(z - T)f\|_{\mathcal{H}}}{\|f\|_{\mathcal{H}}}. \quad (10)$$

If $\Theta(\mu) = 0$, then $\mu = \mu(\mathcal{L})$ is a solution to the Rayleigh-Ritz problem

$$\mu = \min_{\substack{\dim(S)=k \\ S \subseteq \mathcal{L}}} \max_{g \in S} \mathcal{R}(g) = \min_{\substack{\dim(S)=k \\ S \subseteq \mathcal{L}}} \max_{g \in S} \frac{\langle Tg, g \rangle}{\|g\|_{\mathcal{T}}^2}, \quad (11)$$

where the opposite of the assertion is also true. Moreover, by assuming $\Theta(\mu) = 0$, we conclude that there exists $f_0 \in \mathcal{L}$ such that

$$(\mu - T)f_0 \perp \mathcal{L}, \quad (12)$$

which particularly means that $\mathcal{R}(f_0) = \mu$. Thus μ is close to the point spectrum $\sigma_p(T)$. But, generally, as $\|(\mu - T)f\|_{\mathcal{T}}/\|f\|_{\mathcal{T}}$ is not necessary small for $f = f_0$, any other $f \in \mathcal{L}$, or any $f \in \mathcal{T}$, then (12) does not guarantee that μ is close to the spectrum $\sigma(T)$ of T .

To verify the above theory, consider the following operator, see [7],

$$(Tf)(x) = \operatorname{sgn}(x)f(x), \quad (13)$$

defined on $\mathcal{T} = L^2(-\pi, \pi)$, where $\operatorname{sgn}(x) = x/|x|$. Since $\|T\| = 1$, then $\sigma(T) \subseteq [-1, 1]$, but for $\mu \in (-1, 1)$, the resolvent operator $(T - \mu)^{-1}$ is well-defined and bounded, therefore $\sigma(T) \subseteq \{-1, 1\}$. However, it is easy to show that ± 1 are eigenvalues of T , these two eigenvalues are of infinite multiplicity, i.e., $\mathbf{N}(\mu - T)$ is infinite, $\mu = \pm 1$. Thus these two eigenvalues belong to $\sigma_{ess}(T)$. On the other hand, if $\mathcal{L} \subset \mathcal{T}$ is spanned by the set of Fourier basis $\{\varphi_{-n}, \varphi_{-n+1}, \dots, \varphi_{n-1}, \varphi_n\}$, given by

$$\varphi_j(x) = \frac{1}{\sqrt{2\pi}} e^{-ijx}, \quad j = -n, -n+1, \dots, n-1, n, \quad (14)$$

then, the Galerkin approximation applied to T in the finite dimensional subspace \mathcal{L} implies that $\mu_j(T, \mathcal{L})$ are the eigenvalues of the $(2n+1) \times (2n+1)$ matrix A with entries (a_{jk}) defined as

$$a_{jk} = \int_{-\pi}^{\pi} \operatorname{sgn}(x) \varphi_j(x) \varphi_k(-x) dx = \begin{cases} 0, & \text{for } k-j \text{ even,} \\ \frac{-2i}{\pi(k-j)}, & \text{for } k-j \text{ odd.} \end{cases} \quad (15)$$

The matrix A looks like

$$A = \begin{pmatrix} 0 & N & 0 & N & \dots & 0 \\ N & 0 & N & 0 & \dots & N \\ 0 & N & 0 & N & \dots & 0 \\ N & 0 & N & \ddots & \dots & N \\ \vdots & & & & \ddots & \vdots \\ 0 & N & 0 & N & \dots & 0 \end{pmatrix}, \quad (16)$$

here the letter N is used just to refer to a quantity different from zero (i.e., a number) and does not mean that these quantities are equal. It is clearly that A consists of $n + 1$ columns (the first set) whose odd entries are zero, and n columns (the second set) whose even entries are zero. If we disregard the zero entries (which are only $n + 1$ entries) in each element of the first set, then we end with a set $V = \{v_1, v_2, \dots, v_{n+1}\}$ where $v_i \in \mathbb{R}^n, i = 1, 2, \dots, n+1$. The set V is clearly linearly dependent, therefore the columns of the first set of the matrix A is linearly dependent, hence $0 \in \sigma(A)$. This, of course, violates the fact that $0 \in \text{Res}(T)$, where Res denotes the resolvent set. In this case, we conclude that 0 is a spurious eigenvalue that appears in the computed spectrum of the operator T caused by applying the projection method onto the finite dimensional subspace \mathcal{L} .

3.1.2 Spuriousity in the Dirac eigenvalue problem

The occurrence of the instilled spurious eigenvalues is a general phenomenon of the projection method in the numerical computations, thus the previous discussion can be considered as a good explanation for this type of spuriousity. Below we discuss the unphysical coincidence phenomenon as explained in [52].

Consider the radial Dirac eigenvalue problem (8), after applying the shift by $-mc^2$ and assuming $m = 1$, it can be rewritten in the same form as (8) but with

$$H_\kappa = \begin{pmatrix} V(r) & c\left(-\frac{d}{dr} + \frac{\kappa}{r}\right) \\ c\left(\frac{d}{dr} + \frac{\kappa}{r}\right) & -2c^2 + V(r) \end{pmatrix}, \quad (17)$$

where the eigenvalues are also shifted but kept denoted as λ . Define the following transformation

$$\mathcal{U}_\kappa = \begin{pmatrix} 1 & \mathcal{U}_\kappa \\ \mathcal{U}_\kappa & 1 \end{pmatrix}, \quad (18)$$

where $\mathcal{U}_\kappa = \frac{-Z\kappa}{c|\kappa|(|\kappa| + \varsigma)}$, with $\varsigma = \sqrt{\kappa^2 - Z^2/c^2}$. We apply the above transformation to the radial function $\varphi(r)$ given by (9) to get

$$\tilde{\varphi}_\kappa(r) = \mathcal{U}_\kappa \begin{pmatrix} f(r) \\ g(r) \end{pmatrix} = \begin{pmatrix} f(r) + \mathcal{U}_\kappa g(r) \\ g(r) + \mathcal{U}_\kappa f(r) \end{pmatrix} =: \begin{pmatrix} \tilde{f}_\kappa(r) \\ \tilde{g}_\kappa(r) \end{pmatrix}. \quad (19)$$

Using this transformation one can write

$$\mathcal{U}_\kappa^{-1} H_\kappa \mathcal{U}_\kappa^{-1} \tilde{\varphi}_\kappa(r) = \lambda_\kappa \mathcal{U}_\kappa^{-2} \tilde{\varphi}_\kappa(r). \quad (20)$$

By (20), and after adding the term $c^2(1 - \frac{|\kappa|}{\zeta})\mathcal{U}_\kappa^{-2}\tilde{\varphi}_\kappa(r)$ to its both sides, the radial Dirac eigenvalue problem, (8), can be written in the form

$$H_{\kappa,\mu}\tilde{\varphi}_\kappa(r) = \mu_\kappa\mathcal{U}_\kappa^{-2}\tilde{\varphi}_\kappa(r), \quad (21)$$

where the operator $H_{\kappa,\mu}$ is defined by

$$H_{\kappa,\mu} = \mathcal{U}_\kappa^{-1}H_\kappa\mathcal{U}_\kappa^{-1} + \Delta\mu_\kappa\mathcal{U}_\kappa^{-2} = \begin{pmatrix} 0 & cB_\kappa^+ \\ cB_\kappa & -2c^2 \end{pmatrix}, \quad (22)$$

and where $\Delta\mu_\kappa = c^2(1 - \frac{|\kappa|}{\zeta})$, $\mu_\kappa = \lambda_\kappa + \Delta\mu_\kappa$, $B_\kappa = d/dr + \zeta\kappa/(|\kappa|r) - Z/\kappa$, and $B_\kappa^+ = -B_{-\kappa}$. The same projection \mathcal{U}_κ can be applied to the Galerkin formulation of the radial Dirac eigenvalue problem in a finite dimensional subspace. In other words, if both radial functions f and g are expanded in a finite orthonormal basis set (orthonormal is assumed for simplicity, and it is not a requirement, since we can normalize, by a suitable linear transformation, any set of basis functions without changing the spectrum), then the above transformation applied to the discretization of the Galerkin formulation of the radial Dirac eigenvalue problem yields

$$(H_{\kappa,\mu})_{ij}(\tilde{\varphi}_\kappa)_{ij} = \mu_\kappa\mathcal{U}_\kappa^{-2}(\tilde{\varphi}_\kappa)_{ij}. \quad (23)$$

Here we have used the notation $(\)_{ij}$ to denote for the matrices (regardless their sizes) obtained from the Galerkin formulation. The vector $(\tilde{\varphi}_\kappa)_{ij} = ((\tilde{f}_\kappa)_{ij}, (\tilde{g}_\kappa)_{ij})^t$ is the unknowns, and the matrix $(H_{\kappa,\mu})_{ij}$ is given by

$$(H_{\kappa,\mu})_{ij} = \begin{pmatrix} 0 & c(B_\kappa^+)_{ij} \\ c(B_\kappa)_{ij} & -2c^2 \end{pmatrix}, \quad (24)$$

where $(B_\kappa)_{ij}$ is the matrix of elements resulted from the discretization of the Galerkin formulation on the finite basis set.

We multiply (23) from left by the matrix

$$\mathcal{A}_\kappa = \begin{pmatrix} A_\kappa & 0 \\ 0 & -A_\kappa^+ \end{pmatrix}, \quad (25)$$

where $A_\kappa = (B_\kappa)_{ij} - \mu_\kappa\kappa Z/(|\kappa|c^2\zeta)$ and $A_\kappa^+ = (B_\kappa^+)_{ij} - \mu_\kappa\kappa Z/(|\kappa|c^2\zeta)$, to get

$$(H_{-\kappa,\mu})_{ij}\mathcal{A}_\kappa(\tilde{\varphi}_\kappa)_{ij} = \mu_\kappa\mathcal{U}_{-\kappa}^{-2}\mathcal{A}_\kappa(\tilde{\varphi}_\kappa)_{ij}, \quad (26)$$

where we have used the fact that

$$\mathcal{A}_\kappa((H_{\kappa,\mu})_{ij} - \mu_\kappa\mathcal{U}_\kappa^{-2}) = ((H_{-\kappa,\mu})_{ij} - \mu_\kappa\mathcal{U}_{-\kappa}^{-2})\mathcal{A}_\kappa. \quad (27)$$

Now we define the normalization factor \mathcal{N}_κ as

$$\mathcal{N}_\kappa = \langle A_\kappa(\tilde{f}_\kappa)_{ij}, A_\kappa(\tilde{f}_\kappa)_{ij} \rangle + \langle A_\kappa^+(\tilde{g}_\kappa)_{ij}, A_\kappa^+(\tilde{g}_\kappa)_{ij} \rangle, \quad (28)$$

here $\langle \cdot, \cdot \rangle$ is the scalar product of vectors in the Euclidean space. Then for $\mu_\kappa \neq 0$, the eigenfunctions of $(H_{\kappa,\mu})_{ij}$ and $(H_{-\kappa,\mu})_{ij}$ are related by the following equation

$$(\tilde{\varphi}_{-\kappa})_{ij} = A_\kappa(\tilde{\varphi}_\kappa)_{ij} / \sqrt{\mathcal{N}_\kappa}. \quad (29)$$

Substituting (29) in (26) yields

$$(H_{-\kappa,\mu})_{ij}(\tilde{\varphi}_{-\kappa})_{ij} = \mu_\kappa \mathcal{U}_{-\kappa}^{-2}(\tilde{\varphi}_{-\kappa})_{ij}. \quad (30)$$

Thus by (23) and (30), the nonzero eigenvalues of H_κ and $H_{-\kappa}$ would coincide in the finite basis set. Since $(H_{-\kappa,\mu})_{ij}$ and $(H_{-\kappa,\mu})_{ij}$ are of the same size, then the number of their zero eigenvalues is the same. To conclude, the eigenvalues of H_κ and $H_{-\kappa}$ would coincide in the projection method onto the finite dimensional subspaces in the numerical computations.

3.1.3 More on spuriosity in the Dirac eigenvalue problem

Most of computational methods of the eigenvalues of the radial Dirac operator consent that incorrect balancing and symmetric treatment of the large and small components of the wave function are the core of the problem [1, 38, 43]. We relate the occurrence of spuriosity of both categories to unsuitable computational spaces and to the symmetric treatment of the trial and test functions in the weak formulation of the equation. To get more understanding, we rewrite (8) to obtain explicit formulae for the radial functions f and g , see Paper I in the appendix,

$$f''(x) + \gamma_1(x, \lambda)f'(x) + \gamma_2(x, \lambda)f(x) = 0, \quad (31)$$

$$g''(x) + \theta_1(x, \lambda)g'(x) + \theta_2(x, \lambda)g(x) = 0, \quad (32)$$

where

$$\begin{aligned} \gamma_1(x, \lambda) &= -\frac{V'(x)}{w^-(x) - \lambda}, & \theta_1(x, \lambda) &= -\frac{V'(x)}{w^+(x) - \lambda}, \\ \gamma_2(x, \lambda) &= \frac{(w^+(x) - \lambda)(w^-(x) - \lambda)}{c^2} - \frac{\kappa^2 + \kappa}{x^2} - \frac{\kappa V'(x)}{x(w^-(x) - \lambda)}, \\ \theta_2(x, \lambda) &= \frac{(w^+(x) - \lambda)(w^-(x) - \lambda)}{c^2} - \frac{\kappa^2 - \kappa}{x^2} + \frac{\kappa V'(x)}{x(w^+(x) - \lambda)}, \end{aligned}$$

and $w^\pm(x) = \pm mc^2 + V(x)$. It is a well-known fact that the numerical methods are not stable when they are applied to convection dominated problems causing the solution to be disturbed by spurious oscillations. The following two criteria are frequently used to determine whether a given equation is convection dominated. Let

$$Pe_j = \frac{|u_j|h_j}{2K} \quad \text{and} \quad Da_j = \frac{s_j h_j}{|u_j|}, \quad (33)$$

where Pe_j and Da_j are known as the grid Peclet and Damköhler numbers respectively, h_j is the size of the element interval I_j , u_j and s_j are respectively the coefficients of the convection and reaction terms corresponding to I_j , and K is the diffusivity size. In general, when the convection coefficient or the source term is larger than the diffusion coefficient, i.e., when $Pe_j > 1$ or $2Pe_j Da_j = (s_j h_j^2 / K) > 1$, then the associated equation is a convection dominated one.

For both (31) and (32), the quantity $2PeDa$ admits very large values if small number of nodal points in the discretization of the weak form is considered regardless the sizes of $|\lambda|$, Z , and κ . Even with mesh refinement (increasing the number of nodal points), $2PeDa$ still admits very large values. For (31), Pe is always less than one. As for (32), even with mesh refinement, Pe admits a value greater than one, see Paper II in the appendix for more details. Therefore, (31) and (32) are convection dominated equations. This means that the approximated solutions, f and g , will be disturbed by unphysical oscillations, these oscillations in the eigenfunctions are the cause of spurious eigenvalues.

3.2 Stable computation of the eigenvalues

In the coming discussion we present mesh-based and meshfree stable approaches for the approximation of the radial Dirac operator eigenvalues. As a mesh-based approach we use the finite element method (FEM), and as a meshfree approach we apply the hp -cloud method [17, 61]. For the purpose of obtaining stability scheme based on Petrov-Galerkin formulation with stability parameters for the particular problem, the hp -cloud method applied in this work is based on the Galerkin formulation. This means a background mesh must be employed in evaluating the integrals in the weak form, hence, the hp -cloud method used here is not really a truly meshfree method (MM). Therefore, the FEM and Galerkin-based hp -cloud method are similar in principle, while the latter approach can be regarded as a generalization of the FEM.

Based on (31) and (32), the radial functions f and g are continuous and have continuous first derivatives. Thus, the suitable choice of computational spaces

for the radial Dirac eigenvalue problem should possess these properties. Then, with homogeneous Dirichlet boundary condition for both radial functions, the proposed space is $\mathbb{H}(\Omega) := C^1(\Omega) \cap H_0^1(\Omega)$. Note that, except the states $1s_{1/2}$ and $2p_{1/2}$, the radial functions are vanishing on the boundary in a damping way, consequently homogeneous Neumann boundary condition should be taken into account. Meanwhile, the upper boundary of the states $1s_{1/2}$ and $2p_{1/2}$ is treated as the others, but the first derivative of these states at the lower boundary is not zero, see e.g. [41]. For simplicity and to avoid further remarks, in the discussion below, general boundary conditions are assumed for all states, that is, homogeneous Dirichlet boundary condition. Thus the space $\mathbb{H}(\Omega)$ is considered. However, for better rate of convergence of the approximation of the radial Dirac operator eigenvalues, the suitable Neumann boundary conditions, as discussed above, should be also implemented.

In our computation using the FEM, we use cubic Hermite basis functions, these functions treat also the first derivative values of the approximated function at the nodal values. Therefore, homogeneous Neumann boundary condition can be easily implemented by omitting the two basis functions that treat the function first derivative at the boundary nodal points, see the discussion below. Hence, in the approximation of the eigenvalues of the radial Dirac operator using the FEM, homogeneous Neumann boundary condition, as well homogeneous Dirichlet boundary condition, is implemented for all states. For the approximation using hp -cloud method, homogeneous Dirichlet boundary condition is only considered.

Since the radial Dirac eigenvalue problem is a convection dominated problem, the FEM and hp -cloud method for this problem will be unstable, thus the occurrence of spurious eigenvalues. To stabilize the computation and to get rid of spurious eigenvalues completely, finite element Petrov-Galerkin (FEPG) (called also Streamline Upwind Petrov-Galerkin (SUPG)) [2, 14, 27] and hp -cloud Petrov-Galerkin (hp -CPG) (a technique of the general meshfree local Petrov-Galerkin (MLPG) methods [3, 18, 30]) methods are used. Apart from mesh consideration, the principle of FEPG method is similar to that of hp -CPG method, while the two methods mainly vary in the set of basis functions. The FEPG and hp -CPG methods are used to introduce artificial diffusion terms in the weak formulation of the equation to stabilize the approximated solution in a consistent way so that the solution of the original problem is also a solution to the weak form. The size of the added diffusivity is controlled by a stability parameter that is derived for the particular problem we consider.

To set the scheme, let \mathcal{V}_h be a finite dimensional subspace spanned by a suitable C^1 -basis set on a partition k_h of the domain Ω , where exponentially distributed nodal points are assumed to get sufficient information about the radial functions behavior near the origin where they oscillate heavily compared to regions away from it. We consider the weak form of the radial Dirac eigenvalue problem

$$\int_{\Omega} \mathbf{u}^t H_{\kappa} \varphi dr = \lambda \int_{\Omega} \mathbf{u}^t \varphi dr, \quad (34)$$

where, we recall that, H_{κ} is the radial Dirac operator given by

$$H_{\kappa} = \begin{pmatrix} mc^2 + V(r) & c\left(-\frac{d}{dr} + \frac{\kappa}{r}\right) \\ c\left(\frac{d}{dr} + \frac{\kappa}{r}\right) & -mc^2 + V(r) \end{pmatrix}, \quad (35)$$

and φ is the radial function given by

$$\varphi(r) = \begin{pmatrix} f(r) \\ g(r) \end{pmatrix}. \quad (36)$$

The usual Galerkin formulation is to consider the test function \mathbf{u} in the weak form above as $(v, 0)$ and $(0, v)$, where v as well f and g is an element of \mathcal{V}_h . The FEPG and hp -CPG methods are formulated by considering \mathbf{u} in (34) as $(v, \tau v')$ and $(\tau v', v)$, where v' means dv/dr and τ is the stability parameter that controls the size of the artificial diffusivity. The stability parameter τ is the main challenge in constructing the stability scheme and its derivation is the major task.

The derivation of τ assumes leading simplification; the operator limit as the radial variable $r \rightarrow \infty$. This presumable simplification is inevitable and justifiable: The derivation leads to an approximation of the limit point eigenvalue depending on τ which can be compared to the theoretical limit [22]. Thus, minimizing the error between these two limits provides τ . By considering the limit operator at infinity, we consider the part that includes the convection terms of the operator which are mostly needed to be stabilized. Besides that, the stability parameter should be applicable at all positions, particularly for the large values of r . The derivation also considers the dominant terms with respect to the speed of light, c , as another minor simplification.

3.2.1 The FEPG approximation

In the FEPG method we let \mathcal{V}_h be spanned by the cubic Hermite basis functions

$$\phi_{j,1}(x) = \begin{cases} \frac{1}{h_j^2}(x - x_{j-1})^2 - \frac{2}{h_j^3}(x - x_{j-1})^2(x - x_j), & x \in I_j, \\ 1 - \frac{1}{h_{j+1}^2}(x - x_j)^2 + \frac{2}{h_{j+1}^3}(x - x_j)^2(x - x_{j+1}), & x \in I_{j+1}, \end{cases}$$

$$\phi_{j,2}(x) = \begin{cases} \frac{1}{h_j^2}(x - x_{j-1})^2(x - x_j), & x \in I_j, \\ (x - x_j) - \frac{1}{h_{j+1}}(x - x_j)^2 + \frac{1}{h_{j+1}^2}(x - x_j)^2(x - x_{j+1}), & x \in I_{j+1}. \end{cases}$$

These functions are continuous and admit continuous first derivatives, so they satisfy the continuity properties of the space $\mathbb{H}(\Omega)$. Moreover, they consist of two different bases, one treats the function values and the other treats the function first derivative values at the nodal points, see Figure 1. Thus any function $w \in \mathcal{V}_h$ can be written as

$$w(r) = \sum_{j=1}^n w_j \phi_{j,1}(r) + \sum_{j=1}^n w'_j \phi_{j,2}(r), \quad (37)$$

where w_j and w'_j are respectively the function and the function first derivative values at the node r_j , and n is the number of type one basis functions $\phi_{\cdot,1}$ (which is the same as the number of type two basis functions $\phi_{\cdot,2}$) in the basis set.

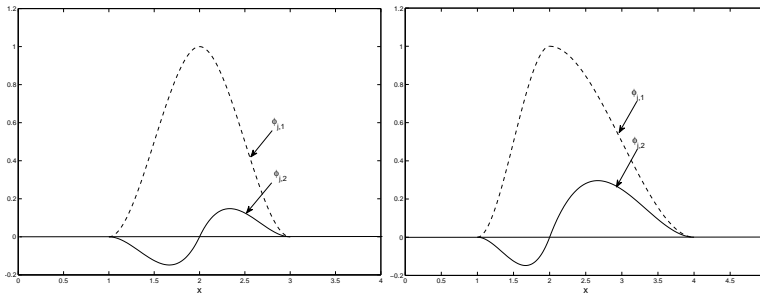


Figure 1: The CH basis functions with uniformly distributed nodal points (to the left), and non-uniformly distributed nodal points (to the right).

To treat the homogeneous Dirichlet boundary condition, the two basis functions of type $\phi_{\cdot,1}$ at the boundary nodal points are omitted. Also, for simplicity, we omit the two basis functions of type $\phi_{\cdot,2}$ at the boundary nodes, thus homogeneous Neumann boundary condition is also implemented. In the weak formulation (34), let $v, f, g \in \mathcal{V}_h$, this leads to the generalized eigenvalue problem

$$\mathbf{A}X = \lambda \mathbf{B}X. \quad (38)$$

The perturbed block matrices are given by $\mathbf{A} = A + \tau \mathcal{A}$ and $\mathbf{B} = B + \tau \mathcal{B}$, where A and B are the matrices obtained from the FEM, and \mathcal{A} and \mathcal{B} are the

matrices obtained as a result of the correction part, $\tau v'$, in the test function. Note that τ must be correlated with the size of the generated mesh, i.e., for a fine-structure mesh we expect τ to be relatively small compared to a coarse mesh. On the other hand, to avoid the occurrence of complex eigenvalues, τ should not be large compared to the mesh size. These properties are clear from the representation of τ given by the following theorem, see Paper I in the appendix.

Theorem 1 Considering the behavior of the eigenvalues as r tends to infinity, together with the dominant terms with respect to the speed of light, the mesh-dependent stability parameter, τ_j , for an arbitrary j^{th} row of the matrices \mathcal{A} and \mathcal{B} in the generalized eigenvalue problem (38) has the form

$$\tau := \tau_j \cong \frac{9}{35} h_{j+1} \frac{(h_{j+1} - h_j)}{(h_{j+1} + h_j)}, \quad (39)$$

where h_j is the displacement between the nodes r_j and r_{j-1} .

Below, a numerical example of the computation of the eigenvalues of the electron in the Hydrogen-like Magnesium ion using the FEPG method is presented for $\kappa = \pm 2$. Note that, in all our computations, the eigenvalues are given in atomic unit. Table 2 shows the computation using the FEM with linear basis functions with 400 interior nodal points for point nucleus. Table 3 shows the same computation with the stability scheme.

Table 2: The first computed eigenvalues of the electron in the Hydrogen-like Magnesium ion using the FEM with linear basis functions for point nucleus.

Level	$\kappa = 2$	$\kappa = -2$	Exact, $\kappa = -2$
1	-18.0086349982	-18.0086349982	-18.0086349982
2	-8.00511829944	-8.00511829944	-8.00511739963
3	-4.50270135222	-4.50270135225	-4.50269856638
⇒	-2.88546212211	-2.88546212205	Spurious Eigenvalue
4	-2.88155295096	-2.88155295095	-2.88154739168
5	-2.00096852250	-2.00096852249	-2.00095939879
6	-1.47003410346	-1.47003410350	-1.47002066823
⇒	-1.13034880166	-1.13034880167	Spurious Eigenvalue
7	-1.12545691681	-1.12545691683	-1.12543844140
8	-.889228944495	-.889228944484	-.889204706429
9	-.720265553198	-.720265553187	-.720234829539
⇒	-.600492562625	-.600492562622	Spurious Eigenvalue
10	-.595258516248	-.595258516277	-.595220579682
11	-.500185771976	-.500185772005	-.500139887884
12	-.426201311278	-.426201311300	-.426146735771

Table 3: The first computed eigenvalues of the electron in the Hydrogen-like Magnesium ion using the stability scheme for point nucleus.

Level	$\kappa = 2$	$\kappa = -2$	Exact, $\kappa = -2$
1		-18.0086349985	-18.0086349982
2	-8.00511739978	-8.00511740020	-8.00511739963
3	-4.50269856669	-4.50269856719	-4.50269856638
4	-2.88154739219	-2.88154739270	-2.88154739168
5	-2.00095939948	-2.00095939991	-2.00095939879
6	-1.47002066888	-1.47002066924	-1.47002066823
7	-1.12543844176	-1.12543844201	-1.12543844140
8	-.889204706068	-.889204706109	-.889204706429
9	-.720234827833	-.720234827687	-.720234829539
10	-.595220575840	-.595220575531	-.595220579682
11	-.500139880950	-.500139880357	-.500139887884
12	-.426146724530	-.426146723650	-.426146735771
13	-.367436809137	-.367436807839	-.367436826403
14	-.320073519367	-.320073498169	-.320073665658
15	-.281295132797	-.281293164731	-.281311119433

In Table 4, the computation is performed for extended nucleus using uniformly distributed charge with 397 interior nodal points, where 16 nodal points are considered in the domain $[0, R]$ (R is the radius of the nucleus).

Table 4: The first computed eigenvalues of the electron in the Hydrogen-like Magnesium ion using the stability scheme for extended nucleus.

Level	$\kappa = 2$	$\kappa = -2$	Exact, $\kappa = -2$
1		-18.0086349986	-18.0086349982
2	-8.00511739975	-8.00511740015	-8.00511739963
3	-4.50269856673	-4.50269856733	-4.50269856638
4	-2.88154739230	-2.88154739279	-2.88154739168
5	-2.00095939956	-2.00095940014	-2.00095939879
6	-1.47002066903	-1.47002066934	-1.47002066823
7	-1.12543844179	-1.12543844207	-1.12543844140
8	-.889204706021	-.889204706003	-.889204706429
9	-.720234827640	-.720234827433	-.720234829539
10	-.595220575309	-.595220574883	-.595220579682
11	-.500139879906	-.500139879215	-.500139887884
12	-.426146722827	-.426146721812	-.426146735771
13	-.367436806543	-.367436805088	-.367436826403
14	-.320073514034	-.320073492344	-.320073665658
15	-.281294966822	-.281292979627	-.281311119433

Note that the exact eigenvalues in the tables above (as well in the computations below) are obtained, of course for point nucleus, using the relativistic formula.

3.2.2 The hp -CPG approximation

The hp -Cloud basis functions are obtained using moving least-squares (MLS) approximation method which allows polynomial enrichment and desired fundamental characters of the sought solution to be constructed in the approximation. The hp -Cloud basis functions take the form

$$\psi_j(r) = P^t(r)M^{-1}(r)\varphi_j\left(\frac{r-r_j}{\rho_j}\right)P(r_j)\psi_j, \quad (40)$$

where $M(r) = \sum_{j=1}^n \varphi_j\left(\frac{r-r_j}{\rho_j}\right)P(r_j)P^t(r_j)$ is the momentum matrix, P is a vector of intrinsic enrichments, φ_j is a weight function, and ρ_j is the dilation parameter that controls the support of the weight functions.

The weight function φ_j is the main feature in the definition of ψ_j , it is needed to be C^1 -function in order to guarantee the continuity property of the space $\mathbb{H}(\Omega)$. For this purpose, we will consider quartic spline (which is a C^2 -function) as a weight function defined as

$$\varphi(\check{r}) = \begin{cases} 1 - 6\check{r}^2 + 8\check{r}^3 - 3\check{r}^4, & \check{r} \leq 1, \\ 0, & \check{r} > 1, \end{cases} \quad (41)$$

where $\check{r} = \frac{|r-r_j|}{\rho_j}$. While the set of functions $\{\psi_j\}_{j=1}^n$ builds a partition of unity (PU) ($\sum_{j=1}^n \psi_j(r) = 1$, for all $r \in \Omega$), the set of their first derivatives $\{\psi_{j,r}\}_{j=1}^n = \left\{\frac{d\psi_j(r)}{dr}\right\}_{j=1}^n$ builds a partition of nullity (PN) ($\sum_{j=1}^n \psi_{j,r}(r) = 0$ for all $r \in \Omega$), see Figure 2.

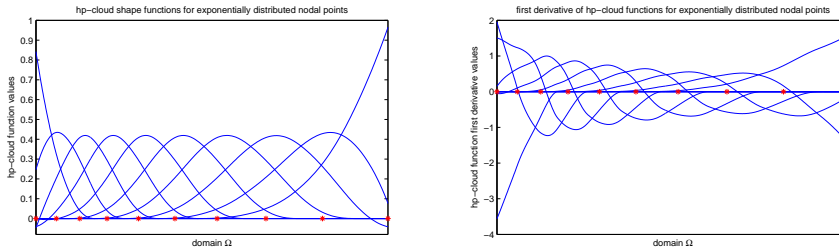


Figure 2: PU hp -clouds (to the left) and their PN first derivatives (to the right). Quartic spline is used as a weight function.

The invertibility of M depends on ρ_j , as ρ_j gets smaller as the matrix M has more tendency to be singular. So, in order to maintain the invertibility of M , it is necessary to keep ρ_j sufficiently large. However, ρ_j can be chosen fixed or

arbitrary, in this work we consider (exponentially distributed nodal points are used)

$$\rho_j = \nu \cdot \max\{h_j, h_{j+1}\} = \nu h_{j+1}, \quad (42)$$

where ν is the dimensionless size of the influence domain [29] which is chosen to be fixed in our computation. Note that the maximum in (42) is crucial to guarantee less possibility for singularity of M . The choices of ν are constrained by two restrictions; the values of ν should not be very small to ensure that any region is covered by at least two clouds, thus the invertibility of M . On the other hand, the values of ν should not be very large to guarantee the local character of the approximation. Noting that as $\nu \rightarrow 1$, the hp -cloud, ψ_j , will act as a finite element basis function, and thus the features of the hp -cloud approximation are gradually lost. The optimal choices of ν are left undetermined in general, but they can be individually specified for each problem by running numerical experiments [32, 59]. For the computation of the radial Dirac eigenvalue problem, for $\nu \in [2.2, 2.7]$ good approximation is achieved, see Figure 5, with complete elimination of the spurious eigenvalues.

The intrinsic enrichment basis vector P is a very important ingredient in the construction of the hp -cloud functions. Using the vector P , all fundamental features of the sought solution as well as singularities and discontinuities can be inherited by the hp -cloud basis functions. This distinguishes the hp -cloud approximation by solving particular problems where much care is needed about the approximated solution such as solving equations with rough coefficients, problems with high oscillatory solutions, or eigenvalue problems that admit spurious eigenvalues. Note that yet another type of enrichment, called extrinsic enrichment, can be considered in the construction of the hp -cloud functions, but this type of enrichment is not adequate when applying the hp -CPG method [3]. Thus, in this work, extrinsic enrichment is not considered.

The number and type of the intrinsic enrichment functions in the basis set P can be chosen arbitrary for each cloud [20, 33], but for practical reasons (lowering both the condition number of M and the computational costs) we shall assume $P(x) = [1, p_1(x)]$, where the choices of $p_1(x)$ follow two main properties; since ψ_j is needed to be a C^1 -function, which is guaranteed only if both the weight function φ_j and the elements of P are also in C^1 , $p_1(x)$ should be a C^1 -function as well. Secondly, $p_1(x)$ should possess the global behavior of the electron motion.

Slater type orbital functions (STOs) and Gaussian type orbital functions (GTOs) provide good description of the electron motion [10, 24]. But the

quadratic term in the exponent of GTOs causes some numerical difficulty, in the sense that, the matrix M rapidly becomes poorly conditioned, this is also what is observed when applying quadratic basis enrichments, see [5]. Consequently, STOs are considered as the intrinsic enrichment of the hp -cloud functions, thus $p_1(x)$ can have, e.g., one of the following forms

$$\exp(-x), x \exp(-x/2), x(1 - x/2) \exp(-x/2), \dots \text{ etc.}$$

Other possible intrinsic enrichments for the computation of the radial Dirac operator eigenvalues can be found in Paper II in the appendix. In the computations presented below, we consider $p_1(x) = x(1 - x/2) \exp(-x/2)$.

The boundary conditions need special treatment: For the computation of the radial Dirac eigenvalue problem we assume homogeneous Dirichlet boundary condition, while it is well-known that imposition of essential boundary conditions (EBCs) in MMs, in general, is a difficulty which needs to be treated with care. The reason is that the meshfree basis functions lack the Kronecker delta property ($\psi_j(r_i) \neq \delta_{ji}$), thus EBCs are not directly imposed as for the FEM. To circumvent this difficulty, a coupling with finite element basis functions is considered, see Figure 3. By coupling with finite element basis functions at the lower and upper boundaries, the imposition of the homogeneous Dirichlet boundary condition is straightforward, e.g., by eliminating the two finite element basis functions at the boundary nodes.

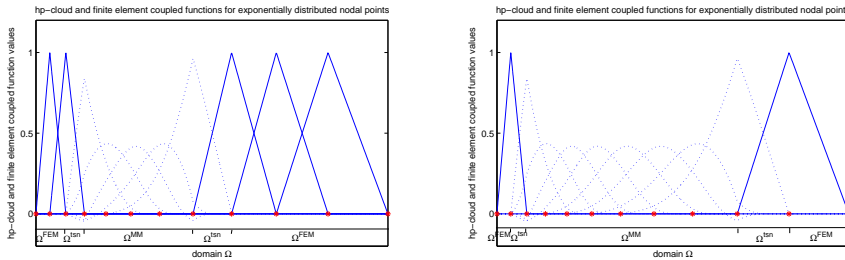


Figure 3: Coupled hp -cloud and finite element functions: general coupling (to the left), and coupling for the purpose of imposing EBCs (to the right) (two finite element shape functions are sufficient). Linear functions are used as finite element functions, and quartic spline as a weight function in the hp -clouds.

Two efficient approaches of coupling MMs with FEM are coupling with Ramp functions [4] and coupling with reproducing conditions [25]. Using the former one, the derivative of the coupled approximation function on the boundary of the interface region, Ω^{tsn} in Figure 3, is discontinuous, for this reason we

use the latter coupling approach, see e.g. [19]. The coupled hp -cloud and finite element function with the reproducing conditions is given as

$$\begin{aligned} \psi_j(r) = & \left(P^t(r) - \mathcal{G}_j(r)P^t(r_j)\chi_{\Omega^{\text{FEM}}}(r_j) \right) M^{-1}(r)\varphi_j\left(\frac{r-r_j}{\rho_j}\right) \times \\ & \times P(r_j)\chi_{\Omega^{\text{MM}}}(r_j)\psi_j + \mathcal{G}_j(r)\chi_{\Omega^{\text{FEM}}}(r_j)\psi_j, \end{aligned} \quad (43)$$

where $\chi_{\Omega^{\text{FEM}}}$ and $\chi_{\Omega^{\text{MM}}}$ are respectively the characteristic functions of the domains Ω^{FEM} and Ω^{MM} , see Figure 3, and \mathcal{G}_j is the finite element function.

To enhance the stability of the computation and to maintain the accuracy that may be affected or lost due to the round-off error, and also to get a lower condition number for the matrix M , the origin should be shifted to the evaluation point in the meshfree basis functions in general [19, 26, 29].

After constructing the hp -cloud basis functions, the hp -CPG method is formulated by assuming the weak form (34) where u , as before, takes the forms $(v, \tau v')$ and $(\tau v', v)$, and $v, f, g \in \mathcal{V}_h$, where \mathcal{V}_h is now spanned by a set of functions of the form (43). This yields similar generalized eigenvalue problem as of (38). The stability parameter, τ , is now different from the one given by Theorem 1, and can be considered as a generalization of it. The same principle as in Theorem 1 is used in deriving τ by using the hp -cloud basis functions. The following theorem provides the representation of τ which will be still denoted by the same notation.

Theorem 2 Let M_{000} and M_{100} be the $n \times n$ matrices (n is the number of hp -cloud basis functions) defined as

$$(M_{000})_{ij} = \int_{\Omega} \psi_j \psi_i dr, \text{ and } (M_{100})_{ij} = \int_{\Omega} \psi_j \psi_i' dr, \quad (44)$$

and let σ_{ji} and η_{ji} be the corresponding entries respectively. Define ϑ as

$$\vartheta_{ji} = \begin{cases} -\sum_{k=i+1}^j h_k, & i < j, \\ 0, & i = j, \\ \sum_{k=j+1}^i h_k, & i > j, \end{cases}$$

where h_k is the displacement between the adjacent nodes r_k and r_{k-1} . Then the stability parameter, τ_j , for an arbitrary j^{th} row of the matrices \mathcal{A} and \mathcal{B} in the generalized eigenvalue problem (38) is given by

$$\tau := \tau_j = \left| \frac{\sum_{i=1}^n \sigma_{ji} \vartheta_{ji}}{\sum_{i=1}^n \eta_{ji} \vartheta_{ji}} \right|. \quad (45)$$

The advantage of the hp -CPG stability parameter (45) is that it can be applied for general basis functions and not for particular ones as of the FEPG stability parameter (39).

Remark 1 To capture the behavior of the radial functions near the origin where they oscillate heavily compared to regions away from it, the computation of the radial Dirac operator eigenvalues requires, as we mentioned before, exponentially distributed nodal points. In this regard, the following formula is used to discretize Ω

$$r_i = \exp \left(\ln(I_a + \varepsilon) + \left(\frac{\ln(I_b + \varepsilon) - \ln(I_a + \varepsilon)}{n} \right) i \right) - \varepsilon, \quad i = 0, 1, 2, \dots, n, \quad (46)$$

where n is the total number of nodal points, I_a and I_b are the lower and upper boundaries of Ω , and $\varepsilon \in [0, 1]$ is the nodes intensity parameter. The main role of ε is to control the intensity of the nodal points close to the origin (I_a). As ε gets smaller as more nodes are dragged to the origin. In Paper II in the appendix, a study is carried out concerning the suitable choices of ε , it is shown that the most appropriate values for ε that provide good results are in the interval $[10^{-6}, 10^{-4}]$.

The results of the computation using the hp -CPG method with the stability parameter (45) are presented in Tables 5 and 6. In Table 5, the approximated eigenvalues of the electron in the Hydrogen-like Ununoctium ion are obtained using the usual and the stabilized hp -cloud methods. The computation is obtained at $\rho_j = 2.2h_{j+1}$, $\varepsilon = 10^{-5}$, and $n = 600$. In the hp -cloud method, the instilled spurious eigenvalues appear for both positive and negative κ (the two shaded values in the fourteenth level). Also the the so-called unphysical coincidence phenomenon occurs for the positive κ (the shaded value in the first level). Note that these spurious eigenvalues are removed by the stability scheme.

Table 6 represents the stabilized hp -cloud approximation of the electron in the Hydrogen-like Ununoctium ion with different numbers of nodal points. The convergence rate of the first five eigenvalues is studied in Figure 4. In Figure 4, h is the maximum of the distances between the adjacent nodes, which equals to $h_n = r_n - r_{n-1}$ for exponentially distributed nodal points. It can be verified from the figure that the convergence rates of the approximation of the first five eigenvalues, $\lambda_1, \lambda_2, \dots, \lambda_5$, are nearly 3.09, 2.66, 2.62, 2.59, and 2.56 respectively.

Table 5: The first computed eigenvalues of the electron in the Hydrogen-like Ununoctium ion using the hp -cloud and hp -CPG methods for point nucleus.

Level	hp -cloud $\kappa = 2$	hp -cloud $\kappa = -2$	Exact $\kappa = -2$	hp -CPG $\kappa = -2$	hp -CPG $\kappa = 2$
1	-1829.6307	-1829.6307	-1829.6307	-1829.6283	
2	-826.76981	-826.76981	-826.76835	-826.77147	-826.77388
3	-463.12149	-463.12149	-463.11832	-463.12471	-463.12611
4	-294.45523	-294.45523	-294.45098	-294.45915	-294.46006
5	-203.24689	-203.24689	-203.24195	-203.25115	-203.25179
6	-148.55882	-148.55882	-148.55344	-148.56324	-148.56372
7	-113.25360	-113.25360	-113.24791	-113.25808	-113.25845
8	-89.163854	-89.163854	-89.157945	-89.168323	-89.168622
9	-72.004533	-72.004533	-71.998465	-72.008947	-72.009194
10	-59.354813	-59.354813	-59.348624	-59.359134	-59.359342
11	-49.764290	-49.764290	-49.758009	-49.768490	-49.768669
12	-42.321471	-42.321471	-42.315117	-42.325523	-42.325679
13	-36.430396	-36.430396	-36.423983	-36.434277	-36.434414
14	-33.965028	-33.965028	-31.681730	-31.691878	-31.692001
15	-31.688189	-31.688189	-27.808134	-27.818109	-27.818219

Table 6: The first computed eigenvalues of the electron in the Hydrogen-like Ununoctium ion for $\kappa = -2$ for point nucleus with different number of nodes, where $\nu = 2.2$ and $\varepsilon = 10^{-5}$ are used.

Level	$n = 200$	$n = 400$	$n = 600$	$n = 800$	$n = 1000$	Exact, $\kappa = -2$
1	-1829.5628	-1829.6224	-1829.6283	-1829.6297	-1829.6302	-1829.6307
2	-826.82670	-826.77726	-826.77147	-826.76987	-826.76923	-826.76835
3	-463.23292	-463.13630	-463.12471	-463.12146	-463.12016	-463.11832
4	-294.59147	-294.47367	-294.45915	-294.45503	-294.45336	-294.45098
5	-203.39386	-203.26721	-203.25115	-203.24654	-203.24466	-203.24195
6	-148.70878	-148.58009	-148.56324	-148.55835	-148.55635	-148.55344
7	-113.40170	-113.27527	-113.25808	-113.25304	-113.25096	-113.24791
8	-89.306709	-89.185557	-89.168323	-89.163201	-89.161076	-89.157945
9	-72.139617	-72.026008	-72.008947	-72.003802	-72.001653	-71.998465
10	-59.480154	-59.375861	-59.359134	-59.354006	-59.351849	-59.348624
11	-49.878353	-49.784751	-49.768490	-49.763410	-49.761256	-49.758009
12	-42.423104	-42.341207	-42.325523	-42.320517	-42.318374	-42.315117
13	-36.518814	-36.449288	-36.434277	-36.429365	-36.427242	-36.423983
14	-31.762955	-31.706134	-31.691878	-31.687081	-31.684984	-31.681730
15	-27.875610	-27.831538	-27.818109	-27.813442	-27.811376	-27.808134

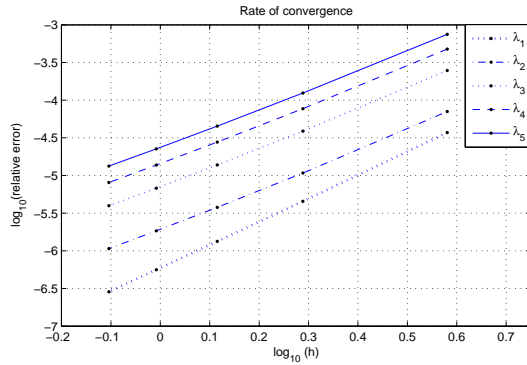


Figure 4: Studying the convergence rate of the first five eigenvalues in Table 6.

In Figure 5, we study the effect of the influence domain factor ν . The comparison is performed for the first five eigenvalues of the electron in the Hydrogen-like Ununoctium ion for $\kappa = -2$ for point nucleus. The computation is obtained at $n = 600$ and $\varepsilon = 10^{-5}$.

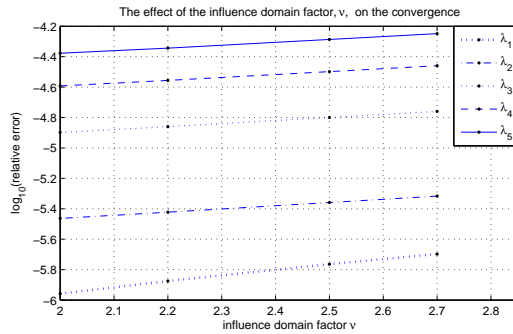


Figure 5: Studying the convergence rate with respect to ν .

Figure 5 shows that smaller ν gives better approximation. However, as we have mentioned, the appropriate values of ν lie in $[2.2, 2.7]$, while other smaller values of ν cause spurious eigenvalues, see Paper II in the appendix. This is seen evident since for small values of ν the cloud is not stretched enough to capture the behavior of the sought solution. Also for small ν , some regions of Ω are covered only with one cloud, which makes the momentum matrix M singular.

It is worth to mention that the FEPG method has a convergence rate higher than that of the hp -CPG method. Further, the hp -CPG method is more expensive due to the time consumption in evaluating the cloud functions that demand more integration points as ν gets larger, which is the main disadvantage of MMs.

4 G-convergence and eigenvalue problems

In this part, we study the convergence of the eigenvalues and the corresponding eigenvalue problems for families of positive definite self-adjoint operators using the theory of G-convergence. First we discuss G-convergence of a class of elliptic and bounded positive definite self-adjoint operators. Then we consider G-convergence of a family of Dirac operators. Using the spectral measure, we consider projected positive definite parts of this family of Dirac operators and then apply the theory of G-convergence.

The theory of G-convergence was introduced in the late 1960's [13, 44, 45, 46] for linear elliptic and parabolic operators with symmetric coefficient matrices. The concept was further extended to non-symmetric coefficient matrices [35, 47, 48, 49] and referred to as H-convergence. The theory was then generalized to positive definite self-adjoint operators [11] under the name G-convergence. The study of G-convergence of positive definite self-adjoint operators is often connected to the study of convergence of the associated quadratic forms in the calculus of variations via the notion of Γ -convergence which was introduced in the mid 1970's [12]. The monographs [8, 11] contain comprehensive material on the topic, where [11] deals with the connection to G-convergence. In this work, we will use the name G-convergence for the case of non-symmetric matrices as well.

4.1 Elliptic operators

4.1.1 An overview

Let Ω be an open bounded set in \mathbb{R}^N , $N \geq 1$. To present the idea of G-convergence, a heat conduction example is considered. The h -dependent stationary heat equation with heat source $f(x) \in H^{-1}(\Omega)$ and periodic heat conductivity matrix $\mathbf{A}_h(x) = \mathbf{A}(hx)$, \mathbf{A} is \mathbf{Y} -periodic, is given by

$$\begin{cases} -\frac{\partial}{\partial x_i}((\mathbf{A}_h(x))_{ij} \frac{\partial u_h}{\partial x_j}) = f(x) & \text{in } \Omega, \\ u_h = 0 & \text{on } \partial\Omega. \end{cases} \quad (47)$$

The operator $-\frac{\partial}{\partial x_i}((\mathbf{A}_h(x))_{ij} \frac{\partial}{\partial x_j})$ is defined on $L^2(\Omega)$ with domain $H_0^1(\Omega)$, $h \in \mathbb{N}$ is a parameter that tends to infinity, and $L^\infty(\Omega)^{N \times N} \ni (\mathbf{A}_h(x))_{ij}$ is positive definite and bounded.

The difficulty arises when h tends to infinity, where the highly oscillating coefficient matrix, \mathbf{A}_h , makes (47) hard to solve with direct numerical methods

with good accuracy. The idea we will advocate is to consider instead the limit equation as $h \rightarrow \infty$ where the material is expected to behave as a homogeneous one. In other words, we are interested in finding the properties of a homogeneous equation that gives the same overall response as the heterogeneous one. This means that we look for the global macroscopic behavior of the solution. The limit problem of (47), as $h \rightarrow \infty$, can formally be written as

$$\begin{cases} -\frac{\partial}{\partial x_i}((\mathbf{B}(x))_{ij} \frac{\partial u}{\partial x_j}) = f(x) & \text{in } \Omega, \\ u = 0 & \text{on } \partial\Omega. \end{cases} \quad (48)$$

In a successful approach, the problem (48) contains no oscillations and hence is easier to be treated numerically. Thus, the task is to characterize the matrix \mathbf{B} .

The way of specifying the limit matrix \mathbf{B} is to let $h \rightarrow \infty$ in the weak form of (47): Find $u_h \in H_0^1(\Omega)$ such that

$$\langle \mathbf{A}_h(x) \nabla u_h(x), \nabla v(x) \rangle = \langle f(x), v(x) \rangle, \quad \forall v \in H_0^1(\Omega). \quad (49)$$

By the boundedness and coercivity of \mathbf{A}_h , the existence and uniqueness of a solution u_h to (47) are guaranteed by the Lax-Milgram theorem. Also these assumptions imply the boundedness of u_h and ∇u_h in $H_0^1(\Omega)$ and $L^2(\Omega)$ respectively. Therefore, up to a subsequence of u_h still denoted by u_h ,

$$u_h(x) \rightharpoonup u(x) \quad \text{in } H_0^1(\Omega), \quad (50)$$

$$\nabla u_h(x) \rightharpoonup \nabla u(x) \quad \text{in } L^2(\Omega)^N, \quad (51)$$

where the notation \rightharpoonup refers to the weak convergence. Since \mathbf{A}_h is an element of $L^\infty(\Omega)^{N \times N}$, then up to a subsequence denoted by \mathbf{A}_h ,

$$\mathbf{A}_h \overset{*}{\rightharpoonup} M(\mathbf{A}), \quad \text{in } L^\infty(\Omega)^{N \times N}, \quad (52)$$

where $M(\mathbf{A}) = \frac{1}{|\Upsilon|} \int_{\Upsilon} \mathbf{A}(y) dy$ is the average of \mathbf{A}_h , and $\overset{*}{\rightharpoonup}$ refers to the weak* convergence. We recall that (52) is also true in the $L^2(\Omega)^{N \times N}$ sense, this is because L^2 is continuously embedded in L^1 , which implies $L^\infty = (L^1)^* \subset \subset (L^2)^* = L^2$ (\star refers to the duality), hence the same topology on $L^\infty(\Omega)$ can be also defined on $L^2(\Omega)$. Thus, we have two sequences, ∇u_h and \mathbf{A}_h , which converge only weakly. This is the intricate task that we face to pass to limit as $h \rightarrow \infty$ in (49) as nothing can be concluded about the limit of the product of two sequences that are only weakly convergent, and generally the following result is not true

$$\mathbf{A}_h(x) \nabla u_h(x) \rightharpoonup M(\mathbf{A}) \nabla u(x), \quad \text{in } L^2(\Omega)^N. \quad (53)$$

Here, another technique is employed to study the existence and characterization of the asymptotic limit of $\mathbf{A}_h(x) \nabla u_h(x)$, namely the theory of G-convergence.

4.1.2 A one dimensional example

Consider the following Dirichlet boundary value problem

$$\begin{cases} -\frac{d}{dx}(\mathbf{A}_h(x)\frac{du_h}{dx}) = f & \text{in } \Omega = (x_0, x_1) \subset \mathbb{R}, \\ u_h \in H_0^1(\Omega), \end{cases} \quad (54)$$

where $f \in L^2(\Omega)$, and $L^\infty(\Omega) \ni \mathbf{A}_h(x) = \mathbf{A}(hx)$, with $\mathbf{A} : \mathbb{R} \rightarrow \mathbb{R}$ is a Y -periodic function satisfying, for $\alpha, \beta \in \mathbb{R}$, $0 < \alpha \leq \mathbf{A}(x) \leq \beta < \infty$ a.e on \mathbb{R} . The bounds for \mathbf{A}_h give the existence and uniqueness of a solution u_h to (54). Moreover the a priori estimate $\|u_h\|_{H_0^1(\Omega)} \leq C$ implies that the sequence u_h is uniformly bounded in $H_0^1(\Omega)$. Hence by Rellich-Kondrachov compactness theorem, up to a subsequence still denoted by u_h , there exists $u_0 \in H_0^1(\Omega)$ such that

$$u_h \rightharpoonup u_0 \text{ in } H_0^1(\Omega). \quad (55)$$

By the periodicity assumption on \mathbf{A} we have

$$\mathbf{A}_h \overset{*}{\rightharpoonup} M(\mathbf{A}) \text{ in } L^\infty(\Omega), \text{ (also weakly in } L^2(\Omega)). \quad (56)$$

One hastily concludes that the asymptotic limit of (54) is

$$\begin{cases} -\frac{d}{dx}(M(\mathbf{A})\frac{du_0}{dx}) = f & \text{in } \Omega, \\ u_0 \in H_0^1(\Omega). \end{cases} \quad (57)$$

But this is not the case in general, since the weak limit of the product of two sequences that are only weakly convergent is not the product of their individual weak limits. Here, the role of G-convergence theory comes in, it gives a strategy of identifying the correct limit of the problem.

In order to get the correct limit problem, we define

$$\xi_h = \mathbf{A}_h(x)\frac{du_h}{dx}. \quad (58)$$

By the boundedness of \mathbf{A}_h and the estimate $\|u_h\|_{H_0^1(\Omega)} \leq C$, ξ_h is uniformly bounded in $L^2(\Omega)$. Since $-\frac{d\xi_h}{dx} = f \in L^2(\Omega)$, we conclude that ξ_h is uniformly bounded in $H_0^1(\Omega)$. By the compact embedding of $H_0^1(\Omega)$ in $L^2(\Omega)$, up to a subsequence still denoted by ξ_h , we have

$$\xi_h \rightarrow \xi_0 \text{ in } L^2(\Omega), \quad (59)$$

for some ξ_0 , consequently

$$\frac{d\xi_h}{dx} \rightharpoonup \frac{d\xi_0}{dx} \text{ in } L^2(\Omega). \quad (60)$$

Note that $0 < \frac{1}{\beta} < \frac{1}{\mathbf{A}_h(x)} < \frac{1}{\alpha} < \infty$, hence

$$\frac{1}{\mathbf{A}_h} \rightharpoonup M\left(\frac{1}{\mathbf{A}}\right) \text{ in } L^\infty(\Omega), \text{ (also weakly in } L^2(\Omega)). \quad (61)$$

Since $\frac{1}{\mathbf{A}_h(x)}\xi_h = \frac{du_h}{dx}$, by (55) and (61) one gets

$$\frac{du_0}{dx} = M\left(\frac{1}{\mathbf{A}}\right)\xi_0. \quad (62)$$

By the result (60) together with (62) and a limit passage of $-\frac{d\xi_h}{dx} = f$, we conclude that u_0 is the solution to the limit problem

$$\begin{cases} -\frac{d}{dx}\left(\frac{1}{M\left(\frac{1}{\mathbf{A}}\right)}\frac{du_0}{dx}\right) = f & \text{in } \Omega, \\ u_0 \in H_0^1(\Omega). \end{cases} \quad (63)$$

By the uniqueness of the solution u_0 to (63), and using Urysohn property, it follows that the whole sequence u_h converges weakly to u_0 . The above conclusion can be summarized as \mathbf{A}_h G-converges to $(1/M(1/\mathbf{A}))$ which is known as the harmonic mean of A_h .

It is important to point out that in the previous example the weak* limit of $\frac{1}{\mathbf{A}_h}$ characterizes the limit problem. This is only true for one dimensional problem, and it is not the case in higher dimensions (\mathbb{R}^N , $n \geq 2$). For more discussion on this issue we refer to [35].

4.1.3 The definition

Let α and β be two real numbers such that $0 < \alpha \leq \beta < \infty$, and let $S(\alpha, \beta, \Omega)$ be defined as $S(\alpha, \beta, \Omega) = \{\mathbf{A} \in L^\infty(\Omega)^{N \times N}; (\mathbf{A}(x, \xi), \xi) \geq \alpha|\xi|^2 \text{ and } |\mathbf{A}(x, \xi)| \leq \beta|\xi|, \forall \xi \in \mathbb{R}^N \text{ and a.e } x \in \Omega\}$.

Definition 1 The sequence $\mathbf{A}_h \subset S(\alpha, \beta, \Omega)$ is G-convergent to $\mathbf{A} \in S(\alpha, \beta, \Omega)$, denoted by $\mathbf{A}_h \xrightarrow{G} \mathbf{A}$, if for every $f \in H^{-1}(\Omega)$, the sequence u_h of solutions to the equation

$$\begin{cases} -\operatorname{div}(\mathbf{A}_h(x, Du_h)) = f & \text{in } \Omega, \\ u_h \in H_0^1(\Omega) \end{cases} \quad (64)$$

satisfies

$$\begin{aligned} u_h &\rightharpoonup u \text{ in } H_0^1(\Omega), \\ \mathbf{A}_h(\cdot, Du_h) &\rightharpoonup \mathbf{A}(\cdot, Du) \text{ in } L^2(\Omega)^N, \end{aligned}$$

where u is the unique solution of the problem

$$\begin{cases} -\operatorname{div}(\mathbf{A}(x, Du)) = f & \text{in } \Omega, \\ u \in H_0^1(\Omega). \end{cases} \quad (65)$$

G-convergence possesses the compactness property, i.e., if $\mathbf{A}_h \in S(\alpha, \beta, \Omega)$, then there exists a subsequence, denoted by \mathbf{A}_h , and $\mathbf{A} \in S(\alpha, \beta, \Omega)$, such that $\mathbf{A}_h \xrightarrow{G} \mathbf{A}$. The G-limit is unique and local, also if $\mathbf{A}_h \xrightarrow{G} \mathbf{A}$, then $\mathbf{A}_h^t \xrightarrow{G} \mathbf{A}^t$, here t denotes the transpose operator.

4.1.4 Convergence of elliptic eigenvalue problems

For elliptic boundary value problems with source function f_h we have

Theorem 3 Consider the Dirichlet boundary value problem

$$\begin{cases} -\operatorname{div}(\mathbf{A}_h(x)\nabla u_h) = f_h & \text{in } \Omega, \\ u_h \in H_0^1(\Omega). \end{cases} \quad (66)$$

If $\mathbf{A}_h \in S(\alpha, \beta, \Omega)$ and f_h converges in $H^{-1}(\Omega)$ to f_0 , then the sequence u_h of solutions to (66) is weakly convergent in $H_0^1(\Omega)$ to the solution of the problem

$$\begin{cases} -\operatorname{div}(\mathbf{A}_0(x)\nabla u_0) = f_0 & \text{in } \Omega, \\ u_0 \in H_0^1(\Omega), \end{cases} \quad (67)$$

where \mathbf{A}_0 is the G-limit of \mathbf{A}_h .

The strength of G-convergence can be evidently seen by applying the concept to elliptic eigenvalue problems. Consider the linear elliptic eigenvalue problem

$$\begin{cases} -\operatorname{div}(\mathbf{A}_h(x)\nabla u_h^k) = \lambda_h^k u_h^k & \text{in } \Omega, \\ u_h^k \in H_0^1(\Omega), \end{cases} \quad (68)$$

where $\mathbf{A}_h \in S(\alpha, \beta, \Omega)$ is symmetric and positive definite. Then, the set of eigenvalues $\{\lambda_h^k\}$ is bounded and $0 < \lambda_h^1 \leq \lambda_h^2 \leq \lambda_h^3 \leq \dots$, also the multiplicity of each λ_h^k is finite.

Theorem 4 The sequences of eigenvalues λ_h^k and the corresponding eigenfunctions u_h^k of (68) converge to λ_0^k in \mathbb{R} and weakly to u_0^k in $H_0^1(\Omega)$ respectively, where the eigencouple $\{\lambda_0^k, u_0^k\}$ is the solution to the G-limit problem

$$\begin{cases} -\operatorname{div}(\mathbf{A}_0(x)\nabla u_0^k) = \lambda_0^k u_0^k & \text{in } \Omega, \\ u_0^k \in H_0^1(\Omega). \end{cases} \quad (69)$$

4.2 Positive definite self-adjoint operators

4.2.1 The definition

Let \mathcal{H} be a Hilbert space and let $\lambda \geq 0$ be a real number, by $\mathcal{P}_\lambda(\mathcal{H})$ we denote the class of self-adjoint operators A on a closed linear subspace $\overline{\mathbf{D}(A)}$ of \mathcal{H} such that $\langle Au, u \rangle \geq \lambda \|u\|_{\mathcal{H}}^2$, $\forall u \in \mathbf{D}(A)$.

Definition 2 Let $\lambda \geq 0$, and let $A_h \in \mathcal{P}_\lambda(\mathcal{H})$. If $\lambda > 0$, we say that $A_h \xrightarrow{G} A \in \mathcal{P}_\lambda(\mathcal{H})$ in \mathcal{H} if $A_h^{-1}P_h u \rightarrow A^{-1}Pu$ in \mathcal{H} , $\forall u \in \mathcal{H}$, where P_h and P are the orthogonal projections onto $\overline{\mathbf{D}(A_h)}$ and $\overline{\mathbf{D}(A)}$ respectively. If $\lambda = 0$, we say that $A_h \in \mathcal{P}_0(\mathcal{H})$ converges to $A \in \mathcal{P}_0(\mathcal{H})$ in the strong resolvent sense (SRS) if $(\mu I + A_h) \xrightarrow{G} (\mu I + A)$ in \mathcal{H} , $\forall \mu > 0$.

G-convergence of positive definite self-adjoint operators can be studied using Γ -convergence of the corresponding quadratic forms [11], where, generally, proving Γ -limits is simpler than proving G-limits. Below we define Γ -convergence and discuss its relation to G-convergence. First we need the following definitions.

Definition 3 A function $F : \mathcal{H} \rightarrow [0, \infty]$ is said to be lower semi-continuous (*lsc*) at $u \in \mathcal{H}$, if

$$F(u) \leq \sup_{U \in \mathcal{N}(u)} \inf_{v \in U} F(v),$$

where $\mathcal{N}(u)$ is the set of all open neighborhoods of u in \mathcal{H} .

Definition 4 A function F in \mathcal{H} is called a quadratic form if there exists a linear dense subspace \mathcal{X} of \mathcal{H} and a symmetric bilinear form $B : \mathcal{X} \times \mathcal{X} \rightarrow [0, \infty)$ such that

$$F(u) = \begin{cases} B(u, u), & \forall u \in \mathcal{X}, \\ \infty, & \forall u \in \mathcal{H} \setminus \mathcal{X}. \end{cases}$$

Let F and B be as in the above definition, where $\mathbf{D}(F) = \{u \in \mathcal{H}; F(u) < \infty\}$. Then the operator associated to F is the linear operator A on $\overline{\mathbf{D}(F)}$ with the domain being the set of all $u \in \mathbf{D}(F)$ such that there exists $v \in \mathbf{D}(F)$ satisfying $B(u, f) = \langle v, f \rangle$, $\forall f \in \mathbf{D}(F)$ and $Au = v$, $\forall u \in \mathbf{D}(A)$. If $f = u$ then $F(u) = \langle Au, u \rangle$, $\forall u \in \mathbf{D}(A)$.

Let $\lambda \geq 0$, by $\tilde{\mathcal{Q}}_\lambda(\mathcal{H})$ we denote the class of quadratic forms $F : \mathcal{H} \rightarrow [0, \infty]$ such that $F(u) \geq \lambda \|u\|_{\mathcal{H}}^2$. And by $\mathcal{Q}_\lambda(\mathcal{H})$ we denote the subset of $\tilde{\mathcal{Q}}_\lambda(\mathcal{H})$ whose elements are *lsc*.

Definition 5 A sequence of functionals $F_h : \mathcal{H} \rightarrow \overline{\mathbb{R}}$ is said to Γ -converge to $F : \mathcal{H} \rightarrow \overline{\mathbb{R}}$, written as $F(u) = \Gamma - \lim_{h \rightarrow \infty} F_h(u)$ and denoted by $F_h \xrightarrow{\Gamma} F$ if

$$F(u) = \Gamma - \liminf_{h \rightarrow \infty} F_h(u) = \Gamma - \limsup_{h \rightarrow \infty} F_h(u),$$

where $\Gamma - \liminf_{h \rightarrow \infty} F_h(u) = \sup_{U \in \mathcal{N}(u)} \liminf_{h \rightarrow \infty} \inf_{v \in U} F_h(v)$ and $\Gamma - \limsup_{h \rightarrow \infty} F_h(u) = \sup_{U \in \mathcal{N}(u)} \limsup_{h \rightarrow \infty} \inf_{v \in U} F_h(v)$.

Note that if \mathcal{H} satisfies the first axiom of countability (the neighborhood system of every point in \mathcal{H} has a countable base), then $F_h \xrightarrow{\Gamma} F$ in \mathcal{H} if and only if the following two conditions are satisfied

- (i) (lim inf-inequality) $\forall u \in \mathcal{H}$ and $\forall u_h$ converging to u , $F(u) \leq \liminf_{h \rightarrow \infty} F_h(u_h)$.
- (ii) (lim-equality) $\forall u \in \mathcal{H}$, $\exists u_h$ converging to u such that $F(u) = \lim_{h \rightarrow \infty} F_h(u_h)$.

It is worth to mention that Γ -limit is always *lsc* and unique, also Γ -limit of non-negative quadratic form is also a non-negative quadratic form. Γ -convergence possesses the compactness property, that is, if \mathcal{H} is a separable metric space, then every sequence $F_h : \mathcal{H} \rightarrow \overline{\mathbb{R}}$ has a Γ -convergent subsequence.

The following theorem is the cornerstone of the relation between G-convergence of operators of the class $\mathcal{P}_\lambda(\mathcal{H})$ for $\lambda \geq 0$ and Γ -convergence of the associated quadratic forms of the class $\mathcal{Q}_\lambda(\mathcal{H})$.

Theorem 5 Let F_h and F be elements of $\mathcal{Q}_0(\mathcal{H})$, and let $A_h, A \in \mathcal{P}_0(\mathcal{H})$ be the associated operators respectively. Then $F_h \xrightarrow{\Gamma} F$ if and only if $A_h \rightarrow A$ in the SRS. Also, for $\mu > 0$, if $F_h, F \in \mathcal{Q}_\mu(\mathcal{H})$, and $A_h, A \in \mathcal{P}_\mu(\mathcal{H})$ are the associated operators respectively, then $F_h \xrightarrow{\Gamma} F$ if and only if $A_h \xrightarrow{G} A$.

4.2.2 G-convergence of positive definite self-adjoint operators

Let H_0 be a positive definite bounded self-adjoint operator defined on $L^2(\Omega)$ and let $\mathbf{D}(H_0) = H_0^1(\Omega)$. Consider the perturbed operator $H_h = H_0 + V_h$ where $V_h(x)$ is a positive bounded real-valued multiplication operator in $L^2(\Omega)$. Using G-convergence together with Γ -convergence, we state the following results, see Paper IV in the appendix.

Theorem 6 Let V_h be a sequence in $L^\infty(\Omega)$ that converges weakly* to V , then H_h G-converges to $H = H_0 + V$.

Theorem 7 If V_h is a weakly convergent sequence in $L^p(\Omega)$ for $2 \leq p < \infty$ with a weak limit denoted by V , then H_h G-converges to $H = H_0 + V$.

Let \mathcal{X} and \mathcal{H} be two Hilbert spaces, and let $\mathcal{B}(\mathcal{H})$ be the set of bounded linear operators on \mathcal{H} . As a generalization of Theorem 4, below we state the relation between the eigenvalue problems of an operator and its G-limit of the class $\mathcal{P}_\lambda(\mathcal{H})$ for $\lambda \geq 0$, see Paper III in the appendix.

Theorem 8 Let $\lambda > 0$, let A_h be a sequence in $\mathcal{P}_\lambda(\mathcal{H})$ G-converging to $A \in \mathcal{P}_\lambda(\mathcal{H})$, and let $\{\mu_h, u_h\}$ be the solution of the eigenvalue problem $A_h u_h = \mu_h u_h$. If $\{\mu_h, u_h\} \rightarrow \{\mu, u\}$ in $\mathbb{R} \times \mathcal{H}$, then the limit couple $\{\mu, u\}$ is the solution of the eigenvalue problem $Au = \mu u$.

