On the Approximation of the Solution of the Schrödinger Equation by Superpositions of Stationary Solutions

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ABSTRACT. Let S be a symmetric operator with gap J. Suppose in addition that the deficiency indices of S are infinite, the Hamiltonian H is a self – adjoint extension of S and the support of the spectral measure $\mu_{f_0,H}$ of the initial state f_0 is a compact subset of J. Then there exist other self – adjoint extensions H_n of S and finite sums f_n of eigenvectors of H_n such that

$$e^{-itH_n} f_n \longrightarrow e^{-itH} f_0, \quad \text{as} \quad n \longrightarrow \infty,$$

locally uniformly in time. Upper estimates for the rate of convergence will be given.

1. Introduction

Obviously $f(t) = e^{-it\lambda} f_0$ is the solution of the Schrödinger equation

$$\begin{aligned} i\frac{d}{dt} f(t) &= Hf(t), \\ f(0) &= f_0, \end{aligned}$$

provided $Hf_0 = \lambda f_0$. Such solutions are called stationary. More generally it is trivial to solve the Schrödinger equation if the initial vector f_0 is a superposition of eigenvectors of H. Note that f_0 is a superposition of eigenvectors of the self – adjoint operator H if and only if f_0 belongs to the space $\mathcal{H}^{pp}(H)$ of vectors whose spectral measure (with respect to H) is a pure point measure.

Now let f_0 be any initial vector. Due to the continuous dependence on the initial conditions one might try to apply the following strategy in order to find the solution of the Schrödinger equation: One approximates f_0 by a sequence (f_n) in the space $\mathcal{H}^{pp}(H)$. Then the solutions $e^{-itH} f_n$ corresponding to the initial vectors f_n converge locally uniformly in t to the solution $e^{-itH} f_0$ corresponding to the initial vector f_0.

I would like to thank N. Elander and P. Kurasov for the organisation of a very pleasant and profitable conference. Financial support by the sponsors of the conference is gratefully acknowledged. I am grateful to H. Neidhardt and J. Weidmann for useful conversations. I would like to thank the anonymous referees for valuable suggestions and corrections.

As it is well known this strategy fails since the space $\mathcal{H}^{pp}(H)$ is closed and for $f_0 \notin \mathcal{H}^{pp}(H)$ the mentioned approximation is not possible.

While the above strategy to solve the Schrödinger equation fails a modification of it might be successful. One chooses self – adjoint operators H_n, $n \in \mathbb{N}$, and $f_n \in \mathcal{H}^{pp}(H_n)$ such that

$$e^{-itH_n} f_n \longrightarrow e^{-itH} f_0, \quad \text{as} \quad n \longrightarrow \infty,$$

locally uniformly in t.

We shall prove that this modified approach works if H is a self – adjoint extension of a densely defined symmetric operator S, the support of the spectral measure $\mu_{f_0,H}$ of f_0 with respect to H is a compact subset of a spectral gap J of S and for one and therefore every λ in J the dimension of the space of solutions of the eigenequation

$$S^* f = \lambda f$$

is infinite dimensional. Since J is a gap of S this last condition is equivalent to the fact that S has infinite deficiency indices.

More precisely we shall give a sequence (f_n) such that

$$e^{-itH_n} f_n \longrightarrow e^{-itH} f_0, \quad \text{as} \quad n \longrightarrow \infty,$$

locally uniformly in t and for every $n \in \mathbb{N}$ the vector f_n is the sum of finitely many, say $N(n)$, eigenvectors of another self – adjoint extension H_n of S.

We shall give upper estimates for the rate of convergence in terms of the numbers $N(n)$. Roughly speaking these estimates will depend on "how fast the spectral measure $\mu_{f_0,H}$ can be approximated by linear combinations of finitely many Dirac measures". Thus we are especially interested in the case when the measure $\mu_{f_0,H}$ is concentrated on a set with small Hausdorff – dimension. We refer to [**6**] and references therein for other results on the solution of the Schrödinger equation if the initial state has a continuous spectral measure concentrated on a set with small Hausdorff – dimension. We refer to [**5**] for the description of an important class of self – adjoint operators with continuous but zero – dimensional spectral measures and a discussion of the relation to the Anderson model.

