Thesis for the Degree of Master of science (20p)

ON EIGENVALUES OF *SCHRÖDINGER* OPERATORS WITH δ-POTENTIALS

Kiumbiro Shirley Murigu
International Masters' Programme in Engineering Mathematics
Department of Mathematics
Chalmers University of Technology and *Göteborg* university
SE-412 96 *Göteborg* , Sweden

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Abstract

In this paper, our main aim is to model both a formulative and elaborate algorithm to approximately get the number of negative eigenvalues of a 1 dimensional *schrödinger* operator. I will hence compare the formulative(theoretical) and the elaborate(computer program) algorithms and briefly explore the possibilities and limitations of such an approach. This research, among other uses, helps to determine the behaviour of atoms and is an interesting study in Quantum Mechanics.

Contents

List of Figures

1 Introduction

In the mathematically rigorous formulation developed by Paul Dirac and John von Neumann, the possible states of a quantum mechanical system are represented by unit vectors (called state vectors) residing in a complex separable Hilbert space(called the state space.) The exact nature of the Hilbert space is dependent on the system; for example, the state space for position and momentum states is the space of square-integrable functions, while the state space for the spin of a single electron is just the product of two complex planes.

The time evolution of a quantum state is described by the Schrödinger equation, in which the Hamiltonian, the operator corresponding to the total energy of the system, generates the time evolution. Each observable is represented by a densely-defined Hermitian linear operator acting on the state space. Each eigenstate of an observable corresponds to an eigenvector of the operator, and the associated eigenvalue corresponds to the value of the observable in that eigenstate. If the operator's spectrum is discrete, the observable can only attain those discrete eigenvalues.

During a measurement, the probability that a system collapses to each eigenstate is given by the absolute square of the inner product between the eigenstate vector and the state vector just before the measurement. The possible results of a measurement are the eigenvalues of the operator - which explains the choice of Hermitian operators - all their eigenvalues are real.

This topic is useful in spectroscopy, where the particle-in-a-box model of quantum mechanics is placed in a context of light absorption by materials. It ties together simple ideas such as the color of material being the complement of that absorbed, with more sophisticated ideas relating to which molecular motions give rise to absorption in different parts of the spectrum. It is also useful in electronics, particularly in the electronic structure and resistivity of copper and copper alloys which can be useful in modern electronics although it farther requires the implementation of the Quantum Monte-Carlo method. Unfortunately, this study usually doesn't give exact results as one can not derive closed formulas for the quantities. However, we are not going to go as far as spectroscopy and electronics is concerned as this is more complex than our topic.

Our main goal is to get the eigenvalues of the schrödinger operator with a delta potential. In order to get an approximate computation of eigenvalues of this 1-D schrödinger operator $-\frac{d^2}{dx^2} + V$, it is sufficient to compute eigenvalues of suitably chosen operators of the form $-\frac{d^2}{dx^2} + \mu$, where μ is a finite linear combination of Dirac measures cf. section 3.

Operators of this form have been discussed in detail in cf.[9]. In [9], a mapping M with values in the set of N-by-N matrices, has been given such that E is an eigenvalue of $-\frac{d^2}{dx^2}+\mu$ if and only if detM(E) = 0. Here N is the number of Dirac measures occuring in the representation of μ. To achieve a good approximation for the eigenvalues of $-\frac{d^2}{dx^2}+V$, one has to choose a large N. For the computation of the zeros of detM(E) one needs about N^3computations. This is a very long method and is not easy to compute.

Therefore, in this thesis, we shall present a **new** method to compute the eigenvalues of $-\frac{d^2}{dx^2}+\mu$ where the number of computations only grow linearly in N.

With this foundational explanation of the motivational background, we are now ready for a reminder of the basic definitions and remarks necessary for this paper.

2 General Theory

Here, we collect various known definitions, remarks and theorems from cf.[2]

2.1 Basic Definitions And Remarks

Let $\mathcal{H}$be the Hilbert Space over $\mathbb{C}$ with scalar product $\langle \cdot, \cdot \rangle$, then:

Definition 2.2 Let $\mathcal{H}_o$ be a linear subspace of $\mathcal{H}$
Let $H : \mathcal{H}_o \mapsto \mathcal{H}$ be linear.
Then H is called an operator in $\mathcal{H}$, $\mathcal{H}_o$ is called the domain of H ie, D(H).

Definition 2.3 let H be an operator in $\mathcal{H}$ and assume that D(H) is dense in $\mathcal{H}$.
Put
$D(H^*) = \{f \in \mathcal{H} : \exists \quad f^* \in \mathcal{H} \quad \forall g \in D(H) : \langle f^*, g \rangle = \langle f, Hg \rangle\}$
$H^* f = f^*; \quad f \in D(H^*)$.
Then H^* is called the adjoint of H.