It is clear that the assertion of Theorem 8 is also true if the sequence $A_h \in \mathcal{P}_0(\mathcal{H})$ is convergent in the SRS to $A \in \mathcal{P}_0(\mathcal{H})$.

Note that if a sequence A_h is convergent in the SRS (or strongly convergent) to A , then every $\lambda \in \sigma(A)$ is the limit of a sequence $\lambda_h \in \sigma(A_h)$, but not the limit of every sequence $\lambda_h \in \sigma(A_h)$ lies in the spectrum of A , see [54]. Despite of this fact, the following theorem provides conditions by which G-convergence of an operator in $\mathcal{P}_\lambda(\mathcal{H})$ (consequently the strong resolvent convergence in $\mathcal{P}_0(Y)$) implies the convergence of the corresponding eigenvalues, see Paper III in the appendix.

Theorem 9 Let \mathcal{X} be compactly and densely embedded in \mathcal{H} , and let A_h be a family of operators in $\mathcal{P}_\lambda(\mathcal{H})$, $\lambda > 0$, with domain \mathcal{X} . If A_h G-converges to $A \in \mathcal{P}_\lambda(\mathcal{H})$, then A_h^{-1} converges in the norm of $\mathcal{B}(\mathcal{H})$ to A^{-1} . Moreover, the k^{th} eigenvalue μ_h^k of A_h converges to the k^{th} eigenvalue μ^k of A , $\forall k \in \mathbb{N}$.

Theorem 9 implies that, for those perturbations considered in Theorems 6 and 7, the eigenvalues of H_h converge to the eigenvalues of the G-limit operator H . Moreover, Theorem 8 guarantees that the eigenvalue problem $H_h u_h = \mu_h u_h$ converges to the limit problem $Hu = \mu u$, where u is the limit of u_h in $L^2(\Omega)$.

Remark 2 Let E^{H_h} and E^H be the spectral measures of H_h and H respectively, then G-convergence of H_h to H implies that $E^{H_h}(\lambda) \rightarrow E^H(\lambda)$ strongly for all $\lambda \in \mathbb{R}$ such that $E^H(\lambda) = E^H(-\lambda)$.

4.3 Families of Dirac operators

Here we consider an h -dependent perturbation added to the Dirac operator with Coulomb potential. The purpose is to apply G-convergence theory for positive definite parts of the perturbed operator and to investigate the asymptotic behavior of the corresponding eigenvalues in the gap.

4.3.1 The Dirac operator with perturbation ($\tilde{\mathcal{H}}_h$)

Let \mathcal{H}_h be defined as

$$\mathcal{H}_h = \mathbf{H} + V_h, \quad (70)$$

where $V_h = V_h(x)$ is a 4×4 matrix-valued function and, as defined before, $\mathbf{H} = \mathbf{H}_0 + V$, where again \mathbf{H}_0 and V are respectively the free Dirac operator and the Coulomb potential. We recall here the spaces $X = H^1(\mathbb{R}^3, \mathbb{C}^4)$ and $Y = L^2(\mathbb{R}^3, \mathbb{C}^4)$.

Recall that a function F is called homogeneous of degree p if for any nonzero scalar a , $F(ax) = a^p F(x)$. The next theorem is of profound importance [53, 55].

Theorem 10 Let, for $h > 0$, V_h be a measurable (-1) -homogeneous Hermitian 4×4 matrix-valued function with entries in $L^p_{loc}(\mathbb{R}^3)$, $p > 3$. Then \mathcal{H}_h is essentially self-adjoint on $C_0^\infty(\mathbb{R}^3; \mathbb{C}^4)$ and self-adjoint on X . Moreover, $\sigma(\mathcal{H}_h) = (-\infty, -mc^2] \cup \{\lambda_h^k\}_{k \in \mathbb{N}} \cup [mc^2, +\infty)$, where $\{\lambda_h^k\}_{k \in \mathbb{N}}$ is a discrete sequence of h -dependent eigenvalues corresponding to the Dirac eigenvalue problem $\mathcal{H}_h u_h = \lambda_h u_h$.

We assume further that the 4×4 matrix-valued function V_h is of the form $V_h(x) = V_1(x)V_2(hx)$, where V_1 is (-1) -homogeneous and where the entries of $V_2(y)$ are 1-periodic in y , i.e.,

$$V_2^{ij}(y+k) = V_2^{ij}(y), \quad k \in \mathbb{Z}^3.$$

We also assume that the entries of V_2 belong to $L^\infty(\mathbb{R}^3)$. It is then well-known that

$$V_2^{ij}(hx) \ast \rightarrow M(V_2^{ij}) = \int_{\mathbb{T}^3} V_2^{ij}(y) dy, \quad \text{in } L^\infty(\mathbb{R}^3), \quad (71)$$

where \mathbb{T}^3 is the unit torus in \mathbb{R}^3 . It easily follows from this mean-value property that

$$V_h \ast \rightarrow V_1 M(V_2), \quad \text{in } L^p(\mathbb{R}^3), \quad p > 3.$$

In the sequel, we consider a shifted family of Dirac operators denoted by $\tilde{\mathcal{H}}_h$ and defined as $\tilde{\mathcal{H}}_h = \tilde{\mathbf{H}} + V_h$, where $\tilde{\mathbf{H}} = \mathbf{H} + mc^2 \mathbf{I}$. Also without loss of generality we set $\hbar = c = m = 1$. By Theorem 10, for $h > 0$, we then get $\sigma(\tilde{\mathcal{H}}_h) = (-\infty, 0] \cup \{\tilde{\lambda}_h^k\}_{k \in \mathbb{N}} \cup [2, \infty)$.

4.3.2 The spectral theorem

Let \mathcal{H} be a Hilbert space, and let $(\mathcal{U}, \mathcal{A})$ be a measurable space where $\mathcal{U} \subseteq \mathbb{C}$ and \mathcal{A} is a σ -algebra on \mathcal{U} . Assume $\mathbb{P}^{\mathcal{H}} = \mathbb{P}(\mathcal{H})$ is the set of orthogonal

projections onto \mathcal{H} , then $E : \mathcal{A} \rightarrow \mathbb{P}^{\mathcal{H}}$ is called a spectral measure if $E(\emptyset) = 0$, $E(\mathcal{U}) = I$ (completeness), and if $\{\Delta_n\} \subset \mathcal{A}$ is a finite or a countable set of disjoint elements and $\Delta = \cup_n \Delta_n$, then $E(\Delta) = \sum_n E(\Delta_n)$ (countable additivity), see e.g. [6, 28, 53]. Further, let $\mathcal{U} = \mathbb{R}$, the spectral measure on the real line corresponding to an operator S is given as $E^S(\lambda) = E^S(\Delta)$ where $\Delta = (-\infty, \lambda)$, $\lambda \in \mathbb{R}$.

Theorem 11 The Spectral Theorem.

For a self-adjoint operator S defined on a Hilbert space \mathcal{H} there exists a unique spectral measure E^S on \mathcal{H} such that $S = \int_{\sigma(S)} \lambda dE^S(\lambda)$.

4.3.3 G-convergence of projected parts of $\tilde{\mathcal{H}}_h$

Let X and Y be defined as before, and let $E^{\tilde{\mathcal{H}}_h}$ and $E^{\tilde{\mathbf{H}}}$ be the spectral measures of the families $\tilde{\mathcal{H}}_h$ and $\tilde{\mathbf{H}}$ respectively, by the spectral theorem

$$\tilde{\mathcal{H}}_h = \int_{\sigma(\tilde{\mathcal{H}}_h)} \lambda dE^{\tilde{\mathcal{H}}_h}(\lambda). \quad (72)$$

Define $X_h^p = \oplus_{k \in \mathbb{N}} \mathcal{N}_h^k$ where $\mathcal{N}_h^k = \{u_h \in X; \tilde{\mathcal{H}}_h u_h = \lambda_h^k u_h\}$. Note that X_h^p is a closed subspace of Y invariant with respect to $\tilde{\mathcal{H}}_h$. Then we have the following theorem, see Paper III in the appendix.

Theorem 12 Let $E^{\tilde{\mathcal{H}}_h, p}$ be the point measure of $\tilde{\mathcal{H}}_h$, and consider the restriction $\tilde{\mathcal{H}}_h^p$ of $\tilde{\mathcal{H}}_h$ to X_h^p defined as

$$\tilde{\mathcal{H}}_h^p = \sum_{\lambda \in \sigma_p(\tilde{\mathcal{H}}_h)} \lambda E^{\tilde{\mathcal{H}}_h, p}(\lambda). \quad (73)$$

The operator $\tilde{\mathcal{H}}_h^p$ is positive definite and self-adjoint on X with compact inverse $(\tilde{\mathcal{H}}_h^p)^{-1}$. Then there exists a positive definite self-adjoint operator $\tilde{\mathcal{H}}^p$ such that, up to a subsequence, $\tilde{\mathcal{H}}_h^p$ G-converges to $\tilde{\mathcal{H}}^p$. The operator $\tilde{\mathcal{H}}^p$ is given by $(\tilde{\mathbf{H}} + V_1 M(V_2))|_{X^p}$, where $\mathbf{D}(\tilde{\mathcal{H}}^p) = X^p = \oplus_{k \in \mathbb{N}} \mathcal{N}^k$ and $\mathcal{N}^k = \{u \in X; \tilde{\mathcal{H}}^p u = \lambda^k u\}$.

Now we can apply Theorem 9 to conclude that the sequence of k^{th} eigenvalues λ_h^k associated to $\tilde{\mathcal{H}}_h^p$ converges to the k^{th} eigenvalue λ^k of $\tilde{\mathcal{H}}^p$.

For the absolutely continuous part of the operator $\tilde{\mathcal{H}}_h$, we let first $X_h^{ac} = X_h^{ac,+} \oplus X_h^{ac,-}$, where $X_h^{ac,+}$ and $X_h^{ac,-}$ are the closed subspaces, invariant with respect to $\tilde{\mathcal{H}}_h$, corresponding respectively to the absolutely continuous

spectra $\sigma_{ac}^+(\tilde{\mathcal{H}}_h) = [2, +\infty)$ and $\sigma_{ac}^-(\tilde{\mathcal{H}}_h) = (-\infty, 0]$. Let $E^{\tilde{\mathcal{H}}_h, ac, +}(\lambda)$ be the absolutely continuous spectral measure corresponding to $\tilde{\mathcal{H}}_h^{ac, +}$ and define

$$\tilde{\mathcal{H}}_h^{ac, +} = \int_{\lambda \in \sigma_{ac}^+(\tilde{\mathcal{H}}_h)} \lambda dE^{\tilde{\mathcal{H}}_h, ac, +}(\lambda). \quad (74)$$

By this construction, the operator $\tilde{\mathcal{H}}_h^{ac, +}$ is the restriction of $\tilde{\mathcal{H}}_h$ to $X_h^{ac, +}$, thus it is positive definite and self-adjoint on X . Therefore, there exists a subsequence of $\tilde{\mathcal{H}}_h^{ac, +}$, still denoted by $\tilde{\mathcal{H}}_h^{ac, +}$, which G-converges to a positive definite self-adjoint operator $\tilde{\mathcal{H}}^{ac, +}$. Moreover, convergence in the SRS can be drawn for $-\tilde{\mathcal{H}}_h^{ac, -}$,

$$\tilde{\mathcal{H}}_h^{ac, -} = \int_{\lambda \in \sigma_{ac}^-(\tilde{\mathcal{H}}_h)} \lambda dE^{\tilde{\mathcal{H}}_h, ac, -}(\lambda), \quad (75)$$

where $E^{\tilde{\mathcal{H}}_h, ac, -}(\lambda)$ is the absolutely continuous spectral measure corresponding to the operator $\tilde{\mathcal{H}}_h^{ac, -}$.

5 The wave operators for \hbar -dependent self-adjoint operators

Scattering theory is a frame for comparing the dynamic behaviors of two quantum systems, and is well-known as perturbation theory of self-adjoint operators on the absolutely continuous spectrum. More specifically, scattering theory concerns studying the behavior, for large times, of the absolutely continuous solution of the convolution equation $i\partial u/\partial t = Hu = (H_0 + \text{Interaction})u$ in terms of the absolutely continuous solution of the simple convolution equation $i\partial u_0/\partial t = H_0u_0$. Here H_0 and H are self-adjoint operators acting on Hilbert spaces \mathcal{H}_0 and \mathcal{H} respectively. That is, for a given initial solution f to the equation with interaction above, if f is an eigenvector corresponding to an eigenvalue μ , then $u(t) = \exp(-i\mu t)f$, so that the time behavior is clear. But if $f \in \mathcal{H}^{(ac)}$ (the absolutely continuous subspace of H), it is not possible, in general, to calculate $u(t)$ explicitly. Using scattering theory, one may study the asymptotic behavior of $u(t) = \exp(-iHt)f$ as $t \rightarrow \pm\infty$, $f \in \mathcal{H}^{(ac)}$, in terms of $u_0(t) = \exp(-iH_0t)f_0$ for $f_0 \in \mathcal{H}_0^{(ac)}$ (the absolutely continuous subspace of H_0).

5.1 A simple overview

Consider a self-adjoint operator H_0 defined in a Hilbert space \mathcal{H}_0 , and assume that its absolutely continuous spectrum can be identified. Let H be another self-adjoint operator defined in a Hilbert space \mathcal{H} so that H is close to H_0 in a certain sense. Scattering theory concerns the study of the absolutely continuous spectrum of the operator H and its connection to that of H_0 . It is generally assumed that $H = H_0 + V$, where V is, in a particular measure, small compared to H_0 , and thus the deduction of the spectral properties of the absolutely continuous spectrum of H depends on the presumed knowledge of the absolutely continuous spectrum for H_0 .

Consider the free evolution problem

$$\begin{cases} i\frac{\partial}{\partial t}u_0(x,t) = H_0u_0(x,t), \\ u_0(x,0) = u_0^0(x) \end{cases} \quad (76)$$

which has the solution $u_0(t) = e^{-iH_0t}u_0^0$. Let now

$$\begin{cases} i\frac{\partial}{\partial t}u(x,t) = Hu(x,t), \\ u(x,0) = u^0(x) \end{cases} \quad (77)$$

be the evolution problem of the perturbed operator $H = H_0 + V$, which has the solution $u(t) = e^{-iHt}u^0$. The main task of scattering theory is to study the conditions under which, for all $u^0 \in \mathcal{H}^{(ac)}$, there exist $u_0^{0,\pm} \in \mathcal{H}_0^{(ac)}$, such that

$$\lim_{t \rightarrow \pm\infty} \|u(t) - \mathcal{J}u_0(t)\|_{\mathcal{H}} = 0, \quad (78)$$

for a bounded operator \mathcal{J} , where $u_0(t) = e^{-iH_0t}u_0^{0,\pm}$. Equivalently, scattering theory concerns the study of existence and completeness of the wave operator (WO) $W_{\pm}(H, H_0; \mathcal{J})$,

$$W_{\pm}(H, H_0; \mathcal{J}) = s\text{-}\lim_{t \rightarrow \pm\infty} e^{iHt}\mathcal{J}e^{-iH_0t}u_0^{0,\pm}, \quad (79)$$

where the letter s refers to the strong sense convergence.

For comprehensive materials on scattering theory we refer to the monographs [39, 56]. Following the general notation in scattering theory, below we use $s\text{-}\lim$ and $w\text{-}\lim$ to denote the strong and weak limits respectively. Let H and H_0 be self-adjoint operators in \mathcal{H} and \mathcal{H}_0 with spectral families E and E_0 respectively, below we define the time-dependent and stationary WOs.

5.2 The time-dependent WO

There are two types of time-dependent WOs, the strong and weak WOs. In what follows, the strong time-dependent WO will be referred to as just WO.

5.2.1 The strong time-dependent WO

The (modified or generalized) strong time-dependent WO W_{\pm} is defined as follows

Definition 6 Let $\mathcal{J} : \mathcal{H}_0 \rightarrow \mathcal{H}$ be a bounded operator (identification), the WO $W_{\pm} = W_{\pm}(H, H_0; \mathcal{J})$ for H and H_0 is the operator

$$W_{\pm}(H, H_0; \mathcal{J}) = s\text{-}\lim_{t \rightarrow \pm\infty} U(-t)\mathcal{J}U_0(t)P_0^{(ac)}, \quad (80)$$

provided that the corresponding strong limits exist (s refers to the strong sense convergence), where $P_0^{(ac)}$ is the orthogonal projection onto the absolutely continuous subspace $\mathcal{H}_0^{(ac)}$ of H_0 , $U(t) = e^{-iHt}$, and $U_0(t) = e^{-iH_0t}$. If $\mathcal{H} = \mathcal{H}_0$ and \mathcal{J} is the identity operator, then the WO is denoted by $W_{\pm}(H, H_0)$.

The WO $W_{\pm} = W_{\pm}(H, H_0; \mathcal{J})$ is bounded, and possesses the intertwining property, that is, for any bounded Borel function ϕ ,

$$\phi(H)W_{\pm}(H, H_0; \mathcal{J}) = W_{\pm}(H, H_0; \mathcal{J})\phi(H_0), \quad (81)$$

also for any Borel set $\Delta \subset \mathbb{R}$,

$$E(\Delta)W_{\pm}(H, H_0; \mathcal{J}) = W_{\pm}(H, H_0; \mathcal{J})E_0(\Delta). \quad (82)$$

The WO W_{\pm} admits the chain rule, i.e., if $W_{\pm}(H, H_1; \mathcal{J}_1)$ and $W_{\pm}(H_1, H_0; \mathcal{J}_0)$ exist, then the WO $W_{\pm}(H, H_0; \mathcal{J}_{1,0}) = W_{\pm}(H, H_1; \mathcal{J}_1)W_{\pm}(H_1, H_0; \mathcal{J}_0)$ also exists, where $\mathcal{J}_{1,0} = \mathcal{J}_1\mathcal{J}_0$.

Note that $U(-t)U_0(t)$ is unitary, thus the operator $W_{\pm}(H, H_0)$ is isometric. To prove that $W_{\pm}(H, H_0; \mathcal{J})$ is isometric is equivalent to prove that for any $u \in \mathcal{H}_0^{(ac)}$, $\lim_{t \rightarrow \pm\infty} \|\mathcal{J}U_0(t)u\|_{\mathcal{H}} = \|u\|_{\mathcal{H}_0}$.

The following remark states the equivalence between WOs with different identifications.

Remark 3 Assume that, with an identification \mathcal{J}_1 , the WO $W_{\pm}(H, H_0; \mathcal{J}_1)$ exists, and suppose that \mathcal{J}_2 is another identification such that $\mathcal{J}_1 - \mathcal{J}_2$ is compact, then the WO $W_{\pm}(H, H_0; \mathcal{J}_2)$ exists and $W_{\pm}(H, H_0; \mathcal{J}_1) = W_{\pm}(H, H_0; \mathcal{J}_2)$. Moreover, the condition that $\mathcal{J}_1 - \mathcal{J}_2$ is compact can be replaced by $s\text{-}\lim_{t \rightarrow \pm\infty} (\mathcal{J}_1 - \mathcal{J}_2)U_0(t)P_0^{(ac)} = 0$.

Assume the existence of the WO W_{\pm} , another task that is not less important is to show the completeness of W_{\pm} .

Definition 7 The WO W_{\pm} is said to be complete if $\mathbf{R}(W_{\pm}) = \mathcal{H}^{(ac)}$.

If the WO W_{\pm} is complete then the absolutely continuous operators $H^{(ac)}$ and $H_0^{(ac)}$ are unitary equivalent. Since, by the chain rule, $P^{(ac)} = W_{\pm}(H, H) = W_{\pm}(H, H_0)W_{\pm}^*(H, H_0)$ where $P^{(ac)}$ is the orthogonal projection onto the absolutely continuous subspace $\mathcal{H}^{(ac)}$ of H , to prove the completeness of the WO $W_{\pm}(H, H_0)$ is equivalent to prove the existence of the WO $W_{\pm}^*(H, H_0) = W_{\pm}^*(H_0, H)$. On the other hand, the completeness of the WO $W_{\pm}(H, H_0; \mathcal{J})$ is equivalent to the existence of $W_{\pm}(H_0, H; \mathcal{J}^*)$ and that the identification \mathcal{J} is boundedly invertible.

5.2.2 The weak time-dependent WO

The weak time-dependent WO \widetilde{W}_{\pm} is defined as follows

Definition 8 Let $\mathcal{J} : \mathcal{H}_0 \rightarrow \mathcal{H}$ be a bounded identification, the weak WO $\widetilde{W}_\pm(H, H_0; \mathcal{J})$ for H and H_0 is the operator

$$\widetilde{W}_\pm(H, H_0; \mathcal{J}) = w\text{-}\lim_{t \rightarrow \pm\infty} P^{(ac)} U(-t) \mathcal{J} U_0(t) P_0^{(ac)}, \quad (83)$$

provided that the corresponding weak limits exist (w refers to the weak sense convergence).

Note that the boundedness and intertwining properties of the WO W_\pm are preserved for the WO \widetilde{W}_\pm , whereas the chain rule property is not valid for the weak WO. This is evident since the weak limit of the product of two sequences that are only weakly convergent is not necessarily the product of their weak limits. On contrast to W_\pm , if the weak WO $\widetilde{W}_\pm(H, H_0; \mathcal{J})$ exists, then it is necessary that $\widetilde{W}_\pm(H_0, H; \mathcal{J}^*)$ also exists.

5.3 The stationary WO

Let $R(z)$ and $R_0(z)$ be the resolvent operators of H and H_0 respectively, and let M_0 and M be dense sets in \mathcal{H}_0 and \mathcal{H} respectively.

Let $\epsilon > 0$, and let $\theta(\lambda, \epsilon)$ be defined as

$$\theta(\lambda, \epsilon) =: (2\pi i)^{-1} (R(\lambda + i\epsilon) - R(\lambda - i\epsilon)) = \pi^{-1} \epsilon R(\lambda + i\epsilon) R(\lambda - i\epsilon). \quad (84)$$

Further, let \mathfrak{H} be an auxiliary Hilbert space, the concept H -smoothness in the strong and weak senses is defined as follows

Definition 9 An H -bounded operator, $A : \mathcal{H} \rightarrow \mathfrak{H}$, is called H -smooth (in the strong sense) if one of the following bounds is satisfied

$$\sup_{\|v\|_{\mathcal{H}}=1, v \in \mathbf{D}(H)} \int_{-\infty}^{\infty} \|Ae^{-iHt}v\|_{\mathfrak{H}}^2 dt < \infty.$$

$$\sup_{\epsilon > 0, \mu \in \mathbb{R}} \|AR(\mu \pm i\epsilon)\|_{\mathfrak{H}}^2 < \infty.$$

Definition 10 An H -bounded operator, $A : \mathcal{H} \rightarrow \mathfrak{H}$, is called H -smooth in the weak sense if

$$w\text{-}\lim_{\epsilon \rightarrow \infty} A\theta(\lambda, \epsilon)A^* \quad (85)$$

exists for a.e. $\lambda \in \mathbb{R}$.

Equivalent conditions for the weak H -smoothness are stated by the following remark (other conditions can be found in [56]).

Remark 4 An operator $A : \mathcal{H} \rightarrow \mathfrak{H}$ is weakly H -smooth if and only if any of the following two conditions is satisfied

$$\|A\theta(\lambda, \epsilon)A^*\|_{\mathfrak{H}} \leq C(\lambda), \quad \text{a.e. } \lambda \in \mathbb{R}. \quad (86)$$

$$\epsilon^{1/2}\|AR(\lambda \pm i\epsilon)\|_{\mathfrak{H}} \leq C(\lambda), \quad \text{a.e. } \lambda \in \mathbb{R}. \quad (87)$$

To define the stationary WO, we first define the following

$$\mathcal{G}_{\pm}(H, H_0; \mathcal{J}) = \lim_{\epsilon \rightarrow 0} \pi^{-1} \epsilon \langle \mathcal{J}R_0(\lambda \pm i\epsilon)u_0, R(\lambda \pm i\epsilon)u \rangle. \quad (88)$$

Let, for all $u_0 \in M_0$ and $u \in M$, the limit (88) exist for a.e. $\lambda \in \mathbb{R}$, then the stationary WO $\mathcal{W}_{\pm} = \mathcal{W}_{\pm}(H, H_0; \mathcal{J})$ for the operators H and H_0 with the identification \mathcal{J} is the operator on $M_0 \times M$ defined by the following sesquilinear form

$$\langle \mathcal{W}_{\pm}u_0, u \rangle = \int_{-\infty}^{\infty} \mathcal{G}_{\pm}(H, H_0; \mathcal{J})d\lambda. \quad (89)$$

The WO \mathcal{W}_{\pm} is bounded, satisfies the intertwining property, and $\mathbf{R}(\mathcal{W}_{\pm}) \subseteq \mathcal{H}^{(ac)}$. Moreover, by the existence of $\mathcal{W}_{\pm}(H, H_0; \mathcal{J})$, then the adjoint WO $\mathcal{W}_{\pm}^*(H, H_0; \mathcal{J})$ also exists and given by

$$\mathcal{W}_{\pm}^*(H, H_0; \mathcal{J}) = \mathcal{W}_{\pm}(H_0, H; \mathcal{J}^*). \quad (90)$$

The importance of the stationary approach in scattering theory can be summarized as:

Let the WOs $\widetilde{\mathcal{W}}_{\pm}(H, H_0; \mathcal{J})$ and $\widetilde{\mathcal{W}}_{\pm}(H_0, H_0; \mathcal{J}^*\mathcal{J})$ exist, and let

$$\mathcal{W}_{\pm}^*(H, H_0; \mathcal{J})\mathcal{W}_{\pm}(H, H_0; \mathcal{J}) = \mathcal{W}_{\pm}(H_0, H_0; \mathcal{J}^*\mathcal{J}) \quad (91)$$

be satisfied, then the WO $\mathcal{W}_{\pm}(H, H_0; \mathcal{J})$ exists.

Below we define a particular class of pseudo-differential operators (PSDOs) necessary to state the results on the convergence of the WOs for a family of Dirac operators.

5.4 Pseudo-differential operators

The class $\mathcal{S}_{\rho, \delta}^r(\mathbb{R}^3, \mathbb{R}^3)$ of symbols is defined as follows

Definition 11 The class $\mathcal{S}_{\rho,\delta}^r(\mathbb{R}^3, \mathbb{R}^3)$ is the vector space of all smooth functions $\mathcal{P}(x, \zeta) : \mathbb{R}^3 \times \mathbb{R}^3 \rightarrow \mathbb{C}$ such that for all multi-indices α and γ

$$|\partial_x^\alpha \partial_\zeta^\gamma \mathcal{P}(x, \zeta)| \leq c_{\alpha,\gamma} \langle x \rangle^{r-\rho|\alpha|+\delta|\gamma|}, \quad (92)$$

where $r \in \mathbb{R}$, $\rho > 0$, $\delta < 1$, and $\langle x \rangle = (1 + |x|^2)^{1/2}$. The function \mathcal{P} is called the symbol of the PSDO and r is called the order of \mathcal{P} .

Let $\mathcal{P}(x, \zeta) \in \mathcal{S}_{\rho,\delta}^r(\mathbb{R}^3, \mathbb{R}^3)$, the associated PSDO, \mathcal{P} , to \mathcal{P} is defined by the following integral

$$(\mathcal{P}f)(x) = (2\pi)^{-3/2} \int_{\mathbb{R}^3} e^{ix \cdot \zeta} \mathcal{P}(x, \zeta) \hat{f}(\zeta) d\zeta, \quad (93)$$

where $f \in \mathcal{H}$ and $\hat{f}(\zeta) = (2\pi)^{-3/2} \int_{\mathbb{R}^3} e^{-ix \cdot \zeta} f(x) dx$ is the Fourier transform of f .

5.5 A family of Dirac operators

Consider the free Dirac operator \mathbf{H}_0 , and let \mathbf{V} be a short-range potential (decaying faster than the Coulomb potential), then the WO $W_\pm(\mathbf{H}_0 + \mathbf{V}, \mathbf{H}_0)$ exists and is complete. The proofs of existence and completeness of $W_\pm(\mathbf{H}_0 + \mathbf{V}, \mathbf{H}_0)$ are similar to that of the Schrödinger operator. For \mathbf{V} being the Coulomb potential, the WO $W_\pm = W_\pm(\mathbf{H}_0 + \mathbf{V}, \mathbf{H}_0; \mathcal{J})$, with a bounded identification \mathcal{J} , has been studied in [15, 16]. If \mathbf{V} is of long-range type (decaying as the Coulomb potential or slower), the existence and completeness of the WO W_\pm have been studied in [21, 36, 37, 51]. The asymptotic behavior of the WO W_\pm with respect to the speed of light, c , as $c \rightarrow \infty$, has been discussed for the short-range potentials in [57] and for the long-range potentials in [58].

5.5.1 An h -dependent perturbation and the WO

Consider the free Dirac operator \mathbf{H}_0 , and let \mathbf{V}_h be an h -dependent potential. We define the following family of Dirac operators

$$\mathbf{H}_h = \mathbf{H}_0 + \mathbf{V}_h. \quad (94)$$

We assume the potential \mathbf{V}_h is real and bounded, thus the operators \mathbf{H}_h and \mathbf{H}_0 have the same domain X and that \mathbf{H}_h is self-adjoint on X , for $h > 0$. Also, for simplicity, we let $\hbar = c = 1$.

We assume further that \mathbf{V}_h is of long-range type for all $h > 0$, that is, for all multi-index α , \mathbf{V}_h fulfills the following condition

$$|\partial^\alpha \mathbf{V}_h(x)| \leq C \langle x \rangle^{-\rho-|\alpha|}, \quad \text{for all } h > 0, \text{ and } \rho \in (0, 1], \quad (95)$$

where again $\langle x \rangle = (1 + |x|^2)^{1/2}$, and C is a constant independent of x and h .

Let $P_h^{(ac)}$ be the orthogonal projection onto the absolutely continuous subspace of \mathbf{H}_h , and define $U_h(t) = e^{-i\mathbf{H}_h t}$ and $U_0(t) = e^{-i\mathbf{H}_0 t}$. Now, by (95), and according to [21], the WOs $W_{\pm, h}$ and $W_{\pm, h}^*$, defined as

$$W_{\pm, h} = W_{\pm}(\mathbf{H}_h, \mathbf{H}_0; \mathcal{J}_{\pm, h}) = s\text{-}\lim_{t \rightarrow \pm\infty} U_h(-t) \mathcal{J}_{\pm, h} U_0(t) \quad (96)$$

and

$$W_{\pm, h}^* = W_{\pm}(\mathbf{H}_0, \mathbf{H}_h; \mathcal{J}_{\pm, h}^*) = s\text{-}\lim_{t \rightarrow \pm\infty} U_0(-t) \mathcal{J}_{\pm, h}^* U_h(t) P_h^{(ac)}, \quad (97)$$

exist, moreover the WO $W_{\pm, h}$ is complete. The identification $\mathcal{J}_{\pm, h}$ is defined by the following PSDO

$$(\mathcal{J}_{\pm, h} g)(x) = (2\pi)^{-3/2} \int_{\mathbb{R}^3} e^{ix \cdot \zeta + i\Phi_{\pm, h}(x, \zeta)} \mathcal{P}_{\pm, h}(x, \zeta) \mathcal{C}_{\pm}(x, \zeta) \psi(|\zeta|^2) \hat{g}(\zeta) d\zeta, \quad (98)$$

where $\psi \in C_0^\infty(\mathbb{R}_+)$ is introduced to localize $\mathcal{J}_{\pm, h}$ in a compact interval of (m, ∞) and where $\mathcal{C}_{\pm}(x, \zeta)$ is a cut-off function defined as

$$\mathcal{C}_{\pm}(x, \zeta) = \theta(x) \omega_{\pm}(\langle \check{x}, \check{\zeta} \rangle), \quad \text{for all } y \in \mathbb{R}^3 \setminus \{0\}, \check{y} = y/|y|. \quad (99)$$

The function θ is smooth and is introduced to avoid the singularity of \check{x} at $x = 0$, and $\omega_{\pm}(\tau) = 1$ near ± 1 and $\omega_{\pm}(\tau) = 0$ near ∓ 1 . Thus the cut-off function \mathcal{C}_{\pm} is supported in the cone

$$\Xi_{\pm}(\varrho) = \{(x, \zeta) \in \mathbb{R}^6 : \pm \langle x, \zeta \rangle \geq \varrho |x| |\zeta|\}, \quad \varrho \in (-1, 1). \quad (100)$$

Below, in a chain of definitions, we give the construction of the phase function $\Phi_{\pm, h}(x, \zeta)$ and the amplitude function $\mathcal{P}_{\pm, h}(x, \zeta)$. The function $\Phi_{\pm, h}(x, \zeta)$ is defined as follows

$$\Phi_{\pm, h}(x, \zeta) = \sum_{n=1}^N \Phi_{\pm, h}^{(n)}(x, \zeta), \quad x \in \Xi_{\pm}(\varrho), \quad (101)$$

where N satisfies $(N+1)\rho > 1$, and for $n \geq 0$, $\Phi_{\pm, h}^{(n+1)}(x, \zeta) = Q_{\pm}(\zeta) F_{\pm, h}^{(n)}$,

$$(Q_{\pm}(\zeta) F)(x) = \pm \int_0^\infty (F(x \pm t\zeta, \zeta) - F(\pm t\zeta, \zeta)) dt. \quad (102)$$

The functions $F_{\pm,h}^{(n)}$ are defined as

$$F_{\pm,h}^{(0)}(x, \zeta) = \eta(\zeta)V_h(x) - \frac{1}{2}V_h^2(x), \quad F_{\pm,h}^{(1)}(x, \zeta) = \frac{1}{2}|\nabla\Phi_{\pm,h}^{(1)}(x, \zeta)|^2, \quad (103)$$

and for $n \geq 2$

$$F_{\pm,h}^{(n)}(x, \zeta) = \sum_{k=1}^{n-1} \langle \nabla\Phi_{\pm,h}^{(k)}(x, \zeta), \nabla\Phi_{\pm,h}^{(n)}(x, \zeta) \rangle + \frac{1}{2}|\nabla\Phi_{\pm,h}^{(n)}(x, \zeta)|^2. \quad (104)$$

The amplitude function $\mathcal{P}_{\pm,h}(x, \zeta)$ is defined by

$$\mathcal{P}_{\pm,h}(x, \zeta) = (I - S_{\pm,h}(x, \zeta))^{-1}p_0(\zeta), \quad x \in \Xi_{\pm}(\varrho), \quad (105)$$

where $p_0(\zeta) = p_{+,0}(\zeta)$, and

$$p_{\pm,0}(\zeta) = \frac{1}{2}(I \pm \eta^{-1}(\zeta)(\zeta_{\alpha} + mc^2\beta)), \quad (106)$$

with $\eta(\zeta) = \sqrt{|\zeta|^2 + m^2c^4}$ and $\zeta_{\alpha} = \alpha \cdot \zeta = \sum_{k=1}^3 \alpha_k \zeta_k$. Finally, $S_{\pm,h}(x, \zeta)$ is given by

$$S_{\pm,h}(x, \zeta) = (2\eta(\zeta))^{-1} \left(V_h(x) + \sum_{k=1}^3 \partial_k \Phi_{\pm,h}(x, \zeta) \alpha_k \right), \quad x \in \Xi_{\pm}(\varrho). \quad (107)$$

Note that the WOs defined above are for positive part of the spectrum (m, ∞) . For the negative part of the spectrum $(-\infty, -m)$, the WOs can be defined in a similar way with minor modifications, see [21]. The asymptotic study carried out below can be applied for the WOs on the negative part as well.

5.5.2 The asymptotics of the WOs and some particular cases

Define the WOs $W_{\pm}^{\dagger} := s\text{-}\lim_{h \rightarrow \infty} W_{\pm,h}$ and $W_{\pm}^{\dagger,*} := s\text{-}\lim_{h \rightarrow \infty} W_{\pm,h}^*$. Let the perturbed Dirac operator \mathbf{H}_h converge in the SRS to \mathbf{H}_{∞} , and assume that the identification $\mathcal{J}_{\pm,h}$ converges strongly to $\mathcal{J}_{\pm,\infty}$, then the WOs W_{\pm}^{\dagger} and $W_{\pm}^{\dagger,*}$ exist. The task now is to characterize the limits, as $h \rightarrow \infty$, of the WOs $W_{\pm,h}$ and $W_{\pm,h}^*$, which is equivalent to the problem of interchanging $s\text{-}\lim_{h \rightarrow \infty}$ and $s\text{-}\lim_{t \rightarrow \pm\infty}$. To this end, we state the following two lemmas.

Lemma 1 Define the function $\mathcal{K}_{u_0,h}^{(1)}$ as

$$\mathcal{K}_{u_0,h}^{(1)}(t) = \left\| \left(H_h \phi(H_h) \mathcal{J}_{\pm,h} \phi(H_0) - \phi(H_h) \mathcal{J}_{\pm,h} H_0 \phi(H_0) \right) U_0(t) u_0 \right\|_Y,$$

where $u_0 \in X$. Then for some continuous function $\phi : \mathbb{R} \rightarrow \mathbb{R}$ such that $x\phi(x)$ is bounded on \mathbb{R} and for any $\varepsilon > 0$ there exist $D_1, D_2 \in \mathbb{R}$ such that $\int_{D_1}^{\infty} \mathcal{K}_{u_0,h}^{(1)}(t) dt \leq \varepsilon$ and $\int_{-\infty}^{D_2} \mathcal{K}_{u_0,h}^{(1)}(t) dt \leq \varepsilon$ for all $h > 0$.

Lemma 2 Define the function $\mathcal{K}_{u,h}^{(2)}$ as

$$\mathcal{K}_{u,h}^{(2)}(t) = \left\| \left(H_0 \phi(H_0) \mathcal{J}_{\pm,h}^* \phi(H_h) - \phi(H_0) \mathcal{J}_{\pm,h}^* H_h \phi(H_h) \right) U_h(t) u \right\|_Y,$$

where $u_0 \in X$. Then for some continuous function $\phi : \mathbb{R} \rightarrow \mathbb{R}$ such that $x\phi(x)$ is bounded on \mathbb{R} and for any $\varepsilon > 0$ there exist $D_3, D_4 \in \mathbb{R}$ such that $\int_{D_3}^{\infty} \mathcal{K}_{u,h}^{(2)}(t) dt \leq \varepsilon$ and $\int_{-\infty}^{D_4} \mathcal{K}_{u,h}^{(2)}(t) dt \leq \varepsilon$ for all $h > 0$.

By Lemmas 1 and 2, and according to [9], the limits $s\text{-}\lim_{h \rightarrow \infty}$ and $s\text{-}\lim_{t \rightarrow \pm\infty}$ in the definition of the WOs W_{\pm}^{\dagger} and $W_{\pm}^{\dagger,*}$ are interchangeable. Thus we have the following result.

Theorem 13 Let the WOs $W_{\pm,h}$ and $W_{\pm,h}^*$ be defined by (96) and (97) respectively. Suppose that, as $h \rightarrow \infty$, the Dirac operator \mathbf{H}_h converges to \mathbf{H}_{∞} in the SRS, and the identification $\mathcal{J}_{\pm,h}$ converges strongly to $\mathcal{J}_{\pm,\infty}$. Then the WOs W_{\pm}^{\dagger} and $W_{\pm}^{\dagger,*}$ exist,

$$W_{\pm}^{\dagger} = W_{\pm}(\mathbf{H}_{\infty}, \mathbf{H}_0; \mathcal{J}_{\pm,\infty}),$$

and

$$W_{\pm}^{\dagger,*} = W_{\pm}(\mathbf{H}_0, \mathbf{H}_{\infty}; \mathcal{J}_{\pm,\infty}^*).$$

Remark 5 In Theorem 13 we assume that $\mathcal{J}_{\pm,h}$ converges strongly to $\mathcal{J}_{\pm,\infty}$, this also implies that $\mathcal{J}_{\pm,h}^*$ converges strongly to $\mathcal{J}_{\pm,\infty}^*$. However, in general, the strong convergence of an operator does not imply the strong convergence of its adjoint operator to the adjoint of its strong limit. Hence, in order to study the convergence of the adjoint WO in the strong sense for other self-adjoint operators, we should assume if necessary, the strong convergence of the identifications adjoint operators as well.

In what follows we assume the hypotheses of Theorem 13 and study different cases of the identification $\mathcal{J}_{\pm,h}$. Noted that, in the first case we also consider short-range potentials, so the identification is just the identity operator. On the other hand, the other two cases are stated briefly, where a dwell-upon discussion is available in Paper V in the appendix.

The case $\rho > 1$.

In this case we can set $\mathcal{J}_{\pm,h} = I$, this due to the fact that for short-range potentials, the WOs $W_{\pm}(\mathbf{H}_h, \mathbf{H}_0)$ and $W_{\pm}(\mathbf{H}_0, \mathbf{H}_h)$ exist and are complete. Therefore the limits $s\text{-}\lim_{h \rightarrow \infty}$ and $s\text{-}\lim_{t \rightarrow \pm\infty}$ are interchangeable in the definitions of the WOs W_{\pm}^{\dagger} and $W_{\pm}^{\dagger,*}$. Thus, if \mathbf{H}_h is convergent to \mathbf{H}_{∞} in the SRS, then

$$W_{\pm}^{\dagger} = W_{\pm}(\mathbf{H}_{\infty}, \mathbf{H}_0) \quad (108)$$

and

$$W_{\pm}^{\dagger,*} = W_{\pm}(\mathbf{H}_0, \mathbf{H}_{\infty}). \quad (109)$$

The case $\rho = 1$.

Let $\Phi_{\pm}(x, \zeta)$ be an h -free function satisfying

$$|\partial_x^{\alpha} \partial_{\zeta}^{\gamma} \Phi_{\pm}(x, \zeta)| \leq c_{\alpha,\gamma} \langle x \rangle^{1-\rho-|\alpha|}, \quad x \in \Xi_{\pm}(\varrho), \quad (110)$$

and let $\mathcal{J}_{\pm}^{(1)}$ (with adjoint denoted by $\mathcal{J}_{\pm}^{(1),*}$) be defined as

$$(\mathcal{J}_{\pm}^{(1)} g)(x) = (2\pi)^{-3/2} \int_{\mathbb{R}^3} e^{ix \cdot \zeta + i\Phi_{\pm}(x, \zeta)} p_0(\zeta) \mathcal{C}_{\pm}(x, \zeta) \psi(|\zeta|^2) \hat{g}(\zeta) d\zeta. \quad (111)$$

Then

$$W_{\pm}^{\dagger} = W_{\pm}(\mathbf{H}_{\infty}, \mathbf{H}_0; \mathcal{J}_{\pm}^{(1)}) \quad (112)$$

and

$$W_{\pm}^{\dagger,*} = W_{\pm}(\mathbf{H}_0, \mathbf{H}_{\infty}; \mathcal{J}_{\pm}^{(1),*}). \quad (113)$$

The case $\rho \in (1/2, 1)$.

Let $\mathcal{J}_{\pm,h}^{(2)}$ (with adjoint denoted by $\mathcal{J}_{\pm}^{(2),*}$) be given by (98), but with $\Phi_{\pm,h}(x, \zeta)$ defined as

$$\Phi_{\pm,h}(x, \zeta) = \pm \eta(\zeta) \int_0^{\infty} (\mathbf{V}_h(x \pm t\zeta) - \mathbf{V}_h(\pm t\zeta)) dt \quad (114)$$

and with $p_0(\zeta)$ instead of $\mathcal{P}_{\pm,h}(x, \zeta)$. Assume further that \mathbf{V}_h is given so that $\mathbf{H}_h = \mathbf{H}_0 + \mathbf{V}_h$ and $\Phi_{\pm,h}(x, \zeta)$ converge in the SRS respectively to $\mathbf{H}_{\infty} = \mathbf{H}_0 + \mathbf{V}_{\infty}$ and

$$\Phi_{\pm,\infty}(x, \zeta) = \pm \eta(\zeta) \int_0^{\infty} (\mathbf{V}_{\infty}(x \pm t\zeta) - \mathbf{V}_{\infty}(\pm t\zeta)) dt. \quad (115)$$

Then

$$W_{\pm}^{\dagger} = W_{\pm}(\mathbf{H}_{\infty}, \mathbf{H}_0; \mathcal{J}_{\pm, \infty}^{(2)}) \quad (116)$$

and

$$W_{\pm}^{\dagger, *} = W_{\pm}(\mathbf{H}_0, \mathbf{H}_{\infty}; \mathcal{J}_{\pm, \infty}^{(2), *}), \quad (117)$$

where

$$(\mathcal{J}_{\pm, \infty}^{(2)}g)(x) = (2\pi)^{-3/2} \int_{\mathbb{R}^3} e^{ix \cdot \zeta + i\Phi_{\pm, \infty}(x, \zeta)} p_0(\zeta) \mathcal{C}_{\pm}(x, \zeta) \psi(|\zeta|^2) \hat{g}(\zeta) d\zeta. \quad (118)$$

5.6 Self-adjoint h -dependent operators

Let \mathcal{H}_0 and \mathcal{H} be two Hilbert spaces, and let M_0 and M be dense sets in \mathcal{H}_0 and \mathcal{H} respectively. Let H_0 and H_h be two self-adjoint operators in \mathcal{H}_0 and \mathcal{H} respectively, with $\mathbf{D}(H_0) = \mathcal{X}_0$ and $\mathbf{D}(H_h) = \mathcal{X}$, and with corresponding resolvent operators R_0 and R_h respectively. Let also $P_0^{(ac)}$ and $P_h^{(ac)}$ be respectively the orthogonal projections onto the absolutely continuous subspaces of H_0 and H_h . Assume that $H_h = H_0 + V_h$, where V_h admits the following factorization

$$V_h = H_h \mathcal{J}_h - \mathcal{J}_h H_0 = A_h^* A_0, \quad (119)$$

where $\mathcal{J}_h : \mathcal{H}_0 \rightarrow \mathcal{H}$ is a bounded identification, and $A_h : \mathcal{H} \rightarrow \mathfrak{H}$ and $A_0 : \mathcal{H}_0 \rightarrow \mathfrak{H}$ are respectively H_h -bounded, for all $h > 0$, and H_0 -bounded operators, where \mathfrak{H} is an auxiliary Hilbert space. Note that (119) is understood as the equalities of the corresponding sesquilinear forms.

Define the time-dependent WO $W_{\pm}^{\dagger}(H, H_0; \mathcal{J})$ as

$$\begin{aligned} W_{\pm}^{\dagger}(H, H_0; \mathcal{J}) &= s\text{-}\lim_{h \rightarrow \infty} W_{\pm}(H_h, H_0; \mathcal{J}_h) \\ &= s\text{-}\lim_{h \rightarrow \infty} s\text{-}\lim_{t \rightarrow \pm\infty} U_h(-t) \mathcal{J}_h U_0(t) P_0^{(ac)}, \end{aligned} \quad (120)$$

where $U_h(t) = e^{-iH_h t}$, $U_0(t) = e^{-iH_0 t}$, and H and \mathcal{J} are limit operators in appropriate sense of H_h and \mathcal{J}_h respectively.

Let $\mathcal{G}_{\pm}^{\dagger}(H, H_0; \mathcal{J})$ be defined as

$$\mathcal{G}_{\pm}^{\dagger}(H, H_0; \mathcal{J}) = \lim_{h \rightarrow \infty} \lim_{\epsilon \rightarrow 0} \pi^{-1} \epsilon \langle \mathcal{J}_h R_0(\lambda \pm i\epsilon) u_0, R_h(\lambda \pm i\epsilon) u \rangle, \quad (121)$$

where $u_0 \in M_0$ and $u \in M$. We define the stationary WO $\mathcal{W}_{\pm}^{\dagger} = \mathcal{W}_{\pm}^{\dagger}(H, H_0; \mathcal{J})$ on $M_0 \times M$ by the sesquilinear form

$$\langle \mathcal{W}_{\pm}^{\dagger} u_0, u \rangle = \int_{-\infty}^{\infty} \mathcal{G}_{\pm}^{\dagger}(H, H_0; \mathcal{J}) d\lambda. \quad (122)$$

We also define the weak WO $\widetilde{W}_{\pm}^{\dagger}(H, H_0; \mathcal{J})$ as

$$\begin{aligned}\widetilde{W}_{\pm}^{\dagger}(H, H_0; \mathcal{J}) &= w\text{-}\lim_{h \rightarrow \infty} \widetilde{W}_{\pm}(H_h, H_0; \mathcal{J}_h) \\ &= w\text{-}\lim_{h \rightarrow \infty} w\text{-}\lim_{t \rightarrow \pm\infty} P_h^{(ac)} U_h(-t) \mathcal{J}_h U_0(t) P_0^{(ac)}.\end{aligned}\quad (123)$$

In the coming discussion we state some results regarding the existence of the WOs $\mathcal{W}_{\pm}^{\dagger}$, $\widetilde{W}_{\pm}^{\dagger}$, W_{\pm}^{\dagger} , and their adjoint operators that are denoted respectively by $\mathcal{W}_{\pm}^{\dagger,*}$, $\widetilde{W}_{\pm}^{\dagger,*}$, and $W_{\pm}^{\dagger,*}$, see Paper VI in the appendix for more details.

Theorem 14 Assume the following

- (i) A_0 is weakly H_0 -smooth.
- (ii) For all $h > 0$, $A_h R_h(\lambda \pm i\epsilon)$ is strongly convergent as $\epsilon \rightarrow 0$ for a.e. $\lambda \in \mathbb{R}$.
- (iii) If T_h is the strong limit of $A_h R_h(\lambda \pm i\epsilon)$ as $\epsilon \rightarrow 0$ obtained in (ii), T_h converges weakly to some T_{∞} for a.e. $\lambda \in \mathbb{R}$.
- (iv) \mathcal{J}_h converges weakly to \mathcal{J}_{∞} .

Then the WO $\mathcal{W}_{\pm}^{\dagger}(H, H_0; \mathcal{J})$ exists, also $\mathcal{W}_{\pm}^{\dagger}(H_0, H; \mathcal{J}^*)$ exists and

$$\mathcal{W}_{\pm}^{\dagger,*}(H, H_0; \mathcal{J}) = \mathcal{W}_{\pm}^{\dagger}(H_0, H; \mathcal{J}^*). \quad (124)$$

Note that the assertions of Theorem 14 remain unchanged if its first three hypotheses are replaced by; for a.e. $\lambda \in \mathbb{R}$, as $\epsilon \rightarrow 0$, the operator $A_0 \theta_0(\lambda, \epsilon)$ is strongly convergent and $T_{h,\epsilon} := A_h R_h(\lambda \pm i\epsilon)$ is weakly convergent to some $T_{h,0}$ for all $h > 0$, and $T_{h,0}$ converges weakly to some $T_{\infty,0}$ as $h \rightarrow \infty$.

Similar assertions as of Theorem 14 can be formulated as in the following theorem.

Theorem 15 Assume the following

- (i) For all $h > 0$, A_h is weakly H_h -smooth.
- (ii) The operator $A_0 R_0(\lambda \pm i\epsilon)$ is strongly convergent as $\epsilon \rightarrow 0$ for a.e. $\lambda \in \mathbb{R}$.
- (iii) If T_h is the weak limit of $A_h \theta_h(\lambda, \epsilon)$ as $\epsilon \rightarrow 0$ obtained in (i), T_h converges weakly to some T_{∞} for a.e. $\lambda \in \mathbb{R}$.
- (iv) If E_h is the spectral family of H_h , then $E_h(\lambda)$ and \mathcal{J}_h converge weakly to $E_{\infty}(\lambda)$ and \mathcal{J}_{∞} respectively for a.e. $\lambda \in \mathbb{R}$.

Then the WO $\mathcal{W}_{\pm}^{\dagger}(H, H_0; \mathcal{J})$ exists, also $\mathcal{W}_{\pm}^{\dagger}(H_0, H; \mathcal{J}^*)$ exists and

$$\mathcal{W}_{\pm}^{\dagger,*}(H, H_0; \mathcal{J}) = \mathcal{W}_{\pm}^{\dagger}(H_0, H; \mathcal{J}^*). \quad (125)$$

The assertions of Theorem 15 are also true if its first three hypotheses are replaced by the following; for a.e. $\lambda \in \mathbb{R}$, as $\epsilon \rightarrow 0$, the operator $A_0 R_0(\lambda \pm i\epsilon)$ is weakly convergent and $S_{h,\epsilon} := A_h \theta_h(\lambda, \epsilon)$ is strongly convergent to some $S_{h,0}$ for all $h > 0$, and $S_{h,0}$ converges weakly to some $S_{\infty,0}$ as $h \rightarrow \infty$.

The existence of $\mathcal{W}_{\pm}^{\dagger}(H, H; \mathcal{J}\mathcal{J}^*)$ and $\mathcal{W}_{\pm}^{\dagger}(H_0, H_0; \mathcal{J}^*\mathcal{J})$ is proved in Theorems 16 and 17 respectively.

Theorem 16 Let the hypotheses of Theorem 14 be satisfied, and let further \mathcal{J}_h^* and R_h be strongly convergent. Then the WO $\mathcal{W}_{\pm}^{\dagger}(H, H; \mathcal{J}\mathcal{J}^*)$ exists and

$$\mathcal{W}_{\pm}^{\dagger}(H, H_0; \mathcal{J})\mathcal{W}_{\pm}^{\dagger,*}(H, H_0; \mathcal{J}) = \mathcal{W}_{\pm}^{\dagger}(H, H; \mathcal{J}\mathcal{J}^*). \quad (126)$$

Theorem 17 Let the hypotheses of Theorem 15 be satisfied, and let \mathcal{J}_h be strongly convergent. Then the WO $\mathcal{W}_{\pm}^{\dagger}(H_0, H_0; \mathcal{J}^*\mathcal{J})$ exists and

$$\mathcal{W}_{\pm}^{\dagger,*}(H, H_0; \mathcal{J})\mathcal{W}_{\pm}^{\dagger}(H, H_0; \mathcal{J}) = \mathcal{W}_{\pm}^{\dagger}(H_0, H_0; \mathcal{J}^*\mathcal{J}). \quad (127)$$

One of the important results is the equivalence between the stationary WO $\mathcal{W}_{\pm}^{\dagger}$ and the weak time-dependent WO $\widetilde{\mathcal{W}}_{\pm}^{\dagger}$, that is, if both $\mathcal{W}_{\pm}^{\dagger}(H, H_0; \mathcal{J})$ and $\widetilde{\mathcal{W}}_{\pm}^{\dagger}(H, H_0; \mathcal{J})$ exist, then their sesquilinear forms are equivalent to each other. The same conclusion can be drawn for the pairs $(H_0, H; \mathcal{J}^*)$, $(H_0, H_0; \mathcal{J}^*\mathcal{J})$, and $(H, H; \mathcal{J}\mathcal{J}^*)$.

Also, by the hypotheses of Theorem 14 (equivalently Theorem 15), the WO $\widetilde{\mathcal{W}}_{\pm}^{\dagger}(H, H_0; \mathcal{J})$ exists, consequently $\widetilde{\mathcal{W}}_{\pm}^{\dagger}(H_0, H; \mathcal{J}^*)$ exists and

$$\widetilde{\mathcal{W}}_{\pm}^{\dagger,*}(H, H_0; \mathcal{J}) = \widetilde{\mathcal{W}}_{\pm}^{\dagger}(H_0, H; \mathcal{J}^*). \quad (128)$$

For the WOs $\widetilde{\mathcal{W}}_{\pm}^{\dagger}(H, H; \mathcal{J}\mathcal{J}^*)$ and $\widetilde{\mathcal{W}}_{\pm}^{\dagger}(H_0, H_0; \mathcal{J}^*\mathcal{J})$, we have the following two theorems.

Theorem 18 Suppose the hypotheses of Theorem 16 are satisfied, then the WO $\widetilde{\mathcal{W}}_{\pm}^{\dagger}(H, H; \mathcal{J}\mathcal{J}^*)$ exists.

Theorem 19 Suppose the hypotheses of Theorem 17 are satisfied, then the WO $\widetilde{\mathcal{W}}_{\pm}^{\dagger}(H_0, H_0; \mathcal{J}^*\mathcal{J})$ exists.

The existence of the time-dependent WOs $W_{\pm}^{\dagger}(H, H_0; \mathcal{J})$ and $W_{\pm}^{\dagger}(H_0, H; \mathcal{J}^*)$ is summarized in the following theorems.

Theorem 20 If the hypotheses of Theorem 16 are satisfied, then $W_{\pm}^{\dagger}(H_0, H; \mathcal{J}^*)$ exists.

Theorem 21 If the hypotheses of Theorem 17 are satisfied, then $W_{\pm}^{\dagger}(H, H_0; \mathcal{J})$ exists.

After proving the existence of the WOs $W_{\pm}^{\dagger}(H, H_0; \mathcal{J})$ and $W_{\pm}^{\dagger}(H_0, H; \mathcal{J}^*)$, we would like to study the asymptotic behavior, as $h \rightarrow \infty$, of the WOs $W_{\pm}(H_h, H_0; \mathcal{J}_h)$ and $W_{\pm}(H_0, H_h; \mathcal{J}_h^*)$. The problem of finding these asymptotic limits is reduced, as we mentioned before, to the problem of interchanging $s\text{-}\lim_{h \rightarrow \infty}$ and $s\text{-}\lim_{t \rightarrow \pm\infty}$. By the existence of $W_{\pm}^{\dagger}(H, H_0; \mathcal{J})$ and $W_{\pm}^{\dagger}(H_0, H; \mathcal{J}^*)$, Lemmas 1 and 2 are satisfied for the collections $(H_h, H_0, \mathcal{J}_h, \mathcal{H})$ and $(H_0, H_h, \mathcal{J}_h^*, \mathcal{H}_0)$ respectively. This implies that, according to [9], in the definitions of $W_{\pm}^{\dagger}(H, H_0; \mathcal{J})$ and $W_{\pm}^{\dagger}(H_0, H; \mathcal{J}^*)$, the limits $s\text{-}\lim_{h \rightarrow \infty}$ and $s\text{-}\lim_{t \rightarrow \pm\infty}$ are interchangeable. Therefore, if H_h converges to H_{∞} in the SRS, and \mathcal{J}_h and \mathcal{J}_h^* converge strongly to \mathcal{J}_{∞} and \mathcal{J}_{∞}^* respectively, then

$$s\text{-}\lim_{h \rightarrow \infty} W_{\pm}(H_h, H_0; \mathcal{J}_h) = W_{\pm}(H_{\infty}, H_0; \mathcal{J}_{\infty}) \quad (129)$$

and

$$s\text{-}\lim_{h \rightarrow \infty} W_{\pm}(H_0, H_h; \mathcal{J}_h^*) = W_{\pm}(H_0, H_{\infty}; \mathcal{J}_{\infty}^*). \quad (130)$$

References

- [1] E. Ackad and M. Horbatsch, *Numerical solution of the Dirac equation by a mapped fourier grid method*, J. Phys. A: Math. Gen., 38(2005), pp. 3157-3171.
- [2] R. C. Almeida and R. S. Silva, *A stable Petrov-Galerkin method for convection-dominated problems*, Comput. Methods Appl. Mech. Engng., 140(1997).
- [3] S. N. Atluri and S. Shen, *The meshless local Petrov-Galerkin (MLPG) method: A simple and less-costly alternative to the finite element and boundary element methods*, CMES, 3(2002), pp. 11-51.
- [4] T. Belytschko, D. Organ, and Y. Krongauz, *A coupled finite element-element-free Galerkin method*, Comput. Mech., 17(1995), pp. 186-195.
- [5] T. Belytschko, Y. Krongauz, D. Organ, M. Fleming, and P. Krysl, *Meshless methods: An overview and recent developments*, Comput. Methods Appl. Mech. Engng., 139(1996), pp. 3-47.
- [6] M. S. Birman and M. Z. Solomjak, *Spectral Theory of Self-adjoint Operators in Hilbert Space*, D. Reidel Publishing Company, Dordrecht, Holland, 1987.
- [7] L. Boulton and M. Levitin, *Trends and Tricks in Spectral Theory*, Ediciones IVIC, Caracas, Venezuela, 2007.
- [8] A. Braides, *Γ -convergence for Beginners*, Oxford University Press Inc., New York, 2002.
- [9] E. Brüning and F. Gesztesy, *Continuity of wave and scattering operators with respect to interactions*, J. Math. Phys., 24(1983), pp. 1516-1528.
- [10] J. S. Chen, W. Hu, and M. A. Puso, *Orbital hp-clouds for solving Schrödinger equation in quantum mechanics*, Comput. Methods Appl. Mech. Engng., 196(2007), pp. 3693-3705.
- [11] G. Dal Maso, *An Introduction to Γ -convergence*, Birkhäuser, Boston, 1993.

- [12] E. De Giorgi and T. Franzoni, *Su un tipo convergenza variazionale*, Atti Accad. Naz. Lincei Rend. Cl. Sci. Mat. 58(1975), pp. 842-850.
- [13] E. De Giorgi and S. Spagnolo, *Sulla convergenze degli integrali dell'energia per operatori ellittici del secondo ordine*, Boll. Un. Mat. Ital., 8(1973), pp. 391-411.
- [14] P. A. B. De Sampaio, *A Petrov-Galerkin/modified operator formulation for convection-diffusion problems*, Int. J. Numer. methods Engng., 30(1990).
- [15] J. Dollard, *Asymptotic convergence and Coulomb interaction*, J. Math. Phys., 5(1964), pp. 729-738.
- [16] J. Dollard and G. Velo, *Asymptotic behaviour of a Dirac particle in a Coulomb field*, Nuovo Cimento, 45(1966), pp. 801-812.
- [17] C. A. Duarte and J. T. Oden, *H-p clouds—An h-p meshless method*, Numer. Meth. Part. D. E., 12(1996), pp. 673-705.
- [18] T. Fries and H. Matthies, *A review of Petrov-Galerkin stabilization approaches and an extension to meshfree methods*, Institute of scientific computing, Technical University Braunschweig, Brunswick, Germany, 2004.
- [19] T. Fries and H. Matthies, *Classification and overview of Meshfree Methods*, Institute of scientific computing, Technical University Braunschweig, Brunswick, Germany, 2004.
- [20] O. Garcia, E. A. Fancello, C. S. de Barcellos, and C. A. Duarte, *hp-Clouds in Mindlin's thick plate model*, Int. J. Numer. methods Engng., 47(2000), pp. 1381-1400.
- [21] Y. Gâtél and D. R. Yafaev, *Scattering theory for the Dirac operator with a long-range electromagnetic potential*, J. Fun. Anal., 184(2001), pp. 136-176.
- [22] M. Griesemer and J. Lutgen, *Accumulation of Discrete Eigenvalues of the Radial Dirac Operator*, J. Funct. Anal., 162(1999).
- [23] H. Haken and H. C. Wolf, *The Physics of Atoms and Quanta, Introduction to Experiments and Theory*, Springer-Verlag, Berlin, 1996.

- [24] W. J. Hehre, L. Radom, P. Schleyer, and J. Pople, *Ab Initio Molecular Orbital Theory*, John Willey & Sons, New York, 1986.
- [25] A. Huerta and S. Fernández-Méndez, *Coupling element free Galerkin and finite element methods*, ECCOMAS, Barcelona, 2000.
- [26] A. Huerta and S. Fernández-Méndez, *Enrichment and coupling of the finite element and meshless methods*, Int. J. Numer. methods Engng., 48(2000), pp. 1615-1636.
- [27] S. Idelsohn, N. Nigro, M. Storti, and G. Buscaglia, *A Petrov-Galerkin formulation for advection-reaction-diffusion problems*, Comput. Methods Appl. Mech. Engng., 136(1996).
- [28] T. Kato, *Perturbation Theory for Linear Operators*, Springer-Verlag, Berlin Heidelberg, 1976.
- [29] C. V. Le, *Novel numerical procedures for limit analysis of structures: Mesh-free methods and mathematical programming*, Ph.D thesis, University of Sheffield, England, 2009.
- [30] H. Lin and S. N. Atluri, *Meshless local Petrov-Galerkin (MLPG) method for convection-diffusion problems*, CMES, 1(2000), pp. 45-60.
- [31] I. Lindgren, S. Salomonson, and B. Åsén, *The covariant-evolution-operator method in bound-state QED*, Physics Reports, 389(2004), pp. 161-261.
- [32] G. R. Liu, *Mesh Free Methods: Moving Beyond the Finite Element Method*, CRC press, 2003.
- [33] P. de T. R. Mendonça, C. S. de Barcellos, A. Duarte, *Investigations on the hp-cloud method by solving Timoshenko beam problems*, Comput. Mech., 25(2000), pp. 286-295.
- [34] G. Mur, *On the causes of spurious solutions in electromagnetics*, Electromagnetic, 22(2002), pp. 357-367.
- [35] F. Murat, *H-convergence*, Séminaire d'Analyse Fonctionnelle et Numérique de l'Université d'Alger, 1977.
- [36] Pl. Muthuramalingam, *Scattering theory by Enss' method for operator valued matrices: Dirac operator in an electric field*, J. Math. Soc. Japan, 37(1985), pp. 415-432.

- [37] P. Muthuramalingam and K. B. Sinha, *Existence and completeness of wave operators for the Dirac operator in an electromagnetic field with long range potentials*, J. Indian Math. Soc. (N.S.), 50(1986), pp. 103-130.
- [38] G. Pestka, *Spurious roots in the algebraic Dirac equation*, Chem. Phys. Lett. 376(2003), pp. 659-661.
- [39] M. Reed and B. Simon, *Methods of Modern Mathematical Physics: Scattering Theory*, Vol. 3, Academic Press, San Diego, CA, 1979.
- [40] L. Rosenberg, *Virtual-pair effects in atomic structure theory*, Phys. Rev. A, 39(1989), pp. 4377-4386.
- [41] S. Salomonson and P. Öster, *Relativistic all-order pair functions from a discretized single-particle Dirac Hamiltonian*, Phys. Rev. A, 40(1989), pp. 5548-5558.
- [42] W. Schroeder and I. Wolf, *The origin of spurious modes in numerical solutions of electromagnetic field eigenvalue problems*, IEEE Tran. on Micr. Theory and Tech., 42(1994), pp. 644-653.
- [43] V. M. Shabaev, I. I. Tupitsyn, V. A. Yerokhin, G. Plunien, and G. Soff, *Dual kinetic balance approach to basis-set expansions for the Dirac equation*, Phys. Rev. Lett., 93(2004).
- [44] S. Spagnolo, *Sul limite delle soluzioni di problemi di Cauchy relativi all'equazione del calore*, Ann. Sc. Norm. Sup. Pisa cl. Sci., 21(1967), pp. 657-699.
- [45] S. Spagnolo, *Sulla convergenza delle soluzioni di equazioni paraboliche ed ellittiche*, Ann. Sc. Norm. Sup. Pisa cl. Sci., 22(1968), pp. 571-597.
- [46] S. Spagnolo, *Convergence in energy for elliptic operators*, Proc. Third Symp. Numer. Solut. Partial Diff. Equat. (College Park, 1975), pp. 469-498, Academic Press, San Diego, 1976.
- [47] L. Tartar, *Quelques remarques sur l'homogénéisation*, Proc. of the Japan-France seminar 1976, "Functional analysis and numerical analysis", pp. 469-482, Japan society for the promotion of science, 1978.

- [48] L. Tartar, *Convergence d'opérateurs différentiels*, Analisi convessa, Roma, 1977.
- [49] L. Tartar, *Cours peccot au collège de France*, Paris, 1977.
- [50] B. Thaller, *The Dirac Equation*, Springer-verlag, Berlin, 1993.
- [51] B. Thaller and V. Enss, *Asymptotic observables and Coulomb scattering for the Dirac equation*, Ann. Inst. H. Poincaré Phys. Theor., 45(1986), pp. 147-171.
- [52] I. I. Tupitsyn and V. M. Shabaev, *Spurious states of the Dirac equation in a finite basis set*, Optika i Spektroskopiya, 105(2008), pp. 203-209.
- [53] J. Weidman, *Linear Operators in Hilbert Spaces*, Springer-verlag, New York, 1980.
- [54] J. Weidman, *Strong operator convergence and spectral theory of ordinary differential operators*, Univ. Lagel. Acta Math. No., 34(1997), pp. 153-163.
- [55] J. Weidman, *Lineare Operatoren in Hilberträumen*, Teubner verlag, Wiesbaden, 2003.
- [56] D. R. Yafaev, *Mathematical Scattering Theory: General Theory*, Amer. Math. Soc., Providence, Rhode Island, 1992.
- [57] K. Yajima, *Nonrelativistic limit of the Dirac theory, scattering theory*, J. Fac. Sci. Univ. Tokyo Sect. 1A, Math., 23(1976), pp. 517-523.
- [58] O. Yamada, *The nonrelativistic limit of modified wave operators for Dirac operators*, Proc. Japan Acad., Ser. A, 59(1983), pp. 71-74.
- [59] Y. You, J. S. Chen, and H. Lu *Filters, reproducing kernel, and adaptive meshfree method*, Comput. Mech., 31(2003), pp. 316-326.
- [60] S. Zhao, *On the spurious solutions in the high-order finite difference methods for eigenvalue problems*, Comp. Meth. Appl. Mech. Engng., 196(2007), pp. 5031-5046.
- [61] C. Zuppa, *Modified Taylor reproducing formulas and h-p clouds*, Math. Comput., 77(2008), pp. 243-264.