Note that both H and H_n, $n \in \mathbb{N}$, are restrictions of the adjoint S^* of S. If S is a differential operator then this implies that both H and the H_n are described via the same differential expression but correspond to different choices of boundary conditions. Thus in many applications it is possible to approximate solutions of the Schrödinger equation by superpositions of stationary solutions via suitable variations of boundary conditions.

There is an intimate relationship between the mentioned result on the solution of the Schrödinger equation and a problem in spectral theory. K.O.

Friedrichs and M. Stone resp. M.G. Krein have shown that the open interval $J = (a, b)$ is a gap of the symmetric operator S, i.e. there exists at least one self – adjoint extension H_∞ of S without spectrum in J, if and only if

$$\begin{aligned} (Sf, f) &\geq b \parallel f \parallel^2, && \text{if} \quad -\infty = a < b < \infty, \\ \parallel \left(S - \frac{a+b}{2}\right) f \parallel &\geq \frac{b-a}{2} \parallel f \parallel, && \text{if} \quad -\infty < a < b < \infty. \end{aligned}$$

In addition to the self – adjoint extensions of S preserving the gap J there might exist other self – adjoint extensions with some spectrum inside J and one might ask about which kinds of spectra inside J these other self – adjoint extensions can have. In 1947 M.G. Krein has given the complete answer to this question in the special case when the deficiency indices of S are finite. In 2000 I have given the complete answer in the general case [**3**].

A key in the prove has been the surprising observation that even certain vectors f in the domain $D(S^*)$ of S^* which can not be represented as

$$f = \sum_{n=1}^{\infty} a_n e_n$$

for some orthonormal family of eigenvectors e_n of S^* can be approximated by finite sums of eigenvectors of S^*. This observation will also play a key role in the mentioned result on the approximative solution of the Schrödinger equation.

2. Approximate solution of the Schrödinger equation

In what follows let S be a symmetric operator in a complex Hilbert space $\mathcal{H}$. Suppose that the open interval J is a gap of S and for one and therefore every λ in J the space of solutions of the eigenequation

$$S^* f = \lambda f$$

is infinite dimensional. Let H be a self – adjoint extension of S and f_0 a vector such that the support of the spectral measure $\mu_{f_0,H}$ of f_0 with respect to H is a compact subset of J. Here $E_H(\cdot)$ denotes the projection – operator – valued measure associated to H and

$$\mu_{f,H}(\cdot) := \parallel E_H(\cdot) f \parallel^2 .$$

The following lemma will play a key role in our proof of the mentioned result on the approximative solution of the Schrödinger equation.

LEMMA 1. *Let $\lambda \in J$ and let P be the orthogonal projection onto the kernel $\mathcal{N}_\lambda$ of $S^* - \lambda$. Then for every h in the domain of the self – adjoint extension*

H of S

$$\| h - Ph \| \leq \frac{1}{dist(\lambda, \partial J)} \sup_{\lambda' \in C_h} |\lambda - \lambda'| \ \| h \|$$

where C_h denotes the support of the spectral measure $\mu_{h,H}$ of h with respect to H.

Proof: We may assume that the operator S is closed. Then the range of $S-\lambda$ is a closed subspace of $\mathcal{H}$ and we have

$$(\operatorname{ran} P)^{\perp} = \mathcal{N}_{\lambda}^{\perp} = \operatorname{ran}(S-\lambda).$$

We choose normalized vectors $e_1 \in (\operatorname{ran} P)^{\perp}$ and $e_2 \in \operatorname{ran} P$ such that

$$h = (e_1, h)\, e_1 + (e_2, h)\, e_2.$$

We have

$$\begin{aligned} \| (S^* - \lambda)\, h \|^2 &= \| (H - \lambda)\, h \|^2 \\ &= \int |\lambda' - \lambda|^2 \mu_{h,H}(d\lambda') \\ &\leq \sup_{\lambda' \in C_h} |\lambda - \lambda'|^2 \ \| h \|^2 \end{aligned}$$

since $\mu_{h,H}$ is supported by C_h.