Definition 2.4 H is selfadjoint if and only if D(H) is dense in $\mathcal{H}$ and $H = H^*$.

Remark 2.5 If H is selfadjoint then H is symmetric :
$\langle Hf, g \rangle = \langle f, Hg \rangle$ where $f, g \in$ D(H).
Note that selfadjointness implies symmetry but not viceversa.

Definition 2.6 Let H be an operator in $\mathcal{H}$, and z $\in \mathbb{C}$.
z belongs to the resolvent set ρ(H) if and only if
(H-zI) : D(H) $\mapsto \mathcal{H}$ is bijective and
$(H - zI)^{-1}$ is bounded.
z belongs to the spectrum $\sigma(H)$ of H if and only if z $\in \mathbb{C} \setminus \rho(H)$.

Remark 2.7

1. $\sigma(H)$ is closed.

2. If H is selfadjoint, then $\sigma(H) \subset \mathbb{R}$.

3. In quantum mechanics, the Hamiltonian H
   of a system is a selfadjoint operator.

   - The probability that the energy of the
     quantum mechanical system with Hamiltonian H belongs to $\mathbb{R} \cap \rho(H)$ is equal to 1 .
     In other words, "every measurement of the energy gives a value E in $\sigma(H)$ ".

- "The energy can have any value inside $\sigma(H)$".
  More precisely: Let E be an element of σ(H),$\epsilon > 0$. Then the system has a state f such that with probability one, the value of the energy of the system, in state f, belongs to $]E-\epsilon, E+\epsilon[$.

4. $\sigma(H)$ contains the set of eigenvalues of H.

Definition 2.8 Let H be selfadjoint.
E belongs to the discrete spectrum σ_d(H) of H if and only if
E is an eigenvalue of H with finite multiplicity and
is also an isolated point of the spectrum of H.
σ(H)$\backslash\sigma_d$(H) is called the essential spectrum, denoted by σ_{ess}(H).

2.2 *Schrödinger* Operators

In what follows:
$\mathcal{H} = L^2(\mathbb{R}), \langle f, g\rangle = \int_{\mathbb{R}} \overline{f(x)} g(x) dx$.
NOTE: Often one uses another not equivalent definition, i.e
$\langle f, g\rangle = \int_{\mathbb{R}} f(x)\overline{g(x)}dx$.
$V : \mathbb{R} \to \mathbb{R}$ such that $\int_{\mathbb{R}} |V(x)|dx < \infty$.

Definition 2.9 The operator $-\Delta + V$ in $L^2(\mathbb{R})$ is defined as follows:
$D(-\Delta + V) = \{f \epsilon L^2(\mathbb{R}) : f \epsilon \mathbb{C}^1(\mathbb{R}), \quad f'$absolutely continuous,
$f, f', -f'' + V \quad f \epsilon L^2(\mathbb{R})\}$.
$(-\Delta + V)f = -f'' + Vf, f \in D(-\Delta + V)$.
$-\Delta + V$ is referred to as "*schrödinger* operator (one dimensional) "
Then the following is known :

Theorem 2.10 a) $-\Delta + V$ is selfadjoint.
b)$\sigma_{ess}(-\Delta + V) = [0, \infty[$.
c) The number $N_-(V)$ of negative eigevalues of $-\Delta + V$, where every eigenvalue is counted as many times as its multiplicity, has the following upper bound :
$N_-(V) \leq 1 + \frac{\frac{1}{2}\int_{\mathbb{R}}\int_{\mathbb{R}} |(x-y)|V_-(x)V_-(y)dxdy}{\int_{\mathbb{R}} V_-(x)dx}, \quad V = V_+ - V_- \quad$ and $\quad V_\pm \geq 0$.
d) If $\int_{\mathbb{R}} V(x)dx < 0, \quad$ then there exists a negative eigenvalue.
The facts above are well known (cf.[3] for a), b) and d). c),has been obtained by cf.[7], cf.[8], and cf.[4]Theorem 3.5, generalised)

Remark 2.11 1. $-\Delta + V$ is the Hamiltonian for a one dimensional quantum mechanical particle interacting with the potential V : $\mathbb{R} \to \mathbb{R}$.

2. The state of the quantum mechanical system, at a fixed time t,
   is described by a function f: $\mathbb{R} \to \mathbb{C}$.
   The interpretation of f is as follows:

- $\int_a^b |f(x)|^2 dx$ is equal to the probability that the particle is in $[a, b]$ ("position").