Paper I

STABILIZED FINITE ELEMENT METHOD FOR THE RADIAL DIRAC EQUATION

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ABSTRACT. A challenging difficulty in solving the radial Dirac eigenvalue problem numerically is the presence of spurious (unphysical) eigenvalues, among the genuine ones, that are neither related to mathematical interpretations nor to physical explanations. Many attempts have been made and several numerical methods have been applied to solve the problem using the finite element method (FEM), the finite difference method, or other numerical schemes. Unfortunately most of these attempts failed to overcome the difficulty. As a FEM approach, this work can be regarded as a first promising scheme to solve the spuriousity problem completely. Our approach is based on an appropriate choice of trial and test function spaces. We develop a Streamline Upwind Petrov-Galerkin method to the equation and derive an explicit stability parameter.

1. INTRODUCTION.

The Dirac equation describes the electron relativistic behavior by means of specifying its energies (eigenvalues) in orbital levels around the nucleus. Approximating the eigenvalues of an electron in the many-electron systems as in Helium-like ions is based on studying the correlation between the existent electrons under the concept of quantum electrodynamic effects (QED-effects). An approach, see e.g. [11, 17], for calculating QED-effects is based on a basis set of eigenstates of the single-electron system (Hydrogen-like ions). Unfortunately, computing the eigenvalues of the electron in the Hydrogen-like ions by numerical methods is upset by the presence of

Key words and phrases. Dirac operator, finite element scheme, spurious eigenvalue, cubic Hermite functions, Petrov-Galerkin, stability parameter.

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spurious solutions (eigenvalues do not match what is physically observed). The spurious solutions annoy the computation, they disturb the solution in a way it becomes no longer reliable. At the time, one can identify the spurious eigenvalues, but there is no efficient method to just remove them from the entire spectrum without affecting the genuine values.

The presence of spurious eigenvalues in the spectrum of the radial Dirac eigenvalue problem and other problems has been addressed in most of numerical computations. In [16], the occurrence of the spurious roots has been related to incorrect balancing of the numerical spaces of the large and small components of the wave function, and has been restricted to the positive quantum number κ . In solving the Dirac eigenvalue problem by a mapped Fourier grid [1], spurious eigenvalues have been detected for positive κ , where their occurrence has been recounted to the symmetric treatment of the large and small components. For eigenvalue problems in general [23], the occurrence of spectrum pollution has been related to the absence of suitable constraints in the mathematical formulations, this results in mismatching of desired physical properties of the problem. Shabaev and Tupitsyn et al. [19, 21] have also allied the presence of spectrum pollution to the symmetric discretization of the small and large components of the wave function. They have pointed out that using the same finite space for both components is the essence of the problem. They have proposed an alternative method to handle the difficulty by an addition of suitable terms to the basis functions known as a basis correction. Also they have explained the coincidence of the eigenvalues of the radial Dirac operator in a finite basis set for each two values of κ that have the same magnitude but are different in sign.

The spuriousity in the eigenvalues computation using spectral Tau method has been studied in [6]. Also the occurrence of the spurious solution in the electromagnetic problems in general has been reported in [14]. To the radial Dirac eigenvalue problem, we refer respectively to [22] and [8, 19] for finite difference and B-splines approximations. For a brief finite element formulation of the Dirac operator see [15].

In the present work, we provide a finite element scheme for solving the radial Coulomb-Dirac operator that guarantees complete treatment of the spurious eigenvalues. This scheme may be considered as the first stable finite element approach for solving the radial Dirac eigenvalue problem. To proceed, we relate the occurrence of spuriousity to the function spaces in the implemented numerical method. What

ever the method is, the finite element method (FEM), the finite difference method (FDM), the spectral domain approach (SDA), the boundary element method (BEM), or the point matching method (PMM), the spuriousity persists. Hence, the spuriousity is priorly understood as not an effect of the applied numerical method, but to a mismatching of some physical properties of the eigenstates in the computation. The present work interprets the existence of spurious eigenvalues and their remedy as:

- (1) The choice of suitable trial function space that meets the physical property of the wave functions in the implemented numerical methods and its role of spuriousity elimination.
- (2) The choice of test function space, this treats what remains of spurious eigenvalues, and on the other hand, solves the coincidence of the eigenvalues of the radial Dirac operator for two different values of κ that differ in sign.

In other words, we classify the spurious eigenvalues in the computation of the radial Dirac eigenvalue problem in two categories. The first is those that appear within the spectrum for all values of κ . We call this type the instilled spurious eigenvalues. It is worth to mention that this type of spuriousity appears not only for positive κ , but for negative κ as well. Instilled spurious eigenvalues affect the genuine eigenvalues or may degenerate with them which results in some perturbed eigenfunctions. However, this will be discussed in detail in the coming section, where, by means of choosing appropriate function spaces, part of the instilled spurious eigenvalues is treated. The second category can be understood as the coincidence of the first eigenvalue of the radial Dirac operator for positive κ to that for the corresponding (has the same magnitude) negative κ . We call this type of spuriousity the unphysical coincidence phenomenon: The eigenvalues of the radial Dirac operator for positive κ have been shown in finite basis sets to be a repetition to those for the corresponding negative κ [21], which is not the case in the usual (infinite) space of the wave functions. To overcome the difficulty, the last (main) section is devoted to set a scheme that removes the spuriousity of both categories.

To present the scheme, consider the radial Coulomb-Dirac eigenvalue problem

$$\underbrace{\begin{pmatrix} mc^2 + V(x) & c(-D_x + \frac{\kappa}{x}) \\ c(D_x + \frac{\kappa}{x}) & -mc^2 + V(x) \end{pmatrix}}_{H_\kappa} \underbrace{\begin{pmatrix} f(x) \\ g(x) \end{pmatrix}}_{\varphi} = \lambda \underbrace{\begin{pmatrix} f(x) \\ g(x) \end{pmatrix}}_{\varphi}.$$

Here m and c are respectively the mass of the electron and the speed of light, the quantum number κ is the spin-orbit coupling parameter defined as $\kappa = (-1)^{j+\ell+\frac{1}{2}}(j+\frac{1}{2})$, where j and ℓ are the total and the orbital angular momentum numbers respectively, and D_x is the derivative with respect to x in \mathbb{R} . The Coulomb potential, $V(x)$, is given by $\frac{-Z}{x}$, where $Z \in [1, 137]$ is the electric charge number. The unknown f and g are the large and small components of the eigenfunction φ with corresponding eigenvalue λ .

The presence of convection terms in the off diagonal and the absence of diffusion terms cause numerical instability in the computation of the eigenvalues. Indeed, in the standard Galerkin finite element solution of the equation one encounters spurious eigenvalues. In order to remove the spuriousity, we derive a stable finite element scheme based on appropriate choice of spaces of the radial Dirac functions. By obtaining the explicit equations of f and g by rewriting the radial Dirac eigenvalue problem, and applying suitable boundary conditions, the proposed space of the radial Dirac wave functions is $\mathcal{H}_0(\Omega) = \{v \in C^1(\Omega) \cap H_0^1(\Omega) : v'|_{\partial\Omega} = 0\}$, where C^1 is the space of continuous functions which possess continuous first derivatives, Ω is an open bounded domain in \mathbb{R}^+ , and $H_0^1(\Omega) = \{v : v \text{ and } v' \text{ are elements of } L^2(\Omega), \text{ and } v|_{\partial\Omega} = 0\}$ (for all values of κ except ± 1 , where for $\kappa = \pm 1$ the lower boundary condition of v' should differ from zero, but for generality and for sake of simplicity it is assumed to vanish, see Remark 1 below). Thus, by this definition, $\mathcal{H}_0(\Omega)$ is the space of continuous functions, v , which admit continuous first derivatives and vanishing smoothly on the boundaries.

Consider the weak form of the radial Dirac eigenvalue problem of finding $\{\lambda, \varphi\} \in \mathbb{R} \times \mathcal{H}_0(\Omega)^2$ such that

$$\int_{\Omega} \mathbf{u}^t H_{\kappa} \varphi dx = \lambda \int_{\Omega} \mathbf{u}^t \varphi dx,$$

where \mathbf{u} is a test function, and the superscript t is the usual matrix transpose. Cubic Hermite (CH) interpolation functions turn out to be a suitable choice which sufficiently fulfill the requirements of $\mathcal{H}_0(\Omega)$. Let \mathcal{V}_h^H be the finite dimensional subspace of \mathcal{H}_0 spanned by the piecewise CH basis functions on a partition k_h . Choosing $\mathbf{u} \in (\mathcal{V}_h^H)^2$ as $(v, 0)^t$ and $(0, v)^t$, where v is an element of \mathcal{V}_h^H , and assuming $f, g \in \mathcal{V}_h^H$, remove partially the first category of spuriousity (only for very small Z) and do not help in solving the coincidence phenomenon.

A complete treatment is achieved by letting the test function to live in another space different from that of the trial function, i.e., applying the Streamline Upwind Petrov-Galerkin (SUPG) method instead of the FEM. Mainly, by assuming \mathbf{u} to be $(v, \tau v')^t$ and $(\tau v', v)^t$ in the variational form above, where $v' = D_x v$. This yields

$$\langle w^+ f, v \rangle + \langle -cg' + \frac{c\kappa}{x} g, v \rangle + \langle R_e^2(f, g), \tau v' \rangle = \lambda \langle f, v \rangle,$$

$$\langle cf' + \frac{c\kappa}{x} f, v \rangle + \langle w^- g, v \rangle + \langle R_e^1(f, g), \tau v' \rangle = \lambda \langle g, v \rangle,$$

where $\langle \cdot, \cdot \rangle$ is the L^2 scalar product. The residuals $R_e^1(f, g)$ and $R_e^2(f, g)$ are defined as follows

$$R_e^1(f, g)(x) = w^+(x)f(x) - cg'(x) + \frac{c\kappa}{x}g(x) - \lambda f(x) = (W^+f - cg' + \frac{c\kappa}{x}g)(x),$$

$$R_e^2(f, g)(x) = cf'(x) + \frac{c\kappa}{x}f(x) + w^-(x)g(x) - \lambda g(x) = (W^-g + cf' + \frac{c\kappa}{x}f)(x),$$

where $W^\pm(x) = w^\pm(x) - \lambda$, and $w^\pm(x) = \pm mc^2 + V(x)$.

The scheme is accomplished by deriving the stability parameter τ , which turns out to have the form $\tau := \tau_j \cong \frac{9}{35} h_{j+1} \left(\frac{h_{j+1} - h_j}{h_{j+1} + h_j} \right)$. The derivation is based on two leading simplifications; to consider the limit operator in the vicinity of x at infinity (i.e., to consider the most numerically unstable part of the operator) and the dominant parts corresponding to the speed of light (c) of the variational system. From the weak form with the modified test function, and after applying these simplifications we obtain an approximation $\lambda(\tau)$ of the accumulation eigenvalue. Knowing that the limit point eigenvalue is mc^2 , we like to minimize the error $|\lambda(\tau) - mc^2|$, which gives the desired formula of τ .

As a numerical method implemented in this work, the FEM is applied, with the usual continuous Galerkin method in Section 2 and the Petrov-Galerkin method in Section 3. For the integrals evaluation, four-point Gaussian quadrature rule is applied. Also, regarding the programming language, the computation provided here is implemented by Matlab.

The paper is arranged as follows: In Section 2 we discuss the first category of the spurious eigenvalues and how to treat it partially via choosing suitable trial function space. A comparison is also performed between the incorrect and the correct function

spaces through numerical examples. In Section 3, we discuss the completion of the treatment. Basically we impose the test function to live in a space different from that of the trial function. This is the well-known SUPG method [2, 7, 10]. Finally a stability parameter is derived to achieve the desired goal.

2. TRIAL FUNCTION SPACE

Recall the radial Dirac eigenvalue problem

$$(1) \quad \begin{pmatrix} mc^2 + V(x) & c(-D_x + \frac{\kappa}{x}) \\ c(D_x + \frac{\kappa}{x}) & -mc^2 + V(x) \end{pmatrix} \begin{pmatrix} f(x) \\ g(x) \end{pmatrix} = \lambda \begin{pmatrix} f(x) \\ g(x) \end{pmatrix},$$

where, then, the two-equation system is

$$(2) \quad (mc^2 + V(x))f(x) + c(-g'(x) + \frac{\kappa}{x}g(x)) = \lambda f(x),$$

$$(3) \quad c(f'(x) + \frac{\kappa}{x}f(x)) + (-mc^2 + V(x))g(x) = \lambda g(x).$$

Since x ranges over $[0, \infty)$, $x = 0$ represents a singularity for the Coulomb potential and hence careful treatment is needed, i.e., one should consider extended nucleus on the entire domain (the case that we want to get the approximation for) or assume point nucleus (the case we can compare our result to, where the exact eigenvalues can be obtained by the relativistic formula) on a cut-off domain. In the extended nucleus case, to avoid the singularity at $x = 0$, the Coulomb potential is modified so that in the range $[0, R]$ (R is the radius of the nucleus) another potential which has no singularity at $x = 0$ is assumed and keeping the Coulomb potential defined on the rest of domain, where the total potential should be at least $C^1([0, \infty))$ -function. Thus, other distributions of the charge along the nucleus are assumed, these distributions can be, e.g., Fermi or uniform distributions, in this work we consider uniform distribution. However, computationally, the same technique is used for both extended and point nucleus cases. For simplicity we will treat point nucleus model in all computations except in the last two tables where we apply the stability scheme for extended nucleus.

To discretize (2) and (3), we divide the domain $\Omega = [a, b]$ into $n + 1$ subintervals with n interior points, x_1, x_2, \dots, x_n , distributed exponentially where $a = x_0 < x_1 < x_2 < \dots < x_{n+1} = b$. Assume k_h is the partition of Ω that consists of the resulted nodal points, with mesh size $h_j = x_j - x_{j-1}$.

The exponential distribution of the nodal points is crucial for solving the radial Dirac eigenvalue problem in order to get more nodal points near the singularity ($x = 0$). This is because the wave function oscillates much more near the nucleus which means more information is needed about its behavior near that region. Whereas the fine grid is not required at the positions away from the nucleus.

The choice of the computational space \mathcal{V} is important and plays the most influential role in the core of the problem. To see that, let us first take the space of only continuous functions as the function space \mathcal{V} . We will show, by means of numerical examples, how this space causes the occurrence of spurious eigenvalues.

For fast and simple algorithm, continuous linear basis functions are considered. So let $\mathcal{V} = \mathcal{V}^l$ be the space of continuous linear polynomials (the superscript l denotes for the linear case), and let $\mathcal{V}_h^l \subset \mathcal{V}^l$ be the finite subspace of piecewise continuous linear polynomials spanned by the usual linear basis functions (ϕ_j) on the partition k_h . The basis function $\phi_j(x)$ has its support in $[x_{j-1}, x_j] =: I_j$ and $[x_j, x_{j+1}] = I_{j+1}$ and defined as

$$\phi_j(x) = \begin{cases} \frac{x-x_{j-1}}{h_j} & x \in I_j, \\ \frac{x_{j+1}-x}{h_{j+1}} & x \in I_{j+1}. \end{cases}$$

Assume that f and g belong to \mathcal{V}_h^l , then they can be written as

$$(4) \quad f(x) = \sum_{j=1}^n \zeta_j \phi_j(x),$$

$$(5) \quad g(x) = \sum_{j=1}^n \xi_j \phi_j(x),$$

where ζ_j and ξ_j are the unknown values of the functions f and g at the nodal point x_j respectively. Since the wave function vanishes in the vicinity of x at infinity and at $x = 0$, homogeneous Dirichlet boundary condition is assumed. The problem is now read as solving (2) and (3) such that $f = 0$ and $g = 0$ at $x = a, b$ (i.e., $\zeta_0 = \zeta_{n+1} = \xi_0 = \xi_{n+1} = 0$). The FEM of the problem is to assume f and g as above in (2) and (3), then multiply by a test function and integrate over the domain Ω

$$(6) \quad \sum_{j=1}^n \langle w^+(x) \phi_j(x), v(x) \rangle \zeta_j + \sum_{j=1}^n \langle -c \phi_j'(x) + \frac{c\kappa}{x} \phi_j(x), v(x) \rangle \xi_j = \lambda \sum_{j=1}^n \langle \phi_j(x), v(x) \rangle \zeta_j$$

and

$$(7) \quad \sum_{j=1}^n \left\langle c\phi_j'(x) + \frac{c\kappa}{x}\phi_j(x), v(x) \right\rangle \zeta_j + \sum_{j=1}^n \left\langle w^-(x)\phi_j(x), v(x) \right\rangle \xi_j = \lambda \sum_{j=1}^n \left\langle \phi_j(x), v(x) \right\rangle \xi_j,$$

where $w^\pm(x) = \pm mc^2 + V(x)$. Let $v = \phi_i$ be an element of the same space \mathcal{V}_h^l in (6) and (7), this leads to the symmetric generalized eigenvalue problem

$$(8) \quad AX = \lambda BX.$$

Here A and B are both symmetric block matrices defined by

$$(9) \quad A = \left(\begin{array}{c|c} mc^2 M_{000} + M_{000}^V & -cM_{010} + c\kappa M_{001} \\ \hline cM_{010} + c\kappa M_{001} & -mc^2 M_{000} + M_{000}^V \end{array} \right)$$

and

$$(10) \quad B = \left(\begin{array}{c|c} M_{000} & 0 \\ \hline 0 & M_{000} \end{array} \right),$$

where M_{rst}^q are $n \times n$ matrices defined as

$$(11) \quad (M_{rst}^q)_{ij} = \int_{\Omega} \phi_j^{(s)} \phi_i^{(r)} x^{-t} q(x) dx, \quad \left(\phi^{(r)}(x) = \frac{d^r}{dx^r} \phi(x) \right).$$

The vector X is the unknowns defined as $(\zeta, \xi)^t$, where

$$\zeta = (\zeta_1, \zeta_2, \dots, \zeta_n) \quad \text{and} \quad \xi = (\xi_1, \xi_2, \dots, \xi_n).$$

In Table 1 the first six computed eigenvalues of the electron in the Hydrogen atom ($Z = 1$) are listed for $|\kappa| = 1$, these eigenvalues are obtained using $n = 100$ interior nodal points and given, as of all other computations in this work, in atomic unit (au). The exact solution for $\kappa = -1$ is shown in the right column of the table. Even with mesh refinement the spuriousity is still present, see Table 2 with $n = 400$.

In Tables 1 and 2, the shaded value in the first level is what we mean by the unphysical coincidence phenomenon, and the two shaded values after the third level are the so-called instilled spuriousity. The spurious eigenvalues appear for both positive and negative values of κ , and they persist despite of mesh refinement. Generally, the spurious eigenvalues can be identified among the genuine ones, but there is no efficient way to just exclude them as a hope of treatment.

TABLE 1. The first six computed eigenvalues of the electron in the Hydrogen atom using linear basis functions with 100 nodal points.

Level	$\kappa = 1$	$\kappa = -1$	Rel. Form. $\kappa = -1$
1	-0.50000665661	-0.50000665659	-0.50000665659
2	-0.12500414297	-0.12500414298	-0.12500208018
3	-0.05556140476	-0.05556140479	-0.05555629517
\Rightarrow	-0.03192157994	-0.03192157993	Spurious Eigenvalue
4	-0.03124489833	-0.03124489832	-0.03125033803
5	-0.01981075633	-0.19810756319	-0.02000018105

TABLE 2. The first six computed eigenvalues of the electron in the Hydrogen atom using linear basis functions with 400 nodal points.

Level	$\kappa = 1$	$\kappa = -1$	Rel. Form. $\kappa = -1$
1	-0.50000665661	-0.50000665659	-0.50000665659
2	-0.12500208841	-0.12500208839	-0.12500208018
3	-0.05555631532	-0.05555631532	-0.05555629517
\Rightarrow	-0.03141172061	-0.03141172060	Spurious Eigenvalue
4	-0.03118772526	-0.03118772524	-0.03125033803
5	-0.01974434510	-0.01974434508	-0.02000018105

The accuracy of the computation in the case of point nucleus can be measured since by relativistic formula we can obtain the exact eigenvalues. But, unfortunately, with the existence of the spurious solutions, it is rather difficult to measure the accuracy of the result in a complete picture. This is obvious because there will be many unrelated eigenvalues in the list of the spectrum for which there are no exact eigenvalues to compare with.

As we mentioned before, the occurrence of spuriousity is an effect of the applied numerical method. Here the numerical scheme we assume for the computation in Tables 1 and 2 is the FEM with the space \mathcal{V}^l . Therefore, either of them holds the responsibility of the spectrum pollution. At this end, it is worth to mention that other methods like the FDM, the method of moments (MoM) [16, 18], and others, have reported the occurrence of spuriousity in many computations for the Dirac operator or else. So we conclude that the problem of spuriousity is certainly

caused by the employed function spaces in the discretization, hence the cause of spuriousity is \mathcal{V}^l -problem and never FEM-problem.

We return to (2) and (3), rewrite both equations to obtain explicit formulae for f and g

$$(12) \quad w^+(x)(w^-(x) - \lambda)^2 f(x) - \frac{c\kappa}{x}(w^-(x) - \lambda)(cf'(x) + \frac{c\kappa}{x}f(x)) + c \left[(w^-(x) - \lambda) \times \right. \\ \left. (cf''(x) + \frac{c\kappa}{x}f'(x) - \frac{c\kappa}{x^2}f(x)) - V'(x)(cf'(x) + \frac{c\kappa}{x}f(x)) \right] = \lambda(w^-(x) - \lambda)^2 f(x)$$

and

$$(13) \quad w^-(x)(w^+(x) - \lambda)^2 g(x) + \frac{c\kappa}{x}(w^+(x) - \lambda)(cg'(x) - \frac{c\kappa}{x}g(x)) + c \left[(w^+(x) - \lambda) \times \right. \\ \left. (cg''(x) - \frac{c\kappa}{x}g'(x) + \frac{c\kappa}{x^2}g(x)) - V'(x)(cg'(x) - \frac{c\kappa}{x}g(x)) \right] = \lambda(w^+(x) - \lambda)^2 g(x).$$

Equations (12) and (13) can be written in simpler forms as

$$(14) \quad f''(x) + \gamma_1(x, \lambda)f'(x) + \gamma_2(x, \lambda)f(x) = 0$$

and

$$(15) \quad g''(x) + \theta_1(x, \lambda)g'(x) + \theta_2(x, \lambda)g(x) = 0,$$

where

$$\gamma_1(x, \lambda) = -\frac{V'(x)}{w^-(x) - \lambda}, \\ \gamma_2(x, \lambda) = \frac{(w^+(x) - \lambda)(w^-(x) - \lambda)}{c^2} - \frac{\kappa^2 + \kappa}{x^2} - \frac{\kappa V'(x)}{x(w^-(x) - \lambda)}, \\ \theta_1(x, \lambda) = -\frac{V'(x)}{w^+(x) - \lambda},$$

and

$$\theta_2(x, \lambda) = \frac{(w^+(x) - \lambda)(w^-(x) - \lambda)}{c^2} - \frac{\kappa^2 - \kappa}{x^2} + \frac{\kappa V'(x)}{x(w^+(x) - \lambda)}.$$

The terms f'' and g'' in (14) and (15) propose further constraint on both components of the wave function. By these equations, f and g are imposed to be twice differentiable. This means that f and g should be continuous and having continuous first derivatives, hence the proposed domain is $C^1(\Omega) \cap H_0^1(\Omega)$.

Instead of regarding \mathcal{V}^l as the space of variational formulation, a space of continuous functions which admit continuous first derivatives is considered to discretize

both components of the wave function. To this end, one can think about a suitable space which meets the properties of f and g ; Lagrange interpolation functions are not suitable in this situation, since their first derivatives do not match the continuity property. So we consider instead a type of Hermite functions (known as a generalization of the Lagrange functions) which are continuous and admit continuous first derivatives.

The boundary conditions need special care. Since the wave functions are assumed to vanish at the boundaries, and by the smooth property of these functions, the way they move toward the boundaries should be in damping manner, i.e., with vanishing velocity. This implies homogeneous Neumann boundary condition should be considered as well (except the case when $\kappa = \pm 1$ at the lower boundary, see Remark 1). thus, after considering the suitable boundary conditions, the proposed space is $\mathcal{H}_0(\Omega) = \{v \in C^1(\Omega) \cap H_0^1(\Omega) : v'|_{\partial\Omega} = 0\}$.

CH interpolation functions turn out to be sufficient to fulfill the requirements. Such functions are third degree piecewise polynomials consisting of two control points and two control tangent points for the interpolation. That means there is a control for both the function values and its first derivative values at the nodal points.

Remark 1.

- (i) For the states $1s_{1/2}$ and $2p_{1/2}$ ($\kappa = -1$ and 1 respectively), the first derivative values of the components of the wave function at the boundaries are partially different, specifically at the lower boundary. For these two states, if $\partial\Omega^{up}$ and $\partial\Omega^{lo}$ denote respectively the upper and lower boundaries, and if v represents the two components of these states, then $v'|_{\partial\Omega^{up}} = 0$ but $v'|_{\partial\Omega^{lo}} \neq 0$. This is due to the fact that the corresponding wave functions do not vanish in a damping way near the origin, see [22] for more details. Thus, for the states $1s_{1/2}$ and $2p_{1/2}$, the same function space $\mathcal{H}_0(\Omega)$ can be considered but with small modification on the functions first derivative at the lower boundary. Here we will keep the same notation $\mathcal{H}_0(\Omega)$ for the space for all states, but when we mean the states $1s_{1/2}$ and $2p_{1/2}$, the right Neumann lower boundary conditions should be considered.
- (ii) For the sake of simplicity and for comparative point of view, in the following computation of the eigenvalues of the electron in the Hydrogen atom, we do not use the right Neumann lower boundary conditions for the states

$1s_{1/2}$ and $2p_{1/2}$ as stated in part (i). Instead we also assume homogeneous Neumann boundary condition for the components of these two states, where the result might be slightly affected but the essence of comparison will not be impacted.

Let \mathcal{V}_h^H be the finite dimensional subspace of $\mathcal{H}_0(\Omega)$ spanned by the CH basis functions on the partition k_h . To summarize, \mathcal{V}_h^H possesses the following properties:

- (i) It is a set of continuous piecewise CH polynomials.
- (ii) $\forall v \in \mathcal{V}_h^H$, v' exists and piecewise continuous.
- (iii) $\forall v \in \mathcal{V}_h^H$, $v|_{\partial\Omega} = v'|_{\partial\Omega} = 0$, where $\partial\Omega = \{a, b\}$.
- (iv) It is a finite dimensional vector space of dimension $2(n + 2)$ with basis $\{\phi_{j,1}\}_{j=0}^{n+1}$ and $\{\phi_{j,2}\}_{j=0}^{n+1}$ given below.

To approximate a function $u_h \in \mathcal{V}_h^H$, where the same partition k_h is considered as before, u_h can be written as

$$(16) \quad u_h = \sum_{j=1}^n \xi_j \phi_{j,1} + \sum_{j=1}^n \xi'_j \phi_{j,2},$$

ξ_j and ξ'_j are the unknown value of the function and its corresponding derivative at the nodal points x_j respectively, and $\phi_{j,1}$ and $\phi_{j,2}$, $j = 1, 2, \dots, n$, are the basis functions of the space \mathcal{V}_h^H having the following properties

$$\phi_{j,1}(x_i) = \begin{cases} 1, & \text{if } j = i, \\ 0, & \text{otherwise,} \end{cases}$$

$$\phi'_{j,2}(x_i) = \begin{cases} 1, & \text{if } j = i, \\ 0, & \text{otherwise,} \end{cases}$$

and

$$\phi'_{j,1}(x_i) = \phi_{j,2}(x_i) = 0 \quad \forall i = 1, 2, \dots, n.$$

It follows from the conditions above that $\phi_{j,1}$ interpolates the function values whereas $\phi_{j,2}$ is responsible of the function first derivatives at the nodal point x_j . For non-uniform mesh, $\phi_{j,1}$ and $\phi_{j,2}$ are given by the following formulae (see Figure 1 below,

where the two basis functions are depicted for uniform and non-uniform meshes)

$$(17) \quad \phi_{j,1}(x) = \begin{cases} \frac{1}{h_j^2}(x - x_{j-1})^2 - \frac{2}{h_j^3}(x - x_{j-1})^2(x - x_j), & x \in I_j, \\ 1 - \frac{1}{h_{j+1}^2}(x - x_j)^2 + \frac{2}{h_{j+1}^3}(x - x_j)^2(x - x_{j+1}), & x \in I_{j+1}, \end{cases}$$

$$(18) \quad \phi_{j,2}(x) = \begin{cases} \frac{1}{h_j^2}(x - x_{j-1})^2(x - x_j), & x \in I_j, \\ (x - x_j) - \frac{1}{h_{j+1}}(x - x_j)^2 + \frac{1}{h_{j+1}^2}(x - x_j)^2(x - x_{j+1}), & x \in I_{j+1}. \end{cases}$$

The approximation error using CH basis functions in the subinterval I_j is given by

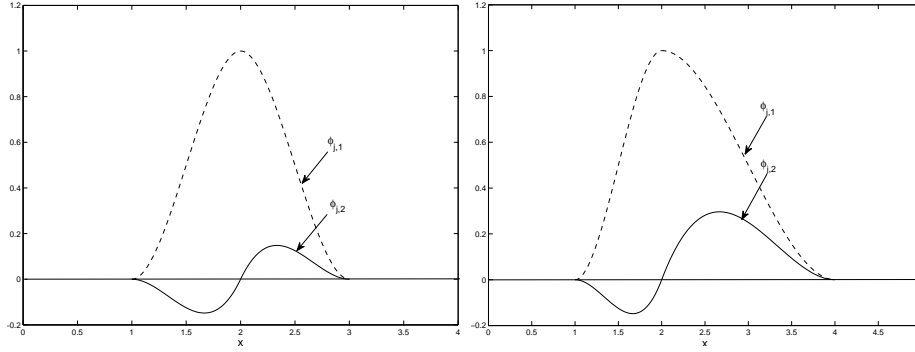


FIGURE 1. CH basis functions with uniformly distributed nodal points(Left) and non-uniformly distributed nodal points(Right).

$$(19) \quad |u - u_h| \leq c_1 h^4 \|u^{(4)}\|_{L^\infty(I_j)},$$

where $c_1 = \frac{1}{384}$, and $h = \max_j h_j$. So the error bound is obtained individually for each subinterval I_j , yielding a fine-grained error bound, which means that the CH basis produces more accuracy compared to the linear or quadratic interpolation function in general. According to Remark 1 part (i), the choice of the CH basis function is also necessary, from simplicity point of view, when the right first derivative of the wave functions at the lower boundary is treated for the states $1s_{1/2}$ and $2p_{1/2}$.

To construct the FEM for the radial Dirac eigenvalue problem using the CH basis functions, we, as usual, multiply (2) and (3) by a test function $v \in \mathcal{H}_0(\Omega)$ and integrate over Ω . To discretize the system, we assume f and g are elements of \mathcal{V}_h^H ,

thus they can be written as

$$(20) \quad f(x) = \sum_{j=1}^n \zeta_j \phi_{j,1}(x) + \sum_{j=1}^n \zeta'_j \phi_{j,2}(x),$$

$$(21) \quad g(x) = \sum_{j=1}^n \xi_j \phi_{j,1}(x) + \sum_{j=1}^n \xi'_j \phi_{j,2}(x),$$

where ζ_j and ζ'_j are the nodal value and the nodal derivative of f respectively at x_j , and ξ_j and ξ'_j are the corresponding ones associated to g . This yields

$$(22) \quad \begin{aligned} & \sum_{j=1}^n \langle -c\phi'_{j,1}(x) + \frac{c\kappa}{x} \phi_{j,1}(x), v(x) \rangle \xi_j + \sum_{j=1}^n \langle -c\phi'_{j,2}(x) + \frac{c\kappa}{x} \phi_{j,2}(x), v(x) \rangle \xi'_j + \\ & + \sum_{j=1}^n \langle w^+(x) \phi_{j,1}(x), v(x) \rangle \zeta_j + \sum_{j=1}^n \langle w^+(x) \phi_{j,2}(x), v(x) \rangle \zeta'_j \\ & = \lambda \left[\sum_{j=1}^n \langle \phi_{j,1}(x), v(x) \rangle \zeta_j + \sum_{j=1}^n \langle \phi_{j,2}(x), v(x) \rangle \zeta'_j \right], \end{aligned}$$

$$(23) \quad \begin{aligned} & \sum_{j=1}^n \langle c\phi'_{j,1}(x) + \frac{c\kappa}{x} \phi_{j,1}(x), v(x) \rangle \zeta_j + \sum_{j=1}^n \langle c\phi'_{j,2}(x) + \frac{c\kappa}{x} \phi_{j,2}(x), v(x) \rangle \zeta'_j + \\ & + \sum_{j=1}^n \langle w^-(x) \phi_{j,1}(x), v(x) \rangle \xi_j + \sum_{j=1}^n \langle w^-(x) \phi_{j,2}(x), v(x) \rangle \xi'_j \\ & = \lambda \left[\sum_{j=1}^n \langle \phi_{j,1}(x), v(x) \rangle \xi_j + \sum_{j=1}^n \langle \phi_{j,2}(x), v(x) \rangle \xi'_j \right]. \end{aligned}$$

Let v be an element of \mathcal{V}_h^H , and consider (22) and (23) first with $v = \phi_{i,1}$ and then with $v = \phi_{i,2}$. This yields the following system

$$(24) \quad \mathcal{A}X = \lambda \mathcal{B}X,$$

where

$$(25) \quad \mathcal{A} = \left(\begin{array}{c|c} mc^2 MM_{000} + MM_{000}^V & -cMM_{010} + c\kappa MM_{001} \\ \hline cMM_{010} + c\kappa MM_{001} & -mc^2 MM_{000} + MM_{000}^V \end{array} \right)$$

and

$$(26) \quad \mathcal{B} = \left(\begin{array}{c|c} MM_{000} & 0 \\ \hline 0 & MM_{000} \end{array} \right).$$

The vector X is the unknowns given by $X = (\zeta, \zeta', \xi, \xi')$, and the general block matrices MM_{rst}^q are defined as

$$(27) \quad MM_{rst}^q = \left(\begin{array}{c|c} M_{rst(1,1)}^q & M_{rst(1,2)}^q \\ \hline M_{rst(2,1)}^q & M_{rst(2,2)}^q \end{array} \right),$$

where

$$(28) \quad (M_{rst(k,l)}^q)_{ij} = \int_{\Omega} \phi_{j,l}^{(s)} \phi_{i,k}^{(r)} x^{-t} q(x) dx.$$

Tables 3 and 4 contain the first six computed eigenvalues of the electron in the Hydrogen atom, with $n = 100$ and 400 interior nodal points using the CH basis functions. The computation is performed for $\kappa = \pm 1$. The right columns of the tables represent the exact solution for $\kappa = -1$ obtained by the relativistic formula.

TABLE 3. The first six computed eigenvalues of the electron in the Hydrogen atom using the CH basis functions with 100 nodal points.

Level	$\kappa = 1$	$\kappa = -1$	Rel. Form. $\kappa = -1$
1	-0.50000632471	-0.50000665659	-0.50000665659
2	-0.12500207951	-0.12500207951	-0.12500208018
3	-0.05555629341	-0.05555629338	-0.05555629517
4	-0.03125018386	-0.03125018404	-0.03125033803
5	-0.01982545837	-0.01982545886	-0.02000018105
6	-0.01085968925	-0.01085968695	-0.01388899674

TABLE 4. The first six computed eigenvalues of the electron in the Hydrogen atom using the CH basis functions with 400 nodal points.

Level	$\kappa = 1$	$\kappa = -1$	Rel. Form. $\kappa = -1$
1	-0.50013790178	-0.50000665659	-0.50000665659
2	-0.12500208021	-0.12500208018	-0.12500208018
3	-0.05555629517	-0.05555629518	-0.05555629517
4	-0.03125027925	-0.03125027916	-0.03125033803
5	-0.01985891281	-0.01985888664	-0.02000018105
6	-0.01116648473	-0.01116629119	-0.01388899674

It is noted, from Tables 3 and 4, that the instilled spurious eigenvalues that were present in Tables 1 and 2 are removed. Also the speed of convergence to the exact eigenvalues is enhanced as the number of nodal points is increased. Unfortunately, part of the instilled spuriousity is still present for most values of Z , also the unphysical coincidence phenomenon remains unsolved. By (19), one argues that the approximation should converge to the exact solution and thus the spurious eigenvalues should disappear if we refine the mesh. This is not the case and the spurious eigenvalues persist even with mesh refinement, see [21], which is costly and also causes numerical deficiencies as refining the mesh where it is not needed.

The unphysical coincidence phenomenon can be simply explained as the following states have respectively almost the same eigenvalue

$$(29) \quad \begin{aligned} np^{\frac{1}{2}}(\kappa = 1) \text{ and } ns^{\frac{1}{2}}(\kappa = -1), \quad n \geq 2, \\ nd^{\frac{3}{2}}(\kappa = 2) \text{ and } np^{\frac{3}{2}}(\kappa = -2), \quad n \geq 3, \\ nf^{\frac{5}{2}}(\kappa = 3) \text{ and } nd^{\frac{5}{2}}(\kappa = -3), \quad n \geq 4, \quad \text{etc.} \end{aligned}$$

The occurrence of this phenomenon is deeply studied for both nonrelativistic and relativistic cases: In [20], the coincidence of the eigenvalues of each two states in (29) is explained by studying the commutation of the Dirac operator with Biedenharn-Johnson-Lippmann operator in the relativistic case. Also in the nonrelativistic case, the eigenvalues dependence on the quantum number $\varrho = n + |\kappa|$ is proved, which implies the eigenvalues independence of the sign of κ . The coincidence of the eigenvalues in the finite dimensional space is also studied in [21], where the spuriousity in general is interpreted as an effect of the same treatment of both components of the wave function.

As it is known that the exact solution of the Dirac operator with Coulomb potential for point nucleus results in different lowest bound eigenvalues for different values of κ . In this work, as it is pointed before, we relate the problem of eigenvalues coincidence to the numerical implementation. Roughly speaking not to the method of approximation, but to the proposed spaces of discretization.

In the previous computation we have imposed the test functions to live in the same space as well as the trial functions, that is the usual Galerkin method. As we have seen, this results in a solution not cleaned from spurious eigenvalues. However, it

is well-known that the Galerkin method when it is applied to convection dominated problem, the solution will be upset by spurious oscillations which are getting worse with the increase in the convection size.

Nevertheless, it is assumed non-uniform mesh (exponentially distributed nodal points) to match desirable requirements of high resolution near the nucleus, where the wave functions oscillate rapidly compared to their oscillations in a region away from it. This means that for each nodal point x_j there are two adjacent systems of what are called fine-mesh grid with much larger coarse mesh. Hence when the wave function crosses the interface between these two regions, its phase is altered to fit the unbalanced change in the displacement size. One can understand the issue by regarding the variant mesh as different media to the generating waves, where most of those waves are not resolvable in two different meshes at the same time. We refer to [5, 12, 13] for more details.

Also, from numerical algebra point of view, one considers the linear system given by (24) and posteriorly notes that the sign of κ that appears as a factor of the block matrix MM_{001} does not contribute in determining the eigenvalues, which is entirely incorrect from physical point of view. So what is needed is to let the sign of κ play a role in eigenvalues definition. This can be achieved by clever and justified addition of terms that include κ without deforming the original equations. These motivations suggest to use an alternative method to the Galerkin formulation that does not admit instability at the time treats the phenomenon of unphysical coincidence.

The SUPG method is used to solve the problem, which consistently introduces additional stability terms in the upwind direction, these terms are based on the residuals of the governing equations and on the modification of the test function space. The latter is understood as adapting the test function \mathbf{u} from $(v, 0)$ and $(0, v)$ to $(v, \tau v')$ and $(\tau v', v)$ respectively. So, the scheme of stability that we consider is a type of residual corrections added to the original equations. The mesh-dependent τ is the stability parameter which we are investigating, where its derivation is the main part of the upcoming section.

3. TEST FUNCTION SPACE

To stabilize the FEM approximation applied to the radial Dirac operator, modified SUPG method is used to formulate the problem. This consists in adding suitable

stability terms to the standard Galerkin method. The SUPG method is designed to maintain consistency, so that the solution of the original equation is still a solution to the variational equation.

The idea of using the SUPG method is to introduce a diffusion term $\langle u', v' \rangle$ which eliminates the instability and enhances the approximation without modifying the equation. Several approaches can be implemented to create such term, to mention, we can just artificially add $\langle au', v' \rangle$, where a is a constant that controls the diffusivity size, this method is first order accurate at most. Or the artificial diffusion term can be added in the direction of the streamlines to avoid excess diffusivity [3, 4], despite this method introduces less crosswind diffusivity than the first mentioned, but it is still inconsistent modification. The methods mentioned above result in modified equations which are different from the original, consequently the exact solution will be no longer satisfying the variational equations.

To formulate the method, consider the radial Dirac eigenvalue problem

$$H_\kappa \varphi = \lambda \varphi, \quad \text{where } \varphi = (f(x), g(x))^t \quad \text{and}$$

$$H_\kappa = \begin{pmatrix} w^+(x) & c(-D_x + \frac{\kappa}{x}) \\ c(D_x + \frac{\kappa}{x}) & w^-(x) \end{pmatrix},$$

which is equivalent to

$$(30) \quad \begin{pmatrix} w^+(x)f(x) - cg'(x) + \frac{c\kappa}{x}g(x) \\ cf'(x) + \frac{c\kappa}{x}f(x) + w^-(x)g(x) \end{pmatrix} = \lambda \begin{pmatrix} f(x) \\ g(x) \end{pmatrix}.$$

Define the residual of each equation as

$$(31) \quad R_e^1(f, g)(x) = w^+(x)f(x) - cg'(x) + \frac{c\kappa}{x}g(x) - \lambda f(x) = (W^+f - cg' + \frac{c\kappa}{x}g)(x),$$

$$(32) \quad R_e^2(f, g)(x) = cf'(x) + \frac{c\kappa}{x}f(x) + w^-(x)g(x) - \lambda g(x) = (W^-g + cf' + \frac{c\kappa}{x}f)(x),$$

where $W^\pm(x) = w^\pm(x) - \lambda$.

The previously derived Galerkin formulation with CH basis functions is

$$(33) \quad \int_\Omega \mathbf{u}^t H_\kappa \varphi dx = \lambda \int_\Omega \mathbf{u}^t \varphi dx,$$

where \mathbf{u} is $(v, 0)^t$ and $(0, v)^t$, and v as well as f and g is an element of \mathcal{V}_h^H . The SUPG method is formulated based on modifying the test function \mathbf{u} to a form that

includes v' as a correction term to introduce the required diffusivity. Hence we assume $v \in \mathcal{V}_h^H$ as well f and g , but $u \notin (\mathcal{V}_h^H)^2$ is just continuous function. In this regard, let u be $(v, \tau v')^t$ and $(\tau v', v)^t$ in (33), where τ is the stability parameter to be studied soon. This leads to

$$(34) \quad \langle w^+ f, v \rangle + \langle -cg' + \frac{c\kappa}{x}g, v \rangle + \langle R_e^2(f, g), \tau v' \rangle = \lambda \langle f, v \rangle$$

and

$$(35) \quad \langle cf' + \frac{c\kappa}{x}f, v \rangle + \langle w^- g, v \rangle + \langle R_e^1(f, g), \tau v' \rangle = \lambda \langle g, v \rangle,$$

Each of the formulations above, using the new test functions, is the usual Galerkin formulation with additional perturbation that consists of the variational form of the residual of the opposite equation with test function $\tau v'$.

In matrix notations, the system $\mathcal{A}X = \lambda \mathcal{B}X$ is obtained as before, but \mathcal{A} and \mathcal{B} are now perturbed by additional matrices factored by τ

$$(36) \quad \mathcal{A} = \left(\begin{array}{c|c} mc^2 MM_{000} + MM_{000}^V + & -cMM_{010} + c\kappa MM_{001} + \\ +c\tau MM_{110} + c\tau\kappa MM_{101} & -mc^2\tau MM_{100} + \tau MM_{100}^V \\ \hline cMM_{010} + c\kappa MM_{001} + & -mc^2 MM_{000} + MM_{000}^V + \\ mc^2\tau MM_{100} + \tau MM_{100}^V & -c\tau MM_{110} + c\tau\kappa MM_{101} \end{array} \right)$$

and

$$(37) \quad \mathcal{B} = \left(\begin{array}{c|c} MM_{000} & \tau MM_{100} \\ \hline \tau MM_{100} & MM_{000} \end{array} \right).$$

The unknowns vector X and the generalized block matrices MM_{rst}^q are as defined before. It is notable from the system above that the resulted block matrices \mathcal{A} and \mathcal{B} are not symmetric any more, in this situation complex eigenvalues may appear, which of course what we should avoid in the computation. To be more precise, the appearance of complex eigenvalues depends on the size of τ , where they do appear for large sizes. For small sizes of τ , one can consider the above system as the usual system that corresponds to the Galerkin approximation (which is symmetric) with an addition of small perturbation of size τ , which still admits real eigenvalues.

Now, the main task is to determine the stability parameter τ that completes the scheme of removing the spuriousity of both categories and improves the convergence.

The derivation of τ assumes non full dependence on the exact solution of the complete operator for point nucleus, instead the limit operator in the vicinity of x at infinity is assumed. Parallel with considering the dominant terms relative to the speed of light (c). Before proceeding into details, we state the following lemmas.

The following lemma provides the approximated values of the radial functions f and g at the nodal point x_j , where backward and forward derivative approximations are used, hence the error is $\mathcal{O}(h)$.

Lemma 1. *For the Dirac functions f and g , let ζ_{j-1} , ζ_{j+1} , ξ_{j-1} , and ξ_{j+1} be the f 's and g 's nodal values at x_{j-1} and x_{j+1} respectively, then the following holds*

$$\begin{aligned}\zeta_{j-1} &\cong \left(1 + \frac{h_j \kappa}{x_j}\right) \zeta_j + \left(\frac{h_j}{c}(-mc^2 + V(x_j)) - \frac{h_j}{c} \lambda\right) \xi_j. \\ \xi_{j-1} &\cong \left(1 - \frac{h_j \kappa}{x_j}\right) \xi_j + \left(-\frac{h_j}{c}(mc^2 + V(x_j)) + \frac{h_j}{c} \lambda\right) \zeta_j. \\ \zeta_{j+1} &\cong \left(1 - \frac{h_{j+1} \kappa}{x_j}\right) \zeta_j + \left(-\frac{h_{j+1}}{c}(-mc^2 + V(x_j)) + \frac{h_{j+1}}{c} \lambda\right) \xi_j. \\ \xi_{j+1} &\cong \left(1 + \frac{h_{j+1} \kappa}{x_j}\right) \xi_j + \left(\frac{h_{j+1}}{c}(mc^2 + V(x_j)) - \frac{h_{j+1}}{c} \lambda\right) \zeta_j.\end{aligned}$$

Proof. Consider the two-equation system of the radial Dirac eigenvalue problem

$$(mc^2 + V(x))f(x) + c(-g'(x) + \frac{\kappa}{x}g(x)) = \lambda f(x)$$

and

$$c(f'(x) + \frac{\kappa}{x}f(x)) + (-mc^2 + V(x))g(x) = \lambda g(x).$$

Assuming the above system for arbitrary $x_j \in k_h$, $j = 1, 2, \dots, n$, and using the backward and forward difference approximations for the derivatives (backward $\Rightarrow f'|_{x_j} \cong \frac{f(x_j) - f(x_{j-1})}{x_j - x_{j-1}} = \frac{\zeta_j - \zeta_{j-1}}{h_j}$ and forward $\Rightarrow f'|_{x_j} \cong \frac{f(x_{j+1}) - f(x_j)}{x_{j+1} - x_j} = \frac{\zeta_{j+1} - \zeta_j}{h_{j+1}}$), one gets the desired results. \blacksquare

For the computed matrices MM_{000} , MM_{100} , MM_{010} , and MM_{110} in the block matrices (36) and (37), the exact element integrals are obtained by the following lemma. For the remaining matrices one can calculate the exact element integrals, but it is rather hard to get them simplified. Therefore, we just write in Remark 3 notations for the desired values without evaluating them.

Lemma 2. *The exact element integrals for some matrices in the generalized system are given in Table 5.*

TABLE 5. The exact element integrals for some matrices in the generalized system. Here M, I, R, and C refer respectively to Matrix, Index, Row, and Column.

$\begin{matrix} I \\ M \end{matrix}$	$\begin{matrix} C \\ R \end{matrix}$	$j-1$	j	$j+1$	$j-1+n$	$j+n$	$j+1+n$
MM_{000}	j	$\frac{9}{70}h_{j+1}$	$\frac{13}{35}(h_{j+1}+h_j)$	$\frac{9}{70}h_{j+1}$	$\frac{13}{420}h_{j+1}^2$	$\frac{11}{210}(h_{j+1}^2-h_j^2)$	$-\frac{13}{420}h_{j+1}^2$
	$j+n$	$-\frac{13}{420}h_{j+1}^2$	$\frac{11}{210}(h_{j+1}^2-h_j^2)$	$\frac{13}{420}h_{j+1}^2$	$-\frac{1}{140}h_{j+1}^3$	$\frac{1}{105}(h_{j+1}^3+h_j^3)$	$-\frac{1}{140}h_{j+1}^3$
MM_{100}	j	$\frac{1}{2}$	0	$-\frac{1}{2}$	$\frac{1}{10}h_{j+1}$	$-\frac{1}{10}(h_{j+1}+h_j)$	$\frac{1}{10}h_{j+1}$
	$j+n$	$-\frac{1}{10}h_{j+1}$	$\frac{1}{10}(h_{j+1}+h_j)$	$-\frac{1}{10}h_{j+1}$	$-\frac{1}{60}h_{j+1}^2$	0	$\frac{1}{60}h_{j+1}^2$
MM_{010}	j	$-\frac{1}{2}$	0	$\frac{1}{2}$	$-\frac{1}{10}h_{j+1}$	$\frac{1}{10}(h_{j+1}+h_j)$	$-\frac{1}{10}h_{j+1}$
	$j+n$	$\frac{1}{10}h_{j+1}$	$-\frac{1}{10}(h_{j+1}+h_j)$	$\frac{1}{10}h_{j+1}$	$\frac{1}{60}h_{j+1}^2$	0	$-\frac{1}{60}h_{j+1}^2$
MM_{110}	j	$-\frac{6}{5}\frac{1}{h_{j+1}}$	$\frac{6}{5}\frac{h_{j+1}+h_j}{h_{j+1}h_j}$	$-\frac{6}{5}\frac{1}{h_{j+1}}$	$-\frac{1}{10}$	0	$\frac{1}{10}$
	$j+n$	$\frac{1}{10}$	0	$-\frac{1}{10}$	$-\frac{1}{30}h_{j+1}$	$\frac{2}{15}(h_{j+1}+h_j)$	$-\frac{1}{30}h_{j+1}$

Proof. The proof is straightforward by evaluating the integrals. ■

Remark 2. The basis functions consist of two parts, one corresponds to the function value and the other to the function derivative at the nodal points. As a first attempt to derive the stability parameter τ , we just take into account the part of the basis functions that contributes to the function values at the nodal points. Thus, the upper left (shaded) three-cell corner of each matrix of Table 5 is considered. This simplification is crucial and justifiable since the basis functions that contribute to the derivative have no considerable contribution to the function values, thus to simplify the derivation we can neglect them, where a complete picture about τ can be obtained by considering the full set of basis functions.

Remark 3. For the other matrices in the block matrix \mathcal{A} , MM_{001} and MM_{101} (where MM_{000}^V and MM_{100}^V can be written respectively as $-ZMM_{001}$ and $-ZMM_{101}$ for $V(x) = \frac{-Z}{x}$), we will use the following notations to denote the element integral obtained using the part of the basis functions that only contributes the function values at the nodal points as indicated in Remark 2. Namely we denote the following

TABLE 6. The element integrals notations of the matrices MM_{001} and MM_{101} for the j^{th} row.

Matrix	Index	$j-1$	j	$j+1$
	MM_{001}		s_{j-1}	s_j
MM_{101}		r_{j-1}	r_j	r_{j+1}

Now we are at the position to state the main theorem of the stability parameter τ . By considering the limit behavior of the eigenvalues in the vicinity of x at infinity, together with the dominant terms with respect to the speed of light we have the following main result

Theorem 1. *The mesh-dependent stability parameter τ that appears in the formulations (34) and (35) is approximated by*

$$(38) \quad \tau := \tau_j \cong \frac{9}{35} h_{j+1} \frac{(h_{j+1} - h_j)}{(h_{j+1} + h_j)}.$$

It is notable that τ is applicable only for non-uniform mesh ($h_j - h_{j-1} \neq 0$ for $j = 1, 2, \dots, n$) and for uniform mesh it is identically zero. This is, of course, of our interest since for the computation of the Dirac operator eigenvalues, the exponential distribution of the nodal points is important and always assumed.

The expression of τ treats the difficulty of the wave transferring between any two adjacent unbalanced mesh steps. The size of τ is proportional to the mesh size, i.e., since we are assuming exponentially distributed points, τ has small sizes near the singularity $x = 0$ due to the small mesh size, while it takes relatively large values in the region away from the origin which is dominated by coarse mesh.

Before proceeding, we introduce the following notations to ease handling the proof.

$$\begin{aligned} c_1 &= -\frac{(h_{j+1} + h_j)}{2c} . \\ c_2 &= -\frac{9}{70}(h_{j+1} - h_j) . \\ c_3 &= \frac{9}{70} \frac{\kappa}{x_j} h_{j+1} (h_{j+1} - h_j) - \kappa s_{j-1} (h_{j+1} - h_j) - \frac{Z}{2cx_j} (h_{j+1} + h_j) \tau_j + \\ &\quad + \frac{Z}{c} (r_{j+1} h_{j+1} - r_{j-1} h_j) \tau_j . \end{aligned}$$

$$\begin{aligned}
 c_4 &= \frac{6c}{5} \frac{(h_{j+1} - h_j)}{h_{j+1}h_j} + \frac{m^2c^3}{2}(h_{j+1} + h_j) + \frac{1}{x_j} \left(\frac{Z^2}{c} - c\kappa^2 \right) (r_{j+1}h_{j+1} - r_{j-1}h_j) . \\
 c_5 &= -\frac{mcZ}{2x_j}(h_{j+1} + h_j) - mcZ(r_{j+1}h_{j+1} - r_{j-1}h_j) + \frac{6c\kappa}{5} \frac{1}{x_j h_{j+1}}(h_{j+1} - h_j) + \\
 &\quad + c\kappa(r_{j-1} + r_j + r_{j+1}) . \\
 c_6 &= mc^2 \frac{9}{70}(h_{j+1} - h_j) . \\
 c_7 &= -Z(2s_{j-1} + s_j) + mc^2\kappa s_{j-1}(h_{j+1} - h_j) + \frac{Z}{2x_j}(h_{j+1} + h_j) + \\
 &\quad - \frac{9}{70} \frac{mc^2\kappa}{x_j} h_{j+1}(h_{j+1} - h_j) . \\
 c_8 &= -\frac{9}{70c} h_{j+1}(h_{j+1} - h_j) . \\
 c_9 &= -\frac{6}{5} \frac{1}{h_{j+1}}(h_{j+1} - h_j)\tau_j . \\
 c_{10} &= \frac{\kappa}{2x_j}(h_{j+1} + h_j)\tau_j - \frac{Zs_{j-1}}{c}(h_{j+1} - h_j) + \kappa(r_{j+1}h_{j+1} - r_{j-1}h_j)\tau_j + \\
 &\quad - \frac{9}{70} \frac{Z}{cx_j} h_{j+1}(h_{j+1} - h_j) . \\
 c_{11} &= -\frac{6mc^2}{5} \frac{1}{h_{j+1}}(h_{j+1} - h_j) . \\
 c_{12} &= -\frac{6}{5} \frac{Z}{x_j} \frac{1}{h_{j+1}}(h_{j+1} - h_j) + mc^2\kappa(r_{j+1}h_{j+1} - r_{j-1}h_j) - Z(r_{j-1} + r_j + r_{j+1}) + \\
 &\quad + \frac{\kappa mc^2}{2x_j}(h_{j+1} + h_j) . \\
 c_{13} &= \frac{9}{70} m^2c^3 h_{j+1}(h_{j+1} - h_j) + \frac{c\kappa^2 s_{j-1}}{x_j}(h_{j+1} - h_j) . \\
 c_{14} &= \frac{9}{70} \frac{mcZ}{x_j} h_{j+1}(h_{j+1} - h_j) + c\kappa(2s_{j-1} + s_j) - \frac{c\kappa}{2x_j}(h_{j+1} + h_j) . \\
 c_{15} &= -\frac{Zs_{j-1}}{c} \left(mc^2 + \frac{Z}{x_j} \right) (h_{j+1} - h_j) . \\
 c_{16} &= -\frac{Zs_{j-1}}{c} \left(mc^2 - \frac{Z}{x_j} \right) (h_{j+1} - h_j) .
 \end{aligned}$$

The following lemma provides the behavior of the eigenvalues in the vicinity of x at infinity.

Lemma 3. *Define the operator*

$$\mathcal{T} = \begin{pmatrix} mc^2 & -cD_x \\ cD_x & -mc^2 \end{pmatrix},$$

then for the radial Coulomb-Dirac eigenvalue problem

$$\left(\mathcal{T} + \begin{pmatrix} V(x) & c\frac{\kappa}{x} \\ c\frac{\kappa}{x} & V(x) \end{pmatrix} \right) \begin{pmatrix} f(x) \\ g(x) \end{pmatrix} = \lambda \begin{pmatrix} f(x) \\ g(x) \end{pmatrix},$$

the only accumulation point of the eigenvalues λ is mc^2 .

Proof. See [9]. ■

We now give the proof of the main theorem.

Proof. Consider the weak formulations (34) and (35), rewrite both of them as the following matrix-system

$$(39) \quad (mc^2 - \lambda)MM_{000}\zeta - cMM_{010}\xi + c\kappa MM_{001}\xi - ZMM_{001}\zeta + \\ + c\tau MM_{110}\zeta + c\kappa\tau MM_{101}\zeta - (mc^2 + \lambda)\tau MM_{100}\xi - Z\tau MM_{101}\xi = 0,$$

$$(40) \quad (mc^2 - \lambda)\tau MM_{100}\zeta - c\tau MM_{110}\xi + c\kappa\tau MM_{101}\xi - Z\tau MM_{101}\zeta + \\ + cMM_{010}\zeta + c\kappa MM_{001}\zeta - (mc^2 + \lambda)MM_{000}\xi - ZMM_{001}\xi = 0,$$

where the unknowns ζ and ξ are given as

$$\zeta = (\zeta_1, \dots, \zeta_{j-1}, \zeta_j, \zeta_{j+1}, \dots, \zeta_n, \zeta'_1, \dots, \zeta'_{j-1}, \zeta'_j, \zeta'_{j+1}, \dots, \zeta'_n)$$

and

$$\xi = (\xi_1, \dots, \xi_{j-1}, \xi_j, \xi_{j+1}, \dots, \xi_n, \xi'_1, \dots, \xi'_{j-1}, \xi'_j, \xi'_{j+1}, \dots, \xi'_n).$$

To get τ locally, that is τ_j , for each element of the mesh, we consider (39) and (40) for arbitrary j cell. Employing Remarks 2 and 3 together with Lemma 2 we end up with

$$(41) \quad (mc^2 - \lambda) \left(\frac{9}{70} h_{j+1} \zeta_{j-1} + \frac{13}{35} (h_{j+1} + h_j) \zeta_j + \frac{9}{70} h_{j+1} \zeta_{j+1} \right) - c \left(-\frac{1}{2} \xi_{j-1} + \frac{1}{2} \xi_{j+1} \right) + \\ + c\kappa \left(s_{j-1} \xi_{j-1} + s_j \xi_j + s_{j+1} \xi_{j+1} \right) - Z \left(s_{j-1} \zeta_{j-1} + s_j \zeta_j + s_{j+1} \zeta_{j+1} \right) + \dots$$

$$\begin{aligned} & \cdots + \tau_j c \left(-\frac{6}{5} \frac{1}{h_{j+1}} \zeta_{j-1} + \frac{6}{5} \frac{(h_{j+1} + h_j)}{h_{j+1} h_j} \zeta_j - \frac{6}{5} \frac{1}{h_{j+1}} \zeta_{j+1} \right) + \tau_j c \kappa \left(r_{j-1} \zeta_{j-1} + r_j \zeta_j + r_{j+1} \zeta_{j+1} \right) \\ & - \tau_j \left(mc^2 + \lambda \right) \left(\frac{1}{2} \xi_{j-1} - \frac{1}{2} \xi_{j+1} \right) - \tau_j Z \left(r_{j-1} \xi_{j-1} + r_j \xi_j + r_{j+1} \xi_{j+1} \right) = 0. \end{aligned}$$

(42)

$$\begin{aligned} & \tau_j \left(mc^2 - \lambda \right) \left(\frac{1}{2} \zeta_{j-1} - \frac{1}{2} \zeta_{j+1} \right) - \tau_j c \left(-\frac{6}{5} \frac{1}{h_{j+1}} \xi_{j-1} + \frac{6}{5} \frac{(h_{j+1} + h_j)}{h_{j+1} h_j} \xi_j - \frac{6}{5} \frac{1}{h_{j+1}} \xi_{j+1} \right) + \\ & + \tau_j c \kappa \left(r_{j-1} \xi_{j-1} + r_j \xi_j + r_{j+1} \xi_{j+1} \right) - \tau_j Z \left(r_{j-1} \zeta_{j-1} + r_j \zeta_j + r_{j+1} \zeta_{j+1} \right) + \\ & + c \left(-\frac{1}{2} \zeta_{j-1} + \frac{1}{2} \zeta_{j+1} \right) + c \kappa \left(s_{j-1} \zeta_{j-1} + s_j \zeta_j + s_{j+1} \zeta_{j+1} \right) - \left(mc^2 + \lambda \right) \left(\frac{9}{70} h_{j+1} \xi_{j-1} + \right. \\ & \left. + \frac{13}{35} (h_{j+1} + h_j) \xi_j + \frac{9}{70} h_{j+1} \xi_{j+1} \right) - Z \left(s_{j-1} \xi_{j-1} + s_j \xi_j + s_{j+1} \xi_{j+1} \right) = 0. \end{aligned}$$

Using Lemma 1 to substitute the nodal values ζ_{j-1} , ζ_{j+1} , ξ_{j-1} , and ξ_{j+1} , and collecting the terms of ζ_j and of ξ_j , (41) and (42) can be written as

(43)

$$\begin{aligned} & \left[\left(\frac{9}{70} h_{j+1} (mc^2 - \lambda) - Z s_{j-1} - \frac{6c}{5} \frac{1}{h_{j+1}} \tau_j \right) \left(2 + \frac{\kappa}{x_j} (h_j - h_{j+1}) \right) + c \kappa (r_{j-1} + r_j + \right. \\ & \left. + r_{j+1} + \frac{\kappa r_{j-1}}{x_j} h_j - \frac{\kappa r_{j+1}}{x_j} h_{j+1}) \tau_j + \frac{6c}{5} \frac{(h_{j+1} + h_j)}{h_{j+1} h_j} \tau_j + \frac{13}{35} (h_{j+1} + h_j) (mc^2 - \lambda) + \right. \\ & \left. - Z s_j + \left(mc^2 - \frac{Z}{x_j} - \lambda \right) \left(-\frac{h_j}{2} - \kappa s_{j-1} h_j + \frac{h_j}{2c} (mc^2 + \lambda) \tau_j + \frac{Z r_{j-1}}{c} h_j \tau_j - \frac{h_{j+1}}{2} + \right. \right. \\ & \left. \left. + \kappa s_{j-1} h_{j+1} + \frac{h_{j+1}}{2c} (mc^2 + \lambda) \tau_j - \frac{Z r_{j+1}}{c} h_{j+1} \tau_j \right) \right] \zeta_j + \left[\left(mc^2 + \frac{Z}{x_j} + \lambda \right) \times \right. \\ & \left. \times \left(-\frac{9}{70c} h_{j+1} h_j (mc^2 - \lambda) + \frac{Z s_{j-1}}{c} h_j + \frac{6}{5} \frac{h_j}{h_{j+1}} \tau_j - \kappa r_{j-1} h_j \tau_j + \frac{9}{70c} h_{j+1}^2 (mc^2 - \lambda) + \right. \right. \\ & \left. \left. - \frac{Z s_{j-1}}{c} h_{j+1} - \frac{6}{5} \tau_j + \kappa r_{j+1} h_{j+1} \tau_j \right) + c \kappa (2s_{j-1} + s_j) - Z (r_{j-1} + r_j + r_{j+1}) \tau_j + \right. \\ & \left. - \frac{c \kappa}{2x_j} (h_j + h_{j+1}) + \frac{\kappa^2 c s_{j-1}}{x_j} (h_{j+1} - h_j) + \frac{\kappa}{2x_j} (mc^2 + \lambda) (h_{j+1} + h_j) \tau_j + \frac{Z r_{j-1} \kappa}{x_j} h_j \tau_j + \right. \\ & \left. - \frac{Z r_{j+1} \kappa}{x_j} h_{j+1} \tau_j \right] \xi_j = 0. \end{aligned}$$

(44)

$$\begin{aligned} & \left[-Z (r_{j-1} + r_j + r_{j+1}) \tau_j + c \kappa (2s_{j-1} + s_j) + \frac{\kappa}{2x_j} (mc^2 - \lambda) (h_{j+1} + h_j) \tau_j - \frac{c \kappa}{2x_j} (h_{j+1} + \right. \\ & \left. + h_j) + \frac{c \kappa^2 s_{j-1}}{x_j} (h_j - h_{j+1}) - \frac{Z r_{j-1} \kappa}{x_j} h_j \tau_j + \frac{Z r_{j+1} \kappa}{x_j} h_{j+1} \tau_j + \left(mc^2 - \frac{Z}{x_j} - \lambda \right) \times \cdots \right. \end{aligned}$$

$$\begin{aligned}
& \cdots \times \left(\frac{9}{70c} h_{j+1} h_j (mc^2 + \lambda) + \frac{Zs_{j-1}}{c} h_j - \frac{6}{5} \frac{h_j}{h_{j+1}} \tau_j - \kappa r_{j-1} h_j \tau_j - \frac{9}{70c} h_{j+1}^2 (mc^2 + \lambda) \right. \\
& \quad \left. - \frac{Zs_{j-1}}{c} h_{j+1} + \frac{6}{5} \tau_j + \kappa r_{j+1} h_{j+1} \tau_j \right) \zeta_j + \left[\left(-\frac{9}{70} h_{j+1} (mc^2 + \lambda) - Zs_{j-1} + \right. \right. \\
& \quad \left. \left. + \frac{6c}{5} \frac{1}{h_{j+1}} \tau_j \right) \left(2 + \frac{\kappa}{x_j} (h_{j+1} - h_j) \right) + c\kappa (r_{j-1} + r_j + r_{j+1} - \frac{\kappa r_{j-1}}{x_j} h_j + \right. \\
& \quad \left. + \frac{\kappa r_{j+1}}{x_j} h_{j+1}) \tau_j - \frac{6c}{5} \frac{(h_{j+1} + h_j)}{h_{j+1} h_j} \tau_j - \frac{13}{35} (h_{j+1} + h_j) (mc^2 + \lambda) - Zs_j + (mc^2 + \right. \\
& \quad \left. + \frac{Z}{x_j} + \lambda) \left(\frac{h_j}{2} - \kappa s_{j-1} h_j - \frac{h_j}{2c} (mc^2 - \lambda) \tau_j + \frac{Zr_{j-1}}{c} h_j \tau_j + \frac{h_{j+1}}{2} + \kappa s_{j-1} h_{j+1} + \right. \right. \\
& \quad \left. \left. - \frac{h_{j+1}}{2c} (mc^2 - \lambda) \tau_j - \frac{Zr_{j+1}}{c} h_{j+1} \tau_j \right) \right] \xi_j = 0.
\end{aligned}$$

Gathering the factors of λ^2 , λ , τ_j , and the free terms in each equation for ζ_j and ξ_j , and using the above defined notations c_i 's, one simplifies (43) and (44) as follows

$$\begin{aligned}
(45) \quad & \left[c_1 \tau_j \lambda^2 + (c_2 + c_3) \lambda + (c_4 + c_5) \tau_j + (c_6 + c_7) \right] \zeta_j + \\
& + \left[c_8 \lambda^2 + (c_9 + c_{10}) \lambda + (c_{11} + c_{12}) \tau_j + (c_{13} + c_{14} + c_{15}) \right] \xi_j = 0.
\end{aligned}$$

$$\begin{aligned}
(46) \quad & \left[-c_8 \lambda^2 + (c_9 - c_{10}) \lambda + (-c_{11} + c_{12}) \tau_j + (-c_{13} + c_{14} + c_{16}) \right] \zeta_j + \\
& + \left[-c_1 \tau_j \lambda^2 + (c_2 - c_3) \lambda + (-c_4 + c_5) \tau_j + (-c_6 + c_7) \right] \xi_j = 0.
\end{aligned}$$

We consider the case where major part of the difficulty of solving the radial Dirac operators comes in. The above formulation is reduced to the operator \mathcal{T} given in Lemma 3, the limit equation at infinity. One can understand the issue as the derived τ_j should guarantee the stability of the computation in the entire domain, particularly for large x , which is the operator \mathcal{T} , and on the other hand, to consider the part of the operator which causes the instability in the computation. These motivations allow to consider (45) and (46) as $x \rightarrow \infty$

$$\begin{aligned}
(47) \quad & \left[-\frac{(h_{j+1} + h_j)}{2c} \tau_j \lambda^2 - \frac{9}{70} (h_{j+1} - h_j) \lambda + \left(\frac{6c}{5} \frac{(h_{j+1} - h_j)}{h_{j+1} h_j} + \frac{m^2 c^3}{2} (h_{j+1} + h_j) \right) \tau_j + \right. \\
& \left. + \frac{9}{70} mc^2 (h_{j+1} - h_j) \right] \zeta_j + \left[-\frac{9}{70c} h_{j+1} (h_{j+1} - h_j) \lambda^2 - \frac{6}{5} \frac{1}{h_{j+1}} (h_{j+1} - h_j) \tau_j \lambda + \right. \\
& \quad \left. - \frac{6mc^2}{5} \frac{1}{h_{j+1}} (h_{j+1} - h_j) \tau_j + \frac{9}{70} m^2 c^3 h_{j+1} (h_{j+1} - h_j) \right] \xi_j = 0.
\end{aligned}$$

$$(48) \quad \left[\frac{9}{70c} h_{j+1} (h_{j+1} - h_j) \lambda^2 - \frac{6}{5} \frac{1}{h_{j+1}} (h_{j+1} - h_j) \tau_j \lambda + \frac{6mc^2}{5} \frac{1}{h_{j+1}} (h_{j+1} - h_j) \tau_j + \right. \\ \left. - \frac{9}{70} m^2 c^3 h_{j+1} (h_{j+1} - h_j) \right] \zeta_j + \left[\frac{(h_{j+1} + h_j)}{2c} \tau_j \lambda^2 - \frac{9}{70} (h_{j+1} - h_j) \lambda + \right. \\ \left. + \left(-\frac{6c}{5} \frac{(h_{j+1} - h_j)}{h_{j+1} h_j} - \frac{m^2 c^3}{2} (h_{j+1} + h_j) \right) \tau_j - \frac{9}{70} m c^2 (h_{j+1} - h_j) \right] \xi_j = 0.$$

Let $m = 1$, and define $\nabla_j = \frac{(h_{j+1} + h_j)}{(h_{j+1} - h_j)}$ and $\rho = -9/70$. Divide (47) and (48) by the quantity $h_{j+1} - h_j$. As c approaches infinity, one gets the following equations

$$(49) \quad [\rho\lambda - a_j]\zeta_j + [d_j\lambda - b_j]\xi_j = 0,$$

$$(50) \quad [d_j\lambda + b_j]\zeta_j + [\rho\lambda + a_j]\xi_j = 0,$$

where $a_j = -\left(\frac{6c}{5} \frac{1}{h_{j+1} h_j} + \frac{c^3}{2} \nabla_j\right) \tau_j + \rho c^2$, $b_j = \frac{6c^2}{5} \frac{1}{h_{j+1}} \tau_j - \frac{9c^3}{70} h_{j+1}$, and $d_j = -\frac{6}{5} \frac{1}{h_{j+1}} \tau_j$.