We choose $g \in D(S)$ such that

$$e_1 = (S - \lambda)\, g.$$

We have

$$\| g \| \leq \| (S-\lambda)^{-1} \| \| e_1 \| \leq \frac{1}{\operatorname{dist}(\lambda, \partial J)}.$$

Thus

$$\begin{aligned} |(e_1, h)| &= |((S-\lambda)\, g, h)| \\ &= |(g, (S^* - \lambda)\, h)| \\ &\leq \frac{1}{\operatorname{dist}(\lambda, \partial J)} \ \| \ (S^* - \lambda)\, h \ \| \\ &\leq \frac{1}{\operatorname{dist}(\lambda, \partial J)} \sup_{\lambda' \in C_h} |\lambda - \lambda'| \ \| \ h \ \| . \end{aligned}$$

Since $h - Ph = (e_1, h)\, e_1$ the assertion is proved.

We shall use the following result from [**1**]:

LEMMA 2. *(*[**1**]*, Lemma 2.2)*

Let S be a symmetric operator in the Hilbert space $\mathcal{H}$. Suppose that the open interval J is a gap of S. Let $\mathcal{H}_0$ be a closed subspace of $\mathcal{H}$ and M a self–adjoint operator in the Hilbert space $\mathcal{H}_0$. Suppose that M is a restriction *of the adjoint S^* of S and the spectrum of M is a subset of the gap J. Then the operator*

$$S_M := S^*_{| D(S)+D(M)}, \tag{1}$$

i. e. the restriction S_M of S^* to the space

$$D(S) + D(M) := \{f + g : f \in D(S), g \in D(M)\},$$

can be represented in the form

$$S_M = M \oplus G_0 \tag{2}$$

for a unique symmetric operator G_0 in the Hilbert space $\mathcal{H}_0^\perp$. Moreover the gap J of S is also a gap of G_0.

By the following theorem, solutions of the Schrödinger equation

$$\begin{aligned} i\frac{d}{dt}f(t) &= Hf(t), \\ f(0) &= f_0, \end{aligned}$$

can be approximated by superpositions of stationary solutions corresponding to other self – adjoint extensions of S provided the support of the measure $\mu_{f_0,H}$ is a compact subset of a gap of S. The theorem gives an upper bound for the rate of convergence and the proof of the theorem a method to construct such approximate solutions.

THEOREM 3. *Suppose that the support of the spectral measure $\mu_{f_0,H}$ of f_0 with respect to H is a compact subset of the gap J of S. Let $B_1, \dots, B_N$ be pairwise disjoint Borel sets which cover the support of $\mu_{f_0,H}$. Let $\lambda_1, \dots, \lambda_N$ be points in J such that*

$$\sup_{\lambda' \in B_j} |\lambda_j - \lambda'| \le d, \quad j = 1, 2, \dots, N,$$

for some constant d. Let D be the distance of the set $\{\lambda_1, \dots, \lambda_N\}$ to the boundary of J. Then there exist an orthonormal family $(e_j)_{j=1}^N$ and a self – adjoint extension $\tilde{H}$ of S such that
(i) $\tilde{H}e_j = \lambda_j e_j, \quad j = 1, 2, \dots, N$, and
(ii) for

$$f := \sum_{j=1}^N \alpha_j e_j, \quad \alpha_j := \sqrt{\mu_{f_0,H}(B_j)}, \ j = 1, 2, \dots, N, \tag{3}$$

the following estimate holds for all $t \in \mathbb{R}$:

$$\| e^{-it\tilde{H}} f - e^{-itH} f_0 \| \le \sqrt{N}\, d \, \| f_0 \| \, (\frac{\sqrt{2}}{D} + |\, t \,|). \tag{4}$$