Equations (49) and (50) can be written in a matrix form as

$$(51) \quad \begin{pmatrix} \rho\lambda - a_j & d_j\lambda - b_j \\ d_j\lambda + b_j & \rho\lambda + a_j \end{pmatrix} \begin{pmatrix} \zeta_j \\ \xi_j \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}.$$

Since ζ_j and ξ_j are not identically zero for all j , then

$$(52) \quad \begin{vmatrix} \rho\lambda - a_j & d_j\lambda - b_j \\ d_j\lambda + b_j & \rho\lambda + a_j \end{vmatrix} = 0,$$

which gives

$$(53) \quad \lambda_{1,2} = \pm \sqrt{(a_j^2 - b_j^2) / (\rho^2 - d_j^2)}.$$

Since c^2 is the accumulation eigenvalue (Lemma 3, with $m = 1$) we will only consider the positive λ in (53) named as λ_1 . Now we would like to have

$$\begin{aligned} |\lambda_1 - c^2| &= 0 \\ \iff \frac{a_j^2 - b_j^2}{c^4} &= \rho^2 - d_j^2 \\ \iff c^4 \left(\rho^2 - \frac{36}{25} \frac{1}{h_{j+1}^2} \tau_j^2 \right) &= \frac{36c^2}{25} \frac{1}{h_{j+1}^2 h_j^2} \tau_j^2 + \frac{c^6}{4} \nabla_j^2 \tau_j^2 + \frac{6c^4}{5} \frac{1}{h_{j+1} h_j} \nabla_j \tau_j^2 + \\ &\quad - \frac{12c^3}{5} \frac{1}{h_{j+1} h_j} \rho \tau_j - \rho c^5 \nabla_j \tau_j - \frac{36c^4}{25} \frac{1}{h_{j+1}^2} \tau_j^2 + \\ &\quad + \rho^2 c^4 + \frac{54c^5}{175} \tau_j - \frac{81c^6}{4900} h_{j+1}^2. \end{aligned}$$

Keeping in mind the c limit at infinity, the above formulation gives

$$(54) \quad \frac{1}{4} \nabla_j^2 \tau_j^2 - \frac{81}{4900} h_{j+1}^2 = 0.$$

The desired result is then obtained straightforward after substituting the value of ∇_j as defined before, which ends the proof. \blacksquare

The derivation of the stability parameter τ mainly depends on the limit behavior of the eigenvalues in the vicinity of x at infinity. This assumption is crucial and inevitable since knowing the theoretical limit of the eigenvalues as $x \rightarrow \infty$, we can compare it to the approximated one that depends on τ , thus minimizing the error between these two accumulation values we get an approximation for τ . For the other simplifications made in the proof of Theorem 1, one can avoid these simplifications to some extent to derive an optimal value of τ or at least to obtain c -based corrections to it, thus better approximation of the eigenvalues will be obtained.

The stability of the SUPG method is mainly measured by complete treatment of the spurious eigenvalues and by the convergence property of the approximated eigenvalues to the exact ones in case of point nucleus. The derived τ provides complete cleaning of spectrum pollution of both categories for all values of $Z \leq 137$ and all $\kappa \in \mathbb{Z} \setminus \{0\}$ without a need to mesh refinement, where the approximated result is compared with the relativistic formula for point nucleus. Moreover, as the mesh is refined a better convergence rate is obtained.

Tables 7, 8, and 9 show the first computed eigenvalues of the electron in the Hydrogen-like Magnesium (Mg) ion for both point and extended nucleus with $\kappa = \pm 2$. Table 7 shows the computed eigenvalues using the FEM with linear basis functions. The number of interior nodal points used is 400. Table 8 shows the same computation using the stability scheme. Table 9 represents the computed eigenvalues for extended nucleus using uniformly distributed charge with interior nodal points 397, where 16 nodal points are considered in the domain $[0, R]$ (R is the radius of the nucleus).

TABLE 7. The first computed eigenvalues of the electron in the Hydrogen-like Mg ion using the FEM with linear basis for point nucleus.

Level	$\kappa = 2$	$\kappa = -2$	Rel. Form. $\kappa = -2$
1	-18.0086349982	-18.0086349982	-18.0086349982
2	-8.00511829944	-8.00511829944	-8.00511739963
3	-4.50270135222	-4.50270135225	-4.50269856638
\Rightarrow	-2.88546212211	-2.88546212205	Spurious Eigenvalue
4	-2.88155295096	-2.88155295095	-2.88154739168
5	-2.00096852250	-2.00096852249	-2.00095939879
6	-1.47003410346	-1.47003410350	-1.47002066823
\Rightarrow	-1.13034880166	-1.13034880167	Spurious Eigenvalue
7	-1.12545691681	-1.12545691683	-1.12543844140
8	-.889228944495	-.889228944484	-.889204706429
9	-.720265553198	-.720265553187	-.720234829539
\Rightarrow	-.600492562625	-.600492562622	Spurious Eigenvalue
10	-.595258516248	-.595258516277	-.595220579682
11	-.500185771976	-.500185772005	-.500139887884
12	-.426201311278	-.426201311300	-.426146735771

TABLE 8. The first computed eigenvalues of the electron in the Hydrogen-like Mg ion using the stability scheme for point nucleus.

Level	$\kappa = 2$	$\kappa = -2$	Rel. Form. $\kappa = -2$
1		-18.0086349985	-18.0086349982
2	-8.00511739978	-8.00511740020	-8.00511739963
3	-4.50269856669	-4.50269856719	-4.50269856638
4	-2.88154739219	-2.88154739270	-2.88154739168
5	-2.00095939948	-2.00095939991	-2.00095939879
6	-1.47002066888	-1.47002066924	-1.47002066823
7	-1.12543844176	-1.12543844201	-1.12543844140
8	-.889204706068	-.889204706109	-.889204706429
9	-.720234827833	-.720234827687	-.720234829539
10	-.595220575840	-.595220575531	-.595220579682
11	-.500139880950	-.500139880357	-.500139887884
12	-.426146724530	-.426146723650	-.426146735771

TABLE 9. The first computed eigenvalues of the electron in the Hydrogen-like Mg ion using the stability scheme for extended nucleus.

Level	$\kappa = 2$	$\kappa = -2$	Rel. Form. $\kappa = -2$
1		-18.0086349986	-18.0086349982
2	-8.00511739975	-8.00511740015	-8.00511739963
3	-4.50269856673	-4.50269856733	-4.50269856638
4	-2.88154739230	-2.88154739279	-2.88154739168
5	-2.00095939956	-2.00095940014	-2.00095939879
6	-1.47002066903	-1.47002066934	-1.47002066823
7	-1.12543844179	-1.12543844207	-1.12543844140
8	-.889204706021	-.889204706003	-.889204706429
9	-.720234827640	-.720234827433	-.720234829539
10	-.595220575309	-.595220574883	-.595220579682
11	-.500139879906	-.500139879215	-.500139887884
12	-.426146722827	-.426146721812	-.426146735771

To study the rate of convergence of the approximation using the derived scheme, we compare the approximated eigenvalues of the electron in the Hydrogen-like Magnesium ion for point nucleus using the FEM as in Table 7, to those eigenvalues obtained by the stability scheme as in Table 8. Ignoring the presence of the spurious eigenvalues, one notes that the relative error of the approximation of the first 12 genuine eigenvalues using the FEM with linear basis functions is nearly 10^{-4} . Whereas the relative error for the same group of eigenvalues using the stability scheme is not exceeding $3 * 10^{-8}$. Thus, the speed of convergence is also enhanced. However, the improvement in the convergence rate is mainly a result of using the CH basis functions which provide better approximation according to (19).

In Table 10, we provide the approximated eigenvalues of the electron in the Hydrogen-like Uranium (U) ion using the stability scheme. The computation is obtained for different values of the quantum number κ for extended nucleus. The number of nodal points used is 203 (13 out of them are used to discretize the segment $[0, R]$).

TABLE 10. The first computed eigenvalues of the electron in the Hydrogen-like U ion using the stability scheme for extended nucleus.

Level	$\kappa = -1$	$\kappa = 1$	$\kappa = -2$	$\kappa = 2$	$\kappa = -3$
1	-4853.62949434				
2	-1255.95827216	-1257.22738641			
3	-538.661380908	-539.033990526	-1089.61141552		
4	-295.078728020	-295.232044507	-489.037085134	-489.037084960	
5	-185.395090636	-185.471947843	-274.407758128	-274.407757668	-476.261594535
6	-127.042256989	-127.086006093	-174.944613694	-174.944613207	-268.965877806
7	-92.4088112704	-92.4360075180	-121.057538281	-121.057537866	-172.155252828
8	-70.2043012114	-70.2223336849	-88.6717487653	-88.6717484812	-119.445272665
9	-55.1286483910	-55.1412076654	-67.7178951387	-67.7178950309	-87.6582879582
10	-44.4301782764	-44.4392710290	-53.3922002629	-53.3922003729	-67.0402332769
11	-36.5662117804	-36.5730039895	-43.1702540865	-43.1702544560	-52.9170997410
12	-30.6178633663	-30.6230696251	-35.6233695209	-35.6233701925	-42.8244637407
13	-26.0103096494	-26.0143875052	-29.8940993552	-29.8941003747	-35.3639479395
14	-22.3691011929	-22.3723545239	-25.4427187732	-25.4427201886	-29.6945373867
15	-19.4418733070	-19.4445102954	-21.9158181718	-21.9158200337	-25.2859399425
16	-17.0535375600	-17.0557046811	-19.0741660324	-19.0741683944	-21.7904231350
17	-15.0795424863	-15.0813452131	-16.7511595194	-16.7511624386	-18.9723111918
18	-13.4293342440	-13.4308500831	-14.8278955863	-14.8278991221	-16.6673054165
19	-12.0358025118	-12.0370894509	-13.2176791341	-13.2176833488	-14.7580403886
20	-10.8483590654	-10.8494611874	-11.8560968516	-11.8561018101	-13.1588737727
21	-9.82828760857	-9.82923891029	-10.6944840991	-10.6944898690	-11.8061295095
22	-8.94555154162	-8.94637858292	-9.69552155807	-9.69552820876	-10.6516697044
23	-8.17655984194	-8.17728361748	-8.83020376778	-8.83021137096	-9.65855817575
24	-7.50257602554	-7.50321330929	-8.07571205220	-8.07572068159	-8.79807266133
25	-6.90856705387	-6.90913137985	-7.41389618253	-7.41390591378	-8.04760687717
26	-6.38235847787	-6.38286086464	-6.83017355332	-6.83018446387	-7.38917199781
27	-5.91400613762	-5.91445563130	-6.31271965872	-6.31273182756	-6.80830955954
28	-5.49532323801	-5.49572732274	-5.85186500024	-5.85187850842	-6.29329159563
29	-5.11952039156	-5.11988530441	-5.43964039565	-5.43965532594	-5.83452444744
30	-4.78092881330	-4.78125978717	-5.06943037836	-5.06944681572	-5.42409906976
31	-4.47478541851	-4.47508687212	-4.73570629156	-4.73572432309	-5.05544809643
32	-4.19706449375	-4.19734018037	-4.43381880272	-4.43383851763	-4.72308165346
33	-3.94434475273	-3.94459787924	-4.15983518735	-4.15985667790	-4.42238191278
34	-3.71370352567	-3.71393684674	-3.91041067459	-3.91043403573	-4.14944192144
35	-3.50263193199	-3.50284782636	-3.68268594092	-3.68271127049	-3.90093812765

Conclusion.

Our computations indicate that the SUPG scheme applied to solve the radial Dirac eigenvalue problem is stable in the sense of complete elimination of spectrum pollution. This approach is mainly compiled of two strategies; the first is the suitable choice of the trial function space. The second is based on varying the test function to live in another space different from that of the trial function. This strongly depends on the derived stability parameter τ . The derived τ is a considerable achievement where its formula is rather easy to implement and, it yields complete treatment of the spuriousity of both categories.

REFERENCES

- [1] E. Ackad and M. Horbatsch, *Numerical solution of the Dirac equation by a mapped fourier grid method*, J. Phys. A: Math. Gen., 38(2005), pp. 3157-3171.
- [2] R. C. Almeida and R. S. Silva, *A stable Petrov-Galerkin method for convection-dominated problems*, Comput. Methods Appl. Mech. Engng., 140(1997).
- [3] A. N. Brooks, *A Petrov-Galerkin finite element formulation for convection dominated flows*, Thesis for the degree of Doctor of Philosophy, California Institute of Technology, California, 1981.
- [4] A. N. Brooks and T. J. R. Hughes, *Streamline Upwind/Petrove-Galerkin formulations for convection dominated flows with particular emphasis on the incompressible Navier-Stokes equations*, Comput. Methods Appl. Mech. Engng., 32(1982).
- [5] M. J. P. Cullin, *A finite element method for a non-linear initial value problem*, J. Inst. Math. Appl., 13(1974), pp. 233-247.
- [6] P. T. Dawkins, S. R. Dunbar, and R. W. Douglass, *The origin and nature of spurious eigenvalues in the spectral Tau method*, J. Comp. Phys., 147(1998), pp. 441-462.
- [7] P. A. B. De Sampaio, *A Petrov-Galerkin/modified operator formulation for convection-diffusion problems*, Int. J. Numer. methods Engng., 30(1990).
- [8] C. F. Fisher and O. Zatsarinny, *A B-splines Galerkin method for the Dirac equation*, Comp. Phys. Comm., 180(2009), pp. 879-886.
- [9] M. Griesemer and J. Lutgen, *Accumulation of Discrete Eigenvalues of the Radial Dirac Operator*, J. Funct. Anal., 162(1999).
- [10] S. Idelsohn, N. Nigro, M. Storti, and G. Buscaglia, *A Petrov-Galerkin formulation for advection-reaction-diffusion problems*, Comput. Methods Appl. Mech. Engng., 136(1996).

- [11] I. Lindgren, S. Salomonson, and B. Åsén, *The covariant-evolution-operator method in bound-state QED*, Physics Reports, 389(2004), pp. 161-261.
- [12] P. E. Lony and W. A. Shaffer, *Some physical and numerical aspects of boundary layer modeling*. Presented at the Second Conference on Numerical Prediction, Montrey, Calif, 37pp, (1973). [Available as NOAA Tech. Memo. NWS TDL-56, Silver Spring, MD.].
- [13] P. E. Lony and W. A. Shaffer, *Boundary layer modeling experiments of the techniques development laboratory*. Presented at the First Conference on Regional and Mesoscale Modeling, Analysis and Prediction, Las Vegas, Nev, (1975), [Abstract in Bull. Amer. Meteor. Soc., 56, 103].
- [14] G. Mur, *On the causes of spurious solutions in electromagnetics*, Electromagnetic, 22(2002), pp. 357-367.
- [15] C. Müller, N. Grün, and W. Scheid, *Finite element formulation of the Dirac equation and the problem of fermion doubling*, Phys. Lett. A, 242(1998), pp. 245-250.
- [16] G. Pestka, *Spurious roots in the algebraic Dirac equation*, Chem. Phys. Lett. 376(2003), pp. 659-661.
- [17] L. Rosenberg, *Virtual-pair effects in atomic structure theory*, Phys. Rev. A, 39(1989), pp. 4377-4386.
- [18] W. Schroeder and I. Wolf, *The origin of spurious modes in numerical solutions of electromagnetic field eigenvalue problems*, IEEE Tran. on Micr. Theory and Tech., 42(1994), pp. 644-653.
- [19] V. M. Shabaev, I. I. Tupitsyn, V. A. Yerokhin, G. Plunien, and G. Soff, *Dual kinetic balance approach to basis-set expansions for the Dirac equation*, Phys. Rev. Lett., 93(2004).
- [20] B. Thaller, *The Dirac Equation*, Springer-Verlag, Berlin, 1993.
- [21] I. I. Tupitsyn and V. M. Shabaev, *Spurious states of the Dirac equation in a finite basis set*, Optika i Spektroskopiya, 105(2008), pp. 203-209.
- [22] S. Salomonson and P. Öster, *Relativistic all-order pair functions from a discretized single-particle Dirac Hamiltonian*, Phys. Rev. A, 40(1989), pp. 5548-5558.
- [23] S. Zhao, *On the spurious solutions in the high-order finite difference methods for eigenvalue problems*, Comp. Meth. Appl. Mech. Engng., 196(2007), pp. 5031-5046.

Paper II

hp-CLOUD APPROXIMATION OF THE DIRAC EIGENVALUE PROBLEM: THE WAY OF STABILITY

HASAN ALMANASREH

ABSTRACT. We apply *hp*-cloud method to the radial Dirac eigenvalue problem. The difficulty of occurrence of spurious eigenvalues among the genuine ones is treated. The method of treatment is based on assuming *hp*-cloud Petrov-Galerkin scheme to construct the weak formulation of the problem which adds a consistent diffusivity to the variational formulation. The size of the artificially added diffusion terms is controlled by a stability parameter (τ). The derivation of τ assumes the limit behavior of the eigenvalues at infinity. The importance of τ is of being applicable for generic basis functions. This is together with choosing appropriate intrinsic enrichments in the construction of the cloud shape functions.

1. INTRODUCTION.

In the last decades, several numerical methods have been derived to compute the eigenvalues of operators. The need of accurate computation of eigenvalues is intensely considered due to their significant applications in many disciplines of science: Mathematically, if a matrix or a linear operator is diagonalized, then by the spectral theorem, it can be analyzed by studying their corresponding eigenvalues, i.e., transforming the matrix or operator to a set of eigenfunctions which can be easily studied. From physical point of view, the eigenvalues could have wide range of information about the behavior of the desired system governed by an operator. This information might be all what is needed to answer many questions regarding the system properties such as stability, positivity, boundedness, asymptotic behavior, etc. In mechanics, eigenvalues play a central role in several aspects such as

Key words and phrases. Dirac operator, spurious eigenvalues, meshfree method, clouds, moving least-squares, intrinsic enrichment, Petrov-Galerkin, stability parameter.

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determining whether the automobile is noisy, whether a bridge will collapse by the water waves, etc. Also, the eigenvalues describe how the quantum state of a physical system changes in time (Schrödinger equation). They represent the electrons energies and describe their motion in the atomic levels, this is the well-known Dirac equation, which is the core of the present work.

The calculation of energy levels in Helium-like ions, where the interaction between two electrons takes place, can be determined by studying the electrons correlation which is part of quantum electrodynamic effects (QED-effects). A scheme for calculating QED-effects [29, 33, 38, 40] is based on a basis set of relativistic Hydrogen-like ion wave eigenfunctions (of the Dirac operator). Meanwhile, the numerical computation of the Dirac operator eigenvalues encounters unphysical values (do not match the physical observations) called spurious eigenvalues or spectrum pollution. The spurious eigenvalues result in rapid oscillations in the wave functions, hence, in many cases, ruining the computation reliability of the basis set (partially or in some cases even completely) in the practical atomic calculations.

The spurious eigenvalues are an effect of the numerical methods and are found in the computation of many problems other than the Dirac eigenvalue problem [1, 2, 37, 41]. For general eigenvalue problems, spurious eigenvalues are reported in [46]. The occurrence of the spuriousity is related to mismatching of desired properties of the original solution in the numerical formulation. Also in the computation of electromagnetic problems the spuriousity is perceived [34, 39]. Two leading approaches are derived to solve this difficulty; Shabaev et al. [41] have related the spuriousity to the same treatment of the large and small components of the Dirac wave function. Their approach for removing the spurious eigenvalues is based on deriving dual kinetic-balance (DKB) basis functions for the large and small components. Almasreth et al. [2] have allied the occurrence of spurious eigenvalues to the same treatment of the trial and test functions in the finite element method (FEM), they proposed stability scheme based on creating a consistent diffusivity by modifying the test function so that it includes a derivative-based correction term.

In this work, we apply *hp*-cloud method [15, 47] to the radial Dirac eigenvalue problem. The technique is known as one of the meshfree methods (MMs) [6, 18, 30, 31, 35] that allows to two different enrichments, intrinsic and extrinsic, to be built in the construction of the basis functions. The method was previously applied for

different problems, e.g., the Schrödinger equation [10], Mindlin's thick plate model [19], and Timoshenko beam problems [32], etc. Here, we apply *hp*-cloud method based on the Galerkin formulation. This means that it is required to evaluate the integrals in the weak formulation of the particular equation, thus a background mesh must be employed in the integration techniques. Therefore, the *hp*-cloud method used here is not really a truly MM. However, all other features of MMs are maintained in our approximation.

In order to treat the spuriousity problem, we stabilize the computation by considering instead *hp*-cloud Petrov-Galerkin (*hp*-CPG) method which may be considered as a new technique of the general meshfree local Petrov-Galerkin (MLPG) [4, 17, 28]. The stability scheme is based on adding consistent diffusion terms without changing the structure of the equation, i.e., the original solution also satisfies the weak formulation. The size of the additional diffusivity is controlled by a stability parameter.

Consider the radial Dirac eigenvalue problem $H_\kappa \Phi(x) = \lambda \Phi(x)$, where $\Phi(x) = (F(x), G(x))^t$ is the radial wave function, λ is the electron relativistic energies (eigenvalues), and H_κ is the radial Dirac operator given as

$$H_\kappa = \begin{pmatrix} mc^2 + V(x) & c(-D_x + \frac{\kappa}{x}) \\ c(D_x + \frac{\kappa}{x}) & -mc^2 + V(x) \end{pmatrix}.$$

The constant c is the speed of light, m is the electron mass, V is the Coulomb potential, $D_x = d/dx$, and κ is the spin-orbit coupling parameter defined as $\kappa = (-1)^{j+\ell+\frac{1}{2}}(j + \frac{1}{2})$, where j and ℓ are the total and the orbital angular momentum quantum numbers respectively. The weak formulation of the problem is to find $\lambda \in \mathbb{R}$ and Φ in a specified functions space such that for every test function Ψ living in some suitable space we have $\int_\Omega \Psi^t H_\kappa \Phi dx = \lambda \int_\Omega \Psi^t \Phi dx$. The usual *hp*-cloud Galerkin approximation is to let Ψ to be $(\psi, 0)^t$ and $(0, \psi)^t$, where ψ lives in the same space as of the two components of Φ . To discretize the weak form, the components of the trial function Φ and the test function ψ are chosen from a finite set of *hp*-cloud basis functions which are constructed using moving least-squares method. Since the radial Dirac operator is dominated by advection (convection) terms, the *hp*-cloud approximation will be upset by spurious eigenvalues.

To stabilize the *hp*-cloud approximation, the *hp*-CPG method is used instead to formulate the problem. In this formulation, the test function Ψ is assumed to live in

a functions space different from that of the trial function Φ , i.e., Ψ is chosen in the form $(\psi, \tau\psi')^t$ and $(\tau\psi', \psi)^t$ where ψ belongs to the same space as the two components of Φ . The correction term $\tau\psi'$ is used to add artificial diffusivity to stabilize the convection terms. The size of the diffusion terms is controlled by the stability parameter τ . The derivation of τ follows the principle used in [2] for the FEM, but a generalization of it. Two simplified leading assumptions are considered in deriving τ ; the operator limit as the radial variable x tends to infinity, thus obtaining an approximation of the limit point of the eigenvalues (depending on τ) which can be compared to the theoretical limit point eigenvalue [20]. Along with considering the dominant terms with respect to the speed of light (c).

The work is organized as follows; in Section 2, some preliminaries about the Dirac equation are presented, also we shed some light over the occurrence of the spuriousity. In Section 3, the construction of the hp -cloud functions is provided, also coupling with the FEM to impose essential boundary conditions (EBCs) is explained. The hp -CPG method and the derivation of the stability parameter are treated in Section 4. In the last section, Section 5, we present some numerical results and provide necessary discussion about the stability scheme.

2. THE RADIAL DIRAC EIGENVALUE PROBLEM AND THE SPURIOUSITY

The free Dirac space-time equation is given by

$$(1) \quad i\hbar \frac{\partial}{\partial t} \mathbf{u}(\mathbf{x}, t) = \mathbf{H}_0 \mathbf{u}(\mathbf{x}, t), \quad \mathbf{u}(\mathbf{x}, 0) = \mathbf{u}_0(\mathbf{x}),$$

where \hbar is the Planck constant divided by 2π , and $\mathbf{H}_0 : H^1(\mathbb{R}^3; \mathbb{C}^4) \longrightarrow L^2(\mathbb{R}^3; \mathbb{C}^4)$ is the free Dirac operator acting on the four-component vector \mathbf{u} , given by

$$(2) \quad \mathbf{H}_0 = -i\hbar c \boldsymbol{\alpha} \cdot \nabla + mc^2 \beta.$$

The 4×4 Dirac matrices $\boldsymbol{\alpha} = (\alpha_1, \alpha_2, \alpha_3)$ and β are given by

$$\alpha_j = \begin{pmatrix} 0 & \sigma_j \\ \sigma_j & 0 \end{pmatrix} \quad \text{and} \quad \beta = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}.$$

Here I and 0 are the 2×2 unity and zeros matrices respectively, and σ_j 's are the 2×2 Pauli matrices

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \text{and} \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Note that separation of variable yields the Dirac eigenvalue problem, i.e., by assuming $\mathbf{u}(\mathbf{x}, t) = u(\mathbf{x})\theta(t)$ in (1) one gets

$$(3) \quad \mathbf{H}_0 u(\mathbf{x}) = \lambda u(\mathbf{x}).$$

The operator \mathbf{H}_0 is self adjoint on $H^1(\mathbb{R}^3; \mathbb{C}^4)$, it describes the motion of the electron that moves freely without external forces. The free Dirac operator with Coulomb potential is given as

$$(4) \quad \mathbf{H} = \mathbf{H}_0 + V(\mathbf{x})I,$$

where $V(\mathbf{x}) = \frac{-Z}{|\mathbf{x}|}$, and I is the 4×4 unity matrix. The spectrum, denoted by σ , of the Coulomb-Dirac operator is $\sigma(\mathbf{H}) = (-\infty, -mc^2] \cup \{\lambda_k\}_{k \in \mathbb{N}} \cup [mc^2, +\infty)$, where $\{\lambda_k\}_{k \in \mathbb{N}}$ is a discrete sequence of eigenvalues in the gap $(-mc^2, mc^2)$ of the continuous spectrum.

The radial Coulomb-Dirac operator (the radial Dirac operator) can be obtained by separation of variables of the radial and angular parts, i.e., by assuming $u(\mathbf{x}) = \frac{1}{x} \begin{pmatrix} F(x)\chi_{\kappa, m}(\varpi, \Theta) \\ iG(x)\chi_{-\kappa, m}(\varpi, \Theta) \end{pmatrix}$, where x is the radial variable. The spherical symmetry property of the angular function χ is the key point in the derivation of the radial part. Let $\Phi(x) = (F(x), G(x))^t$, the radial Dirac eigenvalue problem is given as

$$(5) \quad H_\kappa \Phi(x) = \lambda \Phi(x), \quad \text{where}$$

$$(6) \quad H_\kappa = \begin{pmatrix} mc^2 + V(x) & c(-D_x + \frac{\kappa}{x}) \\ c(D_x + \frac{\kappa}{x}) & -mc^2 + V(x) \end{pmatrix}.$$

The radial functions $F(x)$ and $G(x)$ are called respectively the large and small components of the wave function $\Phi(x)$.

The well-known difficulty of solving the radial Dirac eigenvalue problem numerically is the presence of spurious eigenvalues among the genuine ones that disturb the solution and consequently affect the reliability of the approximated eigenstates. Here we follow [2] for the classification of the spurious eigenvalues; the first category

is the so-called instilled spuriousity, and the second category is the unphysical coincidence phenomenon. The first type is those spurious eigenvalues that may occur within the true eigenvalues (i.e., they occur between the genuine energy levels), this type of spuriousity appears for all values of κ . The second type is the unphysical assigning of almost same first eigenvalue for $2s_{1/2}(\kappa = -1)$ and $2p_{1/2}(\kappa = 1)$, $3p_{3/2}(\kappa = -2)$ and $3d_{3/2}(\kappa = 2)$, $4d_{5/2}(\kappa = -3)$ and $4f_{5/2}(\kappa = 3)$, and so on. This phenomenon is rigorously studied in [42] from theoretical aspect and in [43] from numerical viewpoint.

Apparently, most authors [1, 2, 37, 41] agree that the incorrect balancing and the symmetric treatment of the large and small components of the wave function or of the test and trial functions in the numerical methods are the core of the problem. In the present work, we relate the occurrence of spuriousity, of both categories, to the unsuitable functions spaces and to the symmetric treatment of the trial and test functions in the weak formulation of the equation. To clarify, we rewrite (5) to obtain an explicit formula for each of the two radial functions, so by defining $w^\pm(x) = \pm mc^2 + V(x)$ we have, see [2],

$$(7) \quad F''(x) + \gamma_1(x, \lambda)F'(x) + \gamma_2(x, \lambda)F(x) = 0,$$

$$(8) \quad G''(x) + \theta_1(x, \lambda)G'(x) + \theta_2(x, \lambda)G(x) = 0,$$

where

$$\begin{aligned} \gamma_1(x, \lambda) &= -\frac{V'(x)}{w^-(x) - \lambda}, \quad \theta_1(x, \lambda) = -\frac{V'(x)}{w^+(x) - \lambda}, \\ \gamma_2(x, \lambda) &= \frac{(w^+(x) - \lambda)(w^-(x) - \lambda)}{c^2} - \frac{\kappa^2 + \kappa}{x^2} - \frac{\kappa V'(x)}{x(w^-(x) - \lambda)}, \end{aligned}$$

and

$$\theta_2(x, \lambda) = \frac{(w^+(x) - \lambda)(w^-(x) - \lambda)}{c^2} - \frac{\kappa^2 - \kappa}{x^2} + \frac{\kappa V'(x)}{x(w^+(x) - \lambda)}.$$

According to (7) and (8), the components F and G should be continuous and have continuous first derivatives. Thus, the suitable choices of functions spaces for the computation of the radial Dirac eigenvalue problem are those that possessing these properties. Assuming appropriate spaces helps in partial elimination of spurious eigenvalues, and does not help overcoming the unphysical coincidence phenomenon. In [2], the same argument is accounted, where the FEM is applied to approximate the eigenvalues using linear basis functions.

TABLE 1. This table, taken from [2], shows the first computed eigenvalues of the electron in the Hydrogen atom.

Level	$\kappa = 1$	$\kappa = -1$	Rel. Form. $\kappa = -1$
1	-0.50000665661	-0.50000665659	-0.50000665659
2	-0.12500208841	-0.12500208839	-0.12500208018
3	-0.05555631532	-0.05555631532	-0.05555629517
\Rightarrow	-0.03141172061	-0.03141172060	Spurious Eigenvalue
4	-0.03118772526	-0.03118772524	-0.03125033803
5	-0.01974434510	-0.01974434508	-0.02000018105

In Table 1, 400 nodal points are used to discretize the domain, and the computation is performed for point nucleus. The shaded value in the first level is what meant by the unphysical coincidence phenomenon, and the two shaded values after the third level are the so-called instilled spuriousity. If the basis functions are chosen to be C^1 -functions, then some instilled spurious eigenvalues are avoided as indicated in [2]. Therefore, after applying the boundary conditions, homogeneous Dirichlet boundary condition is assumed for both radial functions, the proposed space is $\mathcal{H}(\Omega) := C^1(\Omega) \cap H_0^1(\Omega)$. Also, the radial functions are mostly like to vanish at the boundaries in a damping way (except some states), consequently homogeneous Neumann boundary condition should be taken into account. The exceptional states are $1s_{1/2}$ and $2p_{1/2}$, in this case at the upper boundary the same treatment is considered as of the other states, but the first derivative of these two states at the lower boundary is not zero. Here we will assume general boundary condition, that is, homogeneous Dirichlet boundary condition. Thus, from now on, the space $\mathcal{H}(\Omega)$ is considered.

What deserves to dwell upon is that numerical methods when they are applied to convection dominated problem, the solution is disturbed by spurious oscillations. This instability gets worse as the convection size increases. The following two numbers are considered as tools to measure the dominance of the convection term

$$(9) \quad Pe_j = \frac{|u_j|h_j}{2K} \quad \text{and} \quad Da_j = \frac{s_j h_j}{|u_j|},$$

where Pe_j and Da_j are known as the grid Peclet and Damköhler numbers respectively, h_j is the size of the element interval I_j , u_j and s_j are respectively the coefficients of the convection and the reaction terms corresponding to I_j , and K is the diffusivity size. The difficulty arises when either the convection coefficient or the source term is larger than the diffusion coefficient, i.e., when $Pe_j > 1$ or when $2Pe_j Da_j = \frac{s_j h_j^2}{K} > 1$ respectively, then the associated equation is a convection dominated one.

For the simplified equations (7) and (8), it is easy to check that $2PeDa$ admits very large values if small number of nodal points is considered regardless the sizes of $|\lambda|$, Z , and κ . Even with mesh refinement, $2PeDa$ still admits very large values at some positions ($2Pe_j Da_j \gg 1$ for some j). The Peclet number, Pe , for the equation that involves the function F , is always less than 1. But for the equation that corresponds to G , Pe admits a value greater than one, exactly at the nodal point where u_j changes its sign, here refining the mesh does not bring Pe below one for all choices of λ , Z , and κ . Hence, (7) and (8) are dominated by convection terms. Thus the approximated solutions F and G , will be upset by unphysical oscillations. The Draw back is that these oscillations in the eigenfunctions result in some unphysical eigenvalues, the spurious eigenvalues. For detailed study on convection dominated problems we refer to [7, 8].

3. MOVING LEAST-SQUARES (MLS) APPROXIMATION

To build the hp -cloud functions, MLS method is applied which allows easily p -enrichment to be implemented and to desired fundamental characters to be enriched in the approximation. MLS is a well-known approximation technique for constructing meshfree shape functions in general. It applies certain least square approach to get the best local approximation, then the local variable is let to 'move' to cover the whole domain.

Consider an open bounded domain $\Omega \subset \mathbb{R}$ with boundary $\partial\Omega$, assume $X = \{x_1, x_2, \dots, x_n\}$ is a set of n arbitrary points in $\bar{\Omega}$. Let $W = \{w_i\}_{i=1}^n$ be a set of open covering of Ω defined by X such that w_i is centered at x_i and $\Omega \subset \cup_{i=1}^n w_i$.

Definition 1. *A set of functions $\{\psi_i\}_{i=1}^n$ is called a partition of unity (PU) subordinated to the cover W if*

- (1) $\sum_{i=1}^n \psi_i(x) = 1$ for all $x \in \Omega$.
(2) $\psi \in C_0^s(w_i)$ for $i = 1, 2, \dots, n$, where $s \geq 0$.

Let $P = \{p_1(x), p_2(x), \dots, p_m(x)\}$ be a set of basis of polynomials (or any basis of suitable intrinsic enrichments). Suppose that $\Psi(x)$ is a continuous function defined on Ω and that its values, Ψ_i , at the points $x_i \in \bar{\Omega}$, $i = 1, 2, \dots, n$, are given. To approximate $\Psi(x)$ globally by $\Psi_h(x)$, firstly $\Psi(x)$ is approximated locally at $\tilde{x} \in \bar{\Omega}$ by $J_{\tilde{x}}\Psi$ defined in terms of the given basis set P as

$$(10) \quad J_{\tilde{x}}\Psi(x) = P^t(x)a(\tilde{x}),$$

where t denotes the usual transpose. The unknown coefficients $a(\tilde{x})$ are chosen so that $J_{\tilde{x}}\Psi$ is the best approximation of Ψ in a certain least squares sense, this is achieved if a is selected to minimize the following weighted least squares L^2 -error norm

$$(11) \quad I_{\tilde{x}}(a) = \sum_{i=1}^n \varphi_i\left(\frac{x-x_i}{\rho_i}\right)(P^t(x_i)a(\tilde{x}) - \Psi_i)^2,$$

where φ_i is a weight function introduced to insure the locality of the approximation, and ρ_i is the dilation parameter which controls the support radius of φ_i at x_i . To minimize $I_{\tilde{x}}$ with respect to the vector a , the first derivative test is applied, i.e., we set $\frac{\partial I_{\tilde{x}}}{\partial a} = 0$ which gives

$$\frac{\partial I_{\tilde{x}}}{\partial a_j} = \sum_{i=1}^n \varphi_i\left(\frac{x-x_i}{\rho_i}\right) 2p_j(x_i)(P^t(x_i)a(\tilde{x}) - \Psi_i) = 0, \quad j = 1, 2, \dots, m.$$

The above system can be written as

$$(12) \quad M(x)a(\tilde{x}) - B(x)\Psi = 0,$$

where $M(x) = \mathcal{P}^t \Upsilon(x) \mathcal{P}$, $B(x) = \mathcal{P}^t \Upsilon(x)$, $\Psi^t = [\Psi_1, \Psi_2, \dots, \Psi_n]$, and $a^t(\tilde{x}) = [a_1(\tilde{x}), a_2(\tilde{x}), \dots, a_m(\tilde{x})]$, with \mathcal{P} and $\Upsilon(x)$ defined as

$$\mathcal{P} = \begin{pmatrix} p_1(x_1) & p_2(x_1) & \dots & p_m(x_1) \\ p_1(x_2) & p_2(x_2) & \dots & p_m(x_2) \\ \vdots & \vdots & \ddots & \vdots \\ p_1(x_n) & p_2(x_n) & \dots & p_m(x_n) \end{pmatrix}$$

and

$$\Upsilon(x) = \begin{pmatrix} \varphi_1\left(\frac{x-x_1}{\rho_1}\right) & 0 & \dots & 0 \\ 0 & \varphi_2\left(\frac{x-x_2}{\rho_2}\right) & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \varphi_n\left(\frac{x-x_n}{\rho_n}\right) \end{pmatrix}.$$

We proceed from equation (12) to get

$$(13) \quad a(\tilde{x}) = M^{-1}(x)B(x)\Psi.$$

Thus

$$J_{\tilde{x}}\Psi(x) = P^t(x)a(\tilde{x}) = P^t(x)M^{-1}(x)B(x)\Psi.$$

The global approximations is then obtained by assuming \tilde{x} arbitrary, i.e., by letting \tilde{x} move over the domain, viz, the solution is globalized by considering $\Psi(x) \approx \lim_{\tilde{x} \rightarrow x} J_{\tilde{x}}\Psi(x) =: \Psi_h(x)$, thus

$$(14) \quad \Psi_h(x) = \sum_{i=1}^n \psi_i(x)\Psi_i$$

with $\psi_i(x) = P^t(x)M^{-1}(x)B_i(x)$, and $B_i(x) = \varphi_i\left(\frac{x-x_i}{\rho_i}\right)P(x_i)$. To sum up, Ψ_h can be written as

$$(15) \quad \Psi_h(x) = P^t(x) \left(\sum_{i=1}^n \varphi_i\left(\frac{x-x_i}{\rho_i}\right)P(x_i)P^t(x_i) \right)^{-1} \sum_{i=1}^n \varphi_i\left(\frac{x-x_i}{\rho_i}\right)P(x_i)\Psi_i.$$

The first derivative of ψ_i is given by $\psi_{i,x} = \frac{d\psi_i(x)}{dx} = P^t M^{-1} B_i - P^t M^{-1} M_x M^{-1} B_i + P^t M^{-1} B_{i,x}$. Below we shall need the consistency concept definition.

Definition 2. A set of functions $\{u_i(x)\}$ is consistent of order m if $\sum_i u_i(x)\mathfrak{P}(x_i) = \mathfrak{P}(x)$ for all $x \in \Omega$, where $\mathfrak{P}(x) = \{x^\varsigma; |\varsigma| \leq m\}$.

To increase the order of consistency of the approximation, the complete representation of the hp -cloud functions consists of the set of PU functions $\psi_i(x)$ and monomial extrinsic enrichment basis functions P as

$$\Psi_h(x) = \sum_{i=1}^n \psi_i(x) \left(\sum_{j=1}^{n_0} P_j(x)\Psi_i^j \right) = \sum_{i=1}^n \sum_{j=1}^{n_0} \psi_i(x)P_j(x)\Psi_i^j.$$

Note that P can be any type of basis functions, but the most used is monomials since they provide good approximation for smooth functions. The monomials $P_j(x)$, due

to [47], should be normalized by the measure of the grid size at x_j to prevent numerical instability. Nevertheless, in applying the *hp*-cloud approximation for the radial Dirac eigenvalue problem, we will use a stability scheme based on the MLPG method, for that we will not be interested in concerning extrinsic enrichments in the computation ($P = \{1\}$, a monomial of degree zero). The point of this setting follows [4], where six different realizations of MLPG restricted only to intrinsic enrichment basis are considered. It is found that extrinsic enrichments in the MLPG method cause numerical stability problems, because the behavior of their derivatives has large oscillations, which is not the case in the usual MMs. Hence, in the present work, only intrinsic enrichments, $P(x)$, are considered, and thus the approximation with the *hp*-clouds is given by (14).

The weight function φ_i plays the most important role in the definition of the *hp*-cloud shape function, it is defined locally on the cover w_i around x_i . The function φ_i can also be chosen the same for all nodes, in this case we write $\varphi_i = \varphi$, which is the case assumed in this work. The *hp*-cloud, ψ_i , inherits the properties of the weight function φ such as continuity, smoothness, and others. In other words, if φ is continuous with continuous first derivative, then so is ψ_i , provided that the continuity of the enrichment basis $P(x)$ and its first derivatives is ensured. As for the Dirac large and small components, F and G , the proposed space is \mathcal{H} , thus, and therefore, the weight function φ should be at least C^1 -function. For this purpose, we will consider quartic spline (C^2 -function) as a weight function defined by

$$(16) \quad \varphi(r) = \begin{cases} 1 - 6r^2 + 8r^3 - 3r^4, & r \leq 1, \\ 0, & r > 1, \end{cases}$$

where $r = \frac{|x-x_i|}{\rho_i}$.

The set functions $\{\psi_i\}_{i=1}^n$ builds a PU, also the set of their first derivatives $\{\psi_{i,x}\}_{i=1}^n$ builds a partition of nullity (PN) ($\sum_{i=1}^n \psi_{i,x}(x) = 0$ for all $x \in \Omega$), see Figure 1. The computational effort of evaluating the integrals in the weak form in the *hp*-cloud approximation is more time consuming compared to mesh-based methods (the shape functions are of the form φ_i only), this is due to the fact that the derivative of the shape function ψ_i tends to have non-polynomial characters, also due to the time needed for matrix inversion in evaluating the shape functions.

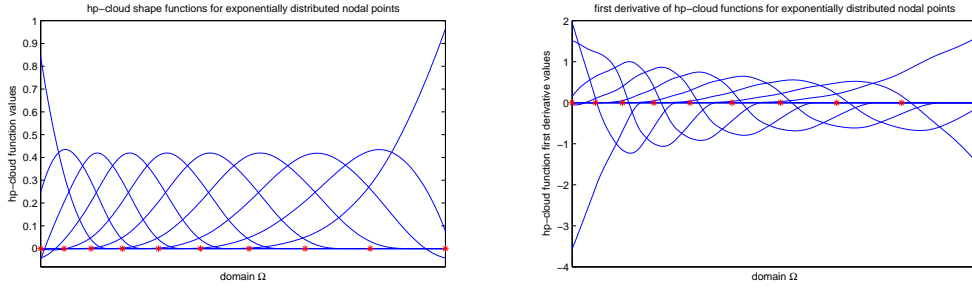


FIGURE 1. PU hp -clouds (to the left) and their PN first derivatives (to the right). Quartic spline is used as a weight function.

Since the Kronecker delta property being not a character of ψ_i ($\psi_i(x_j) \neq \delta_{ij}$), then at each node there are at least two nonzero shape functions. Thus, to have the value of the approximated function at a node, all nonzero shape functions values at that node should be added. The missing of the Kronecker delta property causes a problem in imposing EBCs, and thus other techniques are used to solve this difficulty, see below.

The intrinsic enrichment $P(x)$ has an important effect in the definition of the hp -cloud functions. All known fundamental characters, such as discontinuities and singularities, about the sought solution can be loaded on the intrinsic functions. Consequently, more time is saved; it is not needed, in general, to assume very large number of nodal points to capture a desired behavior of the approximated function while most of the solution features are inserted in the approximation itself. On the other hand, stability is enhanced particularly when there are some crucial characters that can not be captured by usual numerical methods, for example solving equations with rough coefficients that appear, e.g., in composites and materials with micro-structure, problems with high oscillatory solutions, or eigenvalue problems that admit spurious solutions in the computation of the discrete spectrum.

Imposition of essential boundary conditions (EBCs)

The radial Dirac eigenvalue problem assumes homogeneous Dirichlet boundary condition, while it is known that the hp -cloud approximation (MMs in general) can not treat this condition naturally, this is because the lack of the Kronecker

delta property of the shape function. This is in contrast with most mesh-based methods, where the basis functions admit this property, and thus applying EBCs is straightforward (as in FEM) by omitting the first and the last basis functions.

In MMs in general, the widely applied techniques for imposing EBCs are Lagrangian multipliers, penalty condition, and coupling with finite element shape functions. Lagrangian multiplier is a very common and accurate approach for the imposition of EBCs. The disadvantage of this technique, see e.g. [18, 45], is that the resulted discrete equations for a self-adjoint operator are not positive definite (contains zero at the main diagonal) nor banded. Also the structure of the system becomes awkward, i.e., instead of having \mathcal{M} as a resulting matrix of discretization the Galerkin formulation, the system $\begin{pmatrix} \mathcal{M} & lm \\ lm & 0 \end{pmatrix}$ is obtained, where lm is the EBC-enforcement vector. EBCs can also be imposed by penalty condition [18, 36], the problem of applying this technique is the negative effect on the condition number of the resulting discrete equations.

The most powerful and safe method to enforce EBCs is coupling MMs with the FEM, applied for the first time in [26]. With this approach, the meshfree shape functions of the nodes along boundaries are replaced by finite element basis functions. In one dimensional case, the *hp*-cloud functions at the first two and the last two nodes are replaced by finite element functions, and thus EBCs are simply imposed through eliminating the first and last added finite element functions, see Figure 2.

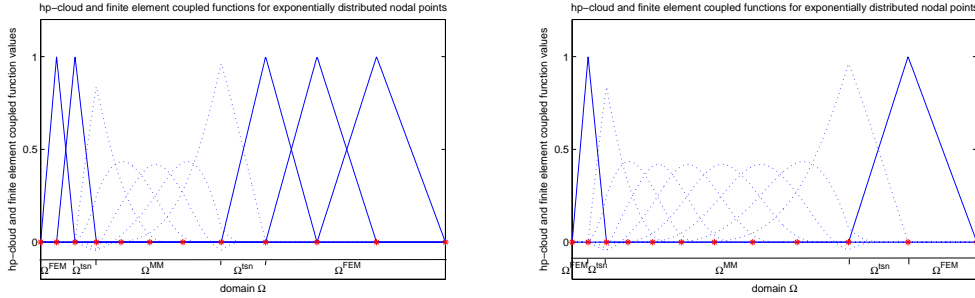


FIGURE 2. Coupled *hp*-cloud and finite element functions: general coupling (to the left), and coupling for the purpose of imposing EBCs (to the right) (two finite element functions are sufficient). Linear (hat) functions are used as finite element functions, and quartic spline as a weight function in the *hp*-clouds.

Two efficient approaches of coupling MMs with the FEM, the first is coupling with Ramp functions [5], and the second is coupling with reproducing conditions [23]. With the first approach, the derivative of the resulting coupled approximation at the boundary of the interface region, Ω^{tsn} in Figure 2, is discontinuous and the consistency is of first order. To ensure the continuity of the first derivative of the coupled function and to obtain consistency of any order, we consider the second approach. Using MLS method, the approximation resulting from coupling hp -cloud and finite element functions with the reproducing conditions is given as (see [18])

$$\begin{aligned}\Psi_h(x) &= \sum_{x_i \in \Omega^{\text{MM}}} \psi_i(x) \Psi_i + \sum_{x_i \in \Omega^{\text{FEM}}} \mathcal{G}_i(x) \Psi_i \\ &= \sum_{x_i \in \Omega^{\text{MM}}} \left(P^t(x) - \sum_{x_i \in \Omega^{\text{FEM}}} \mathcal{G}_i(x) P^t(x_i) \right) M^{-1}(x) \varphi_i \left(\frac{x - x_i}{\rho_i} \right) P(x_i) \Psi_i + \sum_{x_i \in \Omega^{\text{FEM}}} \mathcal{G}_i(x) \Psi_i,\end{aligned}$$

where \mathcal{G}_i are the finite element shape functions, and M is as defined before. From Figure 2, it can be seen that finite element functions are only complete in Ω^{FEM} , and that in Ω^{MM} only hp -clouds are present. In the transition interface region, Ω^{tsn} , the existence of incomplete finite element functions modifies the existed hp -clouds there, and thus coupled hp -cloud and finite element functions are obtained.

4. THE SCHEME AND THE STABILITY PARAMETER

Since the radial Dirac eigenvalue problem is convection dominated, hp -cloud approximation for it will be unstable. As most of applications of numerical methods, certain modifications are used to stabilize solutions [2, 3, 7, 8, 12, 25]. Therefore, instead of considering the hp -cloud approximation for the radial Dirac eigenvalue problem, we will apply the hp -CPG method to create diffusion terms to stabilize the approximation. The hp -CPG method is a consistent method in the sense that the solution of the original problem is also a solution to the weak form. The size of the added diffusivity is controlled by a stability parameter. To set the scheme, consider the radial Dirac eigenvalue problem $H_\kappa \Phi = \lambda \Phi$, the usual hp -cloud method is formulated by multiplying the equation by a test function Ψ and integrating over the domain Ω

$$(17) \quad \int_{\Omega} \Psi^t H_\kappa \Phi dx = \lambda \int_{\Omega} \Psi^t \Phi dx.$$

To discretize (17) let Ψ be defined as $(\psi_i, 0)^t$ and $(0, \psi_i)^t$, $i = 1, 2, \dots, n$, where ψ_i is the *hp*-cloud basis function and

$$(18) \quad \Phi(x) = \begin{pmatrix} F(x) \\ G(x) \end{pmatrix} = \begin{pmatrix} \sum_{j=1}^n f_j \psi_j(x) \\ \sum_{j=1}^n g_j \psi_j(x) \end{pmatrix}.$$

The elements f_j and g_j are the nodal values of F and G respectively. This yields

$$(19) \quad \sum_{j=1}^n \langle w^+(x) \psi_j(x), \psi_i(x) \rangle f_j + \sum_{j=1}^n \langle -c\psi_j'(x) + \frac{c\kappa}{x} \psi_j(x), \psi_i(x) \rangle g_j = \lambda \sum_{j=1}^n \langle \psi_j(x), \psi_i(x) \rangle f_j$$

and

$$(20) \quad \sum_{j=1}^n \langle c\psi_j'(x) + \frac{c\kappa}{x} \psi_j(x), \psi_i(x) \rangle f_j + \sum_{j=1}^n \langle w^-(x) \psi_j(x), \psi_i(x) \rangle g_j = \lambda \sum_{j=1}^n \langle \psi_j(x), \psi_i(x) \rangle g_j,$$

the bracket $\langle \cdot, \cdot \rangle$ is the usual $L^2(\Omega)$ scalar product. After simplifying, equations (19) and (20) lead to the symmetric generalized eigenvalue problem

$$(21) \quad AX = \lambda BX.$$

The block matrices A and B are defined by

$$(22) \quad A = \left(\begin{array}{c|c} mc^2 M_{000} + M_{000}^V & -cM_{010} + c\kappa M_{001} \\ \hline cM_{010} + c\kappa M_{001} & -mc^2 M_{000} + M_{000}^V \end{array} \right), \text{ and } B = \left(\begin{array}{c|c} M_{000} & 0 \\ \hline 0 & M_{000} \end{array} \right),$$

where M_{rst}^q are $n \times n$ matrices given as

$$(23) \quad (M_{rst}^q)_{ij} = \int_{\Omega} \psi_j^{(s)} \psi_i^{(r)} x^{-t} q(x) dx, \quad \left(\psi^{(r)}(x) = \frac{d^r}{dx^r} \psi(x) \right).$$

The vector X is the unknowns defined as $(f, g)^t$, where $f = (f_1, f_2, \dots, f_n)$ and $g = (g_1, g_2, \dots, g_n)$.

To formulate the *hp*-CPG method, the test function Ψ is modified to include the first derivative of the basis function in order to introduce the required diffusivity. This leads to assume Ψ as $(\psi, \tau\psi')^t$ and $(\tau\psi', \psi)^t$ in (17), where τ is the stability parameter that controls the size of the diffusion terms, $\psi = \psi_i$, and the functions F and G are given by (18), thus we get

$$(24) \quad \langle w^+ F, \psi \rangle + \langle -cG' + \frac{c\kappa}{x} G, \psi \rangle + \langle Re^2(F, G), \tau\psi' \rangle = \lambda \langle F, \psi \rangle$$

and

$$(25) \quad \langle cF' + \frac{c\kappa}{x}F, \psi \rangle + \langle w^-G, \psi \rangle + \langle Re^1(F, G), \tau\psi' \rangle = \lambda \langle G, \psi \rangle.$$

The residuals $Re^1(F, G)(x)$ and $Re^2(F, G)(x)$ are defined as

$$(26) \quad Re^1(F, G)(x) = (W^+F - cG' + \frac{c\kappa}{x}G)(x),$$

$$(27) \quad Re^2(F, G)(x) = (W^-G + cF' + \frac{c\kappa}{x}F)(x),$$

where $W^\pm(x) = w^\pm(x) - \lambda$. This results in the usual hp -cloud approximation with addition to perturbations sized by τ as follows

$$(28) \quad \mathbf{A}X = \lambda\mathbf{B}X.$$

The perturbed block matrices, \mathbf{A} and \mathbf{B} , are respectively in the forms $\mathbf{A} = A + \tau\mathcal{A}$ and $\mathbf{B} = B + \tau\mathcal{B}$, where A and B are given by (22),

$$(29) \quad \mathcal{A} = \left(\begin{array}{c|c} cM_{110} + c\kappa M_{101} & -mc^2M_{100} + M_{100}^V \\ \hline mc^2M_{100} + M_{100}^V & -cM_{110} + c\kappa M_{101} \end{array} \right), \text{ and } \mathcal{B} = \left(\begin{array}{c|c} 0 & M_{100} \\ \hline M_{100} & 0 \end{array} \right).$$

The system (28) is not symmetric, thus complex eigenvalues may appear if the size of τ is relatively large. In the FEM, an explicit representation for τ is obtained [2], where the basis functions have the Kronecker delta property, hence the basis functions have regular distribution along the domain and only the adjacent basis functions intersect in one and only one subinterval. Thus the resulted system consists of tridiagonal matrices, this makes the derivation of τ easier and an explicit representation is possible. In MMs in general, a basis function is represented by cloud over a nodal point, with domain of influence, ρ , that may cover many other nodal points. So the resulting matrices can be filled with many nonzero elements, hence the number of non-vanishing diagonals in these matrices is arbitrary (greater than 3) and depending on the size of ρ . Therefore, we can not write an explicit representation for τ that depends only and completely on a given mesh. Instead, τ will be mainly represented by some of the computed matrices obtained from the usual hp -cloud method.

The derivation of τ assumes the limit Dirac operator in the vicinity of x at infinity. This presumable simplification is inevitable and justifiable; the derivation leads to an

approximation of the limit point eigenvalue which depends on τ , where, in [20], the theoretical limit is proved to be mc^2 , hence we can minimize the error between the theoretical and the approximated limits to get τ . By considering the limit operator at infinity, we consider the troublesome part (that includes the convection terms) of the operator which is mostly needed to be stabilized. Besides that, one is obliged to assume that the stability parameter should be applicable at all radial positions $x \in \Omega$, particularly the large values of x .

Theorem 1. *Let M_{000} and M_{100} be the $n \times n$ computed matrices given by (23), and let σ_{ji} and η_{ji} be the corresponding entries respectively. Define ϑ as*

$$(30) \quad \vartheta_{ji} = \begin{cases} -\sum_{k=i+1}^j h_k, & i < j, \\ 0, & i = j, \\ \sum_{k=j+1}^i h_k, & i > j, \end{cases}$$

where h_k is the displacement between the nodes x_k and x_{k-1} . Then the stability parameter, τ_j , for an arbitrary j^{th} row of the matrices in \mathcal{A} and \mathcal{B} is given by

$$(31) \quad \tau_j = \left| \frac{\sum_{i=1}^n \sigma_{ji} \vartheta_{ji}}{\sum_{i=1}^n \eta_{ji} \vartheta_{ji}} \right|.$$

Proof. Consider the limit operator of the radial Dirac eigenvalue problem in the vicinity of x at infinity

$$(32) \quad \begin{pmatrix} mc^2 & -cD_x \\ cD_x & -mc^2 \end{pmatrix} \begin{pmatrix} F(x) \\ G(x) \end{pmatrix} = \lambda \begin{pmatrix} F(x) \\ G(x) \end{pmatrix}.$$

The hp -CPG variational formulation of (32) (which is equivalent to assume a limit passage as $x \rightarrow \infty$ of the equations (24) and (25)) provides

$$(33) \quad (mc^2 - \lambda)M_{000}f + \tau cM_{110}f - (\tau mc^2 - c + \tau\lambda)M_{100}g = 0$$

and

$$(34) \quad (\tau mc^2 - c - \tau\lambda)M_{100}f - \tau cM_{110}g - (mc^2 + \lambda)M_{000}g = 0,$$

where, as defined before, $f = (f_1, f_2, \dots, f_n)$ and $g = (g_1, g_2, \dots, g_n)$. Let σ_k , η_k , and ϱ_k , for $k = 1, 2, \dots, n$, be the corresponding j^{th} row entries of M_{000} , M_{100} , and

M_{110} respectively. To obtain τ_j , we consider the j^{th} rows in (33) and (34), this together with the Lemma 1 below gives

$$(35) \quad \begin{aligned} & \left(mc^2 - \lambda \right) \left(\sum_{k=1}^n \sigma_k f_j + \sum_{k=1}^n \sigma_k (mc\vartheta_k + (\vartheta_k/c)\lambda) g_j \right) + \tau c \left(\sum_{k=1}^n \varrho_k f_j + \sum_{k=1}^n \varrho_k (mc\vartheta_k + \right. \\ & \left. + (\vartheta_k/c)\lambda) g_j \right) - \left(\tau mc^2 - c + \tau \lambda \right) \left(\sum_{k=1}^n \eta_k g_j + \sum_{k=1}^n \eta_k (mc\vartheta_k - (\vartheta_k/c)\lambda) f_j \right) = 0 \end{aligned}$$

and

$$(36) \quad \begin{aligned} & \left(\tau mc^2 - c - \tau \lambda \right) \left(\sum_{k=1}^n \eta_k f_j + \sum_{k=1}^n \eta_k (mc\vartheta_k + (\vartheta_k/c)\lambda) g_j \right) - \tau c \left(\sum_{k=1}^n \varrho_k g_j + \sum_{k=1}^n \varrho_k \times \right. \\ & \left. \times (mc\vartheta_k - (\vartheta_k/c)\lambda) f_j \right) - (mc^2 + \lambda) \left(\sum_{k=1}^n \sigma_k g_j + \sum_{k=1}^n \sigma_k (mc\vartheta_k - (\vartheta_k/c)\lambda) f_j \right) = 0. \end{aligned}$$

Lemma 1. *Let f_i and g_i be respectively the i^{th} nodal values of F and G of the limit equation (32). Freeze j , and let ϑ_i be given by (30) for the given j . Then for $i = 1, 2, \dots, n$*

$$\begin{aligned} f_i &\cong f_j + \left(mc\vartheta_i + (\vartheta_i/c)\lambda \right) g_j. \\ g_i &\cong g_j + \left(mc\vartheta_i - (\vartheta_i/c)\lambda \right) f_j. \end{aligned}$$

Proof. Consider the limit equation (32) which can be written as

$$(37) \quad mc^2 F(x) - cG'(x) = \lambda F(x) \quad \text{and} \quad cF'(x) - mc^2 G(x) = \lambda G(x).$$

If $i = j$, then the result is obvious. So let $i \neq j$, we treat the case $i < j$, where the proof for $i > j$ goes through mutatis mutandis by using forward difference approximations for derivatives. Assume $i < j$, also we prove the first argument of the lemma, the proof of the second argument is similar. Consider the second part of (37) for x_j

$$(38) \quad cF'(x_j) - mc^2 G(x_j) = \lambda G(x_j).$$

Using backward difference approximations for derivatives we can write

$$(39) \quad F'|_{x_j} \cong \frac{F(x_j) - F(x_i)}{-\sum_{k=i+1}^j h_k} = \frac{f_j - f_i}{-\sum_{k=i+1}^j h_k}.$$

Substituting (39) in (38) completes the proof. \blacksquare

We continue the proof of Theorem 1, consider the dominant parts with respect to c , so let $c \rightarrow \infty$ in (35) and (36) and simplify to get

$$(40) \quad \left[\sum_{k=1}^n \left((-\sigma_k - \eta_k \vartheta_k) \lambda + (c \varrho_k - m^2 c^3 \eta_k \vartheta_k) \tau_j + (m c^2 \sigma_k + m c^2 \eta_k \vartheta_k) \right) \right] f_j + \\ + \left[\sum_{k=1}^n \left((\tau_j \varrho_k \vartheta_k - \tau_j \eta_k) \lambda + (m c^2 \varrho_k \vartheta_k - m c^2 \eta_k) \tau_j + (m^2 c^3 \sigma_k \vartheta_k + c \eta_k) \right) \right] g_j = 0$$

and

$$(41) \quad + \left[\sum_{k=1}^n \left((-\tau_j \eta_k + \tau_j \varrho_k \vartheta_k) \lambda + (m c^2 \eta_k - m c^2 \varrho_k \vartheta_k) \tau_j + (-c \eta_k - m^2 c^3 \sigma_k \vartheta_k) \right) \right] f_j + \\ + \left[\sum_{k=1}^n \left((-\eta_k \vartheta_k - \sigma_k) \lambda + (m^2 c^3 \eta_k \vartheta_k - c \varrho_k) \tau_j + (-m c^2 \eta_k \vartheta_k - m c^2 \sigma_k) \right) \right] g_j = 0.$$

To make the derivation simpler, the following notations are introduced

$$a = \sum_{k=1}^n a_k = \sum_{k=1}^n (-\sigma_k - \eta_k \vartheta_k), \quad b = c b_1 - m^2 c^3 b_2 = \sum_{k=1}^n (c \varrho_k - m^2 c^3 \eta_k \vartheta_k), \\ d = m c^2 d_1 = \sum_{k=1}^n m c^2 (\sigma_k + \eta_k \vartheta_k), \quad e = \sum_{k=1}^n e_k = \sum_{k=1}^n (\varrho_k \vartheta_k - \eta_k), \\ q = m c^2 q_1 = \sum_{k=1}^n m c^2 (\varrho_k \vartheta_k - \eta_k), \quad \omega = m^2 c^3 \omega_1 + c \omega_2 = \sum_{k=1}^n (m^2 c^3 \sigma_k \vartheta_k + c \eta_k).$$

By these notations, equations (40) and (41) can be written as

$$(42) \quad \begin{pmatrix} a \lambda + b \tau_j + d & e \tau_j \lambda + q \tau_j + \omega \\ e \tau_j \lambda - q \tau_j - \omega & a \lambda - b \tau_j - d \end{pmatrix} \begin{pmatrix} f_j \\ g_j \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}.$$

Since f_j and g_j are not identically zero for all j , then we expect

$$(43) \quad \det \begin{pmatrix} a \lambda + b \tau_j + d & e \tau_j \lambda + q \tau_j + \omega \\ e \tau_j \lambda - q \tau_j - \omega & a \lambda - b \tau_j - d \end{pmatrix} = 0,$$

where $\det(\cdot)$ is the determinant of matrix. After simplifying, equation (43) leads to

$$(44) \quad \lambda_{\pm}(\tau_j) = \pm \sqrt{\frac{(b\tau_j + d)^2 - (q\tau_j + \omega)^2}{a^2 - e^2\tau_j^2}}.$$

By [20], the only accumulation point for the eigenvalue for the radial Coulomb-Dirac operator in the vicinity of x at infinity is mc^2 . So, we like to have

$$\begin{aligned} |\lambda_+ - mc^2| &= 0 \\ \iff m^2c^4(a^2 - e^2\tau_j^2) &= (b\tau_j + d)^2 - (q\tau_j + \omega)^2 \\ &= (cb_1\tau_j - m^2c^3b_2\tau_j + mc^2d_1)^2 - (mc^2q_1\tau_j + m^2c^3\omega_1 + c\omega_2)^2. \end{aligned}$$

Letting $m = 1$, dividing both sides by c^6 , and taking the limit as $c \rightarrow \infty$, we get

$$(45) \quad b_2^2\tau_j^2 - \omega_1^2 = 0.$$

Substituting back the values of b_2 and ω_1 , the desired consequence is obtained for the fixed j as

$$(46) \quad \tau_j = \left| \frac{\sum_{k=1}^n \sigma_k \vartheta_k}{\sum_{k=1}^n \eta_k \vartheta_k} \right|.$$

The above result can be generalized for arbitrary j as

$$(47) \quad \tau_j = \left| \frac{\sum_{i=1}^n \sigma_{ji} \vartheta_{ji}}{\sum_{i=1}^n \eta_{ji} \vartheta_{ji}} \right|,$$

and this ends the proof. ■

The hp -cloud functions depend strongly on the dilation parameter ρ_j . As ρ_j gets smaller, i.e., $\rho_j \rightarrow \max\{h_j, h_{j+1}\}$ ($= h_{j+1}$ for exponentially distributed nodal points), as the shape functions of MMs in general become closer to the standard finite element functions, see Figure 3. In this case the FEM stability parameter might be applicable for MMs [17]

$$\tau_j^{FEM} \rightarrow \tau_j^{MMs}, \quad \text{as } \rho_j \rightarrow h_{j+1}.$$

On the other hand, one should be careful about the invertibility of the matrix M , i.e., we can not approach $\rho_j = h_{j+1}$ which makes M singular. In Lemma 2, we derive the stability parameter τ_j^{FEM} for the computation of the eigenvalues of the radial Dirac operator, H_κ , using the FEM with quartic spline. The proof of the lemma

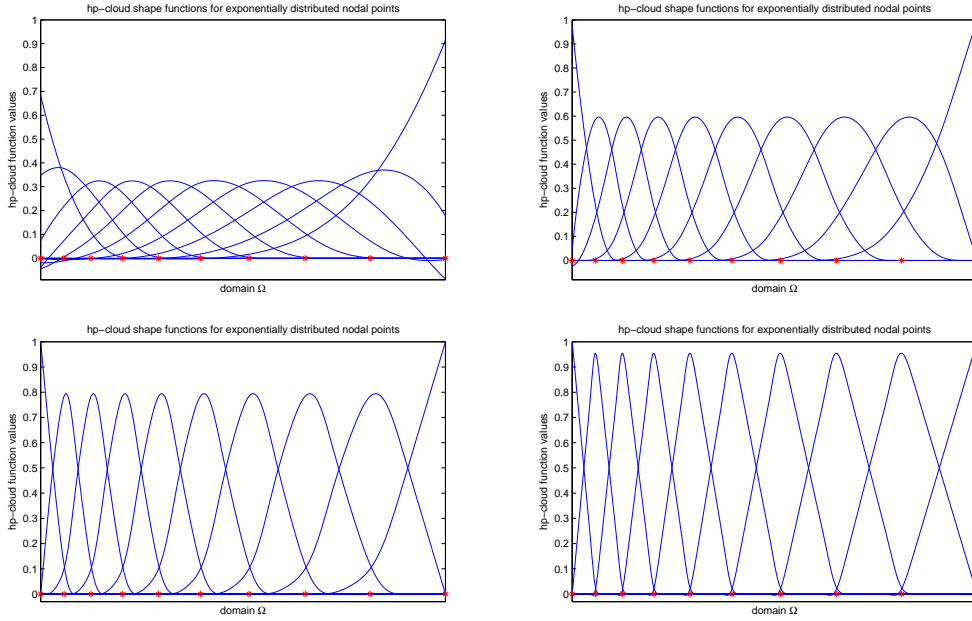


FIGURE 3. PU hp -clouds with different dilation parameters: $\rho_j = 4 \cdot h_{j+1}$ (up to the left), $\rho_j = 2 \cdot h_{j+1}$ (up to the right), $\rho_j = 1.5 \cdot h_{j+1}$ (below to the left), and $\rho_j = 1.2 \cdot h_{j+1}$ (below to the right). Quartic spline is used as a weight function.

is simple and uses the same technique as of the theorem above, thus we directly utilize the result of this theorem with minor modifications. In Table 7, the result of applying τ_j^{FEM} for stabilizing the hp -cloud method with $\rho_j = (1.1) \cdot h_{j+1}$ is obtained, the approximation is good enough and the spuriousity seems to be eliminated. But a difficulty arises, that is, the end of the spectrum (the spectrum tail) behaves in a strange way, which may be regarded as spurious solutions.

Lemma 2. *The FEM stability parameter for the computation of the eigenvalues of the radial Dirac operator using quartic splines as a basis has the form*

$$(48) \quad \tau_j^{FEM} = \frac{3}{17} h_{j+1} \frac{(h_{j+1} - h_j)}{(h_{j+1} + h_j)}.$$

Proof. Consider the general formula derived in Theorem 1

$$(49) \quad \tau_j = \left| \frac{\sum_{i=1}^n \sigma_{ji} \vartheta_{ji}}{\sum_{i=1}^n \eta_{ji} \vartheta_{ji}} \right|,$$

where ϑ_{ji} is defined by (30), and σ_{ji} and η_{ji} are respectively the entries of the matrices M_{000} and M_{100} . Note that in the FEM with quartic spline basis functions, M_{000} and M_{100} are tridiagonal matrices with j^{th} row elements as in Table 2.

TABLE 2. The element integrals of the matrices M_{000} and M_{100} .

Matrix \ Index	$j - 1$	j	$j + 1$
j^{th} row of M_{000}	$\frac{3}{70}h_{j+1}$	$\frac{20}{70}(h_j + h_{j+1})$	$\frac{3}{70}h_{j+1}$
j^{th} row of M_{100}	$\frac{17}{70}$	0	$-\frac{17}{70}$

By Substituting the values of σ_{ji} and η_{ji} from Table 2 in (49) and using the definition of ϑ_{ji} , we get the desired consequence. ■

5. RESULTS AND DISCUSSIONS

Since the main goal of this work is applying the hp -cloud method with the stability scheme, most of the discussion (all figures and tables except Table 7) provided here will be about the main stability parameter τ_j in (31) given in Theorem 1. However, only Table 7 sheds some light on the FEM stability parameter given by Lemma 2. This discussion takes a form of comparison with the main stability parameter.

For point nucleus, the relativistic formula is used to compare our results

$$(50) \quad \lambda_{n_r, \kappa} = \frac{mc^2}{\sqrt{1 + \frac{Z^2 \alpha^2}{(n_r - 1 + \sqrt{\kappa^2 - Z^2 \alpha^2})^2}}},$$

where α is the fine structure constant which has, in atomic unit, the value $1/c$, and the orbital level number n_r takes the values $1, 2, \dots$. To ease performing the comparison, the exact eigenvalues $\lambda_{n_r, \kappa}$ and the positive computed eigenvalues are shifted by $-mc^2$. All computations are performed for the Hydrogen-like Ununoctium ion, where the atomic number and atomic weight for the Ununoctium element are 118 and 294 respectively. Consequently, and since the electron in the Hydrogen-like Ununoctium ion admits relatively large magnitude eigenvalues, for better measuring of the approximation accuracy, through out all computations we shall use the relative error. To treat the singularity of the pure Coulomb potential at $x = 0$, extended nucleus is assumed by modifying the potential to fit the finite nuclear size. The

modified Coulomb potential considers another distribution of the charge along the nucleus (in the region $[0, R]$ where R is the nucleus radius) and pure Coulomb potential in the rest of domain. The continuity and the smoothness property (at least C^1) should be saved for the total modified potential. For the distribution of charge along nucleus, one can consider, e.g., uniform or Fermi distributions, in this work we consider uniformly distributed charge.

As for the boundary conditions, the homogeneous Dirichlet condition is assumed. Note that for better approximation of the eigenstates $1s_{1/2}$ and $2p_{1/2}$, suitable Neumann boundary conditions should also be considered, see [2]. However, here, we do not treat these cases, instead, general computations are performed to account for the essence of discussion. The homogeneous Dirichlet boundary condition is then simply implemented, after coupling with the FEM, by omitting the two finite element functions at the lower and upper boundaries.

As mentioned before, the computation of the radial Dirac operator eigenvalues requires exponential distribution of the nodal points in order to capture desired behavior of the radial functions near the origin. For this purpose, we shall use the following formula

$$(51) \quad x_i = \exp\left(\ln(I_a + \epsilon) + \left(\frac{\ln(I_b + \epsilon) - \ln(I_a + \epsilon)}{n}\right)i\right) - \epsilon, \quad i = 0, 1, 2, \dots, n,$$

where n is the total number of nodal points and $\epsilon \in [0, 1]$ is the nodes intensity parameter. The role of ϵ is to control the intensity of the nodal points close to origin, as smaller ϵ as more nodes are dragged toward the origin, see the discussion below. As for other approximation methods, increasing the number of nodal points provides better approximation, but this, of course, on the account of the computational time. However, we can still obtain a good approximation with relatively less time, compared with increasing the nodal points, if the number of integration points is increased (the same size of the generalized matrices is obtained for a fixed number of nodal points, where increasing the number of integration points means more time is needed for functional evaluations but the same time is used for eigenvalues computation of the generalized system). This does not mean that we do not need to increase the number of nodal points to obtain more computed eigenvalues and improving the approximation, but to get better rate of convergence with less time

consumption, increasing both the numbers of integration points and nodal points are necessary. In this computation, we fix the number of integration points at $10 \cdot n$.

Table 3 shows the approximated eigenvalues of the electron in the Hydrogen-like Ununoctium ion obtained using the usual and the stabilized hp -cloud methods, the computation is obtained at $\rho_j = 2.2h_{j+1}$, $\epsilon = 10^{-5}$, and $n = 600$. The clouds are enriched by $P^t(x) = [1, x(1 - x/2) \exp(-x/2)]$. The eigenvalues, through out the computations in this work, are given in atomic unit. In Table 3, with the usual hp -cloud method, the instilled spurious eigenvalues appear for both positive and negative κ (the two shaded values in the fourteenth level), also the unphysical coincidence phenomenon occurs for the positive κ (the shaded value in the first level). Note that these spuriousity of both categories are removed by the hp -CPG method.

TABLE 3. The first computed eigenvalues of the electron in the Hydrogen-like Ununoctium ion using the usual and the stabilized hp -cloud methods for point nucleus.

Level	hp -cloud $\kappa = 2$	hp -cloud $\kappa = -2$	Exact $\kappa = -2$	hp -CPG $\kappa = -2$	hp -CPG $\kappa = 2$
1	-1829.630750899	-1829.630750902	-1829.630750908	-1829.628309112	
2	-826.7698136330	-826.7698136329	-826.7683539069	-826.7714785272	-826.7738882959
3	-463.1214970564	-463.1214970566	-463.1183252634	-463.1247150569	-463.1261170024
4	-294.4552367950	-294.4552367952	-294.4509801141	-294.4591541031	-294.4600671778
5	-203.2468937049	-203.2468937047	-203.2419549027	-203.2511517040	-203.2517946674
6	-148.5588260984	-148.5588260983	-148.5534402360	-148.5632453116	-148.5637243357
7	-113.2536099083	-113.2536099084	-113.2479180697	-113.2580871797	-113.2584595495
8	-89.16385480233	-89.16385480237	-89.15794547564	-89.16832365853	-89.16862284813
9	-72.00453396071	-72.00453396065	-71.99846504808	-72.00894720487	-72.00919403005
10	-59.35481340095	-59.35481340100	-59.34862423729	-59.35913470352	-59.35934276227
11	-49.76429096817	-49.76429096819	-49.75800915710	-49.76849047005	-49.76866900765
12	-42.32147184311	-42.32147184312	-42.31511730902	-42.32552373918	-42.32567925216
13	-36.43039621976	-36.43039621984	-36.42398370073	-36.43427738957	-36.43441456989
14	-33.96502895994	-33.96502895893	-31.68173025393	-31.69187884728	-31.69200116063
15	-31.68818961940	-31.68818961935	-27.80813459180	-27.81810976712	-27.81821982418

5.1. Integration of hp-cloud functions

To approximate the integrals in the weak form in the Galerkin hp-cloud approximation, we use two-point Gaussian quadrature rule. Gaussian quadrature rules are the most used numerical techniques to evaluate the integrals in MMs due to their exact integrating of polynomials of degree $2m_q - 1$, where m_q is the number of quadrature points [18]. However, using Gaussian quadrature rules yields integration error when the grids are not coincident with the clouds covers, and thus instabilities and spurious modes start to appear. Also for non-uniformly distributed points (the case we assume in this work), Gaussian quadrature rules do not pass the patch test (fail in consistency). Therefore, stabilizing conforming nodal integration (SCNI), see [9], is introduced to overcome these difficulties. The main feature of SCNI is using the divergence theorem to substitute the derivative, i.e., the derivative $\frac{d}{dx}\Psi^h$ in the sub-domain $\Omega_j = [x_j, x_{j+1}]$ is replaced by a smooth derivative (averaging derivative) $\bar{\frac{d}{dx}}\Psi^h$ at $\hat{x} \in \Omega_j$ as

$$\frac{d}{dx}\Psi^h(x) \cong \bar{\frac{d}{dx}}\Psi^h(\hat{x}) = \frac{1}{x_{j+1} - x_j} \int_{x_j}^{x_{j+1}} \frac{d}{dx}\Psi^h(x)dx = \frac{\Psi^h(x_{j+1}) - \Psi^h(x_j)}{x_{j+1} - x_j}.$$

This definition helps stabilizing the integration, further, it saves time in the computation by not calculating the derivatives of the cloud functions. Thus no need to evaluate $(M^{-1})' = -M^{-1}M'M^{-1}$, which is expensive to calculate. For integrating and programming the weak form in MMs, the results from [13, 14] are useful.

The cloud shape functions are evaluated at the integration points (digital evaluation), since, practically, it is somehow impossible to write the cloud functions explicitly without matrix inversion. Also, it is not recommended to obtain the inverse of M directly, instead, LU factorization is better to be used from cost (less time consumption) and numerical stability point of views. Moreover, in MMs generally, to enhance the stability of the computation and to maintain the accuracy (that may be affected or lost due to the round-off error), and to get better conditioning of the matrix M (lower condition number), the origin should be shifted to the evaluation point [18, 24, 27], i.e., x is replaced by the transformation $\bar{x} = x - x_{orig}$, consequently $\psi_i(x) = P^t(0)M^{-1}(x)B_i(x)$ where $M(x) = \sum_{i=1}^n \varphi_i\left(\frac{x - x_i}{\rho_i}\right)P(x_i - x_{orig})P^t(x_i - x_{orig})$ and $B_i(x) = \varphi_i\left(\frac{x - x_i}{\rho_i}\right)P(x_i - x_{orig})$.

5.2. Enrichment basis functions $P(x)$

For the reason discussed before, only intrinsic enrichment, $P(x)$, is considered in the definition of the hp -cloud functions for the computation of the eigenvalues of the radial Dirac operator. The number and the type of enrichment functions in the basis set $P(x)$ can be chosen arbitrary for each cloud [19, 32], but for practical reasons (lowering both the condition number of M and the computational time) we assume $P(x) = [1, p_1(x)]$. For the approximation of the radial Dirac operator eigenvalues, to enrich the cloud with a suitable basis $P(x)$, two main properties should be considered; firstly, and sufficient one, the elements of $P(x)$ ought to have the continuity properties (continuous with continuous first derivatives) of the space \mathcal{H} so that for all j , the cloud ψ_j is a C^1 -function, provided that φ_j is a C^1 -function. Secondly, global behavior and fundamental characters about the electron motion of the Hydrogen-like ion systems should be embedded in $P(x)$. Slater type orbital functions (STOs) and Gaussian type orbital functions (GTOs) provide good description of the electron motion [10, 21]. The quadratic term in the exponent of the GTOs causes numerical difficulty, that is, with the GTOs, the matrix M rapidly becomes poorly conditioned, this is also what is observed when applying quadratic basis enrichments, see [6]. Consequently, the STOs are considered as the enrichment of the hp -cloud functions, thus $p_1(x)$ can have, e.g., the following forms

$$\exp(-x), x \exp(-x/2), x(1-x/2) \exp(-x/2), \dots \text{ etc.}$$

Note that, these functions should be multiplied by normalization parameters, but, computationally, there is no effect of multiplication by these parameters.

Since the global behavior of the eigenstates of the Hydrogen-like ions in the relativistic case (Dirac operator) does not differ much from that of the non-relativistic case (Schrödinger operator), one can also assume the solutions of the radial Coulomb-Schrödinger eigenvalue problem as intrinsic enrichments (see e.g. [22])

$$\mathcal{R}_{n_r \ell}(x) = \mathcal{N}_{n_r \ell} (2Zx/n_r a_0)^\ell \mathbf{L}_{n_r + \ell}^{2\ell + 1}(2Zx/n_r a_0) \exp(-Zx/n_r a_0),$$

where $\mathbf{L}_{n_r + \ell}^{2\ell + 1}(x) = \sum_{k=0}^{n_r + \ell} \frac{(-1)^k}{k!} \binom{n_r + 3\ell + 1}{n_r + \ell - k} x^k$ is the Laguerre polynomial, a_0 is the Bohr radius, $n_r = 1, 2, \dots$ is the orbital level number, and ℓ is, as mentioned

before, the orbital angular momentum number given to be zero for *s*-states, one for *p*-states, two for *d*-states, etc. For general intrinsic enrichment, it is, somehow, tedious to apply the above formula for each level n_r , instead, good results are still achievable even with, e.g., n_r equals the first possible level of the given state (i.e., $n_r = 1$ for all *s*-states, $n_r = 2$ for all *p*-states, $n_r = 3$ for all *d*-states, etc.). Moreover, it is also possible to consider enrichment based on the solution of the radial Dirac eigenvalue problem, see e.g. [11], but the above enrichments are simpler from practical point of view. In the coming discussion, the enrichment basis $P^t(x) = [1, x(1 - x/2) \exp(-x/2)]$ is assumed in all computations.

5.3. Dilation Parameter ρ

The dilation parameter, ρ , plays a crucial role in the approximation accuracy and stability, it serves as the element size in the FEM. The parameter ρ can be chosen fixed or arbitrary, but it is often assumed to be constant for all *hp*-clouds when uniformly distributed nodal points are used. In this work, exponentially distributed nodal points are assumed to get enough information about the radial functions near the origin where they oscillate heavily relative to a region away from it. Thus we consider

$$\rho_j = \nu \cdot \max\{h_j, h_{j+1}\} = \nu h_{j+1},$$

where the maximum is considered to engage sufficiently large region where the cloud function is defined so that possible singularity of the matrix M is substantially decreased, further, ν is the dimensionless size of influence domain [27]. Moreover, for non-uniform mesh, ν can be chosen locally, i.e., $\nu = \nu_j$, where, in this work, we assume fixed ν . Now it remains to determine the value/values of ν taking into account that ρ_j should be large enough ($\nu > 1$) in order to ensure the invertibility of M (to ensure that any region is covered by at least two clouds). On the other hand, ρ_j should not be very large to maintain local character of the approximation. As discussed before (see also Figure 3, the case $\nu = 1.2$), if $\nu \rightarrow 1$, then ψ_j will act as finite element shape function, and thus the features of the *hp*-clouds are gradually lost, also large values of ν make ψ_j to behave like polynomial of higher degree (see Figure 3, the case $\nu = 4$). To conclude, ν should be chosen moderately and such that it guarantees that no integration point is covered by only one cloud [27, 32].

The optimal choices of ν can be determined individually for each problem by carrying out numerical experiments. In [30, 44], it is shown that $\nu \in [2, 3]$ provides nice results for the elasticity problem. For the computation of the radial Dirac operator eigenvalues with the stability scheme, when $\nu \in [2.2, 2.7]$ good results are obtained and the spurious eigenvalues are completely eliminated. Also as ν gets smaller as better approximation is obtained, see Table 4.

TABLE 4. The first computed eigenvalues of the electron in the Hydrogen-like Ununoctium ion for $\kappa = -2$ for point nucleus with different values of ν , where $n = 600$ and $\epsilon = 10^{-5}$ are used.

Level	$\nu = 2.0$	$\nu = 2.2$	$\nu = 2.5$	$\nu = 2.7$	Exact
1	-1829.6287	-1829.6283	-1829.6276	-1829.6270	-1829.6307
2	-826.77119	-826.77147	-826.77197	-826.77233	-826.76835
3	-463.12417	-463.12471	-463.12567	-463.12638	-463.11832
4	-294.45850	-294.45915	-294.46033	-294.46120	-294.45098
5	-203.25046	-203.25115	-203.25244	-203.25340	-203.24195
6	-148.56255	-148.56324	-148.56460	-148.56562	-148.55344
7	-113.25741	-113.25808	-113.25949	-113.26054	-113.24791
8	-89.167688	-89.168323	-89.169756	-89.170831	-89.157945
9	-72.008358	-72.008947	-72.010396	-72.011489	-71.998465
10	-59.358602	-59.359134	-59.360592	-59.361700	-59.348624
11	-49.768025	-49.768490	-49.769950	-49.771070	-49.758009
12	-42.325133	-42.325523	-42.326981	-42.328113	-42.315117
13	-36.433970	-36.434277	-36.435728	-36.436870	-36.423983
14	-31.691663	-31.691878	-31.693318	-31.694472	-31.681730
15	-27.817992	-27.818109	-27.819533	-27.820699	-27.808134

In Figure 4, we study the convergence rate of the first five eigenvalues in Table 4. It is clear how the smaller ν gives the better approximation. One argues, as it is clear from the figure, that ν can be, e.g., of some value less than 2 in order to achieve a better rate of convergence. However, this will be on the account of spurious-ity elimination (the cloud is not stretched enough to capture the desired behavior of the approximated solution) and on the account of the invertibility of the matrix M (for small ν some regions are covered with one cloud). However, as in the FEM, one can apply h -refinement in the hp -cloud method (see e.g. [16, 44]), this can be

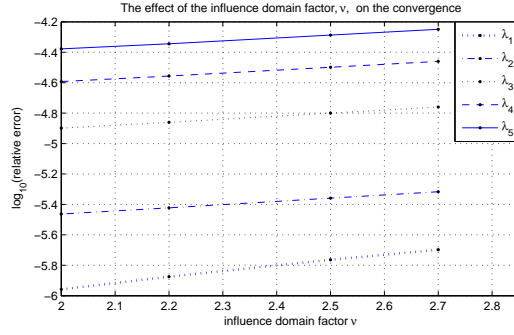


FIGURE 4. Studying the convergence rate with respect to the influence domain factor ν . The comparison is carried out for the first five eigenvalues in Table 4.

done by assuming smaller values of the dilation parameter ρ_j (keeping ν fixed and making h_{j+1} smaller by increasing the number of nodal points). Thus as ρ_j getting smaller, more clouds of smaller domain sizes are added.

The intensity of the exponentially distributed nodal points near the origin has an influence on the convergence rate of the approximation. The intensity of the nodes, near the origin or away from it, is controlled by the nodes intensity parameter, ϵ , via formula (51). As smaller value of ϵ is considered as more concentration of nodes near the origin is obtained, see Figure 5 (the graph to the left).

Table 5 shows the computation of the eigenvalues with different values of ϵ with 600 nodal points. The computation with ϵ smaller than 10^{-7} is almost the same as of $\epsilon = 10^{-7}$, thus it is not required to study smaller values of ϵ than 10^{-7} .

In Figure 5 (the graph to the right), the first computed eigenvalues of Table 5 are studied. It is clear that as ϵ gets larger (up to some limit), better approximation is obtained. However, as mentioned before, the rate of convergence is almost the same when $\epsilon \in (0, 10^{-7})$ ($\epsilon = 0$ is excluded to avoid $\ln(0)$ when extended nucleus is assumed). Also ϵ does not admit relatively large values in order to get enough nodes close to the origin, where the radial functions oscillate relatively more, without increasing the number of nodal points. Therefore, the most appropriate values for ϵ which provide good results, are somewhere in the interval $[10^{-6}, 10^{-4}]$.

TABLE 5. The first computed eigenvalues of the electron in the Hydrogen-like Ununoctium ion for $\kappa = -2$ for point nucleus with different values of ϵ , where $n = 600$ and $\nu = 2.2$ are used.

Level	$\epsilon = 10^{-4}$	$\epsilon = 10^{-5}$	$\epsilon = 10^{-6}$	$\epsilon = 10^{-7}$	Exact
1	-1829.6289	-1829.6283	-1829.6280	-1829.6280	-1829.6307
2	-826.77073	-826.77147	-826.77170	-826.77173	-826.76835
3	-463.12322	-463.12471	-463.12517	-463.12523	-463.11832
4	-294.45726	-294.45915	-294.45973	-294.45981	-294.45098
5	-203.24904	-203.25115	-203.25180	-203.25188	-203.24195
6	-148.56101	-148.56324	-148.56393	-148.56402	-148.55344
7	-113.25578	-113.25808	-113.25879	-113.25888	-113.24791
8	-89.165992	-89.168323	-89.169039	-89.169131	-89.157945
9	-72.006610	-72.008947	-72.009662	-72.009755	-71.998465
10	-59.356811	-59.359134	-59.359844	-59.359936	-59.348624
11	-49.766195	-49.768490	-49.769189	-49.769279	-49.758009
12	-42.323268	-42.325523	-42.326208	-42.326296	-42.315117
13	-36.432073	-36.434277	-36.434943	-36.435030	-36.423983
14	-31.689734	-31.691878	-31.692524	-31.692607	-31.681730
15	-27.816033	-27.818109	-27.818732	-27.818812	-27.808134

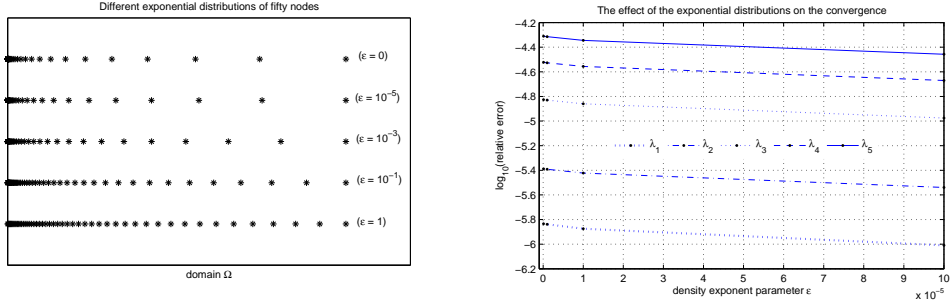


FIGURE 5. To the left, different exponentially distributed nodal points are plotted using the formula (51). To the right, the effect of nodes intensity near the origin on the convergence rate, the comparison is carried out for the first five eigenvalues in Table 5.

The approximation of the stabilized *hp*-cloud scheme with different numbers of nodal points is given in Table 6. The rate of convergence of the corresponding first five eigenvalues is studied in Figure 6, where h is the maximum of all distances between the adjacent nodes which equals to $h_n = x_n - x_{n-1}$, the distance between the last two nodes for exponentially distributed nodes.

TABLE 6. The first computed eigenvalues of the electron in the Hydrogen-like Ununoctium ion for $\kappa = -2$ for point nucleus with different number of nodes, where $\nu = 2.2$ and $\epsilon = 10^{-5}$ are used.

Level	$n = 200$	$n = 400$	$n = 600$	$n = 800$	$n = 1000$	Exact
1	-1829.5628	-1829.6224	-1829.6283	-1829.6297	-1829.6302	-1829.6307
2	-826.82670	-826.77726	-826.77147	-826.76987	-826.76923	-826.76835
3	-463.23292	-463.13630	-463.12471	-463.12146	-463.12016	-463.11832
4	-294.59147	-294.47367	-294.45915	-294.45503	-294.45336	-294.45098
5	-203.39386	-203.26721	-203.25115	-203.24654	-203.24466	-203.24195
6	-148.70878	-148.58009	-148.56324	-148.55835	-148.55635	-148.55344
7	-113.40170	-113.27527	-113.25808	-113.25304	-113.25096	-113.24791
8	-89.306709	-89.185557	-89.168323	-89.163201	-89.161076	-89.157945
9	-72.139617	-72.026008	-72.008947	-72.003802	-72.001653	-71.998465
10	-59.480154	-59.375861	-59.359134	-59.354006	-59.351849	-59.348624
11	-49.878353	-49.784751	-49.768490	-49.763410	-49.761256	-49.758009
12	-42.423104	-42.341207	-42.325523	-42.320517	-42.318374	-42.315117
13	-36.518814	-36.449288	-36.434277	-36.429365	-36.427242	-36.423983
14	-31.762955	-31.706134	-31.691878	-31.687081	-31.684984	-31.681730
15	-27.875610	-27.831538	-27.818109	-27.813442	-27.811376	-27.808134

The lack of error estimates for the approximation of the Dirac eigenvalue problem due to the boundedness problem results in an incomplete picture about the convergence analysis. Nevertheless, from Figure 6, the convergence rate of the approximation of the first five eigenvalues, $\lambda_1, \dots, \lambda_5$, is nearly 3.09, 2.66, 2.62, 2.59, and 2.56 respectively, which it takes a slight decreasing pattern as we go higher in the spectrum levels, see the corresponding table.

With the stability parameter τ^{FEM} , the computation is presented in Table 7. The computation is obtained with 600 nodal points at $\nu = 1.1$ and $\epsilon = 10^{-5}$. The result is compared with the same stability scheme but with the stability parameter τ at the

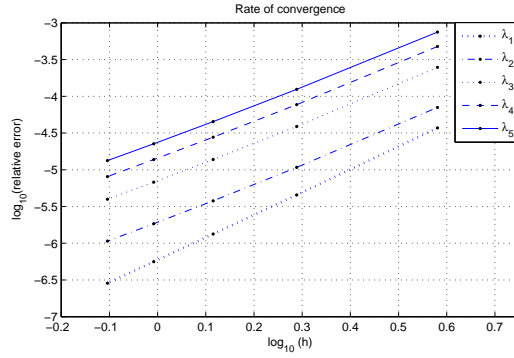


FIGURE 6. Study the convergence rate of the first computed five eigenvalues in Table 6.

same parameters but $\nu = 2.2$, the comparison is also obtained in the non-relativistic limit (very large c).

TABLE 7. The first computed eigenvalues of the electron in the Hydrogen-like Ununoctium ion for $\kappa = -2$ for point nucleus using the stability scheme with the stability parameters τ and τ^{FEM} .

Level	The speed of light			100×The speed of light		
	τ	τ^{FEM}	Exact	τ	τ^{FEM}	Exact
1	-1829.6283	-1829.6304	-1829.6307	-1740.2372	-1740.4777	-1740.5080
2	-826.77147	-826.76993	-826.76835	-773.73860	-773.57259	-773.56033
3	-463.12471	-463.12174	-463.11832	-435.46054	-435.14787	-435.12752
4	-294.45915	-294.45551	-294.45098	-278.88245	-278.49775	-278.48144
5	-203.25115	-203.24715	-203.24195	-193.82362	-193.39522	-193.38978
6	-148.56324	-148.55905	-148.55344	-142.53145	-142.07261	-142.08222
7	-113.25808	-113.25377	-113.24791	-109.23625	-108.75140	-108.78165
8	-89.168323	-89.163916	-89.157945	-86.404375	-85.894382	-85.950912
9	-72.008947	-72.004478	-71.998465	-70.067886	-69.534118	-69.620219
10	-59.359134	-59.354644	-59.348624	-57.975599	-57.420335	-57.537357
11	-49.768490	-49.764010	-49.758009	-48.773149	-48.197640	-48.347352
12	-42.325523	-42.321064	-42.315117	-41.606088	-41.009232	-41.195370
13	-36.434277	-36.429826	-36.423983	-35.913753	-35.292096	-35.520492
14	-31.691878	-31.687405	-31.681730	-31.315908	-30.664671	-30.942291
15	-27.818109	-27.813579	-27.808134	-27.547311	-26.861865	-27.195369

It can be seen from Table 7, the convergence property with τ^{FEM} is slightly better. Unfortunately, the approximation with τ^{FEM} seems to behave strangely at the end of the spectrum, that is, only the spectrum tail has the following behavior (the last eigenvalues of the computation in Table 7 with τ^{FEM} for the relativistic case)

$\lambda_+ - mc^2$	$\lambda_- + mc^2$
207072481.0215	-215565247.3448
211429663.4158*	-220006205.1800*
226003907.3130	-235294474.7992
231896256.0483*	-241138935.9851*
246890583.9362	-257366374.4374
257292411.7094*	-267386241.2969*
267659710.2673*	-279193268.7275*
291928112.6166	-303237209.5231
296228215.8873*	-308029351.9019*

This behavior occurs only for few values at the end of the spectrum, and no such effect is revealed in the rest of the spectrum. To our knowledge, the values marked with * might be spurious eigenvalues for some unknown origins in higher levels, which, in calculating the correlation energy, seem to have no significant effect.

Table 8 shows the computation of the eigenvalues of the electron in the Hydrogen-like Ununoctium ion with $\kappa = -2$. The computation is for extended nucleus obtained using the stability scheme, where the first and the last computed eigenvalues are presented. The number of nodes used is 1000, also the used values of ν and ϵ are respectively 2.2 and 10^{-5} .

Conclusion.

The scheme developed in this work, the *hp*-CPG method, for stabilizing the *hp*-cloud approximation for solving the single-electron Coulomb-Dirac eigenvalue problem ensures complete treatment of the spurious eigenvalues. The scheme strongly depends on the derived stability parameter τ , which is simple to implement and applicable for general finite basis functions. The elimination of the spurious eigenvalues is also affected by the influence domain factor ν , for ν less than 2, spurious eigenvalues start to appear. The convergence rate is high for the first eigenvalues, while it

slowly decreases as the level gets higher. Comparing with the finite element stability approach [2], the scheme convergence rate is lower. We may state that, as the main disadvantage of MMs in general, the *hp*-cloud method is more expensive due to the time consumption in evaluating the shape function which demands more integration point as ν gets larger to obtain the desired accuracy. The number of integration points used here is ten times the number of nodal points (this large number of points is assumed in order to study the effects of the other parameters from a comparative point of view), which can be made smaller, i.e., $\nu \geq 2$ is enough to get sufficient accuracy.

REFERENCES

- [1] E. Ackad and M. Horbatsch, *Numerical solution of the Dirac equation by a mapped fourier grid method*, J. Phys. A: Math. Gen., 38(2005), pp. 3157-3171.
- [2] H. Almasreh, S. Salomonson, and N. Svanstedt, *Stabilized finite element method for the radial Dirac equation*, (submitted).
- [3] R. C. Almeida and R. S. Silva, *A stable Petrov-Galerkin method for convection-dominated problems*, Comput. Methods Appl. Mech. Engng., 140(1997).
- [4] S. N. Atluri and S. Shen, *The meshless local Petrov-Galerkin (MLPG) method: A simple and less-costly alternative to the finite element and boundary element methods*, CMES, 3(2002), pp. 11-51.
- [5] T. Belytschko, D. Organ, and Y. Krongauz, *A coupled finite element-element-free Galerkin method*, Comput. Mech., 17(1995), pp. 186-195.
- [6] T. Belytschko, Y. Krongauz, D. Organ, M. Fleming, and P. Krysl, *Meshless methods: An overview and recent developments*, Comput. Methods Appl. Mech. Engng., 139(1996), pp. 3-47.
- [7] A. N. Brooks, *A Petrov-Galerkin finite element formulation for convection dominated flows*, Thesis for the degree of Doctor of Philosophy, California Institute of Technology, California, 1981.
- [8] A. N. Brooks and T. J. R. Hughes, *Streamline Upwind/Petrove-Galerkin formulations for convection dominated flows with particular emphasis on the incompressible Navier-Stokes equations*, Comput. Methods Appl. Mech. Engng., 32(1982).
- [9] J. S. Chen, C. T. Wu, S. Yoon, and Y. You, *A stabilized conforming nodal integration for Galerkin mesh-free methods*, Int. J. Numer. Methods Engng., 50(2001), pp. 435-466.
- [10] J. S. Chen, W. Hu, and M. A. Puso, *Orbital hp-clouds for solving Schrödinger equation in quantum mechanics*, Comput. Methods Appl. Mech. Engng., 196(2007), pp. 3693-3705.

TABLE 8. The first and the last computed eigenvalues of the electron in the Hydrogen-like Ununoctium ion for $\kappa = -2$ for extended nucleus using the stabilized scheme.

Level	$\lambda_+ - mc^2$	$\lambda_- + mc^2$	Level	$\lambda_+ - mc^2$	$\lambda_- + mc^2$
1	-1829.630099296	-2.434417024833	971	806198985.1845	-814129982.6368
2	-826.7693836687	-2.627617735663	972	825264528.2332	-833843359.2405
3	-463.1204703095	-2.797844649762	973	843910220.2386	-852283956.3394
4	-294.4537598806	-2.957820323769	974	864343472.0411	-873515941.8428
5	-203.2451112716	-3.112227360954	975	884325905.7234	-893193487.1967
6	-148.5568310625	-3.263408080529	976	906287797.8413	-916147241.8477
7	-113.2514598678	-3.412742089389	977	927793189.6390	-937214464.1559
8	-89.16158600002	-3.561138820860	978	951473602.6651	-962134060.6197
9	-72.00216968256	-3.709254718702	979	974736078.1642	-984781962.7117
10	-59.35236884621	-3.857601123902	980	1000361933.873	-1011962889.837
11	-49.76177611950	-4.006600112632	981	1025681563.220	-1036437526.155
12	-42.31889320986	-4.156612122006	982	1053528920.945	-1066240230.486
13	-36.42775793119	-4.307947863723	983	1081298213.911	-1092869973.210
14	-31.68549413213	-4.460872692773	984	1111711637.956	-1125737288.414
15	-27.81188079379	-4.615608997468	985	1142455141.979	-1154979024.500
16	-24.60715078621	-4.772339706105	986	1175881200.913	-1191458619.345
17	-21.92579810728	-4.931213787881	987	1210315776.667	-1223979724.299
18	-19.65981495410	-5.092353196094	988	1247366017.754	-1264753730.099
19	-17.72767091768	-5.255860198286	989	1286494208.919	-1301585190.310
20	-16.06689248232	-5.421824189525	990	1328074902.403	-1347514563.183
21	-14.62895927631	-5.590327472124	991	1373330615.013	-1390354085.681
22	-13.37572611330	-5.761449842514	992	1420940894.294	-1442573015.641
23	-12.27687110094	-5.935272041930	993	1474405770.317	-1494428385.378
24	-11.30804689661	-6.111878218067	994	1530930196.971	-1554661710.974
25	-10.44952215915	-6.291357562437	995	1595537987.175	-1621361454.883
26	-9.685170122048	-6.473805266356	996	1667868144.599	-1693349701.469
27	-9.001706528736	-6.659322921776	997	1746516931.180	-1787808061.719
28	-8.388109077412	-6.848018469445	998	1858171146.415	-1885927735.358
29	-7.835170608265	-7.040005799103	999	1944896072.579	-2040151500.838
30	-7.335151949937	-7.235404092542	1000	2551096858.208	-2992548052.333

- [11] H. Ciftci, R. L. Hall, and N. Saad, *Iterative solutions to the Dirac equation*, Phys. Rev. A, 72(2005).

- [12] P. A. B. De Sampaio, *A Petrov-Galerkin/modified operator formulation for convection-diffusion problems*, Int. J. Numer. methods Engng., 30(1990).
- [13] J. Dolbow and T. Belytschko, *An introduction to programming the meshless element free Galerkin method*, Arch. Comput. Method E., 5(1998), pp. 207-241.
- [14] J. Dolbow and T. Belytschko, *Numerical integration of the Galerkin weak form in meshfree methods*, Comput. Mech., 23(1999), pp. 219-230.
- [15] C. A. Duarte and J. T. Oden, *H-p clouds—An h-p meshless method*, Numer. Meth. Part. D. E., 12(1996), pp. 673-705.
- [16] C. A. Duarte and J. T. Oden, *An h-p adaptive method using clouds*, Comput. Methods Appl. Mech. Engng., 139(1996), pp. 237-262.
- [17] T. Fries and H. Matthies, *A review of Petrov-Galerkin stabilization approaches and an extension to meshfree methods*, Institute of scientific computing, Technical University Braunschweig, Brunswick, Germany, 2004.
- [18] T. Fries and H. Matthies, *Classification and overview of Meshfree Methods*, Institute of scientific computing, Technical University Braunschweig, Brunswick, Germany, 2004.
- [19] O. Garcia, E. A. Fancello, C. S. de Barcellos, and C. A. Duarte, *hp-Clouds in Mindlin's thick plate model*, Int. J. Numer. methods Engng., 47(2000), pp. 1381-1400.
- [20] M. Griesemer and J. Lutgen, *Accumulation of Discrete Eigenvalues of the Radial Dirac Operator*, J. Funct. Anal., 162(1999).
- [21] W. J. Hehre, L. Radom, P. Schleyer, and J. Pople, *Ab initio molecular orbital theory*, John Willey & Sons, New York, 1986.
- [22] W. T. Hill and C. H. Lee, *Light-Matter interaction: Atoms and molecules in external fields and nonlinear optics*, Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim, 2007.
- [23] A. Huerta and S. Fernández-Méndez, *Coupling element free Galerkin and finite element methods*, ECCOMAS, Barcelona, 2000.
- [24] A. Huerta and S. Fernández-Méndez, *Enrichment and coupling of the finite element and meshless methods*, Int. J. Numer. methods Engng., 48(2000), pp. 1615-1636.
- [25] S. Idelsohn, N. Nigro, M. Storti, and G. Buscaglia, *A Petrov-Galerkin formulation for advection-reaction-diffusion problems*, Comput. Methods Appl. Mech. Engng., 136(1996).
- [26] Y. Krongauz and T. Belytschko, *Enforcement of essential boundary conditions in meshless approximations using finite elements*, Comput. Methods Appl. Mech. Engng., 131(1996), pp. 133-145.

- [27] C. V. Le, *Novel numerical procedures for limit analysis of structures: Mesh-free methods and mathematical programming*, Ph.D thesis, University of Sheffield, England, 2009.
- [28] H. Lin and S. N. Atluri, *Meshless local Petrov-Galerkin (MLPG) method for convection-diffusion problems*, CMES, 1(2000), pp. 45-60.
- [29] I. Lindgren, S. Salomonson, and B. Åsén, *The covariant-evolution-operator method in bound-state QED*, Physics Reports, 389(2004), pp. 161-261.
- [30] G. R. Liu, *Mesh Free Methods: Moving Beyond the Finite Element Method*, CRC press, 2003.
- [31] Y. Y. Lu, T. Belytschko, and L. Gu, *A new implementation of the element free Galerkin method*, Comput. Methods Appl. Mech. Engng, 113(1994), pp. 397-414.
- [32] P. de T. R. Mendonça, C. S. de Barcellos, A. Duarte, *Investigations on the hp-cloud method by solving Timoshenko beam problems*, Comput. Mech., 25(2000), pp. 286-295.
- [33] P. J. Mohr, G. Plunien, and G. Soff, *QED corrections in heavy atoms*, Physics Reports, 293(1998), pp. 227-369.
- [34] G. Mur, *On the causes of spurious solutions in electromagnetics*, Electromagnetic, 22(2002), pp. 357-367.
- [35] V. P. Nguyen, T. Rabczuk, S. Bordas, and M. Duflot, *Meshless methods: A review and computer implementation aspects*, Math. Comput. Simulat., 79(2008), pp. 763-813.
- [36] H. Noguchi, T. Kawashima, and T. Miyamura, *Element free analyses of shell and spatial structures*, Int. J. Numer. methods Engng., 47(2000), pp. 1215-1240.
- [37] G. Pestka, *Spurious roots in the algebraic Dirac equation*, Chem. Phys. Lett. 376(2003), pp. 659-661.
- [38] L. Rosenberg, *Virtual-pair effects in atomic structure theory*, Phys. Rev. A, 39(1989), pp. 4377-4386.
- [39] W. Schroeder and I. Wolf, *The origin of spurious modes in numerical solutions of electromagnetic field eigenvalue problems*, IEEE Tran. on Micr. Theory and Tech., 42(1994), pp. 644-653.
- [40] V. M. Shabaev, *Two-time Green's function method in quantum electrodynamics of high-Z few-electron atoms*, Physics Reports, 356(2002), pp. 119-228.
- [41] V. M. Shabaev, I. I. Tupitsyn, V. A. Yerokhin, G. Plunien, and G. Soff, *Dual kinetic balance approach to basis-set expansions for the Dirac equation*, Phys. Rev. Lett., 93(2004).
- [42] B. Thaller, *The Dirac equation*, Springer-Verlag, Berlin, 1993.

- [43] I. I. Tupitsyn and V. M. Shabaev, *Spurious states of the Dirac equation in a finite basis set*, *Optika i Spektroskopiya*, 105(2008), pp. 203-209.
- [44] Y. You, J. S. Chen, and H. Lu *Filters, reproducing kernel, and adaptive meshfree method*, *Comput. Mech.*, 31(2003), pp. 316-326.
- [45] X. Zhang, X. Liu, M. Lu, and Y. Chen, *Imposition of essential boundary conditions by displacement constraint equations in meshless methods*, *Commun. Numer. Meth. Engng.*, 17(2001), pp. 165-178.
- [46] S. Zhao, *On the spurious solutions in the high-order finite difference methods for eigenvalue problems*, *Comput. Methods Appl. Mech. Engng.*, 196(2007), pp. 5031-5046.
- [47] C. Zuppa, *Modified Taylor reproducing formulas and h-p clouds*, *Math. Comput.*, 77(2008), pp. 243-264.

Paper III

G-CONVERGENCE OF DIRAC OPERATORS

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ABSTRACT. We consider the linear Dirac operator with a (-1) -homogeneous locally periodic potential that varies with respect to a small parameter. Using the notation of G-convergence of positive definite self-adjoint operators in Hilbert spaces we prove G-compactness for families of projections of Dirac operators. We also prove convergence of the corresponding point spectrum in the spectral gap.

1. INTRODUCTION

In the present work we study the asymptotic behavior of Dirac operators $\tilde{\mathcal{H}}_h$ with respect to a parameter $h \in \mathbb{N}$ as $h \rightarrow \infty$. We consider Dirac operators $\tilde{\mathcal{H}}_h = \tilde{\mathbf{H}} + V_h$ on $L^2(\mathbb{R}^3; \mathbb{C}^4)$, where $\tilde{\mathbf{H}} = \mathbf{H}_0 + W + \mathbf{I}$ is a shifted Dirac operator. The operators \mathbf{H}_0 , W , \mathbf{I} , and V_h are respectively the free Dirac operator, the Coulomb potential, the 4×4 identity matrix, and a perturbation to $\tilde{\mathbf{H}}$. We will study the asymptotic behavior of $\tilde{\mathcal{H}}_h$ and of the eigenvalues in the gap of the continuous spectrum with respect to the perturbation parameter h .

G-convergence theory which deals with convergence of operators, is well-known for its applications to homogenization of partial differential equations. The concept was introduced in the late 60's by De Giorgi and Spagnolo [5, 9, 10] for linear elliptic and parabolic problems with symmetric coefficients matrices. Later on it was extended to the non-symmetric case by Murat and Tartar [7, 12, 13] under the name of H-convergence. A detailed exposition of G-convergence of positive definite self-adjoint operators can be found in [3]. In the present work we will base a lot of

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our framework on the results in Chapter 12 and 13 in [3]. The Dirac operator is unbounded both from above and below. This means that the theory of G-convergence of positive definite self-adjoint operators is not directly applicable to Dirac operators. In this work we study self-adjoint projections of Dirac operators which satisfy the positivity so that the theory of G-convergence becomes applicable.

We will consider periodic perturbations, i.e., we will assume that the potential V_h is a periodic function with respect to some regular lattice in \mathbb{R}^N . We are then interested in the asymptotic behavior of shifted perturbed Dirac operators $\tilde{\mathcal{H}}_h$. This yields homogenization problems for the evolution equation associated with the Dirac operator $\tilde{\mathcal{H}}_h$

$$\begin{cases} i\hbar \frac{\partial}{\partial t} \mathbf{u}_h(x, t) = \tilde{\mathcal{H}}_h \mathbf{u}_h(x, t), \\ \mathbf{u}_h(\cdot, 0) = \mathbf{u}_h^0 \end{cases}$$

and the corresponding eigenvalue problem

$$\tilde{\mathcal{H}}_h u_h(x) = \lambda_h u_h(x).$$

The paper is arranged as follows: In Section 2 we provide the reader with basic preliminaries on Dirac operators, G-convergence and on the concepts needed from spectral theory. In Section 3 we present and prove the main results.

2. PRELIMINARIES

Let A be a linear operator on a Hilbert space. By $\mathbf{R}(A)$, $\mathbf{D}(A)$, and $\mathbf{N}(A)$ we mean the range, domain, and null-space of A respectively.

2.1. Dirac Operator. We recall some basic facts regarding the Dirac operator. For more details we refer to the monographs [14, 15, 17].

Let X and Y denote the Hilbert spaces $H^1(\mathbb{R}^3; \mathbb{C}^4)$ and $L^2(\mathbb{R}^3; \mathbb{C}^4)$, respectively. The free Dirac evolution equation reads

$$(1) \quad i\hbar \frac{\partial}{\partial t} \mathbf{u}(x, t) = \mathbf{H}_0 \mathbf{u}(x, t),$$

where $\mathbf{H}_0 : Y \rightarrow Y$ is the free Dirac operator with domain $\mathbf{D}(H_0) = X$, which acts on the four-component vector \mathbf{u} . It is a first order linear hyperbolic partial differential equation. The free Dirac operator \mathbf{H}_0 has the form

$$(2) \quad \mathbf{H}_0 = -i\hbar c \boldsymbol{\alpha} \cdot \nabla + mc^2 \beta.$$

Here $\boldsymbol{\alpha} \cdot \nabla = \sum_{i=1}^3 \alpha_i \frac{\partial}{\partial x_i}$, \hbar is the Planck constant divided by 2π , the constant c is the speed of light, m is the particle rest mass and $\boldsymbol{\alpha} = (\alpha_1, \alpha_2, \alpha_3)$ and β are the 4×4 Dirac matrices given by

$$\alpha_j = \begin{pmatrix} 0 & \sigma_j \\ \sigma_j & 0 \end{pmatrix} \quad \text{and} \quad \beta = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}.$$

Here I and 0 are the 2×2 unity and zero matrices, respectively, and the σ_j 's are the 2×2 Pauli matrices

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \text{and} \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Note that a separation of variables in (1) yields the Dirac eigenvalue problem

$$(3) \quad \mathbf{H}_0 u(x) = \lambda u(x),$$

where $u(x)$ is the spatial part of the wave function $\mathbf{u}(x, t)$ and λ is the total energy of the particle. The free Dirac operator \mathbf{H}_0 is essentially self-adjoint on $C_0^\infty(\mathbb{R}^3; \mathbb{C}^4)$ and self-adjoint on X . Moreover, its spectrum, $\sigma(\mathbf{H}_0)$, is purely absolutely continuous (i.e., its spectral measure is absolutely continuous with respect to the Lebesgue measure) and given by

$$\sigma(\mathbf{H}_0) = (-\infty, -mc^2] \cup [mc^2, +\infty).$$

\mathbf{H}_0 describes the motion of an electron that moves freely without external force. Let us now introduce an external field given by a 4×4 matrix-valued function W ,

$$W(x) = W_{ij}(x) \quad i, j = 1, 2, 3, 4.$$

It acts as a multiplication operator in Y , thus the free Dirac operator with additional field W is of the form

$$(4) \quad \mathbf{H} = \mathbf{H}_0 + W.$$

The operator \mathbf{H} is essentially self-adjoint on $C_0^\infty(\mathbb{R}^3; \mathbb{C}^4)$ and self-adjoint on X provided that W is Hermitian and satisfies the following estimate (see e.g. [14])

$$(5) \quad |W_{ij}(x)| \leq a \frac{c}{2|x|} + b, \quad \forall x \in \mathbb{R}^3 \setminus \{0\} \quad i, j = 1, 2, 3, 4,$$

the constant c is the speed of light, $a < 1$, and $b > 0$. From now on we let $W(x)$ be the Coulomb potential $W(x) = \frac{-Z}{|x|} \mathbf{I}$, where Z is the electric charge number

(without ambiguity, \mathbf{I} is usually dropped from the Coulomb term for simplicity). The spectrum of the Dirac operator with Coulomb potential is given by

$$\sigma(\mathbf{H}) = (-\infty, -mc^2] \cup \{\lambda^k\}_{k \in \mathbb{N}} \cup [mc^2, +\infty),$$

where $\{\lambda^k\}_{k \in \mathbb{N}}$ is a discrete sequence of eigenvalues in the "gap" and the remaining part of the spectrum is the continuous part $\sigma(\mathbf{H}_0)$.

In the present paper we consider a parameter-dependent perturbation added to the Dirac operator with Coulomb potential. The purpose is to investigate the asymptotic behavior of the corresponding eigenvalues in the gap and the convergence properties. To this end we introduce a 4×4 matrix-valued function $V_h = V_h(x)$ and define the operator \mathcal{H}_h as

$$(6) \quad \mathcal{H}_h = \mathbf{H} + V_h.$$

We recall that a function F is called homogeneous of degree p if for any nonzero scalar a , $F(ax) = a^p F(x)$. The next theorem is of profound importance for the present work.

Theorem 1. *Let W be Hermitian and satisfy the bound (5) above. Further, for any fixed $h \in \mathbb{N}$, let V_h be a measurable (-1) -homogeneous Hermitian 4×4 matrix-valued function with entries in $L^p_{loc}(\mathbb{R}^3)$, $p > 3$. Then \mathcal{H}_h is essentially self-adjoint on $C_0^\infty(\mathbb{R}^3; \mathbb{C}^4)$ and self-adjoint on X . Moreover*

$$\sigma(\mathcal{H}_h) = (-\infty, -mc^2] \cup \{\lambda_h^k\}_{k \in \mathbb{N}} \cup [mc^2, +\infty),$$

where $\{\lambda_h^k\}_{k \in \mathbb{N}}$ is a discrete sequence of parameter dependent eigenvalues corresponding to the Dirac eigenvalue problem $\mathcal{H}_h u_h(x) = \lambda_h u_h(x)$.

Proof. See [15, 17]. ■

We will as a motivating example consider perturbations which are locally periodic and of the form $V_h(x) = V_1(x)V_2(hx)$. The entries of V_1 are assumed to be (-1) -homogeneous. The entries of $V_2(y)$ are assumed to be periodic with respect to a regular lattice in \mathbb{R}^3 . This can also be phrased that they are defined on the unit torus \mathbb{T}^3 .

The evolution equation associated with the Dirac operator \mathcal{H}_h reads

$$(7) \quad \begin{cases} i\hbar \frac{\partial}{\partial t} \mathbf{u}_h(x, t) = \mathcal{H}_h \mathbf{u}_h(x, t), \\ \mathbf{u}_h(\cdot, 0) = \mathbf{u}_h^0. \end{cases}$$

By the Stone theorem, since \mathcal{H}_h is self-adjoint on X , there exists a unique solution \mathbf{u}_h to (7) given by

$$(8) \quad \mathbf{u}_h(\cdot, t) = \mathcal{U}_h(t) \mathbf{u}_h^0, \quad \forall \mathbf{u}_h^0 \in X,$$

where $\mathcal{U}_h(t) = \exp(-i/\hbar \mathcal{H}_h t)$ is the strongly continuous unitary operator generated by the infinitesimal operator $-(i/\hbar) \mathcal{H}_h$ on Y , see e.g. [6, 14].

In the sequel we will consider a shifted family of Dirac operators denoted by $\tilde{\mathcal{H}}_h$ and defined as $\tilde{\mathcal{H}}_h = \tilde{\mathbf{H}} + V_h$, where $\tilde{\mathbf{H}} = \mathbf{H} + mc^2 \mathbf{I}$. Also without loss of generality we will in the sequel put $\hbar = c = m = 1$. By Theorem 1, for any $h \in \mathbb{N}$, we then get

$$\sigma(\tilde{\mathcal{H}}_h) = (-\infty, 0] \cup \{\tilde{\lambda}_h^k\}_{k \in \mathbb{N}} \cup [2, \infty).$$

2.2. G-convergence. For more detailed information on G-convergence we refer to e.g. [4, 11] for the application to elliptic and parabolic partial differential operators, and to the monograph [3] for the application to general positive definite self-adjoint operators. Here we recall some basic facts about G-convergence of positive definite self-adjoint operators in a Hilbert space \mathcal{Y} .

In the present work we frequently write A_h converges to A when we mean that the sequence $\{A_h\}$ converges to A . Let $\lambda \geq 0$, by $\mathcal{P}_\lambda(\mathcal{Y})$ we denote the class of self-adjoint operators A on a closed linear subspace $\mathcal{V} = \overline{\mathbf{D}(A)}$ of \mathcal{Y} such that $\langle Au, u \rangle \geq \lambda \|u\|_{\mathcal{Y}}^2 \quad \forall u \in \mathbf{D}(A)$.

Definition 1. Let $\lambda > 0$, and let $A_h \in \mathcal{P}_\lambda(\mathcal{Y})$ then we say that A_h G-converges to $A \in \mathcal{P}_\lambda(\mathcal{Y})$, denoted $A_h \xrightarrow[G, w]{G, s} A$ in \mathcal{Y} if $A_h^{-1} P_h u \xrightarrow[w]{s} A^{-1} P u$ in $\mathcal{Y} \quad \forall u \in \mathcal{Y}$, where s and w refer to strong and weak topologies respectively, and P_h and P are the orthogonal projections onto $\mathcal{V}_h := \overline{\mathbf{D}(A_h)}$ and $\mathcal{V} := \overline{\mathbf{D}(A)}$ respectively. Also we say $A_h \in \mathcal{P}_0(\mathcal{Y})$ converges to $A \in \mathcal{P}_0(\mathcal{Y})$ in the strong resolvent sense (SRS) if $(\lambda I + A_h) \xrightarrow[G, s]{G, s} (\lambda I + A)$ in $\mathcal{Y} \quad \forall \lambda > 0$.

The following result provides a useful criterion for G-convergence of self-adjoint operators of the class $\mathcal{P}_\lambda(\mathcal{Y})$, $\lambda > 0$. See [3] for a proof.

Lemma 1. *Given $\lambda > 0$, $A_h \in \mathcal{P}_\lambda(\mathcal{Y})$ and the orthogonal projection P_h onto \mathcal{V}_h . Suppose that for every $u \in \mathcal{Y}$, $A_h^{-1}P_h u$ converges strongly (resp. weakly) in \mathcal{Y} , then there exists an operator $A \in \mathcal{P}_\lambda(\mathcal{Y})$ such that $A_h \xrightarrow{G,s} A$ (resp. $A_h \xrightarrow{G,w} A$) in $\mathcal{P}_\lambda(\mathcal{Y})$.*

From now on we will just use the word "converge" instead of saying "strongly converge", hence $A_h \xrightarrow{G} A$ instead of $A_h \xrightarrow{G,s} A$.

2.3. Some Basic Results in Spectral Theory. For more details see [2, 6, 15]. Given a Hilbert space \mathcal{Y} , let $(\mathcal{U}, \mathcal{A})$ be a measurable space for $\mathcal{U} \subseteq \mathbb{C}$ and \mathcal{A} being a σ -algebra on \mathcal{U} . Let $\mathbb{P}^{\mathcal{Y}} = \mathbb{P}(\mathcal{Y})$ be the set of orthogonal projections onto \mathcal{Y} , then $E : \mathcal{A} \rightarrow \mathbb{P}^{\mathcal{Y}}$ is called a spectral measure if it satisfies the following

- (i) $E(\emptyset) = \mathbf{0}$ (This condition is superfluous given the next properties).
- (ii) Completeness; $E(\mathcal{U}) = \mathbf{I}$.
- (iii) Countable additivity; if $\{\Delta_n\} \subset \mathcal{A}$ is a finite or a countable set of disjoint elements and $\Delta = \cup_n \Delta_n$, then $E(\Delta) = \sum_n E(\Delta_n)$.

If E is spectral measure then $E(\Delta_1 \cap \Delta_2) = E(\Delta_1)E(\Delta_2) = E(\Delta_2)E(\Delta_1)$, also E is modular, i.e., $E(\Delta_1 \cup \Delta_2) + E(\Delta_1 \cap \Delta_2) = E(\Delta_1) + E(\Delta_2)$. For an increasing sequence of sets Δ_n , $\lim_{n \rightarrow \infty} E(\Delta_n) = E(\cup_n \Delta_n)$, while if Δ_n is a decreasing sequence then $\lim_{n \rightarrow \infty} E(\Delta_n) = E(\cap_n \Delta_n)$. Because of the idempotence property of the spectral measure we have $\|E_n u\|_{\mathcal{Y}}^2 = \langle E_n u, E_n u \rangle = \langle E_n^2 u, u \rangle = \langle E_n u, u \rangle \rightarrow \langle E u, u \rangle = \|E u\|_{\mathcal{Y}}^2$, which means that the weak convergence and the strong convergence of a sequence of spectral measures E_n are equivalent.

Let $E_{u,u}(\Delta)$ be the finite scalar measure on \mathcal{A} generated by E ,

$$E_{u,u}(\Delta) = \langle E(\Delta)u, u \rangle = \|E(\Delta)u\|_{\mathcal{Y}}^2$$

and $E_{u,v}(\Delta)$ be the complex measure

$$E_{u,v}(\Delta) = \langle E(\Delta)u, v \rangle, \quad \forall u, v \in \mathcal{Y}.$$

By the above notations $E_{u,v}(\Delta) \leq \|E(\Delta)u\|_{\mathcal{Y}}\|E(\Delta)v\|_{\mathcal{Y}} \leq \|u\|_{\mathcal{Y}}\|v\|_{\mathcal{Y}}$.

Let $\mathcal{U} = \mathbb{R}$. The spectral measure on the real line corresponding to an operator S is denoted by $E^S(\lambda)$ (where the superscript S indicates that the spectral measure E corresponds to a specific operator S)

$$E^S(\lambda) = E^S(\Delta), \quad \text{where } \Delta = (-\infty, \lambda), \text{ for } \lambda \in \mathbb{R}.$$

Clearly $E^S(\lambda)$ is monotonic (nondecreasing), i.e., $E^S(\lambda_1) \leq E^S(\lambda_2)$ for $\lambda_1 \leq \lambda_2$. Also $\lim_{\lambda \rightarrow -\infty} E^S(\lambda) = \mathbf{0}$ and $\lim_{\lambda \rightarrow \infty} E^S(\lambda) = \mathbf{I}$. $E^S(\lambda)$ is self-adjoint, idempotent, positive, bounded, right continuous operator ($\lim_{t \rightarrow 0^+} E^S(\lambda + t) = E^S(\lambda)$), and discontinuous at each eigenvalue of the spectrum. If λ is an eigenvalue, then we define $p(\lambda) = E^S(\lambda) - E^S(\lambda - 0)$ to be the point projection onto the eigenspace of λ . For λ being in the continuous spectrum $p(\lambda) = \mathbf{0}$.

Now we state the spectral theorem for self-adjoint operators.

Theorem 2. *For a self-adjoint operator S defined on a Hilbert space \mathcal{Y} there exists a unique spectral measure E^S on \mathcal{Y} such that*

- (i) $S = \int_{\sigma(S)} \lambda dE^S(\lambda)$.
- (ii) $E(\Delta) = \mathbf{0}$ if $\Delta \cap \sigma(S) = \emptyset$.
- (iii) If $\Delta \subset \mathbb{R}$ is open and $\Delta \cap \sigma(S) \neq \emptyset$, then $E(\Delta) \neq \mathbf{0}$.

Proof. See e.g. [2]. ■

3. THE MAIN RESULTS

Consider the family $\tilde{\mathcal{H}}_h$, $h \in \mathbb{N}$, of Dirac operators with domain $\mathbf{D}(\tilde{\mathcal{H}}_h) = X$. We will state and prove some useful theorems for operators of the class $\mathcal{P}_\lambda(\mathcal{Y})$ for $\lambda \geq 0$, where we use the notations \mathcal{X} and \mathcal{Y} to denote for arbitrary Hilbert spaces.

The following theorem gives a bound for the inverse of operators of the class $\mathcal{P}_\lambda(\mathcal{Y})$ for $\lambda > 0$.

Theorem 3. *Let A be a positive and self-adjoint operator on \mathcal{Y} and put $B = A + \lambda I$. Then for $\lambda > 0$*

- (i) B is injective. Moreover, for every $v \in \mathbf{R}(B)$, $\langle B^{-1}v, v \rangle \geq \lambda \|B^{-1}v\|_{\mathcal{Y}}^2$ and $\|B^{-1}v\|_{\mathcal{Y}} \leq \lambda^{-1} \|v\|_{\mathcal{Y}}$.
- (ii) $\mathbf{R}(B) = \mathcal{Y}$.

Proof. See Propositions 12.1 and 12.3 in [3].

The connection between the eigenvalue problems of the operator and its G-limit (respectively its SRS limit) of the class $\mathcal{P}_\lambda(\mathcal{Y})$ for $\lambda > 0$ (respectively for $\lambda = 0$) is

addressed in the next two theorems. Here we prove the critical case when $\lambda = 0$, where for $\lambda > 0$ the proof is analogous and even simpler.

Theorem 4. *Given a family of operators A_h of the class $\mathcal{P}_0(\mathcal{Y})$ converging to $A \in \mathcal{P}_0(\mathcal{Y})$ in the SRS. Let u_h be the solution of $A_h u_h = f_h$, where f_h is converging to f in \mathcal{Y} . If u_h converges to u in \mathcal{Y} , then u solves the limit problem $Au = f$.*

Proof. Since A_h converges to A in the SRS

$$(9) \quad B_h^{-1} P_h v \rightarrow B^{-1} P v, \quad \forall v \in \mathcal{Y},$$

where B_h and B are $A_h + \lambda I$ and $A + \lambda I$ respectively. Note that by Theorem 4, $\mathbf{D}(B_h^{-1}) = \mathbf{R}(B_h) = \mathcal{Y}$, so the projections P_h and P are unnecessary.

Consider $A_h u_h = f_h$ which is equivalent to $B_h u_h = f_h + \lambda u_h$, by the definition of B_h we have $u_h = B_h^{-1}(f_h + \lambda u_h)$. Define $\mathcal{J}_h = f_h + \lambda u_h$ which is clearly convergent to $\mathcal{J} = f + \lambda u$ in \mathcal{Y} by the assumptions. Therefore $B_h^{-1} \mathcal{J}_h \rightarrow B^{-1} \mathcal{J}$, this is because

$$\begin{aligned} \|B_h^{-1} \mathcal{J}_h - B^{-1} \mathcal{J}\|_{\mathcal{Y}} &= \|B_h^{-1} \mathcal{J}_h - B_h^{-1} \mathcal{J} + B_h^{-1} \mathcal{J} - B^{-1} \mathcal{J}\|_{\mathcal{Y}} \\ &\leq \|B_h^{-1}\|_{\mathcal{Y}} \|\mathcal{J}_h - \mathcal{J}\|_{\mathcal{Y}} + \|B_h^{-1} \mathcal{J} - B^{-1} \mathcal{J}\|_{\mathcal{Y}} \\ &\rightarrow 0. \end{aligned}$$

The convergence to zero follows with help of (9) and the boundedness of the inverse operator B_h^{-1} . Thus, for all $v \in \mathcal{Y}$

$$\langle u, v \rangle = \lim_{h \rightarrow \infty} \langle u_h, v \rangle = \lim_{h \rightarrow \infty} \langle B_h^{-1} \mathcal{J}_h, v \rangle = \langle B^{-1} \mathcal{J}, v \rangle.$$

Hence $\langle u - B^{-1} \mathcal{J}, v \rangle = 0$ for every $v \in \mathcal{Y}$, which implies $Bu = \mathcal{J}$, therefore $Au = f$. ■

Theorem 5. *Let A_h be a sequence in $\mathcal{P}_0(\mathcal{Y})$ converging to $A \in \mathcal{P}_0(\mathcal{Y})$ in the SRS, and let $\{\mu_h, u_h\}$ be the solution of the eigenvalue problem $A_h u_h = \mu_h u_h$. If $\{\mu_h, u_h\} \rightarrow \{\mu, u\}$ in $\mathbb{R} \times \mathcal{Y}$, then the limit couple $\{\mu, u\}$ is the solution of the eigenvalue problem $Au = \mu u$.*

Proof. The proof is straightforward by assuming $f_h = \mu_h u_h$ (which converges to μu in \mathcal{Y}) in the previous theorem. ■

The convergence properties of self-adjoint operators has quite different implications on the asymptotic behavior of the spectrum, in particular on the asymptotic

behavior of the eigenvalues, depending on the type of convergence. For a sequence A_h of operators which converges uniformly to a limit operator A nice results can be drawn for the spectrum. Exactly speaking $\sigma(A_h)$ converges to $\sigma(A)$ including the isolated eigenvalues. The same conclusion holds if the uniform convergence is replaced by the uniform resolvent convergence, see e.g. [6]. In the case of strong convergence (the same for strong resolvent convergence), if the sequence A_h is strongly convergent to A , then every $\lambda \in \sigma(A)$ is the limit of a sequence λ_h where $\lambda_h \in \sigma(A_h)$, but not the limit of every such sequence λ_h lies in the spectrum of A , (see the below example taken from [16]). For weakly convergent sequences of operators no spectral implications can be extracted.

Example. Let $A_{i,h}$ be an operator in $L^2(\mathbb{R})$ defined by

$$A_{i,h} = -\frac{d^2}{dx^2} + V_{i,h}(x), \quad \text{for } h \in \mathbb{N} \text{ and } i = 1, 2,$$

where

$$V_{1,h}(x) = \begin{cases} -1, & \text{if } h \leq x \leq h+1, \\ 0, & \text{Otherwise,} \end{cases} \quad \text{and} \quad V_{2,h}(x) = \begin{cases} -1, & \text{if } x \geq h, \\ 0, & \text{Otherwise.} \end{cases}$$

The operator $A_{i,h}$ converges to $A = -\frac{d^2}{dx^2}$ in the SRS as $h \rightarrow \infty$ for both $i = 1, 2$. One can compute the spectrum for the three operators and obtain $\sigma(A_{1,h}) = [0, \infty) \cup \{\mu_h\}$ for μ_h being a simple eigenvalue in $[-1, 0]$ and $\sigma(A_{2,h}) = [-1, \infty)$, whereas for the unperturbed limit operator A the spectrum consists of just the continuous spectrum, i.e., $\sigma(A) = [0, \infty)$.

Since the uniform convergence is not always the case for operators, the theorem below provides some criteria by which G-convergence of an operator in the set $\mathcal{P}_\lambda(\mathcal{Y})$ (hence convergence in the SRS of operators of the class $\mathcal{P}_0(\mathcal{Y})$) implies the convergence of the corresponding eigenvalues.

Theorem 6. *Let \mathcal{X} be compactly and densely embedded in \mathcal{Y} , and let A_h be a family of operators in $\mathcal{P}_\lambda(\mathcal{Y})$, $\lambda > 0$, with domain \mathcal{X} . If A_h G-converges to $A \in \mathcal{P}_\lambda(\mathcal{Y})$, then $\mathcal{K}_h := A_h^{-1}$ converges in the norm of $\mathcal{B}(\mathcal{Y})$ ($\mathcal{B}(\mathcal{Y})$ is the set of bounded linear operators on \mathcal{Y}) to $\mathcal{K} := A^{-1}$. Moreover the k^{th} eigenvalue μ_h^k of A_h converges to the*

k^{th} eigenvalue μ^k of A and the associated k^{th} eigenvector u_h^k converges to u^k weakly in \mathcal{X} , $\forall k \in \mathbb{N}$.