Proof: We may assume that $E_H(B_j)f_0 \neq 0$ for all j. Then the vectors

$$\tilde{e}_j := \frac{E_H(B_j)f_0}{\| E_H(B_j)f_0 \|}$$

form an orthonormal system and

$$f_0 = \sum_{j=1}^{N} \alpha_j \tilde{e}_j. \tag{5}$$

We shall apply Lemma 2 several times. First set

$$\mathcal{H}_0 := \operatorname{ran} E_H(B_2 \cup \ldots \cup B_N).$$

Without loss of generality we may assume that $B_1 \cup \ldots \cup B_N$ is a relatively compact subset of J. Then the space $\mathcal{H}_0$ is contained in the domain $D(H)$ of H,

$$M := H_{|\mathcal{H}_0}$$

is a self – adjoint operator in $\mathcal{H}_0$, $M \subset S^*$ and the spectrum of M is contained in J. By Lemma 2,

$$S \subset M \oplus G_0$$

for some symmetric operator G_0 in $\mathcal{H}_0^\perp$ and the gap J of S is also a gap of G_0.

Apparently

$$H = M \oplus G$$

for some self – adjoint extension G of G_0. It follows that $\tilde{e}_1 \in D(G)$ and $\mu_{\tilde{e}_1,G} = \mu_{\tilde{e}_1,H}$. Let $P : \mathcal{H}_0^\perp \longrightarrow \ker(G_0^* - \lambda_1)$ be the orthogonal projection onto the kernel of $G_0^* - \lambda_1$. By Lemma 1,

$$\| \tilde{e}_1 - P\tilde{e}_1 \| \leq \frac{d}{D}.$$

Thus there exists a normalized vector $e_1 \in \ker(G_0^* - \lambda_1)$ such that

$$\| e_1 - \tilde{e}_1 \| \leq \sqrt{2}\,\frac{d}{D}.$$

Note that $G_0^* \subset S^*$. Thus $S^* e_1 = \lambda_1 e_1$. Moreover, by construction, e_1 is orthogonal to the space $\operatorname{ran} E_H(B_2 \cup \ldots \cup B_N)$.

Now we change the notation. We set

$$\mathcal{H}_0 := \operatorname{span}\{e_1\} + \operatorname{ran} E_H(B_3 \cup \ldots \cup B_N).$$

Obviously $\mathcal{H}_0 \subset D(S^*)$ and $M := S^*_{|\mathcal{H}_0}$ is a self – adjoint operator in $\mathcal{H}_0$, $M \subset S^*$ and the spectrum of M is contained in J. By Lemma 2,

$$S \subset M \oplus G_0$$

for some symmetric operator G_0 in $\mathcal{H}_0^\perp$ and J is also a gap of G_0.

Apparently G_0 has a self – adjoint extension G such that $\mathrm{ran} E_H(B_2) \subset D(G)$ and $Gh = Hh$ for all $h \in \mathrm{ran} E_H(B_2)$. In particular, $\mu_{\tilde{e}_2,G} = \mu_{\tilde{e}_2,H}$. By applying Lemma 1 in the same way as before, we can show that there exists a normalized vector e_2 in the kernel of $S^* - \lambda_2$ such that

$$\| e_2 - \tilde{e}_2 \| \leq \sqrt{2}\,\frac{d}{D}$$

and e_2 is orthogonal to span$\{e_1\}$+ ran $E_H(B_3 \cup \ldots \cup B_N)$.