Proof. By the definition of supremum norm

$$(10) \quad \|\mathcal{K}_h - \mathcal{K}\|_{\mathcal{B}(\mathcal{Y})} = \sup_{\|v\|_{\mathcal{Y}}=1} \|\mathcal{K}_h v - \mathcal{K}v\|_{\mathcal{Y}} = \sup_{\|v\|_{\mathcal{Y}} \leq 1} \|\mathcal{K}_h v - \mathcal{K}v\|_{\mathcal{Y}}.$$

Also, by the definition of supremum norm there exists a sequence v_h in \mathcal{Y} with $\|v_h\|_{\mathcal{Y}} \leq 1$ such that

$$(11) \quad \|\mathcal{K}_h - \mathcal{K}\|_{\mathcal{B}(\mathcal{Y})} \leq \|\mathcal{K}_h v_h - \mathcal{K}v_h\|_{\mathcal{Y}} + \frac{1}{h}.$$

It is well-known that \mathcal{K}_h and \mathcal{K} are compact self-adjoint operators on \mathcal{Y} . Both are bounded operators, by Theorem 3, with compact range \mathcal{X} of \mathcal{Y} .

Consider now the right hand side of (11). We write this as

$$\|\mathcal{K}_h v_h - \mathcal{K}v_h\|_{\mathcal{Y}} + \frac{1}{h} \leq \|\mathcal{K}_h v_h - \mathcal{K}_h v\|_{\mathcal{Y}} + \|\mathcal{K}_h v - \mathcal{K}v\|_{\mathcal{Y}} + \|\mathcal{K}v_h - \mathcal{K}v\|_{\mathcal{Y}} + \frac{1}{h}.$$

The first and the third terms converge to zero by the compactness of \mathcal{K}_h and \mathcal{K} on \mathcal{Y} and the second term converges to zero by the G-convergence of A_h to A . Consequently

$$(12) \quad \|\mathcal{K}_h - \mathcal{K}\|_{\mathcal{B}(\mathcal{Y})} \rightarrow 0.$$

Consider the eigenvalue problems associated to A_h^{-1} and A^{-1}

$$(13) \quad A_h^{-1} v_h^k = \lambda_h^k v_h^k, \quad k \in \mathbb{N}$$

and

$$(14) \quad A^{-1} v^k = \lambda^k v^k, \quad k \in \mathbb{N}.$$

Since A_h^{-1} and A^{-1} are compact and self-adjoint operators it is well-known that there exist infinite sequences of eigenvalues $\lambda_h^1 \geq \lambda_h^2 \geq \dots$ and $\lambda^1 \geq \lambda^2 \geq \dots$ accumulating at the origin, respectively. Define $\mu_h^k := (\lambda_h^k)^{-1}$ and $\mu^k := (\lambda^k)^{-1}$ for all $k \in \mathbb{N}$. Consider now the spectral problems associated to A_h and A

$$(15) \quad A_h u_h^k = \mu_h^k u_h^k, \quad k \in \mathbb{N}$$

and

$$(16) \quad A u^k = \mu^k u^k, \quad k \in \mathbb{N}.$$

There exist infinite sequences of eigenvalues $0 < \mu_h^1 \leq \mu_h^2 \leq \dots$ and $0 < \mu^1 \leq \mu^2 \leq \dots$ respectively. By the compactness of \mathcal{K}_h and \mathcal{K} the sets $\{\lambda_h^k\}_{k=1}^\infty$ and $\{\lambda^k\}_{k=1}^\infty$ are bounded in \mathbb{R} , thus the proof is complete by virtue of the following lemma. ■

Lemma 2. *Let \mathcal{X} , \mathcal{Y} , \mathcal{K}_h , \mathcal{K} , λ_h^k and λ^k be as in Theorem 6, and let $A_h \in \mathcal{P}_\lambda(\mathcal{Y})$, $\lambda > 0$. There is a sequence r_h^k converging to zero with $0 < r_h^k < \lambda^k$ such that*

$$(17) \quad |\lambda_h^k - \lambda^k| \leq c \frac{\lambda^k}{\lambda^k - r_h^k} \sup_{\substack{u \in \mathcal{N}(\lambda^k, \mathcal{K}) \\ \|u\|_{\mathcal{Y}}=1}} \|\mathcal{K}_h u - \mathcal{K}u\|_{\mathcal{Y}},$$

where c is a constant independent of h , and $\mathcal{N}(\lambda^k, \mathcal{K}) = \{u \in \mathbf{D}(\mathcal{K}); \mathcal{K}u = \lambda^k u\}$ is the eigenspace of \mathcal{K} corresponding to λ^k .

Proof. See Theorem 1.4 and Lemma 1.6 in [8] Chapter 3. ■

We can now complete the proof of Theorem 6. By the G-convergence of A_h to A we obtain, by using Lemma 2 and (12), convergence of the eigenvalues and eigenvectors, i.e., $\mu_h^k \rightarrow \mu^k$ and $u_h^k \rightarrow u^k$ weakly in \mathcal{X} as $h \rightarrow \infty$. ■

Let us now return to the shifted and perturbed Dirac operator $\tilde{\mathcal{H}}_h$. We will throughout this section assume the hypotheses of Theorem 1. We further assume that the 4×4 matrix-valued function V_h is of the form $V_h(x) = V_1(x)V_2(hx)$ where V_1 is (-1)-homogeneous and where the entries of $V_2(y)$ are 1-periodic in y , i.e.,

$$V_2^{ij}(y+k) = V_2^{ij}(y), \quad k \in \mathbb{Z}^3.$$

We also assume that the entries of V_2 belong to $L^\infty(\mathbb{R}^3)$. It is then well-known that

$$(18) \quad V_2^{ij}(hx) \rightarrow M(V_2^{ij}) = \int_{\mathbb{T}^3} V_2^{ij}(y) dy,$$

in $L^\infty(\mathbb{R}^3)$ weakly*, where \mathbb{T}^3 is the unit torus in \mathbb{R}^3 . It easily also follows from this mean-value property that

$$V_h \rightarrow V_1 M(V_2),$$

in $L^p(\mathbb{R}^3)$ weakly for $p > 3$, cf the hypotheses in Theorem 1.

We are now interested in the asymptotic behavior of the operator and the spectrum of the perturbed Dirac operator $\tilde{\mathcal{H}}_h$. We recall the spectral problem for $\tilde{\mathcal{H}}_h$, i.e.,

$$\tilde{\mathcal{H}}_h u_h(x) = \tilde{\lambda}_h u_h(x)$$

where there exists a discrete set of eigenvalues $\tilde{\lambda}_h^k$, $k = 1, 2, \dots$ and a corresponding set of mutually orthogonal eigenfunctions u_h^k . We know, by Theorem 1, that the eigenvalues (or point spectrum) $\sigma_p(\tilde{\mathcal{H}}_h) \subset (0, 2)$. We also know that $\tilde{\mathcal{H}}_h$ has absolutely continuous spectrum $\sigma_{ac}(\tilde{\mathcal{H}}_h) = (-\infty, 0] \cup [2, \infty)$. This means that the Dirac operator is neither a positive or negative (semi-definite) operator and thus G-convergence method introduced in the previous section of positive definite self-adjoint operators is not directly applicable. In order to use G-convergence methods for the asymptotic analysis of $\tilde{\mathcal{H}}_h$ we therefore use spectral projection and study the corresponding asymptotic behavior of projected parts of $\tilde{\mathcal{H}}_h$ which are positive definite so that G-convergence methods apply.

Let \mathcal{A} be a fixed σ -algebra of subsets of \mathbb{R} , and let $(\mathbb{R}, \mathcal{A})$ be a measurable space. Consider the spectral measures $E^{\tilde{\mathcal{H}}_h}$ and $E^{\tilde{\mathbf{H}}}$ of the families of Dirac operators $\tilde{\mathcal{H}}_h$ and $\tilde{\mathbf{H}}$ respectively, each one of these measures maps \mathcal{A} onto \mathbb{P}^Y , where \mathbb{P}^Y is the set of orthogonal projections onto Y . By the spectral theorem

$$(19) \quad \tilde{\mathcal{H}}_h = \int_{\sigma(\tilde{\mathcal{H}}_h)} \lambda dE^{\tilde{\mathcal{H}}_h}(\lambda).$$

By the spectral theorem we can also write

$$(20) \quad \int_{\sigma(\tilde{\mathbf{H}})} \lambda dE^{\tilde{\mathbf{H}}}(\lambda) + V_h,$$

since V_h is a multiplication operator.

We recall that $\mathbf{D}(\tilde{\mathcal{H}}_h) = X$, let now

$$\mathcal{N}_h^k = \{u_h \in X; \tilde{\mathcal{H}}_h u_h = \lambda_h^k u_h\},$$

i.e., the eigenspace of $\tilde{\mathcal{H}}_h$ corresponding to the eigenvalue λ_h^k . Further define the sum of mutual orthogonal eigenspaces

$$X_h^p = \bigoplus_{k \in \mathbb{N}} \mathcal{N}_h^k,$$

where X_h^p is a closed subspace of Y invariant with respect to $\tilde{\mathcal{H}}_h$.

It is clear that for $u_h \in X_h^p$ we have

$$\langle \tilde{\mathcal{H}}_h u_h, u_h \rangle = \lambda_h^k \|u_h\|_Y^2 > 0, \quad k = 1, 2, \dots$$

Let us now consider the restriction $\tilde{\mathcal{H}}_h^p$ of $\tilde{\mathcal{H}}_h$ to X_h^p which can be written as

$$\tilde{\mathcal{H}}_h^p = \sum_{\lambda \in \sigma_p(\tilde{\mathcal{H}}_h)} \lambda E^{\tilde{\mathcal{H}}_h, p}(\lambda),$$

where the spectral measure $E^{\tilde{\mathcal{H}}_h, p}$ is the point measure, i.e., the orthogonal projection onto $\ker(\tilde{\mathcal{H}}_h - \lambda \mathbf{I})$. With this construction, $\tilde{\mathcal{H}}_h^p$ is a positive definite and self-adjoint operator on X with compact inverse $(\tilde{\mathcal{H}}_h^p)^{-1}$. By Lemma 1, we conclude that there exists a positive definite and self-adjoint operator $\tilde{\mathcal{H}}^p$ such that, up to a subsequence, $\tilde{\mathcal{H}}_h^p$ G-converges to $\tilde{\mathcal{H}}^p$, where $\tilde{\mathcal{H}}^p$ has domain $\mathbf{D}(\tilde{\mathcal{H}}^p) = X^p$ where

$$X^p = \bigoplus_{k \in \mathbb{N}} \mathcal{N}^k$$

is a closed subspace of Y and where

$$\mathcal{N}^k = \{u \in X; \tilde{\mathcal{H}}^p u = \lambda^k u\}.$$

Moreover, by Theorem 6, the sequence of k^{th} eigenvalues λ_h^k associated to the sequence $\tilde{\mathcal{H}}_h^p$ converges to the k^{th} eigenvalue λ^k of $\tilde{\mathcal{H}}^p$ and the corresponding sequence u_h^k converges to u^k weakly in X . The limit shifted Dirac operator restricted to X^p is explicitly given by

$$\tilde{\mathcal{H}}^p = (\tilde{\mathbf{H}} + V_1 M(V_2))|_{X^p}.$$

This follows by standard arguments in homogenization theory, see e.g. [1].

We continue now to study the asymptotic analysis of the projection to the closed subspace of Y corresponding to the positive part $[2, +\infty)$ of the continuous spectrum of $\tilde{\mathcal{H}}_h$.

We denote by X_h^{ac} the orthogonal complement in X to the eigenspace X_h^p . Thus, X_h^{ac} is the closed subspace invariant with respect to $\tilde{\mathcal{H}}_h$ corresponding to the absolutely continuous spectrum $\sigma_{ac}(\tilde{\mathcal{H}}_h) = (-\infty, 0] \cup [2, \infty)$. We now define the two

mutually orthogonal subspaces $X_h^{ac,+}$ and $X_h^{ac,-}$ with

$$X_h^{ac} = X_h^{ac,+} \oplus X_h^{ac,-}$$

where $X_h^{ac,+}$ corresponds to the positive part $[2, +\infty)$ and $X_h^{ac,-}$ corresponds to the negative part $(-\infty, 0]$, respectively. Next we define the restriction $\tilde{\mathcal{H}}_h^{ac,+}$ of $\tilde{\mathcal{H}}_h$ to $X_h^{ac,+}$ which can be written as

$$\tilde{\mathcal{H}}_h^{ac,+} = \int_{\lambda \in \sigma_{ac}^+(\tilde{\mathcal{H}}_h)} \lambda dE^{\tilde{\mathcal{H}}_h^{ac,+}}(\lambda),$$

where the spectral measure $E^{\tilde{\mathcal{H}}_h^{ac,+}}(\lambda)$ is the continuous spectral measure corresponding to $\tilde{\mathcal{H}}_h^{ac,+}$. By construction, $\tilde{\mathcal{H}}_h^{ac,+}$ is a positive definite and self-adjoint operator on X . Therefore, by Lemma 1, there exists a subsequence of $\tilde{\mathcal{H}}_h^{ac,+}$ which G-converges to a positive definite and self-adjoint operator $\tilde{\mathcal{H}}^{ac,+}$. Moreover, since λ is not an eigenvalue, the corresponding sequence $E^{\tilde{\mathcal{H}}_h^{ac,+}}(\lambda)$ of spectral measures converges to the spectral measure $E^{\tilde{\mathcal{H}}^{ac,+}}(\lambda)$ corresponding to $\tilde{\mathcal{H}}^{ac,+}$.

Let us consider the evolution equation

$$(21) \quad \begin{cases} i \frac{\partial}{\partial t} \mathbf{u}_h(x, t) = \tilde{\mathcal{H}}_h^{ac,+} \mathbf{u}_h(x, t), \\ \mathbf{u}_h(\cdot, 0) = \mathbf{u}_h^0. \end{cases}$$

By the Stone theorem, there exists a unique solution $\mathbf{u}_h = \mathbf{u}(x, t)$ to (21) given by

$$\mathbf{u}_h(\cdot, t) = \mathcal{U}_h(t) \mathbf{u}_h^0, \quad \forall \mathbf{u}_h^0 \in X_h^{ac,+},$$

where $\mathcal{U}_h(t) = \exp(-i\tilde{\mathcal{H}}_h^{ac,+}t)$ is the strongly continuous unitary group of transformations generated by the infinitesimal operator $-i\tilde{\mathcal{H}}_h^{ac,+}$ on Y . By the G-convergence of a subsequence of $\tilde{\mathcal{H}}_h^{ac,+}$ it follows that the corresponding sequence $\mathcal{U}_h^{ac,+}(t)$ of unitary groups of transformations converges to a unitary group of transformations $\mathcal{U}^{ac,+}(t)$ which for every $\mathbf{u}^0 \in X^{ac,+}$ defines the solution $\mathbf{u}(\cdot, t) = \mathcal{U}(t)\mathbf{u}^0$ to the limit evolution equation

$$\begin{cases} i \frac{\partial}{\partial t} \mathbf{u}(x, t) = \tilde{\mathcal{H}}^{ac,+} \mathbf{u}(x, t), \\ \mathbf{u}(\cdot, 0) = \mathbf{u}^0. \end{cases}$$

Finally, by considering the operator $-\tilde{\mathcal{H}}_h^{ac,-}$ where $\tilde{\mathcal{H}}_h^{ac,-}$ is the restriction to $X_h^{ac,-}$, i.e., the closed subspace corresponding to the negative part $(-\infty, 0]$ of the continuous spectrum we can repeat all arguments from the positive part of the

continuous spectrum, where G-convergence of $-\tilde{\mathcal{H}}_h^{ac,-}$ should be understood as the convergence in the SRS.

REFERENCES

- [1] A. Bensoussan, J. L. Lions, and G. Papanicolaou, *Asymptotic Analysis for Periodic Structures*, North-Holland, 1978.
- [2] M. S. Birman and M. Z. Solomjak, *Spectral Theory of Self-adjoint Operators in Hilbert Space*, D. Reidel Publishing Company, Dordrecht, Holland, 1987.
- [3] G. Dal Maso, *An Introduction to Γ -convergence*, Birkhäuser, Boston, 1993.
- [4] A. Defranceschi, *An Introduction to Homogenization and G-convergence*, Lecture Notes, School of Homogenization, ICTP, Trieste, 1993.
- [5] E. De Giorgi and S. Spagnolo, *Sulla convergenze degli integrali dell'energia per operatori ellittici del secondo ordine*, Boll. Un. Mat. Ital., 8(1973), pp. 391-411.
- [6] T. Kato, *Perturbation Theory for Linear Operators*, Springer-Verlag, Berlin Heidelberg, 1976.
- [7] F. Murat, *H-convergence*, Séminaire d'Analyse Fonctionnelle et Numérique de l'Université d'Alger, 1977.
- [8] O. A. Oleinik, A. S. Shamaev, and G. A. Yosifian, *Mathematical Problems in Elasticity and Homogenization*, Elsevier Science Publishers B.V., Amsterdam, 1992.
- [9] S. Spagnolo, *Sul limite delle soluzioni di problemi di Cauchy relativi all'equazione del calore*, Ann. Sc. Norm. Sup. Pisa cl. Sci., 21(1967), pp. 657-699.
- [10] S. Spagnolo, *Convergence in energy for elliptic operators*, Proc. Third Symp. Numer. Solut. Partial Diff. Equat. (College Park, 1975), pp. 469-498, Academic Press, San Diego, 1976.
- [11] N. Svanstedt, *G-convergence of parabolic operators*, Nonlinear Analysis, 36(1999), pp. 807-843.
- [12] L. Tartar, *Cours peccot au collège de France*, Paris, 1977.
- [13] L. Tartar, *Quelques remarques sur l'homogénéisation*, Proc. of the Japan-France seminar 1976, "Functional analysis and numerical analysis", pp. 469-482, Japan society for the promotion of science, 1978.
- [14] B. Thaller, *The Dirac Equation*, Springer-verlag, Berlin, 1993.
- [15] J. Weidman, *Linear Operators in Hilbert Spaces*, Springer-Verlag, New York, 1980.

- [16] J. Weidman, *Strong operator convergence and spectral theory of ordinary differential operators*, Univ. Lagel. Acta Math. No., 34(1997), pp. 153-163.
- [17] J. Weidman, *Lineare Operatoren in Hilberträumen*, Teubner Verlag, Wiesbaden, 2003.

Paper IV

ON G-CONVERGENCE OF POSITIVE SELF-ADJOINT OPERATORS

HASAN ALMANASREH

ABSTRACT. We apply G-convergence theory to study the asymptotic of the eigenvalue problems of positive definite bounded self-adjoint h -dependent operators as $h \rightarrow \infty$. Two operators are considered; a second order elliptic operator and a general linear operator. Using the definition of G-convergence of elliptic operator, we review convergence results of the elliptic eigenvalue problem as $h \rightarrow \infty$. Also employing the general definition of G-convergence of positive definite self-adjoint operator together with Γ -convergence of the associated quadratic form we characterize the G-limit as $h \rightarrow \infty$ of the general operator with some classes of perturbations. As a consequence, we also prove the convergence of the corresponding spectrum.

1. INTRODUCTION

Heterogeneous structures of materials appear often in physics, chemistry, mechanics, life sciences, and engineering. Very often one is also led to consider heterogeneous structures with a very fine and complicated microstructure. Phenomena like heat conduction or transport phenomenon are such structures which typically modeled by mathematical systems such as ordinary differential equations (ODE's) or partial differential equations (PDE's), where the presence of fine microscopic scale is reflected in rapid oscillations of the coefficients. This situation can in general not be treated directly, and if it could be feasible, the numerical methods employed to solve the problem require very fine degree of resolution so that the mesh can capture the oscillations which of course costs a lot, and in some situations, despite of mesh refinement, the solution will be out of reach.

Key words and phrases. G-convergence, Γ -convergence, quadratic form, elliptic operator, self-adjoint, eigenvalues.

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In the present work we consider the convergence of the eigenvalue problem

$$\mathbf{H}_h u_h = \lambda_h u_h$$

for two different operators \mathbf{H}_h defined in some suitable Hilbert spaces. We first consider an elliptic eigenvalue problem where $\mathbf{H}_h = -\operatorname{div}(\mathbf{A}_h(x)\nabla)$ defined on $L^2(\Omega)$ with domain $H_0^1(\Omega)$ for some admissible coefficient matrix $\mathbf{A}_h(x)$, where Ω is an open bounded subset of \mathbb{R}^N , $N \geq 1$. We also consider another arbitrary operator $\mathbf{H}_h = \mathbf{H}_0 + V_h$ defined on $L^2(\Omega)$, where \mathbf{H}_0 is a positive definite bounded self-adjoint operator and V_h is a positive bounded Hermitian multiplicative perturbation. We are interested in the behavior of the operator \mathbf{H}_h as the parameter $h \rightarrow \infty$, particularly we are interested in the asymptotic behavior of the point spectrum (the eigenvalues).

We will use classical operator and variational convergence theory. G-convergence theory is well-known for its applications in homogenization of partial differential equations. The concept was introduced in the late 1960's [9, 13, 14, 15] for linear elliptic and parabolic problems with symmetric coefficient matrices. Then the concept was extended to non-symmetric coefficient matrices [10, 19, 20, 21] known as H-convergence. The definition was then generalized to positive definite self-adjoint operators [6]. Later on, plenty of invaluable results are achieved for the elliptic and hyperbolic problems. In [2, 4, 5] G-convergence of monotone operators is proved. In [16, 17, 18] G-convergence of nonlinear parabolic operators is studied. The theory of G-convergence of differential operators in general is treated in [23, 24]. Through out this paper, we will use the name G-convergence of the case of non-symmetric matrices as well.

The study of the convergence behavior for sequences of operators is often associated to the study of the asymptotic behavior for the associated quadratic forms in the calculus of variations via the notion of Γ -convergence which was introduced in the mid 1970's [8]. Here, we utilize and combine the two concepts in order to prove G-compactness for the operator $\mathbf{H}_h = \mathbf{H}_0 + V_h$.

For the operator $\mathbf{H}_h = -\operatorname{div}(\mathbf{A}_h(x)\nabla)$, the coefficient matrix \mathbf{A}_h is positive definite and bounded, then by the G-compactness criterion for elliptic operators, \mathbf{H}_h has a G-limit as $h \rightarrow \infty$. The operator $\mathbf{H}_h = \mathbf{H}_0 + V_h$ is positive definite, bounded, and self-adjoint, then using Γ -convergence for its associated quadratic form and the

relation between G-convergence and Γ -convergence, we prove that \mathbf{H}_h admits a G-limit as $h \rightarrow \infty$. Under suitable assumptions on the coefficient matrix $\mathbf{A}_h(x)$ and on the perturbation V_h we characterize the G-limits. Consequently we prove the convergence of the corresponding eigenvalues.

The paper is arranged as follows: In Section 2 we provide the reader with basic preliminaries on G-convergence and Γ -convergence. In Section 3 we discuss and revisit G-convergence theory of elliptic operators, and study the convergence properties of the corresponding eigenvalue problems. In Section 4 we prove the G-limit of the operator $\mathbf{H}_h = \mathbf{H}_0 + V_h$.

2. PRELIMINARIES

In what follows Ω will be an open bounded subset of \mathbb{R}^N , $N \geq 1$, further the notations \rightharpoonup and $*\rightharpoonup$ will denote weak and weak* convergence respectively. The domain is denoted by \mathbf{D} . Also c and C will denote real constants that might be different at each occurrence and are independent of all parameters, unless otherwise explicitly specified. The scalar products and norms are denoted by $\langle \cdot, \cdot \rangle$ and $\| \cdot \|$ respectively, where the norms $\| \cdot \|$ will be given indices to distinguish between them, while $\langle \cdot, \cdot \rangle$ are left without indices and their current definitions are obvious from the content.

2.1. G-convergence. For comprehensive materials on G-convergence we refer to e.g. [7, 11, 12], and for a general setting to positive definite self-adjoint operators to the monograph [6]. Below we state two definitions of G-convergence; of elliptic operators and the general definition of positive definite self-adjoint operators.

Consider two positive real numbers α and β such that $0 < \alpha \leq \beta < \infty$, and define the following set of matrices

$$S(\alpha, \beta, \Omega) = \{ \mathbf{A} \in L^\infty(\Omega)^{N \times N} ; (\mathbf{A}(x, \xi), \xi) \geq \alpha |\xi|^2 \text{ and } |\mathbf{A}(x, \xi)| \leq \beta |\xi|, \forall \xi \in \mathbb{R}^N \text{ and a.e. } x \in \Omega \}.$$

We shall define G-convergence of the following sequence of elliptic Dirichlet boundary

value problem

$$(1) \quad \begin{cases} -\operatorname{div}(\mathbf{A}_h(x, Du_h)) = f \text{ in } \Omega, \\ u_h \in H_0^1(\Omega). \end{cases}$$

Definition 1. The sequence \mathbf{A}_h in $S(\alpha, \beta, \Omega)$ is said to G -converge to $\mathbf{A} \in S(\alpha, \beta, \Omega)$, denoted by $\mathbf{A}_h \xrightarrow{G} \mathbf{A}$, if for every $f \in H^{-1}(\Omega)$, the sequence u_h of solutions of (1) satisfies

$$\begin{aligned} u_h &\rightharpoonup u \text{ in } H_0^1(\Omega), \\ \mathbf{A}_h(\cdot, Du_h) &\rightharpoonup \mathbf{A}(\cdot, Du) \text{ in } [L^2(\Omega)]^N, \end{aligned}$$

where u is the unique solution of the problem

$$(2) \quad \begin{cases} -\operatorname{div}(\mathbf{A}(x, Du)) = f \text{ in } \Omega, \\ u \in H_0^1(\Omega). \end{cases}$$

In the sequel we will only consider the case of linear coefficients matrix \mathbf{A}_h , i.e., from now on $\mathbf{A}_h(x, \xi) = \mathbf{A}_h(x)\xi$.

Here are some results that will be used later. These results are given without proofs, for the proofs we refer to [7, 10].

Theorem 1. *G-compactness Theorem.*

For every sequence \mathbf{A}_h in $S(\alpha, \beta, \Omega)$ there exists a subsequence, still denoted by \mathbf{A}_h , and a map $\mathbf{A} \in S(\alpha, \beta, \Omega)$, such that $\mathbf{A}_h \xrightarrow{G} \mathbf{A}$.

Theorem 2. *Uniqueness and Locality of G-limit.*

(i) \mathbf{A}_h has at most one G -limit.

(ii) If $\mathbf{A}_h = \tilde{\mathbf{A}}_h$ on $\omega \subset\subset \Omega$ and $\mathbf{A}_h \xrightarrow{G} \mathbf{A}$ and $\tilde{\mathbf{A}}_h \xrightarrow{G} \tilde{\mathbf{A}}$ then $\mathbf{A} = \tilde{\mathbf{A}}$ on ω .

Theorem 3. If $\mathbf{A}_h \xrightarrow{G} \mathbf{A}$, then $\mathbf{A}_h^t \xrightarrow{G} \mathbf{A}^t$.

Let \mathcal{Y} be a Hilbert space, we provide below the general definition of G -convergence, first we set some useful definitions.

Definition 2. A function $F : \mathcal{Y} \rightarrow [0, \infty]$ is said to be lower semi-continuous (*lsc*) at $u \in \mathcal{Y}$, if

$$F(u) \leq \sup_{U \in \mathcal{N}(u)} \inf_{v \in U} F(v),$$

where $\mathcal{N}(u)$ is the set of all open neighborhoods of u in \mathcal{Y} .

As a consequence of the above definition we have the following

- (i) The inequality in the above definition can be replaced by equality due to the fact that $F(u) \geq \inf\{F(v), v \in U\}$, $\forall U \in \mathcal{N}(u)$.
- (ii) F is *lsc* on \mathcal{Y} , if it is so at each $u \in \mathcal{Y}$.

Definition 3. A function F in \mathcal{Y} is called quadratic form if there exists a linear dense subspace \mathcal{X} of \mathcal{Y} and a symmetric bilinear form $B : \mathcal{X} \times \mathcal{X} \rightarrow [0, \infty)$ such that

$$F(u) = \begin{cases} B(u, u), & \forall u \in \mathcal{X}, \\ \infty, & \forall u \in \mathcal{Y} \setminus \mathcal{X}. \end{cases}$$

Let F and B be as in the definition above, where $\mathbf{D}(F) = \{u \in \mathcal{Y}; F(u) < \infty\}$. The operator associated to F is the linear operator A on $\overline{\mathbf{D}(F)}$ with domain being the set of all $u \in \mathbf{D}(F)$ such that there exists $v \in \overline{\mathbf{D}(F)}$ satisfying $B(u, f) = \langle v, f \rangle$, $\forall f \in \mathbf{D}(F)$ and $Au = v$, $\forall u \in \mathbf{D}(A)$. If $f = u$ then $F(u) = \langle Au, u \rangle$, $\forall u \in \mathbf{D}(A)$.

For $\lambda \geq 0$ we denote the following

- (1) By $\tilde{\mathcal{Q}}_\lambda(\mathcal{Y})$ we denote the class of quadratic forms $F : \mathcal{Y} \rightarrow [0, \infty]$ such that $F(u) \geq \lambda \|u\|_{\mathcal{Y}}^2$, and by $\mathcal{Q}_\lambda(\mathcal{Y})$ the subset of $\tilde{\mathcal{Q}}_\lambda(\mathcal{Y})$ whose elements are *lsc*.
- (2) By $\mathcal{P}_\lambda(\mathcal{Y})$ we denote the class of self-adjoint operators A on a closed linear subspace $\mathcal{V} = \overline{\mathbf{D}(A)}$ of \mathcal{Y} such that $\langle Au, u \rangle \geq \lambda \|u\|_{\mathcal{Y}}^2$, $\forall u \in \mathbf{D}(A)$.

Definition 4. Let $\lambda \geq 0$, and let $A_h \in \mathcal{P}_\lambda(\mathcal{Y})$. If $\lambda > 0$, we say that $A_h \xrightarrow{\text{G}} A \in \mathcal{P}_\lambda(\mathcal{Y})$ in \mathcal{Y} if $A_h^{-1}P_h u \rightarrow A^{-1}Pu$ in \mathcal{Y} , $\forall u \in \mathcal{Y}$, where P_h and P are the orthogonal projections onto $\mathcal{V}_h := \overline{\mathbf{D}(A_h)}$ and $\mathcal{V} := \overline{\mathbf{D}(A)}$ respectively. If $\lambda = 0$, we say that $A_h \in \mathcal{P}_0(\mathcal{Y})$ converges to $A \in \mathcal{P}_0(\mathcal{Y})$ in the strong resolvent sense (SRS) if $(\mu I + A_h) \xrightarrow{\text{G}} (\mu I + A)$ in \mathcal{Y} , $\forall \mu > 0$.

The following result provides a useful criterion for G-convergence of positive definite self-adjoint operators. See [6] for the proof.

Lemma 1. Given $\lambda > 0$, $A_h \in \mathcal{P}_\lambda(\mathcal{Y})$, and an orthogonal projection P_h onto \mathcal{V}_h . Suppose that for every $u \in \mathcal{Y}$, $A_h^{-1}P_h u$ converges in \mathcal{Y} , then there exists an operator $A \in \mathcal{P}_\lambda(\mathcal{Y})$ such that $A_h \xrightarrow{\text{G}} A$ in \mathcal{Y} .

2.2. Γ -convergence. For comprehensive introductions to Γ -convergence we refer to the monographs [3, 6].

Let \mathcal{Y} be a topological space, and let F_h be a sequence of functionals from \mathcal{Y} to $\overline{\mathbb{R}}$.

Definition 5. A sequence of functionals $F_h : \mathcal{Y} \rightarrow \overline{\mathbb{R}}$ is said to Γ -converge to $F : \mathcal{Y} \rightarrow \overline{\mathbb{R}}$, written as $F(u) = \Gamma - \lim_{h \rightarrow \infty} F_h(u)$ and denoted by $F_h \xrightarrow{\Gamma} F$ if

$$F(u) = \Gamma - \liminf_{h \rightarrow \infty} F_h(u) = \Gamma - \limsup_{h \rightarrow \infty} F_h(u),$$

where $\Gamma - \liminf_{h \rightarrow \infty}$ and $\Gamma - \limsup_{h \rightarrow \infty}$ are the Γ -lower and Γ -upper limits respectively defined by

$$F^i(u) := \Gamma - \liminf_{h \rightarrow \infty} F_h(u) = \sup_{U \in \mathcal{N}(u)} \liminf_{h \rightarrow \infty} \inf_{v \in U} F_h(v)$$

and

$$F^s(u) := \Gamma - \limsup_{h \rightarrow \infty} F_h(u) = \sup_{U \in \mathcal{N}(u)} \limsup_{h \rightarrow \infty} \inf_{v \in U} F_h(v).$$

By the definition, it is obvious that the sequence F_h Γ -converges to F if and only if $F^s \leq F \leq F^i$, this means that Γ -convergence and lower semi-continuity are closely related concepts. If in addition \mathcal{Y} satisfies the first axiom of countability (the neighborhood system of every point in \mathcal{Y} has a countable base), then $F_h \xrightarrow{\Gamma} F$ in \mathcal{Y} if and only if the following two conditions are satisfied

- (i) $\forall u \in \mathcal{Y}$ and $\forall u_h$ converging to u , $F(u) \leq \liminf_{h \rightarrow \infty} F_h(u_h)$.
- (ii) $\forall u \in \mathcal{Y}$, $\exists u_h$ converging to u such that $F(u) = \lim_{h \rightarrow \infty} F_h(u_h)$.

Remark 1. The following are some useful properties of Γ -convergence

- (1) A constant sequence of functionals $F_h = f$ does not necessarily Γ -converge to f , but to the relaxation of f , the largest *lsc* functional below f . This is due to the fact that f might not be *lsc*.
- (2) The Γ -limit is always *lsc*.
- (3) Γ -convergence is stable under continuous perturbation, i.e., if $F_h \xrightarrow{\Gamma} F$ in \mathcal{Y} and $G : \mathcal{Y} \rightarrow [0, \infty]$ is continuous, then $F_h + G \xrightarrow{\Gamma} F + G$.
- (4) The Γ -limit of a non-negative quadratic form is also a non-negative quadratic form.

Γ -convergence possesses the compactness property, that is, if \mathcal{Y} is a separable metric space, then every sequence of functionals $F_h : \mathcal{Y} \rightarrow \overline{\mathbb{R}}$ has a Γ -convergent subsequence.

The following theorem is the cornerstone of the relation between Γ -convergence of quadratic forms of the class $\mathcal{Q}_\lambda(\mathcal{Y})$ (respectively $\mathcal{Q}_0(\mathcal{Y})$) and G -convergence of

the associated operators of the class $\mathcal{P}_\lambda(\mathcal{Y})$ for $\lambda > 0$ (respectively strong resolvent convergence of the associated operators of the class $\mathcal{P}_0(\mathcal{Y})$). For the proof of this theorem we refer to [3, 6].

Theorem 4. Let $\lambda > 0$ be a real number, F_h and F be elements of $\mathcal{Q}_0(\mathcal{Y})$, and let $A_h, A \in \mathcal{P}_0(\mathcal{Y})$ be the associated operators respectively. Then the following are equivalent

- (a) $F_h \xrightarrow{\Gamma} F$.
- (b) $(F_h + \lambda \|\cdot\|_{\mathcal{Y}}^2) \xrightarrow{\Gamma} (F + \lambda \|\cdot\|_{\mathcal{Y}}^2)$.
- (c) $(A_h + \lambda I) \xrightarrow{G} (A + \lambda I)$.
- (d) $A_h \rightarrow A$ in the SRS.

Also if $F_h, F \in \mathcal{Q}_\mu(\mathcal{Y})$ for $\mu > 0$, and $A_h, A \in \mathcal{P}_\mu(\mathcal{Y})$ are the associated operators respectively, then the following are equivalent

- (e) $F_h \xrightarrow{\Gamma} F$.
- (f) $A_h \xrightarrow{G} A$.

3. G-CONVERGENCE OF ELLIPTIC OPERATORS

This section is devoted to review some basic results of G-convergence of elliptic operators with source function f_h , at the same time holding in mind the main task, the discussion of eigenvalue problems ($f_h = \lambda_h u_h$). Before proceeding, a time is devoted to study the Dirichlet boundary value problem with h -dependent source function, which turns out to be useful in setting the results of the homogenized eigenvalue problem. The following two lemmata are employed while proving the main results, we refer to [10] for the proofs.

Lemma 2. Let $\xi_h \in [L^2(\Omega)]^N$ be weakly convergent to u_0 in $[L^2(\Omega)]^N$, and $v_h \in H^1(\Omega)$ weakly convergent to v_0 in $H^1(\Omega)$, if

$$\operatorname{div}(\xi_h) \rightarrow \operatorname{div}(\xi_0) \text{ in } H^{-1}(\Omega),$$

then

$$\langle \xi_h, Dv_h \rangle \rightharpoonup \langle \xi_0, Dv_0 \rangle \text{ in } D^*(\Omega),$$

where $D^*(\Omega)$ is the dual space of the dense space $D(\Omega) = C_0^\infty(\Omega)$.

Lemma 3. Let $\mathbf{A}_h \in S(\alpha, \beta, \Omega)$, and assume u_h and v_h in $H^1(\Omega)$ are weakly convergent to u_0 and v_0 in $H^1(\Omega)$ respectively, and such that

$$\begin{aligned}\xi_h &= \mathbf{A}_h \nabla u_h \rightharpoonup \xi_0 \text{ in } [L^2(\Omega)]^N, \\ \operatorname{div}(\xi_h) &\rightarrow \operatorname{div}(\xi_0) \text{ in } H^{-1}(\Omega), \\ \zeta_h &= \mathbf{A}_h^t \nabla v_h \rightharpoonup \zeta_0 \text{ in } [L^2(\Omega)]^N, \\ \operatorname{div}(\zeta_h) &\rightarrow \operatorname{div}(\zeta_0) \text{ in } H^{-1}(\Omega).\end{aligned}$$

then

$$\langle \xi_0, \nabla v_0 \rangle = \langle \nabla u_0, \zeta_0 \rangle \text{ a.e in } \Omega.$$

The main homogenization results for the linear elliptic eigenvalue problem are stated in the following theorem.

Theorem 5. Consider the linear elliptic eigenvalue problem

$$(3) \quad \begin{cases} -\operatorname{div}(\mathbf{A}_h(x) \nabla u_h^k) = \lambda_h^k u_h^k & \text{in } \Omega, \\ u_h^k \in H_0^1(\Omega), \end{cases}$$

where $\mathbf{A}_h \in S(\alpha, \beta, \Omega)$ is symmetric and positive definite. Then the sequences of eigenvalues λ_h^k and the corresponding eigenfunctions u_h^k of (3) converge to λ_0^k in \mathbb{R} and weakly to u_0^k in $H_0^1(\Omega)$ respectively, where the eigencouple $\{\lambda_0^k, u_0^k\}$ is the solution to the G-limit problem

$$(4) \quad \begin{cases} -\operatorname{div}(\mathbf{A}_0(x) \nabla u_0^k) = \lambda_0^k u_0^k & \text{in } \Omega, \\ u_0^k \in H_0^1(\Omega). \end{cases}$$

Remark 2. For equation (3) the following are well-known facts

- (i) $0 < \lambda_h^1 \leq \lambda_h^2 \leq \lambda_h^3 \leq \dots < \infty$.
- (ii) The multiplicity of λ_h^k is finite.
- (iii) The sequence u_h^k forms an orthonormal basis for $L^2(\Omega)$.

Before proving Theorem 5, we state and prove the following theorem for elliptic boundary value problem with source function f_h .

Theorem 6. For the Dirichlet boundary value problem

$$(5) \quad \begin{cases} -\operatorname{div}(\mathbf{A}_h(x) \nabla u_h) = f_h & \text{in } \Omega, \\ u_h \in H_0^1(\Omega), \end{cases}$$

if $\mathbf{A}_h \in S(\alpha, \beta, \Omega)$ and if f_h converges in $H^{-1}(\Omega)$ to f_0 , then the sequence u_h of solutions to (5) is weakly convergent in $H_0^1(\Omega)$ to the solution of

$$(6) \quad \begin{cases} -\operatorname{div}(\mathbf{A}_0(x)\nabla u_0) = f_0 & \text{in } \Omega, \\ u_0 \in H_0^1(\Omega), \end{cases}$$

where \mathbf{A}_0 is the G-limit of \mathbf{A}_h .

Proof. The weak form of (5) is to find $u_h \in H_0^1(\Omega)$ such that $\forall v \in H_0^1(\Omega)$

$$(7) \quad a_h(u_h, v) = \langle f_h, v \rangle,$$

where $a_h(u_h, v) = \langle \mathbf{A}_h \nabla u_h, \nabla v \rangle$. Since $\mathbf{A}_h \in S(\alpha, \beta, \Omega)$, we have the following a priori estimates

$$\alpha \|u_h\|_{H_0^1(\Omega)}^2 \leq a_h(u_h, u_h) = \langle f_h, u_h \rangle \leq c \|f_h\|_{H^{-1}(\Omega)} \|u_h\|_{H_0^1(\Omega)},$$

hence

$$(8) \quad \|u_h\|_{H_0^1(\Omega)} \leq \frac{C}{\alpha}.$$

By (8) and the upper bound of \mathbf{A}_h

$$(9) \quad \|\mathbf{A}_h \nabla u_h\|_{L^2(\Omega)} \leq C \frac{\beta}{\alpha}.$$

So both u_h and $\mathbf{A}_h \nabla u_h$ are bounded sequences in $H_0^1(\Omega)$ and $[L^2(\Omega)]^N$ respectively, hence up to subsequences still denoted by u_h and $\mathbf{A}_h \nabla u_h$

$$(10) \quad u_h \rightharpoonup u_0 \text{ in } H_0^1(\Omega)$$

and

$$(11) \quad \mathbf{A}_h \nabla u_h \rightharpoonup \mathcal{M} \text{ in } [L^2(\Omega)]^N.$$

Claim: we argue that $\mathcal{M} = \mathbf{A}_0 \nabla u_0$, where \mathbf{A}_0 is the G-limit of \mathbf{A}_h (the existence and uniqueness of \mathbf{A}_0 is guaranteed by virtue of Theorem 1 and 2).

Proof of the claim. By (11) it holds that

$$(12) \quad -\operatorname{div}(\mathbf{A}_h \nabla u_h) \rightharpoonup -\operatorname{div}(\mathcal{M}) \text{ in } H^{-1}(\Omega),$$

which means that $\forall v \in H_0^1(\Omega)$

$$(13) \quad \lim_{h \rightarrow \infty} \langle -\operatorname{div}(\mathbf{A}_h \nabla u_h), v \rangle = \langle -\operatorname{div}(\mathcal{M}), v \rangle.$$

Since f_h converges to f_0 in $H^{-1}(\Omega)$ and by (5)

$$(14) \quad \lim_{h \rightarrow \infty} \langle -\operatorname{div}(\mathbf{A}_h \nabla u_h), v \rangle = \lim_{h \rightarrow \infty} \langle f_h, v \rangle = \langle f_0, v \rangle.$$

By the uniqueness of weak limit, together with (13) and (14) we get

$$(15) \quad -\operatorname{div}(\mathcal{M}) = f_0.$$

Since $\mathbf{A}_h \xrightarrow{G} \mathbf{A}_0$, by Theorem 3 it is also true that $\mathbf{A}_h^t \xrightarrow{G} \mathbf{A}_0^t$. Consider now

$$(16) \quad \langle \mathbf{A}_h \nabla u_h, \nabla v_h \rangle = \langle \nabla u_h, \mathbf{A}_h^t \nabla v_h \rangle$$

for a sequence $v_h \in H_0^1(\Omega)$ converging weakly to v_0 in $H_0^1(\Omega)$. The limit passage of (16) together with Lemma 3 give

$$(17) \quad \langle \mathcal{M}, \nabla v_0 \rangle = \langle \nabla u_0, \mathbf{A}_0^t \nabla v_0 \rangle,$$

hence

$$(18) \quad \langle \mathcal{M}, \nabla v_0 \rangle = \langle \mathbf{A}_0 \nabla u_0, \nabla v_0 \rangle.$$

Take $\omega \subset\subset \Omega$ and v_h such that $\nabla v_0 = z \in \mathbb{R}^N$ on ω , then (18) can be written as

$$(19) \quad \langle \mathcal{M} - \mathbf{A}_0 \nabla u_0, z \rangle = 0,$$

consequently, by the density of v_0 in $H_0^1(\Omega)$ we have

$$(20) \quad \mathcal{M} - \mathbf{A}_0 \nabla u_0 = 0,$$

which completes the proof of the claim.

By virtue of (15) and (20), u_h is convergent to u_0 , where u_0 is the solution of the homogenized equation

$$(21) \quad \begin{cases} -\operatorname{div}(\mathbf{A}_0(x) \nabla u_0) = f_0 & \text{in } \Omega, \\ u_0 \in H_0^1(\Omega), \end{cases}$$

where $\mathbf{A}_0(x)$ is the G-limit of $\mathbf{A}_h(x)$. ■

By the uniqueness of the solution u_0 to (21), one can drop the subsequence assumption and conclude that the whole sequence is convergent to u_0 (any other subsequence of u_h has to converge only to u_0 by the uniqueness of solution, thus the entire sequence converges to the same limit as its all subsequences).

Now we give the proof of the main result of this section: Theorem 5.

Proof of Theorem 5.

By virtue of Theorem 6, it suffices to prove

$$(22) \quad \lambda_h^k \rightarrow \lambda_0^k \text{ in } \mathbb{R},$$

$$(23) \quad u_h^k \rightarrow u_0^k \text{ in } L^2(\Omega).$$

Indeed, since we can set in Theorem 6 $f_h = \lambda_h^k u_h^k$ which, using (22) and (23), converges to $f_0 = \lambda_0^k u_0^k$ in $L^2(\Omega) \forall k$ by the following

$$\begin{aligned} \|f_h - f_0\|_{L^2(\Omega)} &= \|\lambda_h^k u_h^k - \lambda_0^k u_h^k + \lambda_0^k u_h^k - \lambda_0^k u_0^k\|_{L^2(\Omega)} \\ &\leq |\lambda_h^k - \lambda_0^k| \|u_h^k\|_{L^2(\Omega)} + |\lambda_0^k| \|u_h^k - u_0^k\|_{L^2(\Omega)} \\ &\rightarrow 0. \end{aligned}$$

Hence if (22) and (23) are satisfied, then by Theorem 6 the eigencouple $\{\lambda_0^k, u_0^k\}$ is the solution to the homogenized eigenvalue problem

$$(24) \quad \begin{cases} -\operatorname{div}(\mathbf{A}_0(x)\nabla u_0^k) = \lambda_0^k u_0^k & \text{in } \Omega, \\ \{\lambda_0^k, u_0^k\} \in \mathbb{R} \times H_0^1(\Omega). \end{cases}$$

Note that by Remark 2 part (i), the sequence λ_h^k is bounded in \mathbb{R} for all k , so a subsequence, denoted by λ_h^k , can be extracted from λ_h^k such that

$$(25) \quad \lambda_h^k \rightarrow \lambda_0^k \text{ in } \mathbb{R}.$$

Also, since $\mathbf{A}_h(x) \in S(\alpha, \beta, \Omega)$ we have

$$(26) \quad \alpha \|u_h^k\|_{H_0^1(\Omega)}^2 \leq a_h(u_h, u_h) = \langle \mathbf{A}_h u_h, u_h \rangle \leq \beta \lambda_h^k \|u_h^k\|_{L^2(\Omega)}^2,$$

which implies $\|u_h^k\|_{H_0^1(\Omega)} \leq C$ for all k . Thus, up to a subsequence still denoted by u_h^k ,

$$(27) \quad u_h^k \rightharpoonup u_0^k \text{ in } H_0^1(\Omega).$$

Hence (23) is justified for a subsequence by Rellich-Kondrachov compactness theorem. The subsequence assumptions can be dropped by the uniqueness of limits, thus the entire sequences λ_h^k and u_h^k converge to λ_0^k and u_0^k respectively. \blacksquare

4. G-CONVERGENCE OF POSITIVE DEFINITE BOUNDED SELF-ADJOINT OPERATORS

Let \mathbf{H}_0 be a positive definite bounded self-adjoint operator defined on $L^2(\Omega)$ with domain $H_0^1(\Omega)$. Assume that $V_h(x)$, $x \in \Omega$, is a positive bounded real-valued perturbation. In this section we discuss the asymptotic limit of the eigenvalue problem $\mathbf{H}_h u_h = (\mathbf{H}_0 + V_h)u_h = \lambda_h u_h$ as the parameter h tends to infinity. We utilize the general definition of G-convergence of positive definite self-adjoint operator together with Γ -convergence of the associated quadratic form to characterize the G-limit of \mathbf{H}_h and to discuss the asymptotic limit of the corresponding eigenvalue problem.

The following theorem is a general setting for the relation between the eigenvalue problems of an operator and its G-limit in the class $\mathcal{P}_\lambda(\mathcal{Y})$ for $\lambda > 0$. Here we assume general Hilbert spaces \mathcal{X} and \mathcal{Y} .

Theorem 7. Let $\lambda > 0$, let A_h be a sequence in $\mathcal{P}_\lambda(\mathcal{Y})$ G-converging to $A \in \mathcal{P}_\lambda(\mathcal{Y})$, and let $\{\mu_h, u_h\}$ be the solution of the eigenvalue problem $A_h u_h = \mu_h u_h$. If $\{\mu_h, u_h\} \rightarrow \{\mu, u\}$ in $\mathbb{R} \times \mathcal{Y}$, then the limit couple $\{\mu, u\}$ is the solution of the eigenvalue problem $Au = \mu u$.

Proof. See [1]. ■

On contrary to the uniform resolvent convergence (uniform convergence), the strong resolvent convergence (strong convergence) does not imply the convergence of the spectrum, but at most we have that, if a sequence A_h is convergent in the SRS (or strongly convergent) to A , then every $\mu \in \sigma(A)$ is the limit of a sequence μ_h where $\mu_h \in \sigma(A_h)$, but not the limit of every sequence μ_h lies in the spectrum of A , see, e.g., [22]. The theorem below provides conditions on which G-convergence of an operator in $\mathcal{P}_\lambda(\mathcal{Y})$ for $\lambda > 0$ (hence convergence in the SRS of operators of the class $\mathcal{P}_0(\mathcal{Y})$) implies the convergence of the corresponding eigenvalues.

Theorem 8. Let \mathcal{X} be compactly and densely embedded in \mathcal{Y} , and let A_h be a family of operators in $\mathcal{P}_\lambda(\mathcal{Y})$, $\lambda > 0$, with domain \mathcal{X} . If A_h G-converges to $A \in \mathcal{P}_\lambda(\mathcal{Y})$, then $\mathcal{K}_h := A_h^{-1}$ converges in the norm of $\mathcal{B}(\mathcal{Y})$ ($\mathcal{B}(\mathcal{Y})$ is the set of bounded linear operators on \mathcal{Y}) to $\mathcal{K} := A^{-1}$. Moreover the k^{th} eigenvalue μ_h^k of A_h converges to the k^{th} eigenvalue μ^k of A , $\forall k \in \mathbb{N}$.

Proof. See [1]. ■

The following lemma provides sufficient conditions for which Γ -convergence and pointwise convergence are equivalent.

Lemma 4. Let \mathcal{Y} be a normed vector space and let F_h be a sequence of convex functions on \mathcal{Y} . Suppose that F_h is equi-bounded in a neighborhood of $u \in \mathcal{Y}$ (i.e., there exists $U \in \mathcal{N}(u)$ such that $|F_h(v)| \leq C$ for every $v \in U$ and all h), then

$$F^i(u) = \liminf_{h \rightarrow \infty} F_h(u), \quad \text{and} \quad F^s(u) = \limsup_{h \rightarrow \infty} F_h(u).$$

For the operators $\mathbf{H}_h = \mathbf{H}_0 + V_h$ and $\mathbf{H} = \mathbf{H}_0 + V$ we define respectively the corresponding quadratic forms

$$F_h(u) = \begin{cases} \langle \mathbf{H}_h u, u \rangle, & u \in H_0^1(\Omega), \\ \infty, & u \in L^2(\Omega) \setminus H_0^1(\Omega), \end{cases}$$

and

$$F(u) = \begin{cases} \langle \mathbf{H} u, u \rangle, & u \in H_0^1(\Omega), \\ \infty, & u \in L^2(\Omega) \setminus H_0^1(\Omega). \end{cases}$$

Theorem 9. Let V_h be a sequence in $L^\infty(\Omega)$ that converges weakly* to V . Then \mathbf{H}_h G-converges to $\mathbf{H} = \mathbf{H}_0 + V$.

Proof. By Theorem 4, it suffices to prove that the associated quadratic form $\mathbf{F}_h(u)$ of H_h Γ -converges to the associated quadratic form $F(u)$ of \mathbf{H} . The convergence of the quadratic form is clear since by the weak* convergence of V_h to V in $L^\infty(\Omega)$ we have

$$\begin{aligned} \lim_{h \rightarrow \infty} F_h(u) &= \lim_{h \rightarrow \infty} \left(\langle \mathbf{H}_0 u, u \rangle + \langle V_h u, u \rangle \right) \\ &= \langle \mathbf{H}_0 u, u \rangle + \langle V u, u \rangle \\ &= F(u). \end{aligned}$$

Then using Lemma 4 above we conclude the proof. ■

The following lemma proves the continuity of F_h in $H_0^1(\Omega)$.

Lemma 5. $F_h(u)$ is continuous in $H_0^1(\Omega)$.

Proof. Let $u, v \in H_0^1(\Omega)$ be such that $\|u - v\|_{H_0^1(\Omega)} < \varepsilon$, then

$$\begin{aligned} |F_h(u) - F_h(v)| &= \left| \langle \mathbf{H}_h u, u \rangle - \langle \mathbf{H}_h v, v \rangle \right| \\ &\leq \left| \langle \mathbf{H}_h(u + v), (u - v) \rangle \right| \\ &\leq \|\mathbf{H}_h(u + v)\|_{L^2(\Omega)} \|u - v\|_{L^2(\Omega)} \\ &\leq \varepsilon \|\mathbf{H}_h(u + v)\|_{L^2(\Omega)}. \end{aligned}$$

The term in the last inequality approaches zero as $\varepsilon \rightarrow 0$, thus the lemma is proved. ■

The following theorem proves and characterizes the G-limit of \mathbf{H}_h for another class of potentials V_h .

Theorem 10. If V_h is a weakly convergent sequence in $L^p(\Omega)$, $2 \leq p < \infty$, with a weak limit denoted by V , then \mathbf{H}_h G-converges to \mathbf{H} .

Proof. Let F_h and F be the quadratic forms corresponding to \mathbf{H}_h and \mathbf{H} respectively. Following Theorem 4, to prove that \mathbf{H}_h G-converges to \mathbf{H} , is equivalent to show that F_h Γ -converges to F . To this end, we consider the quadratic form F_h of \mathbf{H}_h ,

$$F_h(u) = \begin{cases} \langle \mathbf{H}_h u, u \rangle, & u \in H_0^1(\Omega), \\ \infty, & u \in L^2(\Omega) \setminus H_0^1(\Omega). \end{cases}$$

By the definition of Γ -convergence, to prove that F is the Γ -limit of F_h , is equivalent to justify the following two conditions

- (i) lim inf-inequality: For every sequence u_h converging to u in $L^2(\Omega)$, $F(u) \leq \liminf_{h \rightarrow \infty} F_h(u_h)$.
- (ii) lim-equality: There exists a sequence u_h converging to u in $L^2(\Omega)$ such that $F(u) = \lim_{h \rightarrow \infty} F_h(u_h)$.

To prove the lim inf-inequality we assume that $u_h \in H_0^1(\Omega)$. Otherwise the proof is obvious. By the continuity of F_h in $H_0^1(\Omega)$ and since piecewise affine functions are dense in $H_0^1(\Omega)$, it suffices to prove the inequality for this class of functions (the same holds true for the lim-equality).

Let $\Omega = \cup_{j=1}^m \Omega^j$ where Ω^j are disjoint sets, and let u_h be linear in each Ω^j converging in $L^2(\Omega)$ to $u = \sum_{j=1}^m (a_j x + b_j) \chi_{\Omega^j}$, where a_j and b_j are elements of \mathbb{C}^3

and the product $a_j x$ is understood to be componentwise. Consider now F_h with the sequence u_h ,

$$(28) \quad F_h(u_h) = \langle \mathbf{H}_0 u_h, u_h \rangle + \langle V_h u_h, u_h \rangle.$$

Since $u_h \rightarrow u$ in $L^2(\Omega)$,

$$(29) \quad \langle \mathbf{H}_0 u, u \rangle = \|\mathbf{H}_0^{1/2} u\|_{L^2(\Omega)}^2 \leq \liminf_{h \rightarrow \infty} \|\mathbf{H}_0^{1/2} u_h\|_{L^2(\Omega)}^2 = \liminf_{h \rightarrow \infty} \langle \mathbf{H}_0 u_h, u_h \rangle.$$

Hence

$$(30) \quad \liminf_{h \rightarrow \infty} F_h(u_h) \geq \langle \mathbf{H}_0 u, u \rangle + \liminf_{h \rightarrow \infty} \int_{\Omega} V_h |u_h|^2 dx.$$

For the last term of (30)

$$(31) \quad \begin{aligned} \liminf_{h \rightarrow \infty} \int_{\Omega} V_h |u_h|^2 dx &= \liminf_{h \rightarrow \infty} \int_{\Omega} V_h |u + u_h - u|^2 dx \\ &\geq \liminf_{h \rightarrow \infty} \int_{\Omega} V_h |u|^2 dx + \liminf_{h \rightarrow \infty} \int_{\Omega} V_h u^* (u_h - u) dx + \\ &\quad + \liminf_{h \rightarrow \infty} \int_{\Omega} V_h u (u_h - u)^* dx. \end{aligned}$$

The symbol $*$ in (31) refers to the complex conjugate. The first term to the right of the inequality of (31) converges to $\int_{\Omega} V |u|^2 dx$ by the weak convergence of V_h to V in $L^p(\Omega)$, $2 \leq p < \infty$. Since $u_h \rightarrow u$ in $L^2(\Omega)$, the second and third terms to the right of the inequality of (31) are vanishing as $h \rightarrow \infty$. Thus we have the lim inf-inequality, namely

$$(32) \quad \liminf_{h \rightarrow \infty} F_h(u_h) \geq \langle \mathbf{H}_0 u, u \rangle + \langle V u, u \rangle = F(u).$$

To prove the lim-equality for some convergent sequence, again by the continuity argument it is enough to justify the equality for a piecewise affine sequence. So consider $u_h = u = (ax + b)\chi_{\Omega}$, then

$$\begin{aligned} \lim_{h \rightarrow \infty} F_h(u_h) &= \langle \mathbf{H}_0 u, u \rangle + \lim_{h \rightarrow \infty} \langle V_h u, u \rangle \\ &= \langle \mathbf{H}_0 u, u \rangle + \langle V u, u \rangle, \end{aligned}$$

the resulted limit is due to the boundedness of the set Ω and the linearity of u . ■

By Theorem 8, the eigenvalues of the operator \mathbf{H}_h converge to the eigenvalues of the G-limit operator \mathbf{H} for those types of potentials considered in the last two theorems. Also employing Theorem 7, the eigenvalue problem $\mathbf{H}_h \varphi_h^k = \tilde{\lambda}_h^k \varphi_h^k$ converges to the limit problem $\mathbf{H} \varphi^k = \tilde{\lambda}^k \varphi^k$ for all $k \in \mathbb{N}$.

As a consequence of G-convergence, if $E^{\mathbf{H}_h}$ and $E^{\mathbf{H}}$ are the continuous spectral measures of \mathbf{H}_h and \mathbf{H} respectively, then

$$E^{\mathbf{H}_h}(\lambda) \rightarrow E^{\mathbf{H}}(\lambda) \text{ strongly, for all } \lambda \in \mathbb{R} \text{ such that } E^{\mathbf{H}}(\lambda) = E^{\mathbf{H}}(-\lambda).$$

For the convergence of the associated unitary group, if $\mathcal{U}^{\mathbf{H}_h}(t)$ and $\mathcal{U}^{\mathbf{H}}(t)$ are the unitary operators generated by \mathbf{H}_h and \mathbf{H} respectively, then $\mathcal{U}_h^{\mathbf{H}_h}(t) \rightarrow \mathcal{U}^{\mathbf{H}}(t)$ for all $t \in \mathbb{R}^+$.

REFERENCES

- [1] H. Almanasreh, N. Svanstedt, *G-convergence of Dirac operators*, J. Funct. Spaces Appl., 2012(2012).
- [2] A. Braides, V. Chiado-Piat, and A. Defranceschi, *Homogenization of almost periodic monotone operators*, Ann. Inst. H. Poincaré, Anal. Nonlinear, 9(1992), pp. 399-432.
- [3] A. Braides, *Γ -convergence for Beginners*, Oxford University Press Inc., New York, 2002.
- [4] V. Chiado-Piat, G. Dal Maso and A. Defranceschi, *G-convergence of monotone operators*, Ann. Inst. H. Poincaré, Anal. Non Lineaire, 7(1990), pp. 123-160.
- [5] V. Chiado-Piat and A. Defranceschi, *Homogenization of monotone operators*, Nonlinear Anal., 14(1990), pp. 717-732.
- [6] G. Dal Maso, *An Introduction to Γ -convergence*, Birkhäuser, Boston, 1993.
- [7] A. Defranceschi, *An Introduction to Homogenization and G-convergence*, Lecture Notes, School of Homogenization, ICTP, Trieste, 1993.
- [8] E. De Giorgi and T. Franzoni, *Su un tipo convergenza variazionale*, Atti Accad. Naz. Lincei Rend. Cl. Sci. Mat. 58(1975), pp. 842-850.
- [9] E. De Giorgi and S. Spagnolo, *Sulla convergenze degli integrali dell'energia per operatori ellittici del secondo ordine*, Boll. Un. Mat. Ital., 8(1973), pp. 391-411.
- [10] F. Murat, *H-convergence*, Séminaire d'Analyse Fonctionnelle et Numérique de l'Université d'Alger, 1977.

- [11] M. Olsson, *G-convergence and homogenization of some monotone operators*, Thesis of the degree of Doctor of Philosophy, Mid Sweden University, Östersund, 2008.
- [12] J. Silver, *G-convergence and homogenization involving operators compatible with two-scale convergence*, Thesis of the degree of Doctor of Philosophy, Mid Sweden University, Östersund, 2007.
- [13] S. Spagnolo, *Sul limite delle soluzioni di problemi di Cauchy relativi all'equazione del calore*, Ann. Sc. Norm. Sup. Pisa cl. Sci., 21(1967), pp. 657-699.
- [14] S. Spagnolo, *Sulla convergenza delle soluzioni di equazioni paraboliche ed ellittiche*, Ann. Sc. Norm. Sup. Pisa cl. Sci., 22(1968), pp. 571-597.
- [15] S. Spagnolo, *Convergence in energy for elliptic operators*, Proc. Third Symp. Numer. Solut. Partial Diff. Equat. (College Park, 1975), pp. 469-498, Academic Press, San Diego, 1976.
- [16] N. Svanstedt, *G-convergence of parabolic operators*, Nonlinear Analysis, 36(1999), pp. 807-843.
- [17] N. Svanstedt, *Correctors for the homogenization of monotone parabolic operators*, J. Nonlinear Math. Phys., 7(2000), pp. 268-283.
- [18] N. Svanstedt, *Multiscale stochastic homogenization of monotone operators*, Networks and Heterogeneous Media, 2(2007), pp. 181-192.
- [19] L. Tartar, *Cours peccot au collège de France*, Paris, 1977.
- [20] L. Tartar, *Convergence d'opérateurs différentiels*, Analisi convessa, Roma, 1977.
- [21] L. Tartar, *Quelques remarques sur l'homogénéisation*, Proc. of the Japan-France seminar 1976, "Functional analysis and numerical analysis", pp. 469-482, Japan society for the promotion of science, 1978.
- [22] J. Weidman, *Strong operator convergence and spectral theory of ordinary differential operators*, Univ. Lagel. Acta Math. No., 34(1997), pp. 153-163.
- [23] V. V. Zikov, S. M. Kozlov, and O. A. Oleinik, *G-convergence of parabolic operators*, Russian Math. Surveys, 36(1981).
- [24] V. V. Zikov, S. M. Kozlov, and O. A. Oleinik, T. Kha, and Aben Noan, *Averaging and G-convergence of differential operators*, Russian Math. Surveys, 34(1979), pp. 69-147.

Paper V

STRONG CONVERGENCE OF WAVE OPERATORS FOR A FAMILY OF DIRAC OPERATORS

HASAN ALMANASREH

ABSTRACT. We consider a family of Dirac operators with potentials varying with respect to a parameter h . The set of potentials has different power-like decay independent of h . The proofs of existence and completeness of the wave operators are similar to that given in [4]. We are mainly interested in the asymptotic behavior of the wave operators as $h \rightarrow \infty$.

1. INTRODUCTION

In quantum mechanics, it is important to compare a given interacted operator with a simpler (free) operator for which many spectral features are known. Scattering theory is part of perturbation theory that concerns a comparative study of the absolutely continuous spectrum of operators. That is, for two self-adjoint operators T and T_0 that are close to each other in an appropriate sense, scattering theory is mainly the study of existence of $s\text{-}\lim_{t \rightarrow \pm\infty} e^{iTt} \mathcal{J} e^{-iT_0 t}$ where \mathcal{J} is some bounded operator (identification) and s refers to the strong convergence sense. Another important issue is the case studied in the present work, where the operator T is h -dependent, with h a parameter allowed to grow to infinity. For such operators, in addition to study the existence of the time limit, a parallel question also emerges whether or not the limit $s\text{-}\lim_{h \rightarrow \infty} s\text{-}\lim_{t \rightarrow \pm\infty} e^{iT_h t} \mathcal{J}_h e^{-iT_0 t}$ exists, where now \mathcal{J}_h is an h -dependent bounded identification.

Scattering theory for the Dirac operator with potentials decaying faster than the Coulomb potential (short-range potentials) goes straightforward. In this case,

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the proofs of existence and completeness of the wave operator (WO) $W(H, H_0) = s\text{-}\lim_{t \rightarrow \pm\infty} e^{iHt} e^{-iH_0 t}$, where H_0 and H are respectively the free and the interacted Dirac operators, are similar to that of the Schrödinger operator. In the Coulomb interaction case, the modified WO $W_{\pm} = W_{\pm}(H, H_0, \mathcal{J}) = s\text{-}\lim_{t \rightarrow \pm\infty} e^{iHt} \mathcal{J} e^{-iH_0 t}$ has been constructed in [2, 3], where \mathcal{J} is a bounded identification. For potentials decaying as the Coulomb potential or slower (long-range potentials), the existence and completeness of the modified WO W_{\pm} have been studied in [4, 8, 9, 12, 18]. The study of the asymptotic behavior of the WO W_{\pm} with respect to the speed of light (c), as $c \rightarrow \infty$, has been studied for short-range potential in [17] and for long-range potential in [18].

Consider the family of Dirac operators $H_h = H_0 + V_h$ defined on the same space and with the same domain as of H_0 , where H_0 is the free Dirac operator defined on the Hilbert space $L^2(\mathbb{R}^3, \mathbb{C}^4)$ with domain $H^1(\mathbb{R}^3, \mathbb{C}^4)$, and V_h is a bounded interaction to H_0 . Under suitable power-like decay assumption on the potential V_h the WO $W_{\pm, h} := W(H_h, H_0; \mathcal{J}_{\pm, h}) = s\text{-}\lim_{t \rightarrow \pm\infty} e^{iH_h t} \mathcal{J}_{\pm, h} e^{-iH_0 t}$ exists and is complete [4], where $\mathcal{J}_{\pm, h}$ is a bounded identification. In other words, if for all $h > 0$, $|V_h| \leq \langle x \rangle^{-\rho}$, where $\langle x \rangle = (1 + |x|^2)^{1/2}$, then the WO $W_{\pm, h}$ exists and is complete where $\mathcal{J}_{\pm, h}$ being just the identity operator for $\rho > 1$ (short-range). For $0 < \rho \leq 1$ (long-range), the identification $\mathcal{J}_{\pm, h}$ is a pseudo-differential operator (PSDO) defined as

$$(\mathcal{J}_{\pm, h} g)(x) = (2\pi)^{-3/2} \int_{\mathbb{R}^3} e^{ix \cdot \zeta + i\Phi_{\pm, h}(x, \zeta)} \mathcal{P}_{\pm, h}(x, \zeta) \mathcal{C}_{\pm}(x, \zeta) \psi(|\zeta|^2) \hat{g}(\zeta) d\zeta,$$

where $\Phi_{\pm, h}$ is a phase function, $\mathcal{P}_{\pm, h}$ is an amplitude function, \mathcal{C}_{\pm} is a cut-off function, and ψ is a smooth function introduced to localize $\mathcal{J}_{\pm, h}$ in compact intervals from the continuous spectrum.

The goal of the present work is to study the asymptotic behavior of the WO $W_{\pm, h}$ and its adjoint $W_{\pm, h}^* = W_{\pm}(H_0, H_h; \mathcal{J}_{\pm, h}^*)$ as $h \rightarrow \infty$. By the existence of $W_{\pm, h}$, the convergence of H_h in the strong resolvent sense (SRS), and the strong convergence of the identification $\mathcal{J}_{\pm, h}$ we prove that the two strong limits $s\text{-}\lim_{h \rightarrow \infty}$ and $s\text{-}\lim_{t \rightarrow \pm\infty}$ are interchangeable. Hence, if the Dirac operator H_h converges in the SRS to H_{∞} and $\mathcal{J}_{\pm, h}$ converges strongly $\mathcal{J}_{\pm, \infty}$, then we have

$$s\text{-}\lim_{h \rightarrow \infty} W_{\pm, h} = W_{\pm}(H_{\infty}, H_0; \mathcal{J}_{\pm, \infty}).$$

By the strong convergence of the identification $\mathcal{J}_{\pm,h}$ to $\mathcal{J}_{\pm,\infty}$, then also $\mathcal{J}_{\pm,h}^*$ converges strongly to $\mathcal{J}_{\pm,\infty}^*$ (this is not true in general, but it is valid for the type of identifications we consider in this work), hence we also have

$$s\text{-}\lim_{h \rightarrow \infty} W_{\pm,h}^* = W_{\pm}(H_0, H_{\infty}; \mathcal{J}_{\pm,\infty}^*).$$

Further, we consider different cases of potential decay, for these cases, the identification $\mathcal{J}_{\pm,h}$ is simplified so that its strong convergence is easy to work out. In the case $\rho = 1$, we prove that the phase and amplitude functions, $\Phi_{\pm,h}$ and $\mathcal{P}_{\pm,h}$, can be chosen independent of h , thus the convergence of the WOs $W_{\pm,h}$ and $W_{\pm,h}^*$, as $h \rightarrow \infty$, is reduced to the convergence of the Dirac operator H_h in the SRS. In the case $\rho \in (1/2, 1)$, the amplitude function can be chosen independent of h , but not the phase function. In this case, even that the phase function still depends on h , but it can be simplified so that the convergence of the identification $\mathcal{J}_{\pm,h}$ is simpler to consider.

The paper is arranged as follows; in Section 2 we provide the reader with brief preliminaries about the Dirac operator, scattering theory in general setting, basic calculus of PSDO, and the existence and completeness of the WO $W_{\pm,h}$. In Section 3, we state and prove the main results of the asymptotic limit of the WO $W_{\pm,h}$ as $h \rightarrow \infty$, also different cases of potential decay are discussed.

2. PRELIMINARIES

By $\mathbf{R}(A)$, $\mathbf{D}(A)$, and $\mathbf{N}(A)$ we refer respectively to the range, domain, and null space of a given operator A , also we denote by X and Y the Hilbert spaces $H^1(\mathbb{R}^3, \mathbb{C}^4)$ and $L^2(\mathbb{R}^3, \mathbb{C}^4)$ respectively.

2.1. The Dirac operator with an h -dependent potential. The free Dirac evolution equation is given by

$$(1) \quad i\hbar \frac{\partial}{\partial t} u(x, t) = H_0 u(x, t), \quad u(x, 0) = u^0(x),$$

where $H_0 : X \rightarrow Y$ is the free Dirac operator defined as

$$(2) \quad H_0 = \hbar c D_{\alpha} + mc^2 \beta.$$

Here, \hbar is the Planck constant divided by 2π , $D_\alpha = \alpha \cdot D$ where $D = (D_1, D_2, D_3)$ and $D_j = -i\frac{\partial}{\partial x_j}$ for $j = 1, 2, 3$, the constant c is the speed of light, and m is the particle rest mass. The notations $\alpha = (\alpha_1, \alpha_2, \alpha_3)$ and β are the 4×4 Dirac matrices given by

$$\alpha_j = \begin{pmatrix} 0 & \sigma_j \\ \sigma_j & 0 \end{pmatrix} \quad \text{and} \quad \beta = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}.$$

Here I and 0 are the 2×2 unity and zero matrices respectively, and σ_j 's are the 2×2 Pauli matrices

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \text{and} \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Note that separation of the variables x and t in (1) yields the free Dirac eigenvalue problem

$$(3) \quad H_0 u(x) = \lambda u(x),$$

where $u(x)$ is the spatial part of the wave function $u(x, t)$, and λ is the total energy of the particle. The free operator H_0 is essentially self-adjoint on $C_0^\infty(\mathbb{R}^3 \setminus \{0\}, \mathbb{C}^4)$ and self-adjoint on X , its spectrum, $\sigma(H_0)$, is purely absolutely continuous and is given by

$$\sigma(H_0) = (-\infty, -mc^2] \cup [mc^2, +\infty).$$

Let \mathcal{F} be the Fourier transform operator

$$(4) \quad (\mathcal{F}u)(\zeta) = (2\pi)^{-3/2} \int_{\mathbb{R}^3} e^{-ix \cdot \zeta} u(x) dx =: \hat{u}(\zeta),$$

then $\mathcal{F}H_0\mathcal{F}^*$ is the multiplication operator given by the matrix

$$(5) \quad h_0(\zeta) = \zeta_\alpha + mc^2\beta,$$

known as the symbol of H_0 , where $\zeta_\alpha = \alpha \cdot \zeta = \sum_{k=1}^3 \alpha_k \zeta_k$. The symbol $h_0(\zeta)$ can be written as

$$(6) \quad h_0(\zeta) = \eta(\zeta)p_{+,0}(\zeta) - \eta(\zeta)p_{-,0}(\zeta),$$

where $p_{\pm,0}(\zeta)$ are the orthogonal projections onto the eigenspaces of $h_0(\zeta)$ and are given by

$$(7) \quad p_{\pm,0}(\zeta) = \frac{1}{2}(I \pm \eta^{-1}(\zeta)(\zeta_\alpha + mc^2\beta)),$$

and $\pm\eta(\zeta) = \pm\sqrt{|\zeta|^2 + m^2c^4}$ are the corresponding eigenvalues.

We consider an h -dependent potential, $V_h(x)$, added to the free Dirac operator and define

$$(8) \quad H_h = H_0 + V_h.$$

The potential V_h is assumed to be real and say bounded, thus, for all $h > 0$, H_h and H_0 have the same domain X and H_h is self-adjoint on X . For simplicity we assume $\hbar = c = 1$. The corresponding evolution equation reads

$$(9) \quad \begin{cases} i\frac{\partial}{\partial t}u_h(x, t) = H_h u_h(x, t), \\ u_h(x, 0) = u_h^0(x). \end{cases}$$

By the Stone theorem, there exists a unique solution to (9) given by

$$(10) \quad u_h(x, t) = U_h(t)u_h^0(x), \quad u_h^0 \in X,$$

where the strongly continuous unitary operator $U_h(t) = \exp(-iH_h t)$ is generated by the operator $-iH_h$, see e.g. [6, 11].

The potential V_h is assumed to fulfill the following condition for all multi-index α

$$(11) \quad |\partial^\alpha V_h(x)| \leq C\langle x \rangle^{-\rho-|\alpha|}, \quad \text{for all } h > 0, \text{ and } \rho \in (0, 1],$$

the constant C is independent of x and h , and recall that $\langle x \rangle = (1 + |x|^2)^{1/2}$. This condition simply means that V_h is of long-range type for all $h > 0$.

2.2. Basic setting of scattering theory. Given self-adjoint operators H_0 and H in Hilbert spaces \mathcal{H}_0 and \mathcal{H} respectively. Let $P_0^{(ac)}$ and $P^{(ac)}$ be the orthogonal projections onto the absolutely continuous subspaces, $\mathcal{H}_0^{(ac)}$ and $\mathcal{H}^{(ac)}$, of H_0 and H respectively.

Definition 1. The WO for H and H_0 , with a bounded identification $\mathcal{J} : \mathcal{H}_0 \rightarrow \mathcal{H}$ is denoted by $W_\pm(H, H_0; \mathcal{J})$ and defined as

$$(12) \quad W_\pm(H, H_0; \mathcal{J}) = s\text{-}\lim_{t \rightarrow \pm\infty} U(-t)\mathcal{J}U_0(t)P_0^{(ac)},$$

provided that the corresponding strong limits exist, where again the letter s refers to the strong convergence sense, $U(t) = e^{-iHt}$ and $U_0(t) = e^{-iH_0t}$. If $\mathcal{H} = \mathcal{H}_0$ and \mathcal{J} is the identity operator, then the WO is denoted by $W_\pm(H, H_0)$. Also if H_0 has only absolutely continuous spectrum, then $P_0^{(ac)}$ is superfluous.

If the WO exists, then it is bounded. Since the operator $U(-t)U_0(t)$ is unitary, the WO $W_{\pm}(H, H_0)$ is isometric. In the case that \mathcal{J} is not the identity operator, the WO $W_{\pm}(H, H_0; \mathcal{J})$ is isometric if $\lim_{t \rightarrow \pm\infty} \|\mathcal{J}U_0(t)u_0\|_{\mathcal{H}} = \|u_0\|_{\mathcal{H}_0}$ for any $u_0 \in \mathcal{H}_0^{(ac)}$. The WO admits the chain rule, i.e., if $W_{\pm}(H, H_1; \mathcal{J}_1)$ and $W_{\pm}(H_1, H_0; \mathcal{J}_0)$ exist, then the WO $W_{\pm}(H, H_0; \mathcal{J}_{10}) = W_{\pm}(H, H_1; \mathcal{J}_1)W_{\pm}(H_1, H_0; \mathcal{J}_0)$ also exists, where $\mathcal{J}_{10} = \mathcal{J}_1\mathcal{J}_0$. The WO possesses the intertwining property, that is

$$(13) \quad \phi(H)W_{\pm}(H, H_0; \mathcal{J}) = W_{\pm}(H, H_0; \mathcal{J})\phi(H_0),$$

for any bounded Borel function ϕ . Also for any Borel set $\Delta \subset \mathbb{R}$

$$(14) \quad E(\Delta)W_{\pm}(H, H_0; \mathcal{J}) = W_{\pm}(H, H_0; \mathcal{J})E_0(\Delta),$$

where E and E_0 are the spectral families of H and H_0 respectively. The following remark is about the equivalence between WOs with different identifications.

Remark 1. Assume that the WO $W_{\pm}(H, H_0; \mathcal{J}_1)$ exists with an identification \mathcal{J}_1 , and let \mathcal{J}_2 be another identification such that $\mathcal{J}_1 - \mathcal{J}_2$ is compact, then the WO $W_{\pm}(H, H_0; \mathcal{J}_2)$ exists and $W_{\pm}(H, H_0; \mathcal{J}_1) = W_{\pm}(H, H_0; \mathcal{J}_2)$. Moreover, the condition that $\mathcal{J}_1 - \mathcal{J}_2$ is compact can be replaced by $s\text{-}\lim_{t \rightarrow \pm\infty} (\mathcal{J}_1 - \mathcal{J}_2)U_0(t)P_0^{(ac)} = 0$.

Another task of scattering theory is to study the completeness of WOs.

Definition 2. The WO W_{\pm} is said to be complete if $\mathbf{R}(W_{\pm}) = \mathcal{H}^{(ac)}$.

If the WO $W_{\pm}(H, H_0; \mathcal{J})$ is complete, then the absolutely continuous part of H_0 is unitary equivalent to that of H . We refer to [14] for the completeness criteria. For comprehensive materials on scattering theory we refer to [5, 6, 7, 10, 13, 14, 16].

Definition 3. Given a self-adjoint operator H in a Hilbert space \mathcal{H} . An H -bounded operator, $A : \mathcal{H} \rightarrow \mathfrak{H}$, where \mathfrak{H} is an auxiliary Hilbert space, is called H -smooth if one of the following properties is fulfilled

$$\sup_{\|v\|_{\mathcal{H}}=1, v \in \mathbf{D}(H)} \int_{-\infty}^{\infty} \|Ae^{-iHt}v\|_{\mathfrak{H}}^2 dt < \infty,$$

$$\sup_{\varepsilon > 0, \mu \in \mathbb{R}} \|AR_H(\mu \pm i\varepsilon)\|_{\mathfrak{H}}^2 < \infty,$$

where $R_H(\mu \pm i\varepsilon)$ is the resolvent operator of H .

2.3. Preliminaries regarding pseudo-differential operators. In this subsection we will introduce basic calculus about pseudo-differential operators (PSDO's) with symbols belonging to the class $\mathcal{S}_{\rho,\delta}^r(\mathbb{R}^3, \mathbb{R}^3)$.

Definition 4. The class $\mathcal{S}_{\rho,\delta}^r(\mathbb{R}^3, \mathbb{R}^3)$ is the vector space of all smooth functions $\mathcal{P}(x, \zeta) : \mathbb{R}^3 \times \mathbb{R}^3 \rightarrow \mathbb{C}$ such that for all multi-indices α and γ

$$(15) \quad |\partial_x^\alpha \partial_\zeta^\gamma \mathcal{P}(x, \zeta)| \leq c_{\alpha,\gamma} \langle x \rangle^{r-\rho|\alpha|+\delta|\gamma|},$$

where $r \in \mathbb{R}$, $\rho > 0$, and $\delta < 1$. The function \mathcal{P} is called the symbol of the PSDO and r is called the order of \mathcal{P} .

Let $\mathcal{P}(x, \zeta) \in \mathcal{S}_{\rho,\delta}^r(\mathbb{R}^3, \mathbb{R}^3)$, the associated PSDO, \mathcal{P} , to \mathcal{P} in Y is defined as the following inverse Fourier integral

$$(16) \quad (\mathcal{P}f)(x) = (2\pi)^{-3/2} \int_{\mathbb{R}^3} e^{ix \cdot \zeta} \mathcal{P}(x, \zeta) \hat{f}(\zeta) d\zeta,$$

where $f \in Y$ and $\hat{f}(\zeta) = (2\pi)^{-3/2} \int_{\mathbb{R}^3} e^{-ix \cdot \zeta} f(x) dx$ its Fourier transform.

Definition 5. The class $C^r(\Phi) \subset \mathcal{S}_{1-s,s}^r$, $s \in [0, 1)$, consists of all oscillating symbols \mathcal{P} that have the representation $\mathcal{P}(x, \zeta) = e^{i\Phi(x,\zeta)} b(x, \zeta)$, where $\Phi \in \mathcal{S}_{1,0}^s$ and $b \in \mathcal{S}_{1,0}^r$.

The following two propositions are important, their proofs can be found in [15].

Proposition 1. Let $\mathcal{P} \in \mathcal{S}_{0,0}^r$ be compactly supported in x , then the associated PSDO \mathcal{P} is bounded in Y if $r = 0$ and compact if $r < 0$.

Proposition 2. Let $\mathcal{P} \in C^r(\Phi)$ be compactly supported in x , then the associated PSDO \mathcal{P} is bounded in Y if $r = 0$ and compact if $r < 0$.

2.4. The wave operator. In this subsection we adapt the proofs derived in [4] for the class of potentials that we intend to study. Since the potentials we assume are of long-range type for all $h > 0$, there is no need to discuss the construction of the identification \mathcal{J}_h upon the eikonal equation, and thus most of the materials set in this subsection are similar to that given in [4].

Let $\mathcal{E}_\pm(x, \zeta)$ be a cut-off function defined as

$$(17) \quad \mathcal{E}_\pm(x, \zeta) = \theta(x) \omega_\pm(\langle \check{x}, \check{\zeta} \rangle), \quad \text{for all } y \in \mathbb{R}^3 \setminus \{0\}, \check{y} = y/|y|.$$

The function θ is a $C^\infty(\mathbb{R}^3)$ -function such that $\theta(x) = 0$ near $x = 0$ and $\theta(x) = 1$ for large x , thus $\theta(x)$ is introduced to avoid the singularity of \tilde{x} at $x = 0$. The function $\omega_\pm \in C^\infty(-1, 1)$ is such that $\omega_\pm(\tau) = 1$ near ± 1 and $\omega_\pm(\tau) = 0$ near ∓ 1 . Thus the cut-off function \mathcal{C}_\pm is supported in the cone

$$(18) \quad \Xi_\pm(\nu) = \{(x, \zeta) \in \mathbb{R}^6 : \pm \langle x, \zeta \rangle \geq \nu |x| |\zeta|\}, \quad \nu \in (-1, 1).$$

The purpose of defining the cut-off function is that the eikonal equation of the phase function of the approximated eigenfunction of the Dirac equation is not solvable, and thus it is obliged to remove a neighborhood of $-\zeta$ or ζ in order to find a global solution, see [4] for more clarification. Let now $\Phi_{\pm, h}(x, \zeta)$ be defined as

$$(19) \quad \Phi_{\pm, h}(x, \zeta) = \sum_{n=1}^N \Phi_{\pm, h}^{(n)}(x, \zeta), \quad x \in \Xi_\pm(\nu),$$

where N satisfies $(N + 1)\rho > 1$, and for $n \geq 0$

$$(20) \quad \Phi_{\pm, h}^{(n+1)}(x, \zeta) = Q_\pm(\zeta) F_{\pm, h}^{(n)},$$

where

$$(21) \quad (Q_\pm(\zeta)F)(x) = \pm \int_0^\infty (F(x \pm t\zeta, \zeta) - F(\pm t\zeta, \zeta)) dt.$$

Let $F_{\pm, h}^{(n)}$'s be defined as

$$(22) \quad F_{\pm, h}^{(0)}(x, \zeta) = \eta(\zeta) V_h(x) - \frac{1}{2} V_h^2(x), \quad F_{\pm, h}^{(1)}(x, \zeta) = \frac{1}{2} |\nabla \Phi_{\pm, h}^{(1)}(x, \zeta)|^2,$$

and for $n \geq 2$

$$(23) \quad F_{\pm, h}^{(n)}(x, \zeta) = \sum_{k=1}^{n-1} \langle \nabla \Phi_{\pm, h}^{(k)}(x, \zeta), \nabla \Phi_{\pm, h}^{(n)}(x, \zeta) \rangle + \frac{1}{2} |\nabla \Phi_{\pm, h}^{(n)}(x, \zeta)|^2.$$

Define the amplitude function $\mathcal{P}_{\pm, h}(x, \zeta)$ as

$$(24) \quad \mathcal{P}_{\pm, h}(x, \zeta) = (I - S_{\pm, h}(x, \zeta))^{-1} p_0(\zeta), \quad x \in \Xi_\pm(\nu),$$

where $p_0(\zeta) = p_{+, 0}(\zeta)$ and

$$(25) \quad S_{\pm, h}(x, \zeta) = (2\eta(\zeta))^{-1} \left(V_h(x) + \sum_{k=1}^3 \partial_k \Phi_{\pm, h}(x, \zeta) \alpha_k \right), \quad x \in \Xi_\pm(\nu).$$

Note that, all estimates are uniform in ζ through out the paper for $0 < c_1 \leq \zeta \leq c_2 < \infty$. By the definitions of the phase function $\Phi_{\pm,h}(x, \zeta)$ and the amplitude function $\mathcal{P}_{\pm,h}(x, \zeta)$ we have for all multi-indices α and γ

$$(26) \quad |\partial_x^\alpha \partial_\zeta^\gamma \Phi_{\pm,h}(x, \zeta)| \leq c_{\alpha,\gamma} \langle x \rangle^{1-\rho-|\alpha|}, \quad x \in \Xi_\pm(\nu),$$

and

$$(27) \quad |\partial_x^\alpha \partial_\zeta^\gamma \mathcal{P}_{\pm,h}(x, \zeta)| \leq c_{\alpha,\gamma} \langle x \rangle^{-\rho-|\alpha|}, \quad x \in \Xi_\pm(\nu).$$

Hence, the approximation

$$(28) \quad u_{\pm,h}(x, \zeta) = e^{i\varphi_{\pm,h}(x,\zeta)} \mathcal{P}_{\pm,h}(x, \zeta) := e^{ix \cdot \zeta + i\Phi_{\pm,h}(x,\zeta)} \mathcal{P}_{\pm,h}(x, \zeta)$$

of the corresponding eigenvalue problem of (8) satisfies, as $|x| \rightarrow \infty$,

$$(29) \quad (H_h - \eta(\zeta))u_{\pm,h}(x, \zeta) = \mathcal{O}(|x|^{-1-\varepsilon}), \quad \varepsilon = (N+1)\rho - 1 > 0.$$

Consider the identification $\mathcal{J}_{\pm,h}$ given by the following PSDO

$$(30) \quad (\mathcal{J}_{\pm,h}g)(x) = (2\pi)^{-3/2} \int_{\mathbb{R}^3} e^{ix \cdot \zeta + i\Phi_{\pm,h}(x,\zeta)} \mathcal{P}_{\pm,h}(x, \zeta) \mathcal{C}_\pm(x, \zeta) \psi(|\zeta|^2) \hat{g}(\zeta) d\zeta,$$

where $\psi \in C_0^\infty(\mathbb{R}_+)$ is introduced to localize the identification in a compact interval of (m, ∞) . Consider the WOs $W_{\pm,h}$ and $W_{\pm,h}^*$ defined as

$$(31) \quad W_{\pm,h} = W_\pm(H_h, H_0; \mathcal{J}_{\pm,h}) = s\text{-}\lim_{t \rightarrow \pm\infty} U_h(-t) \mathcal{J}_{\pm,h} U_0(t)$$

and

$$(32) \quad W_{\pm,h}^* = W_\pm(H_0, H_h; \mathcal{J}_{\pm,h}^*) = s\text{-}\lim_{t \rightarrow \pm\infty} U_0(-t) \mathcal{J}_{\pm,h}^* U_h(t) P_h^{(ac)},$$

where $P_h^{(ac)}$ is the orthogonal projection onto the absolutely continuous subspace of H_h , $U_0(t) = e^{-iH_0 t}$, and $U_h(t) = e^{-iH_h t}$. Note that the free Dirac operator has only absolutely continuous spectrum, so there is no need to write the corresponding orthogonal projection onto the absolutely continuous subspace in the definition of the WO $W_{\pm,h}$. For the existence and completeness of the WO $W_{\pm,h}$ we have the following theorem.

Theorem 1. Let V_h satisfy (11), and let $\mathcal{J}_{\pm,h}$ be as defined in (30) where the functions $\Phi_{\pm,h}(x, \zeta)$ and $\mathcal{P}_{\pm,h}(x, \zeta)$ are given by (19) and (24) respectively. Then the WOs $W_\pm(H_h, H_0; \mathcal{J}_{\pm,h})$ and $W_\pm(H_0, H_h; \mathcal{J}_{\pm,h}^*)$ exist for all $h > 0$ and $W_\pm^*(H_h, H_0; \mathcal{J}_{\pm,h}) = W_\pm(H_0, H_h; \mathcal{J}_{\pm,h}^*)$. Moreover if $\Delta \subset (m, \infty)$ is a compact interval and $\psi(\mu^2 -$

$m^2) = 1$ for all $\mu \in \Delta$, then the WO $W_{\pm,h}(H_h, H_0; \mathcal{J}_{\pm,h})$, for all $h > 0$, is isometric on the subspace $E_0(\Delta)\mathcal{H}$ and is complete.

Proof. See [4]. ■

Remark 2. It is worth to mention that the WOs defined above are for positive part of the spectrum (m, ∞) . For the negative part of the spectrum $(-\infty, -m)$, the WOs operator can be defined in the same way as above but $\eta(\zeta)$ in the definition of $\Phi_{\pm,h}(x, \zeta)$ is replaced by $-\eta(\zeta)$, and $\eta(\zeta)$ and $p_0(\zeta) = p_{+,0}(\zeta)$ in the definition of $\mathcal{P}_{\pm,h}(x, \zeta)$ are replaced respectively by $-\eta(\zeta)$ and $p_0(\zeta) = p_{-,0}(\zeta)$. Consequently, and therefore, the corresponding identification $\mathcal{J}_{\pm,h}^-$ is given by the following PSDO

$$(33) \quad (\mathcal{J}_{\pm,h}^- g)(x) = (2\pi)^{-3/2} \int_{\mathbb{R}^3} e^{ix \cdot \zeta + i\Phi_{\mp,h}(x, \zeta)} \mathcal{P}_{\mp,h}(x, \zeta) \mathcal{C}_{\mp}(x, \zeta) \psi(|\zeta|^2) \hat{g}(\zeta) d\zeta.$$

In this work, we consider the WOs corresponding to the positive part of the spectrum. However, the asymptotic study below can be carried out to the WOs on the negative part of the spectrum in a similar way.

3. ASYMPTOTIC LIMIT OF THE WO

We study the existence of the WOs $W_{\pm}^{\dagger} := s\text{-}\lim_{h \rightarrow \infty} W_{\pm,h}$ and $W_{\pm}^{\dagger,*} := s\text{-}\lim_{h \rightarrow \infty} W_{\pm,h}^*$ given the existence of the WOs $W_{\pm,h}$ and $W_{\pm,h}^*$. We refer to [1] for comprehensive materials on the asymptotic study of WOs.

Let the perturbed Dirac operator H_h be convergent in the SRS, and let the identification $\mathcal{J}_{\pm,h}$ given by (30) be strongly convergent, then the WOs W_{\pm}^{\dagger} and $W_{\pm}^{\dagger,*}$ exist, i.e., the strong limits as $h \rightarrow \infty$ exist for both WOs $W_{\pm,h}$ and $W_{\pm,h}^*$. The question now is about characterizing W_{\pm}^{\dagger} and $W_{\pm}^{\dagger,*}$, in other words, characterizing the strong limits of the WOs $W_{\pm,h}$ and $W_{\pm,h}^*$ as $h \rightarrow \infty$.

Theorem 2. Let the WOs $W_{\pm,h}$ and $W_{\pm,h}^*$ be defined by (31) and (32) respectively, where the identification $\mathcal{J}_{\pm,h}$, the amplitude $\mathcal{P}_{\pm,h}$, and the phase $\Phi_{\pm,h}$ are given respectively by (30), (24), and (19). Suppose that, as $h \rightarrow \infty$, the Dirac operator H_h converges to H_{∞} in the SRS, and $\mathcal{J}_{\pm,h}$ converges strongly to $\mathcal{J}_{\pm,\infty}$. Then the WOs W_{\pm}^{\dagger} and $W_{\pm}^{\dagger,*}$ exist,

$$W_{\pm}^{\dagger} = s\text{-}\lim_{h \rightarrow \infty} W_{\pm}(H_h, H_0; \mathcal{J}_{\pm,h}) = W_{\pm}(H_{\infty}, H_0; \mathcal{J}_{\pm,\infty}),$$

and

$$W_{\pm}^{\dagger,*} = s\text{-}\lim_{h \rightarrow \infty} W_{\pm}(H_0, H_h; \mathcal{J}_{\pm,h}^*) = W_{\pm}(H_0, H_{\infty}; \mathcal{J}_{\pm,\infty}^*).$$

The proof follows Theorem 2.1 in [1], and is divided into several steps given by the following lemmas, corollaries, and discussion. Firstly, by [4],

$$(34) \quad H_h \mathcal{J}_{\pm,h} - \mathcal{J}_{\pm,h} H_0 = \sum_{j=1}^3 T_j^* B_{1,h} T_j + \langle x \rangle^{-(1+\rho)/2} B_{2,h} \langle x \rangle^{-(1+\rho)/2},$$

where $T_j = \langle x \rangle^{-1/2} \nabla_j$, $(\nabla_j v)(x) = \partial_j v(x) - |x|^2 x_j \sum_{k=1}^3 x_k (\partial_k v)(x)$, and $B_{1,h}$ and $B_{2,h}$ are bounded operators. Note that for all $h > 0$, $\langle x \rangle^{-(1+\rho)/2}$ for all $\rho > 0$ and T_j for $j=1,2,3$, are H_0 -smooth and H_h -smooth on any compact set $\Delta \subset (-\infty, -m) \cup (m, \infty)$ such that $\Delta \cap \sigma_p(H_h) = \emptyset$. The H_0 -smoothness and H_h -smoothness of $\langle x \rangle^{-(1+\rho)/2}$ and of T_j are known respectively as the limiting absorption principle and the radiation estimate. It is a fact that operator-smoothness is invariant under the multiplication by a bounded operator from left (or a bounded operator from right provided it commutes with the spectral family of the given operator), thus we can rewrite (34) as

$$(35) \quad H_h \mathcal{J}_{\pm,h} - \mathcal{J}_{\pm,h} H_0 = \sum_{i=1}^2 K_{2,i,h}^* K_{1,i,h}.$$

The operators $K_{2,1,h}$ and $K_{2,2,h}$ are H_h -smooth for all $h > 0$, and $K_{1,1,h}$ and $K_{1,2,h}$ are H_0 -smooth for all $h > 0$. Without loss of generality, we assume that

$$(36) \quad H_h \mathcal{J}_{\pm,h} - \mathcal{J}_{\pm,h} H_0 = G_h^* G_{0,h}$$

such that G_h and $G_{0,h}$ are H_h -smooth and H_0 -smooth respectively for all $h > 0$.

Lemma 1. For all $h > 0$ and for all $u_0 \in X$ the function

$$(37) \quad \mathcal{K}_{u_0,h}^{(1)}(t) = \| (H_h \phi(H_h) \mathcal{J}_{\pm,h} \phi(H_0) - \phi(H_h) \mathcal{J}_{\pm,h} H_0 \phi(H_0)) U_0(t) u_0 \|_Y$$

belongs to $L^1([-\infty, \infty); dt)$ for some continuous function $\phi : \mathbb{R} \rightarrow \mathbb{R}$ such that $x\phi(x)$ is bounded on \mathbb{R} .

Proof. Let $\phi(x) = (x - z)^{-1}$, $z \in \text{Res}(H_h) \cap \text{Res}(H_0)$ where Res denotes the resolvent set. Therefore, and since

$$(38) \quad \mathcal{K}_{u_0,h}^{(1)}(t) = \| ((H_h - z) \phi(H_h) \mathcal{J}_{\pm,h} \phi(H_0) - \phi(H_h) \mathcal{J}_{\pm,h} (H_0 - z) \phi(H_0)) U_0(t) u_0 \|_Y,$$

to prove the assertion of the lemma, it is enough to prove that

$$(39) \quad \mathcal{K}_{u_0, h}(t) = \|(\phi(H_h)\mathcal{J}_{\pm, h} - \mathcal{J}_{\pm, h}\phi(H_0))U_0(t)u_0\|_Y$$

belongs to $L^1((-\infty, \infty); dt)$. To this end, for all $u_0, u \in X$ we have

$$(40) \quad \langle \mathcal{J}_{\pm, h}u_0, H_h u \rangle - \langle \mathcal{J}_{\pm, h}H_0u_0, u \rangle = \langle G_{0, h}u_0, G_h u \rangle.$$

By (40) we have for any $v_0, v \in Y$

$$(41) \quad \begin{aligned} \langle G_{0, h}R_0(z)v_0, G_h R_h(\bar{z})v \rangle &= \langle \mathcal{J}_{\pm, h}R_0(z)v_0, H_h R_h(\bar{z})v \rangle - \langle \mathcal{J}_{\pm, h}H_0R_0(z)v_0, R_h(\bar{z})v \rangle \\ &= \langle \mathcal{J}_{\pm, h}R_0(z)v_0, v \rangle - \langle \mathcal{J}_{\pm, h}v_0, R_h(\bar{z})v \rangle + \\ &\quad + \langle \mathcal{J}_{\pm, h}R_0(z)v_0, \bar{z}R_h(\bar{z})v \rangle - \langle \mathcal{J}_{\pm, h}R_0(z)v_0, R_h(\bar{z})v \rangle. \end{aligned}$$

Since G_h and $G_{0, h}$ are H_h -bounded and H_0 -bounded respectively for all $h > 0$, all operators in (41) are well-defined and bounded, thus for all $v_0, v \in Y$,

$$(42) \quad \langle (\mathcal{J}_{\pm, h}R_0(z) - R_h(z)\mathcal{J}_{\pm, h})v_0, v \rangle = \langle (G_h R_h(\bar{z}))^* G_{0, h} R_0(z)v_0, v \rangle.$$

Hence

$$(43) \quad \mathcal{J}_{\pm, h}R_0(z) - R_h(z)\mathcal{J}_{\pm, h} = (G_h R_h(\bar{z}))^* G_{0, h} R_0(z).$$

Therefore we have for all $w_0 \in X$ and for all $h > 0$,

$$\begin{aligned} \int_0^{\pm\infty} \|(R_h(z)\mathcal{J}_{\pm, h} - \mathcal{J}_{\pm, h}R_0(z))U_0(t)w_0\|_Y dt &= \int_0^{\pm\infty} \|(G_h R_h(\bar{z}))^* G_{0, h} R_0(z)U_0(t)w_0\|_Y dt \\ &\leq C \int_0^{\pm\infty} \|G_{0, h}U_0(t)w_0\|_Y dt \\ &< \infty \end{aligned}$$

where $u_0 = R_0(z)w_0$ and $C \in \mathbb{R}$. Here we have used the H_h -boundedness of G_h and in the last inequality the H_0 -smoothness of $G_{0, h}$ for all $h > 0$. \blacksquare

The following corollary is a direct consequence of Lemma 1.

Corollary 1. Given the hypotheses of Lemma 1, then for any $\varepsilon > 0$ there exist $D_1, D_2 \in \mathbb{R}$ such that $\int_{D_1}^{\infty} \mathcal{K}_{u_0, h}^{(1)}(t) dt \leq \varepsilon$ and $\int_{-\infty}^{D_2} \mathcal{K}_{u_0, h}^{(1)}(t) dt \leq \varepsilon$.

Lemma 2. For all $h > 0$ and for all $u \in X$ the function

$$(44) \quad \mathcal{K}_{u, h}^{(2)}(t) = \| (H_0\phi(H_0)\mathcal{J}_{\pm, h}^*\phi(H_h) - \phi(H_0)\mathcal{J}_{\pm, h}^*H_h\phi(H_h))U_h(t)u \|_Y$$

belongs to $L^1([-\infty, \infty); dt)$ for some continuous function $\phi : \mathbb{R} \rightarrow \mathbb{R}$ such that $x\phi(x)$ is bounded on \mathbb{R} .

Proof. The proof is similar to that of Lemma 1. ■

The following corollary is a direct consequence of Lemma 2.

Corollary 2. Given the hypotheses of Lemma 2, then for any $\varepsilon > 0$ there exist $D_3, D_4 \in \mathbb{R}$ such that $\int_{D_3}^{\infty} \mathcal{K}_{u,h}^{(2)}(t) dt \leq \varepsilon$ and $\int_{-\infty}^{D_4} \mathcal{K}_{u,h}^{(2)}(t) dt \leq \varepsilon$.

Since H_h is convergent to H_∞ in the SRS, then for any continuous bounded function F on \mathbb{R} , $F(H_h)$ is strongly convergent to $F(H_\infty)$, thus $e^{-iH_h t}$ is strongly convergent to $e^{-iH_\infty t}$ for all $t \in \mathbb{R}$. Moreover, since $\mathcal{J}_{\pm,h}$ is convergent strongly to $\mathcal{J}_{\pm,\infty}$, then W_\pm^\dagger and $W_\pm^{\dagger,*}$ exist, and the characterization of the asymptotic limits of $W_{\pm,h}$ and $W_{\pm,h}^*$ is reduced to the problem of interchanging $s\text{-}\lim_{t \rightarrow \pm\infty}$ and $s\text{-}\lim_{h \rightarrow \infty}$. In this context, the following theorem is important, it is an adaptation of a result achieved in [1].

Theorem 3. Given self-adjoint operators T_h and T_0 defined in Hilbert spaces \mathcal{H} and \mathcal{H}_0 respectively, let the WOs $W_\pm(T_h, T_0; J_h)$ and $W_\pm(T_0, T_h; J_h^*)$ exist, where J_h is some bounded identification. Assume that, as $h \rightarrow \infty$, the operator T_h is convergent in the SRS to T_∞ and that J_h and J_h^* converge strongly to J_∞ and J_∞^* respectively. If, for $T_h, T_0, \mathcal{H}, \mathcal{H}_0$ and J_h , the functions $\mathcal{K}_{u_0,h}^{(1)}(t)$ and $\mathcal{K}_{u,h}^{(2)}(t)$, given respectively by (37) and (44), satisfy the conclusions of Corollaries 1 and 2 respectively, then

$$(45) \quad s\text{-}\lim_{h \rightarrow \infty} W_\pm(T_h, T_0; J_h) = W_\pm(T_\infty, T_0; J_\infty)$$

and

$$(46) \quad s\text{-}\lim_{h \rightarrow \infty} W_\pm(T_0, T_h; J_h^*) = W_\pm(T_0, T_\infty; J_\infty^*).$$

Proof. See Theorem 2.1 and Remark 2.3 in [1]. ■

Since, in general, the strong convergence of an operator does not imply the strong convergence of its adjoint to the adjoint of its strong limit, therefore we have assumed the strong convergence of J_h^* to J_∞^* parallel to the strong convergence of J_h to J_∞ in

Theorem 3. Fortunately, the identification operator $\mathcal{J}_{\pm,h}$ defined by (30) is a PSDO with the adjoint, $\mathcal{J}_{\pm,h}^*$, given by

$$(47) \quad (\mathcal{J}_{\pm,h}^*g)(\zeta) = (2\pi)^{-3/2} \int_{\mathbb{R}^3} e^{-ix \cdot \zeta - i\Phi_{\pm,h}(x,\zeta)} \mathcal{P}_{\pm,h}(x,\zeta) \mathcal{C}_{\pm}(x,\zeta) \psi(|\zeta|^2) g(x) dx.$$

This implies that if $\mathcal{J}_{\pm,h}$ is strongly convergent to $\mathcal{J}_{\pm,\infty}$ as $h \rightarrow \infty$, then $\mathcal{J}_{\pm,h}^*$ is also strongly convergent to $\mathcal{J}_{\pm,\infty}^*$.

The proof of Theorem 2 follows from Lemmas 1-2, Corollaries 1-2, and Theorem 3. Thus, we may conclude that the strong convergence as $h \rightarrow \infty$ of $W_{\pm,h} = W(H_h, H_0; \mathcal{J}_{\pm,h})$ and its adjoint $W_{\pm,h}^* = W(H_0, H_h; \mathcal{J}_{\pm,h}^*)$ to the WO $W_{\pm,\infty} = W(H_\infty, H_0; \mathcal{J}_{\pm,\infty})$ and $W_{\pm,\infty}^* = W(H_0, H_\infty; \mathcal{J}_{\pm,\infty}^*)$ respectively is guaranteed if H_h is convergent to H_∞ in the SRS and $\mathcal{J}_{\pm,h}$ is strongly convergent to $\mathcal{J}_{\pm,\infty}$.

In the coming discussion we assume convergence in the SRS of H_h to H_∞ , and study cases of the identification $\mathcal{J}_{\pm,h}$. In the second case we assume particular condition so that $\Phi_{\pm,h}$ is replaced with some h -free functions in the definition of $\mathcal{J}_{\pm,h}$ to obtain new equivalent identification $\tilde{\mathcal{J}}_{\pm,h}$. Even that this condition is stringent, but this replacement is advantageous if we can also replace the amplitude functions $\mathcal{P}_{\pm,h}$ of the identification $\tilde{\mathcal{J}}_{\pm,h}$ with h -free function $\tilde{\mathcal{P}}_{\pm}$ so that the difference $(\tilde{\mathcal{J}}_{\pm,h}(\mathcal{P}_{\pm,h}) - \tilde{\mathcal{J}}_{\pm}(\tilde{\mathcal{P}}_{\pm}))$ is compact for all $h > 0$, and then applying Remark 1. In this case the study of the asymptotic behavior of the WO $W_{\pm}(H_h, H_0; \tilde{\mathcal{J}}_{\pm,h}(\mathcal{P}_{\pm,h}))$ is reduced to study the asymptotic behavior of the WO $W_{\pm}(H_h, H_0; \tilde{\mathcal{J}}_{\pm}(\tilde{\mathcal{P}}_{\pm}))$. Thus no convergence conditions are needed on the identification operator in finding the asymptotic limits of the WOs.

3.0.1. *The case $\rho > 1$.* Note that here we consider short-range potentials, while our main assumption, (11), assumes potentials of long-range type. However, for $\rho > 1$, we can set $\mathcal{J}_{\pm,h} = I$, this is because for short-range potentials, the WOs $W_{\pm}(H_h, H_0)$ and $W_{\pm}(H_0, H_h)$ exist and are complete. The proofs of existence and completeness of the WOs for the Dirac operator with short-range potential are similar to that for the Schrödinger operator. Hence, the strong convergence of the WOs $W_{\pm}(H_h, H_0)$ and $W_{\pm}(H_0, H_h)$, as $h \rightarrow \infty$, is reduced to the convergence of the Dirac operator H_h in the SRS. Therefore, by assuming the convergence in the SRS of H_h to H_∞ ,

we have

$$(48) \quad W_{\pm}^{\dagger} = W_{\pm}(H_{\infty}, H_0)$$

and

$$(49) \quad W_{\pm}^{\dagger,*} = W_{\pm}(H_0, H_{\infty}).$$

3.0.2. *The case $\rho = 1$.* In this case, one can replace the h -dependent phase function $\Phi_{\pm,h}(x, \zeta)$ with an h -free function by virtue of Remark 1 and Proposition 1 as follows.

Theorem 4. Let $\Phi_{\pm}(x, \zeta)$ be an h -free function satisfying estimate (26), and let the identification $\mathcal{J}_{\pm,h}^{(1)}$ be given by (30) but where $\Phi_{\pm,h}(x, \zeta)$ is replaced by $\Phi_{\pm}(x, \zeta)$. Then for $\rho > 0$ such that $\rho/(1 - \rho) > |\gamma|/(1 + |\alpha|)$, the operator $\mathcal{J}_{\pm,h}^{(1)} - \mathcal{J}_{\pm,h}$ is compact.

Proof. By the estimate (27) the function $\mathcal{P}_{\pm,h}$ belongs to the class $\mathcal{S}_{1,0}^{-\rho}(\mathbb{R}^3, \mathbb{R}^3)$ which is a subset of $\mathcal{S}_{\rho,\delta}^{-\rho}(\mathbb{R}^3, \mathbb{R}^3)$ for $\delta = 1 - \rho$. Since both $\Phi_{\pm,h}(x, \zeta)$ and $\Phi_{\pm}(x, \zeta)$ satisfy the estimate (26), for $x \in \Xi_{\pm}(\nu)$,

$$(50) \quad |\partial_x^{\alpha} \partial_{\zeta}^{\gamma} e^{i\Phi_{\pm,h}(x,\zeta)}| \leq c_{\alpha,\gamma} \langle x \rangle^{-\rho|\alpha| + \delta|\gamma|}$$

and

$$(51) \quad |\partial_x^{\alpha} \partial_{\zeta}^{\gamma} e^{i\Phi_{\pm}(x,\zeta)}| \leq c_{\alpha,\gamma} \langle x \rangle^{-\rho|\alpha| + \delta|\gamma|}.$$

Thus $e^{i\Phi_{\pm,h}} \mathcal{P}_{\pm,h}$ and $e^{i\Phi_{\pm}} \mathcal{P}_{\pm,h}$ are elements of $\mathcal{S}_{\rho,\delta}^{-\rho}(\mathbb{R}^3, \mathbb{R}^3)$, consequently the difference is also an element of $\mathcal{S}_{\rho,\delta}^{-\rho}(\mathbb{R}^3, \mathbb{R}^3)$. By Proposition 1, the operator $\mathcal{J}_{\pm,h}^{(1)} - \mathcal{J}_{\pm,h}$ is compact if its symbol belongs to $\mathcal{S}_{0,0}^r(\mathbb{R}^3, \mathbb{R}^3)$ for $r < 0$. This is achieved if $-\rho - \rho|\alpha| + \delta|\gamma| < 0$ where again $\delta = 1 - \rho$, i.e., $\mathcal{J}_{\pm,h}^{(1)} - \mathcal{J}_{\pm,h}$ is compact if $\rho/(1 - \rho) > |\gamma|/(1 + |\alpha|)$. \blacksquare

According to Theorem 4, it is noted that if $\rho = 1$ (also if $\rho \rightarrow 1^-$), then $\rho/(1 - \rho) > |\gamma|/(1 + |\alpha|)$ is satisfied for all multi-indices α and γ .

Regarding the amplitude function, we shall need the following proposition which is due to Gâtel and Yafaev [4]. This proposition is an important tool in the convergence results in the sense that it replaces the h -dependent amplitude function, $\mathcal{P}_{\pm,h}(x, \zeta)$, with another h -free function.

Proposition 3. For the identification

$$(52) \quad (\mathcal{J}_{\pm,h}g)(x) = (2\pi)^{-3/2} \int_{\mathbb{R}^3} e^{ix \cdot \zeta + i\Phi_{\pm,h}(x,\zeta)} p_0(\zeta) \mathcal{C}_{\pm}(x, \zeta) \psi(|\zeta|^2) \hat{g}(\zeta) d\zeta$$

the difference $\mathcal{J}_{\pm,h} - \mathcal{J}_{\pm,h}$ is a compact PSDO.

Proof. Note that the operator $\mathcal{J}_{\pm,h} - \mathcal{J}_{\pm,h}$ is a PSDO with symbol

$$(53) \quad e^{i\Phi_{\pm,h}(x,\zeta)} (p_0(\zeta) - \mathcal{P}_{\pm,h}(x, \zeta)) \mathcal{C}_{\pm}(x, \zeta) \psi(|\zeta|^2).$$

It is clear that for all $h > 0$, $|\partial_x^\alpha \partial_\zeta^\gamma (p_0(\zeta) - \mathcal{P}_{\pm,h}(x, \zeta))| \leq C_{\alpha,\gamma} \langle x \rangle^{-\rho - |\alpha|}$, thus the symbol of $\mathcal{J}_{\pm,h} - \mathcal{J}_{\pm,h}$ belongs to $C^{-\rho}(\Phi_{\pm,h})$ for all $h > 0$. By Proposition 2, $\mathcal{J}_{\pm,h} - \mathcal{J}_{\pm,h}$ is compact. \blacksquare

According to Remark 1, the WOs $W_{\pm}(H_h, H_0; \mathcal{J}_{\pm,h})$ and $W_{\pm}(H_0, H_h; \mathcal{J}_{\pm,h}^*)$ exist and $W_{\pm}(H_h, H_0; \mathcal{J}_{\pm,h}) = W_{\pm}(H_h, H_0; \mathcal{J}_{\pm,h})$ and $W_{\pm}(H_0, H_h; \mathcal{J}_{\pm,h}^*) = W_{\pm}(H_0, H_h; \mathcal{J}_{\pm,h}^*)$. To this end, if $\rho = 1$ (or $\rho \rightarrow 1^-$), we have after applying Remark 1 and Proposition 3

$$(54) \quad W_{\pm}^{\dagger} = s\text{-}\lim_{h \rightarrow \infty} W_{\pm}(H_h, H_0; \mathcal{J}_{\pm,h}) = W_{\pm}(H_{\infty}, H_0; \mathcal{J}_{\pm}^{(2)})$$

and

$$(55) \quad W_{\pm}^{\dagger,*} = s\text{-}\lim_{h \rightarrow \infty} W_{\pm}(H_0, H_h; \mathcal{J}_{\pm,h}^*) = W_{\pm}(H_0, H_{\infty}; \mathcal{J}_{\pm}^{(2),*}),$$

where $\mathcal{J}_{\pm}^{(2)}$ (with adjoint denoted by $\mathcal{J}_{\pm}^{(2),*}$) is given by

$$(56) \quad (\mathcal{J}_{\pm}^{(2)}g)(x) = (2\pi)^{-3/2} \int_{\mathbb{R}^3} e^{ix \cdot \zeta + i\Phi_{\pm}(x,\zeta)} p_0(\zeta) \mathcal{C}_{\pm}(x, \zeta) \psi(|\zeta|^2) \hat{g}(\zeta) d\zeta.$$

Example 1. The function

$$(57) \quad \Phi_{\pm}(x, \zeta) = \pm \eta(\zeta) \int_0^{\infty} (\langle x \pm t\zeta \rangle^{-\rho} - \langle \pm t\zeta \rangle^{-\rho}) dt$$

satisfies estimate (26). The proof is just a simple elementary calculus, where it is simpler to show first

$$(58) \quad |\partial_x^\alpha \partial_\zeta^\gamma \Phi_{\pm}(x, \zeta)| \leq c_{\alpha,\gamma} (1 + |x|)^{1-\rho-|\alpha|}, \quad x \in \Xi_{\pm}(\nu),$$

and then use the inequalities

$$(59) \quad \langle x \rangle \leq (1 + |x|) \leq \sqrt{2} \langle x \rangle.$$

3.0.3. *The case $\rho \in (1/2, 1)$.* According to the definition of the phase function $\Phi_{\pm, h}(x, \zeta)$ given by (19), if $\rho \in (1/2, 1)$ then $N = 1$ satisfies the condition $(N+1)\rho > 1$. In this case $\Phi_{\pm, h}(x, \zeta)$ can be chosen as, after neglecting the quadratic terms,

$$(60) \quad \Phi_{\pm, h}(x, \zeta) = \pm \eta(\zeta) \int_0^\infty (V_h(x \pm t\zeta) - V_h(\pm t\zeta)) dt.$$

By Proposition 3, to study the strong convergence of $W_{\pm, h}$ with the identification $\mathcal{J}_{\pm, h}$ (respectively $W_{\pm, h}^*$ with $\mathcal{J}_{\pm, h}^*$) is equivalent to study its strong convergence with $\mathcal{J}_{\pm, h}^{(3)}$ (respectively with $\mathcal{J}_{\pm, h}^{(3),*}$, where $\mathcal{J}_{\pm, h}^{(3),*}$ is the adjoint operator of $\mathcal{J}_{\pm, h}^{(3)}$),

$$(61) \quad (\mathcal{J}_{\pm, h}^{(3)}g)(x) = (2\pi)^{-3/2} \int_{\mathbb{R}^3} e^{ix \cdot \zeta + i\Phi_{\pm, h}(x, \zeta)} p_0(\zeta) \mathcal{C}_\pm(x, \zeta) \psi(|\zeta|^2) \hat{g}(\zeta) d\zeta,$$

where $\Phi_{\pm, h}$ is given by (60). By dominated convergence theorem, and since the integrand in (61) is bounded, then if $\Phi_{\pm, h}(x, \zeta)$, given by (60), converges to $\Phi_{\pm, \infty}(x, \zeta)$ in the SRS, then the identification $\mathcal{J}_{\pm, h}^{(3)}$ is strongly convergent to $\mathcal{J}_{\pm, \infty}^{(3)}$, where

$$(62) \quad (\mathcal{J}_{\pm, \infty}^{(3)}g)(x) = (2\pi)^{-3/2} \int_{\mathbb{R}^3} e^{ix \cdot \zeta + i\Phi_{\pm, \infty}(x, \zeta)} p_0(\zeta) \mathcal{C}_\pm(x, \zeta) \psi(|\zeta|^2) \hat{g}(\zeta) d\zeta.$$

Therefore, for those types of potentials V_h that satisfy (11) with $\rho \in (1/2, 1)$ and such that $H_h = H_0 + V_h$ and $\Phi_{\pm, h}(x, \zeta)$ are convergent in the SRS respectively to $H_\infty = H_0 + V_\infty$ and

$$(63) \quad \Phi_{\pm, \infty}(x, \zeta) = \pm \eta(\zeta) \int_0^\infty (V_\infty(x \pm t\zeta) - V_\infty(\pm t\zeta)) dt,$$

we have

$$(64) \quad W_\pm^\dagger = s\text{-}\lim_{h \rightarrow \infty} W_\pm(H_h, H_0; \mathcal{J}_{\pm, h}) = W_\pm(H_\infty, H_0; \mathcal{J}_{\pm, \infty}^{(3)})$$

and

$$(65) \quad W_\pm^{\dagger,*} = s\text{-}\lim_{h \rightarrow \infty} W_\pm(H_0, H_h; \mathcal{J}_{\pm, h}^*) = W_\pm(H_0, H_\infty; \mathcal{J}_{\pm, \infty}^{(3),*}).$$

REFERENCES

- [1] E. Brüning and F. Gesztesy, *Continuity of wave and scattering operators with respect to interactions*, J. Math. Phys., 24(1983), pp. 1516-1528.
- [2] J. Dollard, *Asymptotic convergence and Coulomb interaction*, J. Math. Phys., 5(1964), pp. 729-738.
- [3] J. Dollard and G. Velo, *Asymptotic behaviour of a Dirac particle in a Coulomb field*, Nuovo Cimento, 45(1966), pp. 801-812.

- [4] Y. Gâtel and D. R. Yafaev, *Scattering theory for the Dirac operator with a long-range electromagnetic potential*, J. Fun. Anal., 184(2001), pp. 136-176.
- [5] T. Kato, *Scattering theory with two Hilbert spaces*, J. Fun. Anal., 1(1967), pp. 342-369.
- [6] T. Kato, *Perturbation Theory for Linear Operators*, Springer-Verlag, Berlin Heidelberg, 1976.
- [7] T. Kato and S. T. Kuroda, *The abstract theory of scattering*, Rocky Mt. J. Math., 1(1971), pp. 127-171.
- [8] Pl. Muthuramalingam, *Scattering theory by Enss' method for operator valued matrices: Dirac operator in an electric field*, J. Math. Soc. Japan, 37(1985), pp. 415-432.
- [9] Pl. Muthuramalingam and K. B. Sinha, *Existence and completeness of wave operators for the Dirac operator in an electro-magnetic field with long range potentials*, J. Indian Math. Soc. (N.S.), 50(1986), pp. 103-130.
- [10] M. Reed and B. Simon, *Methods of Modern Mathematical Physics: Scattering Theory*, Vol. 3, Academic Press, San Diego, CA, 1979.
- [11] B. Thaller, *The Dirac Equation*, Springer-verlag, Berlin, 1993.
- [12] B. Thaller and V. Enss, *Asymptotic observables and Coulomb scattering for the Dirac equation*, Ann. Inst. H. Poincaré Phys. Theor., 45(1986), pp. 147-171.
- [13] J. Weidman, *Linear Operators in Hilbert Spaces*, Springer-verlag, New York, 1980.
- [14] D. R. Yafaev, *Mathematical Scattering Theory: General Theory*, Amer. Math. Soc., Providence, Rhode Island, 1992.
- [15] D. R. Yafaev, *A class of Pseudo-differential operators with oscillating symbols*, St. Petersburg Math. J., 11(2000), pp. 375-403.
- [16] D. R. Yafaev, *Scattering Theory: Some Old and New Problems*, Lecture Notes in Mathematics, Vol. 1735, Springer-Verlag, Berlin/New York, 2000.
- [17] K. Yajima, *Nonrelativistic limit of the Dirac theory, scattering theory*, J. Fac. Sci. Univ. Tokyo Sect. 1A, Math., 23(1976), pp. 517-523.
- [18] O. Yamada, *The nonrelativistic limit of modified wave operators for Dirac operators*, Proc. Japan Acad., Ser. A, 59(1983), pp. 71-74.

Paper VI

EXISTENCE AND ASYMPTOTICS OF WAVE OPERATORS FOR SELF-ADJOINT OPERATORS

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ABSTRACT. We consider a family of h -dependent self-adjoint operators, $H_h = H_0 + V_h$, where H_0 is a self-adjoint operator and V_h is some admissible h -dependent interaction, and study the existence of the stationary wave operator (WO) W_{\pm}^{\dagger} defined by the form $\langle W_{\pm}^{\dagger} u_0, u \rangle = \int_{-\infty}^{\infty} \lim_{h \rightarrow \infty} \lim_{\epsilon \rightarrow 0} \pi^{-1} \epsilon \langle \mathcal{J}_h (H_0 - (\lambda \pm i\epsilon))^{-1} u_0, (H_h + (\lambda \pm i\epsilon))^{-1} u \rangle d\lambda$, where \mathcal{J}_h is a bounded identification. Also we study the existence of the weak WO $\widetilde{W}_{\pm}^{\dagger}(H, H_0; \mathcal{J}) = w\text{-}\lim_{h \rightarrow \infty} w\text{-}\lim_{t \rightarrow \pm\infty} P_h^{(ac)} \exp(iH_h t) \times \mathcal{J}_h \exp(-iH_0 t) P_0^{(ac)}$, where $P_0^{(ac)}$ and $P_h^{(ac)}$ are respectively the orthogonal projections onto the absolutely continuous subspaces of H_0 and H_h . Using the existence of the stationary and weak WOs and under additional conditions, we prove the existence of the time-dependent WO $W_{\pm}^{\dagger}(H, H_0; \mathcal{J}) = s\text{-}\lim_{h \rightarrow \infty} s\text{-}\lim_{t \rightarrow \pm\infty} \exp(iH_h t) \times \mathcal{J}_h \exp(-iH_0 t) P_0^{(ac)} = s\text{-}\lim_{h \rightarrow \infty} W_{\pm}(H_h, H_0; \mathcal{J}_h)$. Moreover, we study the asymptotic behavior of the WO $W_{\pm}(H_h, H_0; \mathcal{J}_h)$ as $h \rightarrow \infty$.

1. INTRODUCTION

In the present work we consider a self-adjoint operator H_h , defined in a Hilbert space \mathcal{H} , written in terms of a free self-adjoint operator H_0 defined in \mathcal{H}_0 and an h -dependent perturbation V_h as $H_h = H_0 + V_h$, where $h > 0$. Given a bounded operator (identification) $\mathcal{J}_h : \mathcal{H}_0 \rightarrow \mathcal{H}$, and let $A_h : \mathcal{H} \rightarrow \mathfrak{H}$ and $A_0 : \mathcal{H}_0 \rightarrow \mathfrak{H}$ be H_h -bounded for all $h > 0$ and H_0 -bounded operators respectively, where \mathfrak{H} is some auxiliary Hilbert space, we assume that the perturbation V_h admits the following factorization

$$V_h = H_h \mathcal{J}_h - \mathcal{J}_h H_0 = A_h^* A_0$$

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which is understood as the equalities of the corresponding sesquilinear forms. Following [12], we study sufficient conditions under which the stationary wave operator (WO) $\mathcal{W}_{\pm}^{\dagger} = \mathcal{W}_{\pm}^{\dagger}(H, H_0; \mathcal{J})$ (where H and \mathcal{J} are used to indicate to h -free operators and they can be regarded as some appropriate limits of H_h and \mathcal{J}_h respectively), defined by the sesquilinear form

$$\langle \mathcal{W}_{\pm}^{\dagger} u_0, u \rangle = \int_{-\infty}^{\infty} \lim_{h \rightarrow \infty} \lim_{\epsilon \rightarrow 0} \pi^{-1} \epsilon \langle \mathcal{J}_h R_0(\lambda \pm i\epsilon) u_0, R_h(\lambda \pm i\epsilon) u \rangle d\lambda,$$

exists, where u_0 and u belong to some dense sets M_0 and M in \mathcal{H}_0 and \mathcal{H} respectively, and R_0 and R_h are the resolvent operators of H_0 and H_h respectively. We prove that if A_0 is weakly H_0 -smooth, for a.e. $\lambda \in \mathbb{R}$, $S_{h,\epsilon} := A_h R_h(\lambda \pm i\epsilon)$ is strongly convergent as $\epsilon \rightarrow 0$ to some $S_{h,0}$ for all $h > 0$, and the operators $S_{h,0}$ and \mathcal{J}_h are weakly convergent, then the WOs $\mathcal{W}_{\pm}^{\dagger}(H, H_0; \mathcal{J})$ and $\mathcal{W}_{\pm}^{\dagger}(H_0, H; \mathcal{J}^*)$ exist, and $\mathcal{W}_{\pm}^{\dagger,*}(H, H_0; \mathcal{J}) = \mathcal{W}_{\pm}^{\dagger}(H_0, H; \mathcal{J}^*)$. Other equivalent conditions are also proved to ensure the existence of these WOs.

Also we study the existence of the weak time-dependent WO $\widetilde{\mathcal{W}}_{\pm}^{\dagger} = \widetilde{\mathcal{W}}_{\pm}^{\dagger}(H, H_0; \mathcal{J})$ defined as

$$\begin{aligned} \widetilde{\mathcal{W}}_{\pm}^{\dagger}(H, H_0; \mathcal{J}) &= w\text{-}\lim_{h \rightarrow \infty} \widetilde{\mathcal{W}}_{\pm}^{\dagger}(H_h, H_0; \mathcal{J}_h) \\ &= w\text{-}\lim_{h \rightarrow \infty} w\text{-}\lim_{t \rightarrow \pm\infty} P_h^{(ac)} \exp(iH_h t) \mathcal{J}_h \exp(-iH_0 t) P_0^{(ac)}, \end{aligned}$$

where $P_0^{(ac)}$ and $P_h^{(ac)}$ are the orthogonal projections onto the absolutely continuous subspaces of H_0 and H_h respectively, and w refers to the weak convergence. Under the same conditions of existence of $\mathcal{W}_{\pm}^{\dagger}(H, H_0; \mathcal{J})$ and $\mathcal{W}_{\pm}^{\dagger}(H_0, H; \mathcal{J}^*)$, we prove the existence of the WOs $\widetilde{\mathcal{W}}_{\pm}^{\dagger} = \widetilde{\mathcal{W}}_{\pm}^{\dagger}(H, H_0; \mathcal{J})$ and $\widetilde{\mathcal{W}}_{\pm}^{\dagger} = \widetilde{\mathcal{W}}_{\pm}^{\dagger}(H_0, H; \mathcal{J}^*)$. We discuss the relation between the stationary and the weak time-dependent WOs, in particular, if both WOs $\mathcal{W}_{\pm}^{\dagger}$ and $\widetilde{\mathcal{W}}_{\pm}^{\dagger}$ exist then their corresponding sesquilinear forms are equal.

To use the stationary method for proving the existence of the strong time-dependent WOs, we further study the existence of the WOs $\mathcal{W}_{\pm}^{\dagger}(H, H; \mathcal{J}\mathcal{J}^*)$ and $\mathcal{W}_{\pm}^{\dagger}(H_0, H_0; \mathcal{J}^*\mathcal{J})$, and discuss the validity of the relations

$$\mathcal{W}_{\pm}^{\dagger}(H, H_0; \mathcal{J}) \mathcal{W}_{\pm}^{\dagger,*}(H, H_0; \mathcal{J}) = \mathcal{W}_{\pm}^{\dagger}(H, H; \mathcal{J}\mathcal{J}^*)$$

and

$$\mathcal{W}_{\pm}^{\dagger,*}(H, H_0; \mathcal{J}) \mathcal{W}_{\pm}^{\dagger}(H, H_0; \mathcal{J}) = \mathcal{W}_{\pm}^{\dagger}(H_0, H_0; \mathcal{J}^*\mathcal{J}).$$

Also the existence of the WOs $\widetilde{W}_\pm^\dagger(H, H; \mathcal{J}\mathcal{J}^*)$ and $\widetilde{W}_\pm^\dagger(H_0, H_0; \mathcal{J}^*\mathcal{J})$ is studied for this purpose. In this issue, we prove the existence of $\mathcal{W}_\pm^\dagger(H, H; \mathcal{J}\mathcal{J}^*)$, $\mathcal{W}_\pm^\dagger(H_0, H_0; \mathcal{J}^*\mathcal{J})$, $\widetilde{W}_\pm^\dagger(H, H; \mathcal{J}\mathcal{J}^*)$, $\widetilde{W}_\pm^\dagger(H_0, H_0; \mathcal{J}^*\mathcal{J})$, and the validity of the relations above under the same conditions of existence of $\mathcal{W}_\pm^\dagger(H, H_0; \mathcal{J})$ and $\mathcal{W}_\pm^\dagger(H_0, H; \mathcal{J}^*)$ and the strong convergence of the operators \mathcal{J}_h , \mathcal{J}_h^* , and R_h . Finally, by the existence of the stationary and weak time-dependent WOs and the relations above, we extend the stationary approach for proving the time-dependent WOs for general h -dependent self-adjoint operators, and prove the existence of the strong time-dependent WOs

$$W_\pm^\dagger := s\text{-}\lim_{h \rightarrow \infty} W_\pm(H_h, H_0; \mathcal{J}_h) = s\text{-}\lim_{h \rightarrow \infty} s\text{-}\lim_{t \rightarrow \pm\infty} \exp(iH_h t) \mathcal{J}_h \exp(-iH_0 t) P_0^{(ac)}$$

and

$$W_\pm^{\dagger,*} := s\text{-}\lim_{h \rightarrow \infty} W_\pm(H_0, H_h; \mathcal{J}_h^*) = s\text{-}\lim_{h \rightarrow \infty} s\text{-}\lim_{t \rightarrow \pm\infty} \exp(iH_0 t) \mathcal{J}_h^* \exp(-iH_h t) P_h^{(ac)},$$

where s refers to the strong convergence. At the last, we discuss the limit behavior of $W_{\pm,h} := W_\pm(H_h, H_0; \mathcal{J}_h)$ and $W_{\pm,h}^* := W_\pm(H_0, H_h; \mathcal{J}_h^*)$ as $h \rightarrow \infty$, and consider some examples.

For general scattering theory we refer to [2, 3, 7, 9, 11, 12, 13], also for general perturbation theory we refer to [8, 10]. Asymptotic analysis of WOs is rarely studied, and for simple and particular cases we refer to [1, 5, 6, 14, 15], also [4] is a crucial reference regarding the continuity of the strong time-dependent WO.

The paper is arranged as follows; in Section 2 we give necessary and basic preliminaries on scattering theory for both the time-dependent and stationary approaches. In Section 3 we state and prove the main results about the existence of the WOs \mathcal{W}_\pm^\dagger , $\widetilde{W}_\pm^\dagger$, and W_\pm^\dagger , also we study the asymptotic behavior of the time-dependent WO $W_\pm(H_h, H_0; \mathcal{J}_h)$ as $h \rightarrow \infty$.

2. PRELIMINARIES

In the sequel we use \mathcal{H} and \mathcal{H}_0 as notations for Hilbert spaces, and \mathbf{D} and \mathbf{R} as notations for the domain and range of operators respectively. We assume self-adjoint operators H and H_0 in \mathcal{H} and \mathcal{H}_0 respectively. To simplify the notations we define $U(t) = \exp(-iHt)$ and $U_0(t) = \exp(-iH_0t)$, also we use $P_H^{(ac)}$, simply $P^{(ac)}$, and $P_{H_0}^{(ac)}$, simply $P_0^{(ac)}$, to denote for the orthogonal projections onto the absolutely

continuous subspaces $\mathcal{H}^{(ac)}$ and $\mathcal{H}_0^{(ac)}$ of H and H_0 respectively. To $\mathcal{H}^{(ac)}$ and $\mathcal{H}_0^{(ac)}$ we define the restrictions $H^{(ac)}$ and $H_0^{(ac)}$ respectively, which are known as the absolutely continuous operators of H and H_0 respectively.

2.1. Basic Setting. Let $\mathcal{J} : \mathcal{H}_0 \rightarrow \mathcal{H}$ be a bounded operator (identification), the (modified or generalized) strong time-dependent WO $W_{\pm} = W_{\pm}(H, H_0; \mathcal{J})$ is defined as follows.

Definition 1. The strong time-dependent WO for H and H_0 , with identification \mathcal{J} , is the operator W_{\pm} defined as

$$(1) \quad W_{\pm}(H, H_0; \mathcal{J}) = s\text{-}\lim_{t \rightarrow \pm\infty} U(-t)\mathcal{J}U_0(t)P_0^{(ac)},$$

provided that the corresponding strong limits exist, where again the letter s refers to the strong convergence sense. If $\mathcal{H} = \mathcal{H}_0$ and \mathcal{J} is the identity operator, the WO is then denoted by $W_{\pm}(H, H_0)$.

Remark 1. As for the usual WO W_{\pm} , we define the weak time-dependent WO $\widetilde{W}_{\pm}(H, H_0; \mathcal{J})$ as follows

$$(2) \quad \widetilde{W}_{\pm}(H, H_0; \mathcal{J}) = w\text{-}\lim_{t \rightarrow \pm\infty} P_0^{(ac)}U(-t)\mathcal{J}U_0(t)P_0^{(ac)}.$$

provided that the corresponding weak limits exist, where again the letter w refers to the weak convergence sense.

To study the properties of the WO $W_{\pm}(H, H_0; \mathcal{J})$, we assume first that this operator exists. By $\|W_{\pm}(H, H_0; \mathcal{J})u\|_{\mathcal{H}} \leq \|\mathcal{J}\| \|P_0^{(ac)}u\|_{\mathcal{H}_0}$, the WO $W_{\pm}(H, H_0; \mathcal{J})$ is bounded. Since $U(-t)U_0(t)$ is unitary, the operator $W_{\pm}(H, H_0)$ is isometric. To prove that $W_{\pm}(H, H_0; \mathcal{J})$ is isometric, it is necessary and sufficient to prove that for any $u \in \mathcal{H}_0^{(ac)}$, $\lim_{t \rightarrow \pm\infty} \|\mathcal{J}U_0(t)u\|_{\mathcal{H}} = \|u\|_{\mathcal{H}_0}$. The WO W_{\pm} possesses the intertwining property, that is, for any bounded Borel function ϕ ,

$$(3) \quad \phi(H)W_{\pm}(H, H_0; \mathcal{J}) = W_{\pm}(H, H_0; \mathcal{J})\phi(H_0),$$

also for any Borel set $\Delta \subset \mathbb{R}$,

$$(4) \quad E(\Delta)W_{\pm}(H, H_0; \mathcal{J}) = W_{\pm}(H, H_0; \mathcal{J})E_0(\Delta),$$

where E and E_0 are the spectral families of H and H_0 respectively. The WO W_{\pm} admits the chain rule property, i.e., if $W_{\pm}(H, H_1; \mathcal{J}_1)$ and $W_{\pm}(H_1, H_0; \mathcal{J}_0)$ exist,

then the WO $W_{\pm}(H, H_0; \mathcal{J}_{1,0}) = W_{\pm}(H, H_1; \mathcal{J}_1)W_{\pm}(H_1, H_0; \mathcal{J}_0)$ also exists where $\mathcal{J}_{1,0} = \mathcal{J}_1\mathcal{J}_0$.