Proceeding in this way, we get an orthonormal system $\{e_j\}_{j=1}^N$ such that

$$S^* e_j = \lambda_j e_j, \quad j = 1, \ldots, N,$$

and

$$\| e_j - \tilde{e}_j \| \leq \sqrt{2}\,\frac{d}{D}, \quad j = 1, \ldots, N. \tag{6}$$

Since $S^* e_j = \lambda_j e_j$ and the e_j are pairwise orthogonal, there exists a self – adjoint extension $\tilde{H}$ of S such that $\tilde{H} e_j = \lambda_j e_j$ for all j, cf., e.g., [**1**]. Since the measure $\mu_{\tilde{e}_j,H}$ is concentrated on B_j

$$\| e^{-itH}\tilde{e}_j - e^{-it\lambda_j}\tilde{e}_j \|^2 = \int | e^{-it\lambda} - e^{-it\lambda_j} |^2 \, \mu_{\tilde{e}_j,H}(d\lambda) \;\leq\; d^2\, t^2. \tag{7}$$

By (6) and (7),

$$\| e^{-itH}\tilde{e}_j - e^{-it\lambda_j} e_j \| \leq d\,(\frac{\sqrt{2}}{D} + |\,t\,|). \tag{8}$$

By (3), (5) and (8),

$$\| e^{-itH} f_0 - e^{-it\tilde{H}} f \|^2 \leq \left(\sum_{j=1}^N \alpha_j^2 \right) \sum_{j=1}^N d^2\,(\frac{\sqrt{2}}{D} + |\,t\,|)^2$$

and, by (3), the theorem is proved.

Remark 4. Generalizing the construction of the Cantor measure one gets for arbitrarily small $c > 0$ examples of continuous measures μ_c such that for each $n \in \mathbb{N}$ one can choose $N = 2^n$ and $d = c^n$ in the above theorem (with $\mu_{f_0,H} = \mu_c$). For c sufficiently small one gets a good appoximation of the solution of the Schrödinger equation by superpositions of stationary solutions. Obviously, the smaller c is, the smaller is the Hausdorff dimensionality of the measure μ_c. Recently a lot of work has been done in order to investigate Hamiltonians which have continuous spectral measures concentrated on sets of small Hausdorff dimension (often even Hausdorff dimension 0), cf. [**5**], [**6**],[**8**] and references given therein.

Remark 5. In the above proof we have used the fact that the support of the spectral measure $\mu_{f_0,H}$ is contained in a gap of the symmetric operator S. It might be possible to weaken this hypothesis but one cannot completely omit it. E.g. let $\mathcal{H} = L^2(\mathbb{R}^d)$, $d > 1$. Let Γ be a closed subset of $\mathbb{R}$ such that Γ has Lebesgue measure zero and its complement $\mathbb{R}^d \setminus \Gamma$ is connected. Define the symmetric operator S in $L^2(\mathbb{R}^d)$ as follows:

$$D(S) := C_0^\infty(\mathbb{R}^d \setminus \Gamma), \quad Sf := -\Delta f, \quad f \in D(S).$$

It is a well known consequence of Kato's inequality that the adjoint S^* of S does not have nonnegative eigenvalues. Thus the method described in the proof of the above theorem cannot be applied if the support of the spectral measure $\mu_{f_0,H}$ contains positive real numbers. Note that the operator S has infinite deficiency indices if the set Γ is sufficiently big, e.g. if Γ has infinitely many points and its Hausdorff dimension is larger than $d-4$.

3. A result in Inverse Spectral Theory

Let A be a self – adjoint operator in a Hilbert space $\mathcal{H}$. It easily follows from the spectral theorem, that for every Borel set $B \subset \mathbb{R}$ we have

$$\mathcal{H} = \operatorname{ran} E_A(B) \oplus \operatorname{ran} E_A(\mathbb{R} \setminus B)$$

and there exist unique self – adjoint operators A_B in $\operatorname{ran}(E_A(B))$ and $A_{\mathbb{R}\setminus B}$ in $\operatorname{ran}(E_A(\mathbb{R} \setminus B))$ such that

$$A = A_B \oplus A_{\mathbb{R}\setminus B}.$$

Inside B the operators A and A_B have the same eigenvalues and for every eigenvalue $\lambda \in B$ of A the multiplicity $\operatorname{mult}(\lambda, A)$ of λ as an eigenvalue of A equals $\operatorname{mult}(\lambda, A_B)$.