Remark 2. The WO $\widetilde{W}_{\pm}(H, H_0; \mathcal{J})$ is bounded and $\|\widetilde{W}_{\pm}(H, H_0; \mathcal{J})u\|_{\mathcal{H}} \leq \|\mathcal{J}\| \times \|P_0^{(ac)}u\|_{\mathcal{H}_0}$. The intertwining property is preserved for the WO \widetilde{W}_{\pm} , but the chain rule is lost since, in general, the weak limit of the product of two sequences that are only weakly convergent is not the product of their weak limits. On contrast of the WO W_{\pm} , the WO \widetilde{W}_{\pm} withstands conjugation, this means that $\widetilde{W}_{\pm}(H_0, H; \mathcal{J}^*) = \widetilde{W}_{\pm}^*(H, H_0; \mathcal{J})$ necessarily exists alongside with $\widetilde{W}_{\pm}(H, H_0; \mathcal{J})$.

After proving the existence of the WO $W_{\pm}(H, H_0; \mathcal{J})$, the main task is to show its completeness.

Definition 2. The WO W_{\pm} is said to be complete if $\mathbf{R}(W_{\pm}) = \mathcal{H}^{(ac)}$.

The completeness of W_{\pm} guarantees unitary equivalence of the operators $H^{(ac)}$ and $H_0^{(ac)}$. For the WO $W_{\pm}(H, H_0)$, the proof of completeness is equivalent to the existence of $W_{\pm}^*(H, H_0) = W_{\pm}(H_0, H)$. This is clear because, by the chain rule, we have $P^{(ac)} = W_{\pm}(H, H) = W_{\pm}(H, H_0)W_{\pm}^*(H, H_0)$. The completeness of the WO $W_{\pm}(H, H_0; \mathcal{J})$ is equivalent to the existence of $W_{\pm}(H_0, H; \mathcal{J}^*)$ provided that the identification \mathcal{J} is boundedly invertible.

2.2. The stationary approach. On contrast to the time-dependent approach of scattering theory, the stationary approach is comparably simpler. This is seen evident in general because dealing with resolvent operators in the mathematical analysis is easier than treating unitary groups. For this reason, and others, the stationary approach is often used to prove the existence and other properties of the time-dependent WO $W_{\pm}(H, H_0; \mathcal{J})$.

In this subsection we overview some basic definitions and results on the stationary approach of scattering theory. Let $R(z)$ and $R_0(z)$ be the resolvent operators of H and H_0 respectively, we define $\theta(\lambda, \epsilon)$ as

$$(5) \quad \theta(\lambda, \epsilon) = (2\pi i)^{-1}(R(\lambda + i\epsilon) - R(\lambda - i\epsilon)) = \pi^{-1}\epsilon R(\lambda + i\epsilon)R(\lambda - i\epsilon).$$

Note that it is not difficult to prove that $\lim_{\epsilon \rightarrow 0} \langle \theta(\lambda, \epsilon)u, v \rangle = \frac{d}{d\lambda} \langle E(\lambda)u, v \rangle$ for a.e. $\lambda \in \mathbb{R}$ and all $u, v \in \mathcal{H}$.

Let \mathfrak{H} be an auxiliary Hilbert space, the concept H -smoothness in the weak sense is defined as follows.

Definition 3. An H -bounded operator $A : \mathcal{H} \rightarrow \mathfrak{H}$ is called H -smooth in the weak sense if

$$(6) \quad w\text{-}\lim_{\epsilon \rightarrow \infty} A\theta(\lambda, \epsilon)A^*$$

exists for a.e. $\lambda \in \mathbb{R}$.

It is clear that if the limit (6) exists then so is $w\text{-}\lim_{\epsilon \rightarrow \infty} A\theta(\lambda, \epsilon)$. There are other equivalent conditions for the weak H -smoothness, here we are interested in the following two conditions: An operator $A : \mathcal{H} \rightarrow \mathfrak{H}$ is weakly H -smooth if and only if any of the following conditions is satisfied

$$(7) \quad \|A\theta(\lambda, \epsilon)A^*\|_{\mathfrak{H}} \leq C(\lambda), \quad \text{a.e. } \lambda \in \mathbb{R}.$$

$$(8) \quad \epsilon^{1/2}\|AR(\lambda \pm i\epsilon)\|_{\mathfrak{H}} \leq C(\lambda), \quad \text{a.e. } \lambda \in \mathbb{R}.$$

Let M_0 and M be dense sets in \mathcal{H}_0 and \mathcal{H} respectively, and let that for any $u_0 \in M_0$ and $u \in M$ the following limit exists for a.e. $\lambda \in \mathbb{R}$

$$(9) \quad \mathcal{G}_{\pm}(H, H_0; \mathcal{J}) = \lim_{\epsilon \rightarrow 0} \pi^{-1} \epsilon \langle \mathcal{J}R_0(\lambda \pm i\epsilon)u_0, R(\lambda \pm i\epsilon)u \rangle,$$

then the stationary WO $\mathcal{W}_{\pm} = \mathcal{W}_{\pm}(H, H_0; \mathcal{J})$ for the operators H and H_0 with the identification \mathcal{J} is the operator defined on $M_0 \times M$ by the sesquilinear form

$$(10) \quad \langle \mathcal{W}_{\pm}u_0, u \rangle = \int_{-\infty}^{\infty} \mathcal{G}_{\pm}(H, H_0; \mathcal{J})d\lambda.$$

Remark 3.

(i) If $u_0 \in \mathcal{H}_0^{(ac)}$ and $u \in \mathcal{H}^{(ac)}$, then the limit with respect to ϵ and the integration over λ in the equality (10) are interchangeable.

(ii) For a.e. $\lambda \in \mathbb{R}$, the limit (9) has the same value if $\{u_0, u\}$ is replaced by either $\{P_0^{(ac)}u_0, u\}$, $\{u_0, P^{(ac)}u\}$, or $\{P_0^{(ac)}u_0, P^{(ac)}u\}$.

The WO \mathcal{W}_{\pm} possesses most properties of the time-dependent WO; it is bounded, satisfies the intertwining property, and $\mathbf{R}(\mathcal{W}_{\pm}) \subseteq \mathcal{H}^{(ac)}$. Also by the existence of the limit (9), the WO

$$(11) \quad \mathcal{W}_{\pm}^*(H, H_0; \mathcal{J}) = \mathcal{W}_{\pm}(H_0, H; \mathcal{J}^*)$$

exists.

The stationary approach for proving the existence of the time-dependent WO $W_{\pm}(H, H_0; \mathcal{J})$ is based on the existence of the WOs $\widetilde{W}_{\pm}(H, H_0; \mathcal{J})$ and $\widetilde{W}_{\pm}(H_0, H_0; \mathcal{J}^*\mathcal{J})$, and on the stationary proof of

$$(12) \quad \mathcal{W}_{\pm}^*(H, H_0; \mathcal{J})\mathcal{W}_{\pm}(H, H_0; \mathcal{J}) = \mathcal{W}_{\pm}(H_0, H_0; \mathcal{J}^*\mathcal{J}).$$

3. THE MAIN RESULTS

Define the self-adjoint operator H_h as

$$(13) \quad H_h = H_0 + V_h$$

in the Hilbert space \mathcal{H} with domain $\mathbf{D}(H_h) = X$ independent of h , where the parameter $h > 0$ grows to infinity, H_0 is a self-adjoint operator defined in \mathcal{H}_0 with domain $\mathbf{D}(H_0) = X_0$, and V_h is some admissible h -dependent perturbation chosen so that H_h is self-adjoint on X . Let \mathfrak{H} be an auxiliary Hilbert space, and let M and M_0 be dense sets in \mathcal{H} and \mathcal{H}_0 respectively. Assume that V_h admits the factorization

$$(14) \quad V_h = H_h\mathcal{J}_h - \mathcal{J}_hH_0 = A_h^*A_0.$$

The equalities in (14) should be understood as the equalities of the corresponding sesquilinear forms. The operator $\mathcal{J}_h : \mathcal{H}_0 \rightarrow \mathcal{H}$ is a bounded identification, and $A_h : \mathcal{H} \rightarrow \mathfrak{H}$ and $A_0 : \mathcal{H}_0 \rightarrow \mathfrak{H}$ are respectively H_h -bounded for all $h > 0$ and H_0 -bounded operators.

Let $\mathcal{G}_{\pm}^{\dagger}(H, H_0; \mathcal{J})$ be defined by

$$(15) \quad \mathcal{G}_{\pm}^{\dagger}(H, H_0; \mathcal{J}) = \lim_{h \rightarrow \infty} \lim_{\epsilon \rightarrow 0} \pi^{-1} \epsilon \langle \mathcal{J}_h R_0(\lambda \pm i\epsilon)u_0, R_h(\lambda \pm i\epsilon)u \rangle,$$

where H and \mathcal{J} are limit operators in appropriate sense of H_h and \mathcal{J}_h respectively, R_0 and R_h are the resolvent operators of H_0 and H_h respectively, and $u_0 \in M_0$ and $u \in M$. Then we define the stationary WO $\mathcal{W}_{\pm}^{\dagger} = \mathcal{W}_{\pm}^{\dagger}(H, H_0; \mathcal{J})$ on $M_0 \times M$ by the sesquilinear form

$$(16) \quad \langle \mathcal{W}_{\pm}^{\dagger}u_0, u \rangle = \int_{-\infty}^{\infty} \mathcal{G}_{\pm}^{\dagger}(H, H_0; \mathcal{J}) d\lambda.$$

Also, we define the weak time-dependent WO $\widetilde{W}_{\pm}^{\dagger}(H, H_0; \mathcal{J})$ as

$$(17) \quad \begin{aligned} \widetilde{W}_{\pm}^{\dagger}(H, H_0; \mathcal{J}) &= w\text{-}\lim_{h \rightarrow \infty} \widetilde{W}_{\pm}(H_h, H_0; \mathcal{J}_h) \\ &= w\text{-}\lim_{h \rightarrow \infty} w\text{-}\lim_{t \rightarrow \pm\infty} P_h^{(ac)} U_h(-t) \mathcal{J}_h U_0(t) P_0^{(ac)}, \end{aligned}$$

where $U_h(t) = \exp(-iH_h t)$, $U_0(t) = \exp(-iH_0 t)$, and $P_0^{(ac)}$ and $P_h^{(ac)}$ are respectively the orthogonal projections onto the absolutely continuous subspaces of H_0 and H_h . The strong time-dependent WO $W_{\pm}^{\dagger}(H, H_0; \mathcal{J})$ is defined as

$$(18) \quad W_{\pm}^{\dagger}(H, H_0; \mathcal{J}) = s\text{-}\lim_{h \rightarrow \infty} W_{\pm}(H_h, H_0; \mathcal{J}_h) = s\text{-}\lim_{h \rightarrow \infty} s\text{-}\lim_{t \rightarrow \pm\infty} U_h(-t) \mathcal{J}_h U_0(t) P_0^{(ac)},$$

Before proceeding, we should mention that some materials and helpful settings are used from [12] for the construction of proofs of some results in this section. The following two theorems provide sufficient conditions for the existence of the WO W_{\pm}^{\dagger} and its adjoint $W_{\pm}^{\dagger,*}$.

Theorem 1. Assume the following

- (i) A_0 is weakly H_0 -smooth.
- (ii) For all $h > 0$, $A_h R_h(\lambda \pm i\epsilon)$ is strongly convergent as $\epsilon \rightarrow 0$ for a.e. $\lambda \in \mathbb{R}$.
- (iii) If T_h is the strong limit of $A_h R_h(\lambda \pm i\epsilon)$ as $\epsilon \rightarrow 0$ obtained in (ii), then T_h converges weakly as $h \rightarrow \infty$ for a.e. $\lambda \in \mathbb{R}$.
- (iv) \mathcal{J}_h is weakly convergent.

Then the WO $W_{\pm}^{\dagger}(H, H_0; \mathcal{J})$ exists, also $W_{\pm}^{\dagger}(H_0, H; \mathcal{J}^*)$ exists and $W_{\pm}^{\dagger,*}(H, H_0; \mathcal{J}) = W_{\pm}^{\dagger}(H_0, H; \mathcal{J}^*)$.

Proof. To prove the existence of $W_{\pm}^{\dagger}(H, H_0; \mathcal{J})$, it is equivalent to prove the existence of the operator $\mathcal{G}_{\pm}^{\dagger}(H, H_0; \mathcal{J})$ for a.e. $\lambda \in \mathbb{R}$, see definition (15). Using the factorization (14), then for every $z \in \mathbb{C}$ such that the imaginary part of z , $Im(z)$, is different from zero,

$$(19) \quad \mathcal{J}_h R_0(z) - R_h(z) \mathcal{J}_h = R_h(z) A_h^* A_0 R_0(z)$$

which implies

$$(20) \quad \mathcal{J}_h^* R_h(z) = R_0(z) \mathcal{J}_h^* - R_0(z) A_0^* A_h R_h(z).$$

Let $z = \lambda \pm i\epsilon$ in (20), then for $u_0 \in M_0$ and $u \in M$ we simplify

$$\begin{aligned}
(21) \quad & \pi^{-1}\epsilon \langle \mathcal{J}_h R_0(\lambda \pm i\epsilon)u_0, R_h(\lambda \pm i\epsilon)u \rangle = \\
& = \pi^{-1}\epsilon \langle R_0(\lambda \pm i\epsilon)u_0, R_0(\lambda \pm i\epsilon)\mathcal{J}_h^* u \rangle + \\
& \quad - \pi^{-1}\epsilon \langle R_0(\lambda \pm i\epsilon)u_0, R_0(\lambda \pm i\epsilon)A_0^* A_h R_h(\lambda \pm i\epsilon)u \rangle \\
& = \langle \mathcal{J}_h \theta_0(\lambda, \epsilon)u_0, u \rangle - \langle A_0 \theta_0(\lambda, \epsilon)u_0, A_h R_h(\lambda \pm i\epsilon)u \rangle.
\end{aligned}$$

Thus, the existence of $\mathcal{G}_\pm^\dagger(H, H_0; \mathcal{J})$ is equivalent to the existence of the limit

$$(22) \quad \lim_{h \rightarrow \infty} \lim_{\epsilon \rightarrow 0} (\langle \mathcal{J}_h \theta_0(\lambda, \epsilon)u_0, u \rangle - \langle A_0 \theta_0(\lambda, \epsilon)u_0, A_h R_h(\lambda \pm i\epsilon)u \rangle).$$

Note that $\lim_{\epsilon \rightarrow 0} \langle \mathcal{J}_h \theta_0(\lambda, \epsilon)u_0, u \rangle = \frac{d}{d\lambda} \langle \mathcal{J}_h E_0(\lambda)u_0, u \rangle$ for a.e. $\lambda \in \mathbb{R}$, where E_0 is the spectral family of H_0 . Also condition (i) implies the existence of $w\text{-}\lim_{\epsilon \rightarrow \infty} A_0 \theta_0(\lambda, \epsilon)$, which together with condition (ii) imply the existence of the limit of the second scalar product of (22) as $\epsilon \rightarrow 0$. The limits as $h \rightarrow \infty$ also exist for the already found two ϵ -limits by virtue of conditions (iii) and (iv). Therefore, for a.e. $\lambda \in \mathbb{R}$, the operator $\mathcal{G}_\pm^\dagger(H, H_0; \mathcal{J})$ exists, which implies the existence of the WO $\mathcal{W}_\pm^\dagger(H, H_0; \mathcal{J})$. The existence of the WO $\mathcal{W}_\pm^\dagger(H_0, H; \mathcal{J}^*)$ is a consequence of the existence of $\mathcal{W}_\pm^\dagger(H, H_0; \mathcal{J})$. Moreover

$$\begin{aligned}
(23) \quad & \langle \mathcal{W}_\pm^{\dagger,*}(H, H_0; \mathcal{J})u, u_0 \rangle = \langle u, \mathcal{W}_\pm^\dagger(H, H_0; \mathcal{J})u_0 \rangle \\
& = \langle \mathcal{W}_\pm^\dagger(H, H_0; \mathcal{J})u_0, u \rangle^* \\
& = \frac{\int_{-\infty}^{\infty} \lim_{h \rightarrow \infty} \lim_{\epsilon \rightarrow 0} \pi^{-1}\epsilon \langle \mathcal{J}_h R_0(\lambda \pm i\epsilon)u_0, R_h(\lambda \pm i\epsilon)u \rangle d\lambda}{\int_{-\infty}^{\infty} \lim_{h \rightarrow \infty} \lim_{\epsilon \rightarrow 0} \pi^{-1}\epsilon \langle \mathcal{J}_h R_0(\lambda \pm i\epsilon)u_0, R_h(\lambda \pm i\epsilon)u \rangle^* d\lambda} \\
& = \frac{\int_{-\infty}^{\infty} \lim_{h \rightarrow \infty} \lim_{\epsilon \rightarrow 0} \pi^{-1}\epsilon \langle \mathcal{J}_h^* R_h(\lambda \pm i\epsilon)u, R_0(\lambda \pm i\epsilon)u_0 \rangle d\lambda}{\int_{-\infty}^{\infty} \lim_{h \rightarrow \infty} \lim_{\epsilon \rightarrow 0} \pi^{-1}\epsilon \langle \mathcal{J}_h^* R_h(\lambda \pm i\epsilon)u, R_0(\lambda \pm i\epsilon)u_0 \rangle d\lambda} \\
& = \langle \mathcal{W}_\pm^\dagger(H_0, H; \mathcal{J}^*)u, u_0 \rangle.
\end{aligned}$$

This implies $\mathcal{W}_\pm^{\dagger,*}(H, H_0; \mathcal{J}) = \mathcal{W}_\pm^\dagger(H_0, H; \mathcal{J}^*)$ which ends the proof. \blacksquare

The assertions of the previous theorem are still valid under some modifications of its hypotheses, namely we have the following corollary.

Corollary 1. The assertions of Theorem 1 remain in force if its hypotheses (i)-(iii) are replaced by the following; for a.e. $\lambda \in \mathbb{R}$

- (i) The operator $A_0 \theta_0(\lambda, \epsilon)$ is strongly convergent as $\epsilon \rightarrow 0$.

- (ii) $A_h R_h(\lambda \pm i\epsilon)$ is weakly convergent as $\epsilon \rightarrow 0$ for all $h > 0$.
- (iii) If T_h is the weak limit of $A_h R_h(\lambda \pm i\epsilon)$ as $\epsilon \rightarrow 0$ obtained in (ii), then T_h converges weakly as $h \rightarrow \infty$.

Proof. The proof is similar to that of Theorem 1 and mainly depends on (21). ■

Similar statement as that of Theorem 1 can be formulated as the following.

Theorem 2. Assume that

- (i) For all $h > 0$, A_h is weakly H_h -smooth.
- (ii) The operator $A_0 R_0(\lambda \pm i\epsilon)$ is strongly convergent as $\epsilon \rightarrow 0$ for a.e. $\lambda \in \mathbb{R}$.
- (iii) If T_h is the weak limit of $A_h \theta_h(\lambda, \epsilon)$ as $\epsilon \rightarrow 0$ obtained in (i), then T_h converges weakly as $h \rightarrow \infty$ for a.e. $\lambda \in \mathbb{R}$.
- (iv) If E_h is the spectral family of H_h , $E_h(\lambda)$ and \mathcal{J}_h are weakly convergent for a.e. $\lambda \in \mathbb{R}$.

Then the WO $\mathcal{W}_{\pm}^{\dagger}(H, H_0; \mathcal{J})$ exists, also $\mathcal{W}_{\pm}^{\dagger}(H_0, H; \mathcal{J}^*)$ exists and $\mathcal{W}_{\pm}^{\dagger,*}(H, H_0; \mathcal{J}) = \mathcal{W}_{\pm}^{\dagger}(H_0, H; \mathcal{J}^*)$.

Proof. The proof is similar to that of Theorem 1, therefore we only prove the existence of the WO $\mathcal{W}_{\pm}^{\dagger}(H, H_0; \mathcal{J})$. To complete the proof of the assertions, the proof of Theorem 1 is considered. Using (19) with $z = \lambda \pm i\epsilon$, then for $u_0 \in M_0$ and $u \in M$ we have

$$(24) \quad \pi^{-1} \epsilon \langle \mathcal{J}_h R_0(\lambda \pm i\epsilon) u_0, R_h(\lambda \pm i\epsilon) u \rangle = \langle \theta_h(\lambda, \epsilon) \mathcal{J}_h u_0, u \rangle + \langle A_0 R_0(\lambda, \epsilon) u_0, A_h \theta_h(\lambda, \epsilon) u \rangle.$$

By (24), the existence of $\mathcal{G}_{\pm}^{\dagger}(H, H_0; \mathcal{J})$ is equivalent to the existence of

$$(25) \quad \lim_{h \rightarrow \infty} \lim_{\epsilon \rightarrow 0} \left(\langle \theta_h(\lambda, \epsilon) \mathcal{J}_h u_0, u \rangle + \langle A_0 R_0(\lambda, \epsilon) u_0, A_h \theta_h(\lambda, \epsilon) u \rangle \right).$$

The first term, $\langle \theta_h(\lambda, \epsilon) \mathcal{J}_h u_0, u \rangle$, converges to $\frac{d}{d\lambda} \langle E_h(\lambda) \mathcal{J}_h u_0, u \rangle$, as $\epsilon \rightarrow 0$, for a.e. $\lambda \in \mathbb{R}$. By condition (iv), if E_{∞} and \mathcal{J}_{∞} are the weak limits of E_h and \mathcal{J}_h respectively, then $\frac{d}{d\lambda} \langle E_h(\lambda) \mathcal{J}_h u_0, u \rangle$ converges to $\frac{d}{d\lambda} \langle E_{\infty}(\lambda) \mathcal{J}_{\infty} u_0, u \rangle$ as $h \rightarrow \infty$. Thus the first term has a limit as both $\epsilon \rightarrow 0$ and then as $h \rightarrow \infty$. Using conditions (i) – (iii), the limit of the second scalar product exists as both $\epsilon \rightarrow 0$ and then as $h \rightarrow \infty$. Thus we conclude the existence of $\mathcal{G}_{\pm}^{\dagger}(H, H_0; \mathcal{J})$ for a.e. $\lambda \in \mathbb{R}$, consequently the

existence of the WO $\mathcal{W}_{\pm}^{\dagger}(H, H_0; \mathcal{J})$. ■

The following corollary replaces some hypotheses of Theorem 2.

Corollary 2. The assertions of Theorem 2 remain in force if its hypotheses (i)-(iii) are replaced by the following; for a.e. $\lambda \in \mathbb{R}$

- (i) For all $h > 0$, $A_h \theta_h(\lambda, \epsilon)$ is strongly convergent as $\epsilon \rightarrow 0$.
- (ii) $A_0 R_0(\lambda \pm i\epsilon)$ is weakly convergent as $\epsilon \rightarrow 0$.
- (iii) If T_h is the strong limit of $A_h \theta_h(\lambda, \epsilon)$ as $\epsilon \rightarrow 0$ obtained in (i), then T_h converges weakly as $h \rightarrow \infty$.

Proof. The proof is straightforward by considering (24). ■

In the coming discussion we mainly assume Theorems 1 and 2, while some of the results below can be also proved depending on Corollaries 1 or 2 instead of Theorems 1 or 2 respectively.

Theorem 3. Let the hypotheses of Theorem 1 be satisfied, and let further \mathcal{J}_h^* and R_h be strongly convergent. Then the WO $\mathcal{W}_{\pm}^{\dagger}(H, H; \mathcal{J}\mathcal{J}^*)$ exists and

$$(26) \quad \mathcal{W}_{\pm}^{\dagger}(H, H_0; \mathcal{J})\mathcal{W}_{\pm}^{\dagger,*}(H, H_0; \mathcal{J}) = \mathcal{W}_{\pm}^{\dagger}(H, H; \mathcal{J}\mathcal{J}^*).$$

Proof. First we prove (26), and the existence of $\mathcal{W}_{\pm}^{\dagger}(H, H; \mathcal{J}\mathcal{J}^*)$ will be a direct consequence of it. Since, for all $u_0, v_0 \in M_0$, $\lim_{\epsilon \rightarrow 0} \langle \theta_0(\lambda, \epsilon) u_0, v_0 \rangle = \frac{d}{d\lambda} \langle E_0(\lambda) u_0, v_0 \rangle$ for a.e. $\lambda \in \mathbb{R}$, we have for $u_0 \in M_0$ and $u \in M$,

$$(27) \quad \langle u_0, E_0(\Delta) \mathcal{W}_{\pm}^{\dagger,*} u \rangle = \int_{\Delta} \lim_{h \rightarrow \infty} \lim_{\epsilon \rightarrow 0} \langle u_0, \theta_0(\lambda, \epsilon) \mathcal{W}_{\pm}^{\dagger,*} u \rangle d\lambda,$$

this is also due to the existence of $\mathcal{W}_{\pm}^{\dagger} = \mathcal{W}_{\pm}^{\dagger}(H, H_0; \mathcal{J})$. On the other hand

$$(28) \quad \begin{aligned} \langle u_0, E_0(\Delta) \mathcal{W}_{\pm}^{\dagger,*} u \rangle &= \langle \mathcal{W}_{\pm}^{\dagger} E_0(\Delta) u_0, u \rangle \\ &= \int_{\Delta} \lim_{h \rightarrow \infty} \lim_{\epsilon \rightarrow 0} \pi^{-1} \epsilon \langle \mathcal{J}_h R_0(\lambda \pm i\epsilon) u_0, R_h(\lambda \pm i\epsilon) u \rangle d\lambda. \end{aligned}$$

Thus we have the following equality

$$(29) \quad \lim_{h \rightarrow \infty} \lim_{\epsilon \rightarrow 0} \langle u_0, \theta_0(\lambda, \epsilon) \mathcal{W}_{\pm}^{\dagger,*} u \rangle = \lim_{h \rightarrow \infty} \lim_{\epsilon \rightarrow 0} \pi^{-1} \epsilon \langle u_0, R_0(\lambda \mp i\epsilon) \mathcal{J}_h^* R_h(\lambda \pm i\epsilon) u \rangle.$$

By (29), the quantities $\theta_0(\lambda, \epsilon)\mathcal{W}_\pm^{\dagger,*}u$ and $\pi^{-1}\epsilon R_0(\lambda \mp i\epsilon)\mathcal{J}_h^*R_h(\lambda \pm i\epsilon)u$ are equivalent in the limits first as $\epsilon \rightarrow 0$ and then as $h \rightarrow \infty$. Note that by (14), (20), and defining $J_h^\epsilon = \mathcal{J}_h^* - V_h^*R_h(\lambda \pm i\epsilon)$, we have

$$(30) \quad \mathcal{J}_h^*R_h(\lambda \pm i\epsilon) = R_0(\lambda \pm i\epsilon)J_h^\epsilon$$

which provides

$$(31) \quad \pi^{-1}\epsilon \langle \mathcal{J}_h R_0(\lambda \pm i\epsilon)u_0, R_h(\lambda \pm i\epsilon)u \rangle = \langle \theta_0(\lambda, \epsilon)u_0, J_h^\epsilon u \rangle.$$

Note that, by Theorem 1, $\lim_{h \rightarrow \infty} \lim_{\epsilon \rightarrow 0} \langle \theta_0(\lambda, \epsilon)u_0, J_h^\epsilon u \rangle$ is well-defined. Also, by the strong convergence of \mathcal{J}_h^* and R_h , the limit $\lim_{h \rightarrow \infty} \lim_{\epsilon \rightarrow 0} \langle R_0(\lambda \mp i\epsilon)\mathcal{J}_h^*R_h(\lambda \pm i\epsilon)v, J_h^\epsilon u \rangle$ is well-defined. Now, by the existence of the WO $\mathcal{W}_\pm^{\dagger,*}$, and assuming that $u_0 = \mathcal{W}_\pm^{\dagger,*}v$ in (31) with $v \in M$, we have using the notation $\mathcal{K}_{h,\epsilon}(u, v) = \pi^{-1}\epsilon \langle \mathcal{J}_h R_0(\lambda \pm i\epsilon)\mathcal{W}_\pm^{\dagger,*}v, R_h(\lambda \pm i\epsilon)u \rangle$ and the equality (29),

$$(32) \quad \begin{aligned} \lim_{h \rightarrow \infty} \lim_{\epsilon \rightarrow 0} \mathcal{K}_{h,\epsilon}(u, v) &= \lim_{h \rightarrow \infty} \lim_{\epsilon \rightarrow 0} \langle \theta_0(\lambda, \epsilon)\mathcal{W}_\pm^{\dagger,*}v, J_h^\epsilon u \rangle \\ &= \lim_{h \rightarrow \infty} \lim_{\epsilon \rightarrow 0} \pi^{-1}\epsilon \langle R_0(\lambda \mp i\epsilon)\mathcal{J}_h^*R_h(\lambda \pm i\epsilon)v, J_h^\epsilon u \rangle \\ &= \lim_{h \rightarrow \infty} \lim_{\epsilon \rightarrow 0} \pi^{-1}\epsilon \langle \mathcal{J}_h^*R_h(\lambda \pm i\epsilon)v, \mathcal{J}_h^*R_h(\lambda \pm i\epsilon)u \rangle \\ &= \lim_{h \rightarrow \infty} \lim_{\epsilon \rightarrow 0} \pi^{-1}\epsilon \langle \mathcal{J}_h \mathcal{J}_h^*R_h(\lambda \pm i\epsilon)v, R_h(\lambda \pm i\epsilon)u \rangle. \end{aligned}$$

Therefore

$$(33) \quad \begin{aligned} \langle \mathcal{W}_\pm^{\dagger,*}\mathcal{W}_\pm^{\dagger,*}v, u \rangle &= \int_{-\infty}^{\infty} \lim_{h \rightarrow \infty} \lim_{\epsilon \rightarrow 0} \pi^{-1}\epsilon \langle \mathcal{J}_h R_0(\lambda \pm i\epsilon)\mathcal{W}_\pm^{\dagger,*}v, R_h(\lambda \pm i\epsilon)u \rangle d\lambda \\ &= \int_{-\infty}^{\infty} \lim_{h \rightarrow \infty} \lim_{\epsilon \rightarrow 0} \pi^{-1}\epsilon \langle \mathcal{J}_h \mathcal{J}_h^*R_h(\lambda \pm i\epsilon)v, R_h(\lambda \pm i\epsilon)u \rangle d\lambda \\ &= \langle \mathcal{W}_\pm^{\dagger,*}(H, H; \mathcal{J}\mathcal{J}^*)v, u \rangle. \end{aligned}$$

Thus, the proof is complete. ■

The existence of $\mathcal{W}_\pm^{\dagger,*}(H_0, H_0; \mathcal{J}^*\mathcal{J})$ is summarized in the following theorem.

Theorem 4. Let the hypotheses of Theorem 2 be satisfied, and let \mathcal{J}_h be strongly convergent. Then the WO $\mathcal{W}_\pm^{\dagger,*}(H_0, H_0; \mathcal{J}^*\mathcal{J})$ exists and

$$(34) \quad \mathcal{W}_\pm^{\dagger,*}(H, H_0; \mathcal{J})\mathcal{W}_\pm^{\dagger,*}(H, H_0; \mathcal{J}) = \mathcal{W}_\pm^{\dagger,*}(H_0, H_0; \mathcal{J}^*\mathcal{J}).$$

Proof. We establish the proof of the equality (34), and the proof of the existence of the WO $\mathcal{W}_\pm^{\dagger,*}(H_0, H_0; \mathcal{J}^*\mathcal{J})$ will be a consequence of (34) as indicated in the proof of

Theorem 3. By condition (iv) of Theorem 2 and since the WO $\mathcal{W}_\pm^\dagger = \mathcal{W}_\pm^\dagger(H, H_0; \mathcal{J})$ exists,

$$(35) \quad \langle E_\infty(\Delta) \mathcal{W}_\pm^\dagger u_0, u \rangle = \int_\Delta \lim_{h \rightarrow \infty} \lim_{\epsilon \rightarrow 0} \langle \theta_h(\lambda, \epsilon) \mathcal{W}_\pm^\dagger u_0, u \rangle d\lambda.$$

for $u_0 \in M_0$ and $u \in M$. Also by the definition of \mathcal{W}_\pm^\dagger

$$(36) \quad \langle E_\infty(\Delta) \mathcal{W}_\pm^\dagger u_0, u \rangle = \int_\Delta \lim_{h \rightarrow \infty} \lim_{\epsilon \rightarrow 0} \pi^{-1} \epsilon \langle \mathcal{J}_h R_0(\lambda \pm i\epsilon) u_0, R_h(\lambda \pm i\epsilon) u \rangle d\lambda.$$

Thus the following equality holds

$$(37) \quad \lim_{h \rightarrow \infty} \lim_{\epsilon \rightarrow 0} \langle \theta_h(\lambda, \epsilon) \mathcal{W}_\pm^\dagger u_0, u \rangle = \lim_{h \rightarrow \infty} \lim_{\epsilon \rightarrow 0} \pi^{-1} \epsilon \langle R_h(\lambda \mp i\epsilon) \mathcal{J}_h R_0(\lambda \pm i\epsilon) u_0, u \rangle.$$

According to (37), the quantity $\theta_h(\lambda, \epsilon) \mathcal{W}_\pm^\dagger u_0$ is equivalent in the limits to the quantity $\pi^{-1} \epsilon R_h(\lambda \mp i\epsilon) \mathcal{J}_h R_0(\lambda \pm i\epsilon) u_0$ first as $\epsilon \rightarrow 0$ and then as $h \rightarrow \infty$. Define $\mathcal{S}_h^\epsilon = \mathcal{J}_h + V_h R_0(\lambda \pm i\epsilon)$, then by virtue of (14) and (19) the following is obtained

$$(38) \quad \pi^{-1} \epsilon \langle \mathcal{J}_h R_0(\lambda \pm i\epsilon) u_0, R_h(\lambda \pm i\epsilon) u \rangle = \langle \mathcal{S}_h^\epsilon u_0, \theta_h(\lambda, \epsilon) u \rangle.$$

Note that the hypotheses of Theorem 2 imply the existence of $\lim_{h \rightarrow \infty} \lim_{\epsilon \rightarrow 0} \langle \mathcal{S}_h^\epsilon u_0, \theta_h(\lambda, \epsilon) u \rangle$, thus, by also the strong convergence of \mathcal{J}_h , the limits in (39) and (40) are well-defined. Let now $u = \mathcal{W}_\pm^\dagger v_0$ in (38), and consider the limit first as $\epsilon \rightarrow 0$ and then as $h \rightarrow \infty$, then using (14) and (37) we arrive at

$$(39) \quad \begin{aligned} \lim_{h \rightarrow \infty} \lim_{\epsilon \rightarrow 0} \pi^{-1} \epsilon \langle \mathcal{J}_h R_0(\lambda \pm i\epsilon) u_0, R_h(\lambda \pm i\epsilon) \mathcal{W}_\pm^\dagger v_0 \rangle &= \\ &= \lim_{h \rightarrow \infty} \lim_{\epsilon \rightarrow 0} \pi^{-1} \epsilon \langle \mathcal{J}_h^* \mathcal{J}_h R_0(\lambda \pm i\epsilon) u_0, R_0(\lambda \pm i\epsilon) v_0 \rangle. \end{aligned}$$

Therefore

$$(40) \quad \begin{aligned} \langle \mathcal{W}_\pm^{\dagger,*} \mathcal{W}_\pm^\dagger u_0, v_0 \rangle &= \langle \mathcal{W}_\pm^\dagger u_0, \mathcal{W}_\pm^\dagger v_0 \rangle \\ &= \int_{-\infty}^{\infty} \lim_{h \rightarrow \infty} \lim_{\epsilon \rightarrow 0} \pi^{-1} \epsilon \langle \mathcal{J}_h R_0(\lambda \pm i\epsilon) u_0, R_h(\lambda \pm i\epsilon) \mathcal{W}_\pm^\dagger v_0 \rangle d\lambda \\ &= \int_{-\infty}^{\infty} \lim_{h \rightarrow \infty} \lim_{\epsilon \rightarrow 0} \pi^{-1} \epsilon \langle \mathcal{J}_h^* \mathcal{J}_h R_0(\lambda \pm i\epsilon) u_0, R_0(\lambda \pm i\epsilon) v_0 \rangle d\lambda \\ &= \langle \mathcal{W}_\pm^\dagger(H_0, H_0; \mathcal{J}^* \mathcal{J}) u_0, v_0 \rangle. \end{aligned}$$

Thus the proof of the theorem is complete. ■

Theorem 5. If both $\mathcal{W}_\pm^\dagger = \mathcal{W}_\pm^\dagger(H, H_0; \mathcal{J})$ and $\widetilde{\mathcal{W}}_\pm^\dagger = \widetilde{\mathcal{W}}_\pm^\dagger(H, H_0; \mathcal{J})$ exist, then they coincide with each other. This coincidence is understood of the corresponding sesquilinear forms.

Proof. Recall the definition of the WO $\widetilde{W}_\pm^\dagger = \widetilde{W}_\pm^\dagger(H, H_0; \mathcal{J})$ given by (17) as

$$(41) \quad \widetilde{W}_\pm^\dagger(H, H_0; \mathcal{J}) = w\text{-}\lim_{h \rightarrow \infty} w\text{-}\lim_{t \rightarrow \pm\infty} P_h^{(ac)} U_h(-t) \mathcal{J}_h U_0(t) P_0^{(ac)}.$$

By the existence of $\widetilde{W}_\pm^\dagger$, we can replace $w\text{-}\lim_{t \rightarrow \pm\infty}$ by its equivalent weak Abelian limit (see e.g. [9, 12]) as

$$(42) \quad w\text{-}\lim_{t \rightarrow \pm\infty} P_h^{(ac)} U_h(-t) \mathcal{J}_h U_0(t) P_0^{(ac)} = w\text{-}\lim_{\epsilon \rightarrow 0} \int_0^\infty 2\epsilon e^{-2\epsilon t} P_h^{(ac)} U_h(\mp t) \mathcal{J}_h U_0(\pm t) P_0^{(ac)} dt.$$

By the definition of $\widetilde{W}_\pm^\dagger$ we have

$$(43) \quad \langle \widetilde{W}_\pm^\dagger(H, H_0; \mathcal{J}) u_0, u \rangle = \lim_{h \rightarrow \infty} \lim_{t \rightarrow \pm\infty} \langle P_h^{(ac)} U_h(-t) \mathcal{J}_h U_0(t) P_0^{(ac)} u_0, u \rangle,$$

where u_0 and u belong respectively to \mathcal{H}_0 and \mathcal{H} . By (42) the right hand side of (43) can be transformed equivalently to

$$(44) \quad \lim_{h \rightarrow \infty} \lim_{\epsilon \rightarrow 0} 2\epsilon \int_0^\infty e^{-2\epsilon t} \langle \mathcal{J}_h U_0(\pm t) P_0^{(ac)} u_0, U_h(\pm t) P_h^{(ac)} u \rangle dt$$

which can be written as

$$(45) \quad \lim_{h \rightarrow \infty} \lim_{\epsilon \rightarrow 0} \int_0^\infty 2\epsilon \langle \mathcal{J}_h e^{-\epsilon t} U_0(\pm t) P_0^{(ac)} u_0, e^{-\epsilon t} U_h(\pm t) P_h^{(ac)} u \rangle dt.$$

Let \mathcal{F} denote the Fourier transform operator, $(\mathcal{F}f)(\lambda) = (2\pi)^{-1/2} \int_{-\infty}^\infty e^{-i\lambda t} f(t) dt$, then by $\langle f(t), g(t) \rangle = \langle (\mathcal{F}f)(\lambda), (\mathcal{F}g)(\lambda) \rangle$, (45) is equivalent to

$$(46) \quad \lim_{h \rightarrow \infty} \lim_{\epsilon \rightarrow 0} \int_{-\infty}^\infty 2\epsilon \langle \mathcal{J}_h (\mathcal{F} e^{-\epsilon t} U_0(\pm t)) P_0^{(ac)} u_0, (\mathcal{F} e^{-\epsilon t} U_h(\pm t)) P_h^{(ac)} u \rangle d\lambda.$$

Using the identities

$$(47) \quad R_0(\lambda \pm i\epsilon) = \pm \int_{-\infty}^\infty e^{(i\epsilon \pm \lambda)it} U_0(\pm t) dt \quad \text{and} \quad R_h(\lambda \pm i\epsilon) = \pm \int_{-\infty}^\infty e^{(i\epsilon \pm \lambda)it} U_h(\pm t) dt$$

we write (46) as

$$(48) \quad \lim_{h \rightarrow \infty} \lim_{\epsilon \rightarrow 0} \int_{-\infty}^\infty \pi^{-1} \epsilon \langle \mathcal{J}_h \mathcal{R}_0(\lambda \pm i\epsilon) P_0^{(ac)} u_0, R_h(\lambda \pm i\epsilon) P_h^{(ac)} u \rangle d\lambda.$$

Note that the integrand of (48) is in $L^1(\mathbb{R}; d\lambda)$ for all $h > 0$ and all $\epsilon > 0$. Also By the existence of the WO W_\pm^\dagger , the limits firstly as $\epsilon \rightarrow 0$ and then as $h \rightarrow \infty$ of the integrand exist. Thus using Lebesgue dominated convergence theorem we can move

the limits with respect to ϵ first and then h under the integral sign in (48). Hence (48) can be written equivalently as

$$(49) \quad \int_{-\infty}^{\infty} \lim_{h \rightarrow \infty} \lim_{\epsilon \rightarrow 0} \pi^{-1} \epsilon \langle \mathcal{J}_h \mathcal{R}_0(\lambda \pm i\epsilon) P_0^{(ac)} u_0, R_h(\lambda \pm i\epsilon) P_h^{(ac)} u \rangle d\lambda.$$

Remark 3 part (ii) implies that (49) is equivalent to

$$(50) \quad \int_{-\infty}^{\infty} \lim_{h \rightarrow \infty} \lim_{\epsilon \rightarrow 0} \pi^{-1} \epsilon \langle \mathcal{J}_h \mathcal{R}_0(\lambda \pm i\epsilon) u_0, R_h(\lambda \pm i\epsilon) u \rangle d\lambda = \langle \mathcal{W}_{\pm}^{\dagger}(H, H_0; \mathcal{J}) u_0, u \rangle,$$

and this ends the proof. \blacksquare

Similar to Theorem 5, it is clear that if $\mathcal{W}_{\pm}^{\dagger}(H_0, H; \mathcal{J}^*)$ and $\widetilde{\mathcal{W}}_{\pm}^{\dagger}(H_0, H; \mathcal{J}^*)$ exist, then their corresponding sesquilinear forms are equivalent to each other. The same argument can be drawn for the pair $\mathcal{W}_{\pm}^{\dagger}(H, H; \mathcal{J}\mathcal{J}^*)$ and $\widetilde{\mathcal{W}}_{\pm}^{\dagger}(H, H; \mathcal{J}\mathcal{J}^*)$ and the pair $\mathcal{W}_{\pm}^{\dagger}(H_0, H_0; \mathcal{J}^*\mathcal{J})$ and $\widetilde{\mathcal{W}}_{\pm}^{\dagger}(H_0, H_0; \mathcal{J}^*\mathcal{J})$.

For the WOs $\widetilde{\mathcal{W}}_{\pm}^{\dagger}(H, H_0; \mathcal{J})$ and $\widetilde{\mathcal{W}}_{\pm}^{\dagger}(H_0, H; \mathcal{J}^*)$ we use the following result.

Proposition 1. Let M_1 and M_2 be dense linear manifolds in the Hilbert spaces \mathcal{H}_1 and \mathcal{H}_2 respectively, and let H_1 and $H_2 = H_1 + V$ be self-adjoint operators in \mathcal{H}_1 and \mathcal{H}_2 respectively, where V is some admissible perturbation. Suppose that for a.e. $\lambda \in \mathbb{R}$, $w\text{-}\lim_{\epsilon \rightarrow 0} A_1 \theta_1(\lambda, \epsilon) u_1$ and $w\text{-}\lim_{\epsilon \rightarrow 0} A_2 \theta_2(\lambda, \epsilon) u_2$ exist for all $u_1 \in M_1$ and $u_2 \in M_2$, where $A_2^* A_1 = H_2 \mathcal{J} - \mathcal{J} H_1 = V$, $\mathcal{J} : \mathcal{H}_1 \rightarrow \mathcal{H}_2$ is a bounded identification, and $A_2 : \mathcal{H}_2 \rightarrow \mathfrak{H}$ and $A_1 : \mathcal{H}_1 \rightarrow \mathfrak{H}$ are respectively H_2 -bounded and H_1 -bounded operators, then the WO $\widetilde{\mathcal{W}}_{\pm}^{\dagger}(H_2, H_1; \mathcal{J})$ exists.

Proof. See [12]. \blacksquare

Lemma 1. Suppose that the hypotheses of Theorem 1 are satisfied, then the WO $\widetilde{\mathcal{W}}_{\pm}^{\dagger}(H, H_0; \mathcal{J})$ exists, consequently $\widetilde{\mathcal{W}}_{\pm}^{\dagger}(H_0, H; \mathcal{J}^*)$ exists and

$$(51) \quad \widetilde{\mathcal{W}}_{\pm}^{\dagger,*}(H, H_0; \mathcal{J}) = \widetilde{\mathcal{W}}_{\pm}^{\dagger}(H_0, H; \mathcal{J}^*).$$

Proof. By conditions (i) and (ii) of Theorem 1, and according to Proposition 1, the WO $\widetilde{\mathcal{W}}_{\pm}^{\dagger}(H_h, H_0; \mathcal{J}_h)$ exists for all $h > 0$. By the existence of the WO $\mathcal{W}_{\pm}^{\dagger}(H, H_0; \mathcal{J})$, the following limit is well-defined

$$(52) \quad \int_{-\infty}^{\infty} \lim_{h \rightarrow \infty} \lim_{\epsilon \rightarrow 0} \pi^{-1} \epsilon \langle \mathcal{J}_h \mathcal{R}_0(\lambda \pm i\epsilon) u_0, R_h(\lambda \pm i\epsilon) u \rangle d\lambda,$$

where $u_0 \in M_0$ and $u \in M$. Following the proof of Theorem 5 but in the reverse way, the existence of (52) implies the existence of the following limit

$$(53) \quad \lim_{h \rightarrow \infty} \lim_{\epsilon \rightarrow 0} 2\epsilon \int_0^\infty e^{-2\epsilon t} \langle \mathcal{J}_h U_0(\pm t) P_0^{(ac)} u_0, U_h(\pm t) P_h^{(ac)} u \rangle dt.$$

Since the WO $\widetilde{W}_\pm(H_h, H_0; \mathcal{J}_h)$ exists, then by (42) the following limit also exists

$$(54) \quad \lim_{h \rightarrow \infty} \lim_{t \rightarrow \pm\infty} \langle P_h^{(ac)} U_h(-t) \mathcal{J}_h U_0(t) P_0^{(ac)} u_0, u \rangle,$$

consequently the existence of the WO $\widetilde{W}_\pm^\dagger(H, H_0; \mathcal{J})$.

The conditions of Theorem 1 can be applied for the collection H_0, H_h , and \mathcal{J}_h^* in Lemma 2 to prove the existence of $\widetilde{W}_\pm^\dagger(H_0, H; \mathcal{J}^*)$. Clearly that the equality (51) is a direct consequence of the definition of the weak WO. \blacksquare

Lemma 2. The assertions of Lemma 1 remain in force if its hypotheses are replaced with the hypotheses of Theorem 2.

Proof. The proof is similar to that of Lemma 1. \blacksquare

Theorem 6. Suppose the hypotheses of Theorem 3 are satisfied, then the WO $\widetilde{W}_\pm^\dagger(H, H; \mathcal{J}\mathcal{J}^*)$ exists.

Proof. First we prove the existence of $\widetilde{W}_\pm(H_h, H_h; \mathcal{J}_h \mathcal{J}_h^*)$ for all $h > 0$. In this regard, let $u, v \in X$, then by virtue of (14)

$$(55) \quad \begin{aligned} \langle (H_h \mathcal{J}_h \mathcal{J}_h^* - \mathcal{J}_h \mathcal{J}_h^* H_h) u, v \rangle &= \langle (H_h \mathcal{J}_h \mathcal{J}_h^* - \mathcal{J}_h \mathcal{J}_h^* H_h + \mathcal{J}_h H_0 \mathcal{J}_h^* - \mathcal{J}_h H_0 \mathcal{J}_h^*) u, v \rangle \\ &= \langle \mathcal{J}_h (H_0 \mathcal{J}_h^* - \mathcal{J}_h^* H_h) u, v \rangle - \langle (\mathcal{J}_h H_0 - H_h \mathcal{J}_h) \mathcal{J}_h^* u, v \rangle \\ &= \langle V_h \mathcal{J}_h^* u, v \rangle - \langle \mathcal{J}_h V_h^* u, v \rangle \\ &= \langle A_h^* A_0 \mathcal{J}_h^* u, v \rangle - \langle \mathcal{J}_h A_0^* A_h u, v \rangle \\ &= \langle A_h^* (A_0 \mathcal{J}_h^*) u, v \rangle - \langle (A_0 \mathcal{J}_h^*)^* A_h u, v \rangle. \end{aligned}$$

Hence, we have the equality

$$(56) \quad H_h \mathcal{J}_h \mathcal{J}_h^* - \mathcal{J}_h \mathcal{J}_h^* H_h = A_h^* (A_0 \mathcal{J}_h^*) - (A_0 \mathcal{J}_h^*)^* A_h.$$

Using the representation (56), we apply Proposition 1 to the collection H_h, H_h , and $\mathcal{J}_h \mathcal{J}_h^*$. By Condition (ii) of Theorem 1, the operator A_h is weakly H_h -smooth for all $h > 0$. What remains to prove is the weak H_h -smoothness of $\check{A}_h = A_0 \mathcal{J}_h^*$ for all $h > 0$. Apply A_0 to both sides of (20) provides

$$(57) \quad \check{A}_h R_h(z) = A_0 R_0(z) \mathcal{J}_h^* - A_0 R_0(z) A_0^* A_h R_h(z).$$

Thus, for $u \in M$, we get for a.e. $\lambda \in \mathbb{R}$

$$(58) \quad \begin{aligned} \epsilon^{1/2} \|\check{A}_h R_h(\lambda + i\epsilon)u\|_{\mathfrak{H}} &\leq \epsilon^{1/2} \|A_0 R_0(\lambda + i\epsilon)\|_{\mathfrak{H}} \|\mathcal{J}_h^* u\|_{\mathfrak{H}} + \\ &\quad + \|A_0 R_0(\lambda + i\epsilon)A_0^*\|_{\mathfrak{H}} \|A_h R_h(\lambda + i\epsilon)u\|_{\mathfrak{H}} \\ &\leq C(\lambda). \end{aligned}$$

Note that the boundedness in (58) by $C(\lambda)$ is due to the hypotheses of Theorem 1 and the H_0 -boundedness of A_0 . This proves the existence of $\widetilde{W}_{\pm}(H_h, H_h; \mathcal{J}_h \mathcal{J}_h^*)$ for all $h > 0$.

To prove the existence of $\widetilde{W}_{\pm}^{\dagger}(H, H; \mathcal{J} \mathcal{J}^*)$ we use the same technique as of Lemma 1. By the hypotheses of Theorem 1, the WO $\mathcal{W}_{\pm}^{\dagger}(H, H; \mathcal{J} \mathcal{J}^*)$ exists, thus the following limit is well-defined

$$(59) \quad \int_{-\infty}^{\infty} \lim_{h \rightarrow \infty} \lim_{\epsilon \rightarrow 0} \pi^{-1} \epsilon \langle \mathcal{J}_h^* R_h(\lambda \pm i\epsilon)u, \mathcal{J}_h^* R_h(\lambda \pm i\epsilon)v \rangle d\lambda,$$

where $u, v \in M$. By the existence of (59), and as a result of the proof of Theorem 5, the following limit is also well-defined

$$(60) \quad \lim_{h \rightarrow \infty} \lim_{\epsilon \rightarrow 0} 2\epsilon \int_0^{\infty} e^{-2\epsilon t} \langle \mathcal{J}_h^* U_h(\pm t) P_h^{(ac)} u, \mathcal{J}_h^* U_h(\pm t) P_h^{(ac)} v \rangle dt.$$

Since the WO $\widetilde{W}_{\pm}(H_h, H_h; \mathcal{J}_h \mathcal{J}_h^*)$ exists for all $h > 0$, by virtue of (42) the following limit exists

$$(61) \quad \lim_{h \rightarrow \infty} \lim_{t \rightarrow \pm\infty} \langle P_h^{(ac)} U_h(-t) \mathcal{J}_h \mathcal{J}_h^* U_h(t) P_h^{(ac)} u, v \rangle,$$

thus the existence of $\widetilde{W}_{\pm}^{\dagger}(H, H; \mathcal{J} \mathcal{J}^*)$. ■

Theorem 7. Suppose the hypotheses of Theorem 4 are satisfied, then the WO $\widetilde{W}_{\pm}^{\dagger}(H_0, H_0; \mathcal{J}^* \mathcal{J})$ exists.

Proof. The proof is similar to that of Theorem 6. ■

Theorem 8. If the hypotheses of Theorem 4 are satisfied, then the WO $W_{\pm}^{\dagger}(H, H_0; \mathcal{J})$ exists.

Proof. By Theorem 7 which assumes Theorem 4, the WO $\widetilde{W}_{\pm}^{\dagger}(H_0, H_0; \mathcal{J}^* \mathcal{J})$ exists. Also Theorem 4 assumes the hypotheses of Theorem 2 which imply the existence of $\mathcal{W}_{\pm}^{\dagger}(H, H_0; \mathcal{J})$ and $\mathcal{W}_{\pm}^{\dagger}(H_0, H; \mathcal{J}^*)$. By Lemma 2 the WOs $\widetilde{W}_{\pm}^{\dagger}(H, H_0; \mathcal{J})$ and $\widetilde{W}_{\pm}^{\dagger}(H_0, H; \mathcal{J}^*)$ exist, and $\widetilde{W}_{\pm}^{\dagger,*}(H, H_0; \mathcal{J}) = \widetilde{W}_{\pm}^{\dagger}(H_0, H; \mathcal{J}^*)$. Moreover, by Theorem 4, the WO $\mathcal{W}_{\pm}^{\dagger}(H_0, H_0; \mathcal{J}^* \mathcal{J})$ exists and equality (34) holds. Applying Theorem 5

which implies the equivalence between the stationary WO W_{\pm}^{\dagger} and the weak WO $\widetilde{W}_{\pm}^{\dagger}$, together with (34) we arrive at

$$(62) \quad \widetilde{W}_{\pm}^{\dagger,*}(H, H_0; \mathcal{J})\widetilde{W}_{\pm}^{\dagger}(H, H_0; \mathcal{J}) = \widetilde{W}_{\pm}^{\dagger}(H_0, H_0; \mathcal{J}^*\mathcal{J}).$$

Let $\widetilde{W}_{\pm}^{\dagger} = \widetilde{W}_{\pm}^{\dagger}(H, H_0; \mathcal{J})$ and $P_{\infty}^{(ac)} = \lim_{h \rightarrow \infty} P_h^{(ac)}$, then by the existence of $\widetilde{W}_{\pm}^{\dagger}$ we have

$$(63) \quad \begin{aligned} & \lim_{h \rightarrow \infty} \lim_{t \rightarrow \pm\infty} \operatorname{Re}\langle (P_{\infty}^{(ac)} - P_h^{(ac)})U_h(-t)\mathcal{J}_h U_0(t)P_0^{(ac)}, \widetilde{W}_{\pm}^{\dagger}u_0 \rangle \\ & \leq \lim_{h \rightarrow \infty} \lim_{t \rightarrow \pm\infty} \|U_h(-t)\mathcal{J}_h U_0(t)P_0^{(ac)}\|_{\mathcal{H}} \|(P_{\infty}^{(ac)} - P_h^{(ac)})\widetilde{W}_{\pm}^{\dagger}u_0\|_{\mathcal{H}} \\ & \rightarrow 0. \end{aligned}$$

Without loss of generality we assume $\operatorname{Re}\langle (P_{\infty}^{(ac)} - P_h^{(ac)})U_h(-t)\mathcal{J}_h U_0(t)P_0^{(ac)}, \widetilde{W}_{\pm}^{\dagger}u_0 \rangle \geq 0$, therefore in the limits first as $t \rightarrow \pm\infty$ and then as $h \rightarrow \infty$ we have the equality

$$(64) \quad \operatorname{Re}\langle P_h^{(ac)}U_h(-t)\mathcal{J}_h U_0(t)P_0^{(ac)}, \widetilde{W}_{\pm}^{\dagger}u_0 \rangle = \operatorname{Re}\langle P_{\infty}^{(ac)}U_h(-t)\mathcal{J}_h U_0(t)P_0^{(ac)}, \widetilde{W}_{\pm}^{\dagger}u_0 \rangle.$$

Now, for $u_0 \in \mathcal{H}_0$,

$$(65) \quad \begin{aligned} & \lim_{h \rightarrow \infty} \lim_{t \rightarrow \pm\infty} \|U_h(-t)\mathcal{J}_h U_0(t)P_0^{(ac)}u_0 - \widetilde{W}_{\pm}^{\dagger}u_0\|_{\mathcal{H}}^2 = \\ & = \lim_{h \rightarrow \infty} \lim_{t \rightarrow \pm\infty} \langle P_0^{(ac)}U_0(-t)\mathcal{J}_h^* \mathcal{J}_h U_0(t)P_0^{(ac)}u_0, u_0 \rangle + \\ & \quad - \lim_{h \rightarrow \infty} \lim_{t \rightarrow \pm\infty} 2\operatorname{Re}\langle U_h(-t)\mathcal{J}_h U_0(t)P_0^{(ac)}u_0, \widetilde{W}_{\pm}^{\dagger}u_0 \rangle + \|\widetilde{W}_{\pm}^{\dagger}u_0\|_{\mathcal{H}}^2 \\ & = \lim_{h \rightarrow \infty} \lim_{t \rightarrow \pm\infty} \langle P_0^{(ac)}U_0(-t)\mathcal{J}_h^* \mathcal{J}_h U_0(t)P_0^{(ac)}u_0, u_0 \rangle + \\ & \quad - 2\|\widetilde{W}_{\pm}^{\dagger}u_0\|_{\mathcal{H}}^2 + \|\widetilde{W}_{\pm}^{\dagger}u_0\|_{\mathcal{H}}^2 \\ & = \langle \widetilde{W}_{\pm}^{\dagger}(H_0, H_0; \mathcal{J}^*\mathcal{J})u_0, u_0 \rangle - \|\widetilde{W}_{\pm}^{\dagger}u_0\|_{\mathcal{H}}^2. \end{aligned}$$

By (62), $\langle \widetilde{W}_{\pm}^{\dagger}(H_0, H_0; \mathcal{J}^*\mathcal{J})u_0, u_0 \rangle = \|\widetilde{W}_{\pm}^{\dagger}u_0\|_{\mathcal{H}}^2$, thus the last equality is equal to zero. Note that we have used the fact that $P_{\infty}^{(ac)}\widetilde{W}_{\pm}^{\dagger} = \widetilde{W}_{\pm}^{\dagger}$ together with (64) to get the second term of the equality before the last one. Therefore, and as a consequence of (65), $s\text{-}\lim_{h \rightarrow \infty} s\text{-}\lim_{t \rightarrow \pm\infty} U_h(-t)\mathcal{J}_h U_0(t)P_0^{(ac)}$ exists, i.e., the existence of the WO $W_{\pm}^{\dagger}(H, H_0; \mathcal{J})$. \blacksquare

Theorem 9. Assume the hypotheses of Theorem 3. Then the WO $W_{\pm}^{\dagger}(H_0, H; \mathcal{J}^*)$ exists.

Proof. The proof is similar to that of Theorem 8 but now using the assertions of Theorem 3, Lemma 1, and Theorem 6 instead of those of Theorem 4, Lemma 2, and

Theorem 7 respectively. ■

It is worth to mention that the equality in the limits of both sides of (64) in the proof of Theorem 8 is not needed in the proof of Theorem 9. This is because (64) is needed to guarantee the equality

$$(66) \quad \lim_{h \rightarrow \infty} \lim_{t \rightarrow \pm\infty} \operatorname{Re} \langle U_h(-t) \mathcal{J}_h U_0(t) P_0^{(ac)} u_0, \widetilde{W}_{\pm}^{\dagger}(H, H_0; \mathcal{J}) u_0 \rangle = \|\widetilde{W}_{\pm}^{\dagger}(H, H_0; \mathcal{J}) u_0\|_{\mathcal{H}}^2.$$

In a similar way to the proof of Theorem 8, in the proof of Theorem 9 we have the following term instead

$$(67) \quad \lim_{h \rightarrow \infty} \lim_{t \rightarrow \pm\infty} \operatorname{Re} \langle U_0(-t) \mathcal{J}_h^* U_h(t) P_h^{(ac)} u, \widetilde{W}_{\pm}^{\dagger}(H_0, H; \mathcal{J}^*) u \rangle,$$

where $u \in \mathcal{H}$. By the fact that $\widetilde{W}_{\pm}^{\dagger}(H_0, H; \mathcal{J}^*) = P_0^{(ac)} \widetilde{W}_{\pm}^{\dagger}(H_0, H; \mathcal{J})$, then as a direct consequence, (67) is equal to $\|\widetilde{W}_{\pm}^{\dagger}(H_0, H; \mathcal{J}^*) u\|_{\mathcal{H}_0}^2$.

Once the existence of the WOs $W_{\pm}^{\dagger}(H, H_0; \mathcal{J})$ and $W_{\pm}^{\dagger}(H_0, H; \mathcal{J}^*)$ is established, the remaining question is to characterize these operators as $h \rightarrow \infty$. In other words, we would like to study the asymptotic behavior as $h \rightarrow \infty$ of the WOs $W_{\pm}(H_h, H_0; \mathcal{J}_h)$ and $W_{\pm}(H_0, H_h; \mathcal{J}_h^*)$. To this end, by the existence of $W_{\pm}^{\dagger}(H, H_0; \mathcal{J})$, for all $h > 0$ and $u_0 \in X_0$, the function

$$(68) \quad \mathcal{T}_{u_0, h}(t) = \|(H_h \phi(H_h) \mathcal{J}_h \phi(H_0) - \phi(H_h) \mathcal{J}_h H_0 \phi(H_0)) U_0(t) u_0\|_{\mathcal{H}}$$

is in $L^1([-\infty, \infty); dt)$ for some continuous function $\phi : \mathbb{R} \rightarrow \mathbb{R}$ such that $x\phi(x)$ is bounded on \mathbb{R} , see [1]. This means that for any $\varepsilon > 0$, there exist $s_1, s_2 \in \mathbb{R}$ such that $\int_{s_1}^{\infty} \mathcal{T}_{u_0, h}(t) dt \leq \varepsilon$ and $\int_{-\infty}^{s_2} \mathcal{T}_{u_0, h}(t) dt \leq \varepsilon$.

Similarly, by the existence of $W_{\pm}^{\dagger}(H_0, H; \mathcal{J}^*)$, for a function ϕ as above, and for all $h > 0$ and $u \in X$, the function

$$(69) \quad \mathcal{S}_{u, h}(t) = \|(H_0 \phi(H_0) \mathcal{J}_h^* \phi(H_h) - \phi(H_0) \mathcal{J}_h^* H_h \phi(H_h)) U_h(t) u\|_{\mathcal{H}_0}$$

belongs to $L^1([-\infty, \infty); dt)$. This also implies that for any $\varepsilon > 0$, there exist $r_1, r_2 \in \mathbb{R}$ such that $\int_{r_1}^{\infty} \mathcal{S}_{u, h}(t) dt \leq \varepsilon$ and $\int_{-\infty}^{r_2} \mathcal{S}_{u, h}(t) dt \leq \varepsilon$. Therefore by (68) and (69), and according to [4], if $H_h \rightarrow H_{\infty}$ in the strong resolvent sense (SRS), $\mathcal{J}_h \rightarrow \mathcal{J}_{\infty}$ strongly, and $\mathcal{J}_h^* \rightarrow \mathcal{J}_{\infty}^*$ strongly, then $s\text{-}\lim_{h \rightarrow \infty}$ and $s\text{-}\lim_{t \rightarrow \pm\infty}$ are interchangeable in

the definition of the WOs $W_{\pm}^{\dagger}(H, H_0; \mathcal{J})$ and $W_{\pm}^{\dagger}(H_0, H; \mathcal{J}^*)$. Thus we can state the following results.

Proposition 2. Assume the assertions of Theorems 8 and 9. Suppose that $H_h = H_0 + V_h$ converges in the SRS to $H_{\infty} = H_0 + V_{\infty}$, where V_h and V_{∞} are H_0 -bounded operators. Let $\mathcal{J}_h = I$, then $W_{\pm}^{\dagger}(H, H_0) = W_{\pm}(H_{\infty}, H_0)$ and $W_{\pm}^{\dagger}(H_0, H) = W_{\pm}(H_0, H_{\infty})$.

Also for an identity identification we have the following

Proposition 3. Assume the assertions of Theorems 8 and 9. Suppose that $H_h = H_0 + A_h^* A_0$ where A_h is H_h -bounded for all $h > 0$ and A_0 is H_0 -bounded, and suppose that $\|A_0\| < \infty$, $\sup_h \|A_h\| < \infty$, and $\lim_{h \rightarrow \infty} \|A_h\| = 0$, then $W_{\pm}^{\dagger}(H, H_0) = I$, also $W_{\pm}^{\dagger}(H_0, H) = I$.

In fact instead of strong convergence in Proposition 2 we have uniform convergence of the WO $W_{\pm, h}$, i.e., given the hypotheses of Proposition 2, then $W_{\pm}(H_h, H_0)$ and $W_{\pm}(H_0, H_h)$ converge in norm to the identity operator. For a non-identity identification \mathcal{J}_h , we have the following

Proposition 4. Assume the assertions of Theorems 8 and 9. Suppose that $H_h = H_0 + V_h$ converges in the SRS to $H_{\infty} = H_0 + V_{\infty}$, where V_h and V_{∞} are H_0 -bounded operators. If the identification \mathcal{J}_h converges strongly to \mathcal{J}_{∞} , then $W_{\pm}^{\dagger}(H, H_0; \mathcal{J}) = W_{\pm}(H_{\infty}, H_0; \mathcal{J}_{\infty})$. Also if \mathcal{J}_h^* converges strongly to \mathcal{J}_{∞}^* , then $W_{\pm}^{\dagger}(H_0, H; \mathcal{J}^*) = W_{\pm}(H_0, H_{\infty}; \mathcal{J}_{\infty}^*)$.

REFERENCES

- [1] H. Almasreah, *Strong convergence of wave operators for a family of Dirac operators*, (submitted).
- [2] M. Sh. Birman and S. B. Entina, *Stationary approach in abstract scattering theory*, Math. USSR-Izv, 1(1967), pp. 391-420.
- [3] M. Sh. Birman and M. G. Kreĭn, *On the theory of wave operators and scattering operators*, Soviet Math. Dokl, 3(1962), pp. 740-744.
- [4] E. Brüning and F. Gesztesy, *Continuity of wave and scattering operators with respect to interactions*, J. Math. Phys., 24(1983), pp. 1516-1528.

- [5] M. Demuth, *On scattering for Schrödinger operators with anisotropic and singular potentials*, Math. Nachr., 129(1986), pp. 185-196.
- [6] T. Kako, *Approximation of exterior Dirichlet Problems; convergence of wave and scattering operators*, Publ. RIMS, Kyoto Univ., 10(1975), pp. 359-366.
- [7] T. Kato, *Scattering theory with two Hilbert spaces*, J. Fun. Anal., 1(1967), pp. 342-369.
- [8] T. Kato, *Perturbation Theory for Linear Operators*, Springer-Verlag, Berlin Heidelberg, 1976.
- [9] T. Kato and S. T. Kuroda, *The abstract theory of scattering*, Rocky Mt. J. Math., 1(1971), pp. 127-171.
- [10] M. Reed and B. Simon, *Methods of Modern Mathematical Physics: Analysis of Operators*, Vol. 4, Academic Press, San Diego, CA, 1978.
- [11] M. Reed and B. Simon, *Methods of Modern Mathematical Physics: Scattering Theory*, Vol. 3, Academic Press, San Diego, CA, 1979.
- [12] D. R. Yafaev, *Mathematical Scattering Theory: General Theory*, Amer. Math. Soc., Providence, Rhode Island, 1992.
- [13] D. R. Yafaev, *Scattering Theory: Some Old and New Problems*, Lecture Notes in Mathematics, Vol. 1735, Springer-Verlag, Berlin/New York, 2000.
- [14] K. Yajima, *Nonrelativistic limit of the Dirac theory, scattering theory*, J. Fac. Sci. Univ. Tokyo Sect. 1A, Math., 23(1976), pp. 517-523.
- [15] O. Yamada, *The nonrelativistic limit of modified wave operators for Dirac operators*, Proc. Japan Acad., Ser. A, 59(1983), pp. 71-74.