For open sets J we have in addition that

$$\mu_{f,A}(B) = \mu_{f,A_J}(B)$$

for every Borel set $B \subset J$ and every $f \in \mathcal{H}$. In particular, we have

$$\sigma(A) \cap J = \sigma(A_J) \cap J,\ \sigma_{ac}(A) \cap J = \sigma_{ac}(A_J) \cap J,\ \sigma_{sc}(A) \cap J = \sigma_{sc}(A_J) \cap J,$$

and for every $\alpha \in [0, 1]$

$$\sigma_\alpha(A) \cap J = \sigma_\alpha(A_J) \cap J.$$

Here σ, σ_{ac}, σ_{sc} and σ_α denote the spectrum, the absolutely continuous spectrum, the singular continuous spectrum and the α – dimensional spectrum (cf. [**5**]), respectively.

Let S be a symmetric operator with deficiency indices (n, n). Suppose that the open interval J is a gap of S. It easily follows from von Neumann's extension theory that

$$\dim \operatorname{ran} E_A(J) \leq n$$

for every self – adjoint extension A of S; "dim" means dimension in the sense of Hilbert space theory, i.e. the cardinality of any orthonormal base. Up to unitary equivalence this is the only restriction for the operators A_J, A being a self – adjoint extension of S:

THEOREM 6. *([**3**], Theorem 1) Let S be a symmetric operator in the Hilbert space $\mathcal{H}$. Suppose that the open interval J is a gap of S and the deficiency indices of S equal (n, n). Let A^{aux} be any self – adjoint operator such that*

$$\dim \operatorname{ran} E_{A^{aux}}(J) \leq n.$$

Then there exists a self – adjoint extension A of S such that

$$A_J \simeq A_J^{aux},$$

i.e. $A_J = U^{-1} A_J^{aux} U$ for some unitary operator U.

REMARK 7. In particular, A and A^{aux} have the same eigenvalues inside J and for every eigenvalue $\lambda \in J$ of A we have

$$\operatorname{mult}(\lambda, A) = \operatorname{mult}(\lambda, A^{aux}).$$

Moreover

$$\sigma(A) \cap J = \sigma(A^{aux}) \cap J, \ \sigma_{ac}(A) \cap J = \sigma_{ac}(A^{aux}) \cap J, \ \sigma_{sc}(A) \cap J = \sigma_{sc}(A^{aux}) \cap J,$$

and for every $\alpha \in [0, 1]$

$$\sigma_\alpha(A) \cap J = \sigma_\alpha(A^{aux}) \cap J.$$

REMARK 8. The theorem had been formulated as a conjecture in [**1**].

REMARK 9. In the special case when the deficiency index n is finite the theorem has already been proved by M.G.Krein ([**7**]).

Let S be a symmetric operator with infinite deficiency indices and J a gap of S. Let μ be a finite measure with compact support inside J. Let A^{aux} be the operator of multiplication by the independent variable in the Hilbert space $L^2(\mathbb{R}, \mu)$. Then $A_J^{aux} = A^{aux}$ and, by the above theorem, there exist a self – adjoint extension A of S and a unitary transformation U such that $A_J = U^{-1} A^{aux} U$.

Let $f := U^{-1} 1$, 1 being (the μ – equivalence class of) the function which equals 1 everywhere. Since the support of μ is compact and A a restriction of

S^*, the vector f belongs to the domain of S^{*k} for every k and

$$(S^{*k}f, S^{*j}f) = \int \lambda^{k+j}\mu(d\lambda), \quad k, j = 0, 1, 2, \dots \tag{9}$$

One of the key problems in the proof of the above theorem has been to show the existence of a vector f satisfying these equations (9). This could be done by a construction which is similar to the one in the proof of Theorem 3 but more complicated. Once this problem was solved the proof of the theorem could be completed by applying ideas and results from [**1**], [**2**] and [**4**], cf. [**3**] for the details.

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