- $\int_c^d |\hat{f}(p)|^2 dp =$ probability that the momentum of the particle is in $[c, d]$.

3. f is a bound state i.e,
   If the state of the system at time t, t=0, equals f,
   then for every $\epsilon > 0$ there exists a compact set $\mathbb{C} \subset \mathbb{R}$, such that for every $t \in \mathbb{R}$, the following holds:
   The probability that the particle is outside $\mathbb{C}$ at time t is less than ϵ.

4. f is a bound state if and only if f is a superposition of eigenfunctions of H.

5. If $(-\Delta + V)f = Ef$ and $\|f\| = 1$
   then every measurement of the energy of the system in the state gives the value E (with probability 1, "sharp measurement").
   PS: If one gets the same value E at every measurement,
   then E is an eigenvalue.

6. Often one cannot compute the eigenvalue of $-\Delta + V$ explicitly.

We refer to cf.[5], chapter 6, and references given therein for a detailed discussion of the assertion in this remark.

3 Aim Of The Thesis

Now that we understand most of the mathematical terminology
that we will use in the thesis, we get to briefly explain our goal.
This is to derive, approximately, the
negative eigenvalues of the *schrödinger* operator .
This in essence is computing the number E, given $V : \mathbb{R} \to \mathbb{R}$,
such that $-u'' + Vu = Eu$ has a nontrivial, square integrable[1] solution.
These numbers, E, are the energy levels of the
quantum mechanical system with Hamiltonian
$H = -\frac{d^2}{dx^2} + V$.
But we know it is almost impossible to compute this explicitly.
We thus work with an approximate operator called the H_{app}.

- *Definition of* H_{app}
  We begin by stating that the domain of H_{app} is given by :
  $D(H_{app}) = \{f \in L^2(\mathbb{R}) : f$ is absolutely continuous [2], $f' \in L^2(\mathbb{R})$,
  f' is absolutely continuous on $\mathbb{R} \setminus \{x_1, x_2, ..., x_N\}$,
  $\int_{-\infty}^{x_1} |f''(x)|^2 dx + \int_{x_1}^{x_2} |f''(x)|^2 dx + ... + \int_{x_{N-1}}^{x_N} |f''(x)|^2 dx + \int_{x_N}^{\infty} |f''(x)|^2 dx < \infty$,
  $f'(x_k+) - f'(x_k-) = M_k f(x_k)\}$.
  $H_{app} f(x) = -f''(x)$ a.e[3] on $\mathbb{R} \setminus \{x_1, x_2, ..., x_N\}$.
  We know that,
  $H_{app} f = -\frac{d^2}{dx^2} + \sum_{k=1}^{N} M_k \delta_{x_k} f$ in the distributional sense
  and so for this reason H_{app} is also denoted by $-\frac{d^2}{dx^2} + \sum_{k=1}^{N} M_k \delta_{x_k}$
  .

3.1 The Mathematical Structure Of Quantum Mechanics

We had mentioned earlier that every system in quantum mechanics
is described by a selfadjoint operator, the Hamiltonian H, in a hilbert space $\mathcal{H}$.
Now, consider just one particle on the real line. Then $\mathcal{H} = L^2(\mathbb{R})$.
In Quantum Mechanics one does not know the position of the particle
but can give the probability $P(a, b)$ that the particle is inside
(a, b) for all $-\infty \leq a < b \leq +\infty$.
Here the state $f : \mathbb{R} \to \mathbb{C}$ refers to :
$P(a, b) = \int_a^b |f(x)|^2 dx$
$1 = P(-\infty, \infty) = \int_{-\infty}^{\infty} |f(x)|^2 dx = 1$

Now, if f = g a.e, then
$\int_a^b |f(x)|^2 dx = \int_a^b |g(x)|^2 dx$ for all a, b.
Infact, f and g describe the same physically. In addition,

[1] $\int_{-\infty}^{\infty} |u(x)|^2 dx < \infty$

[2] $g : \mathbb{R} \to \mathbb{R}$ is absolutely continuous,if there exists $h : \mathbb{R} \to \mathbb{R}$ integrable over bounded intervals such that $g(x) = \int_a^x h(t)dt$

[3] almost everywhere

$\langle f, Hf\rangle = \int_{-\infty}^{\infty} \overline{f(x)} Hf(x)dx$ equals the mean value for the energy.
In particular, if $H = -\frac{d^2}{dx^2} + V$, then
$\langle f, Hf\rangle = \int_{-\infty}^{\infty} |f'(x)|^2 dx + \int_{-\infty}^{\infty} |f(x)|^2 V dx$.
Integrating by parts we get:

$$\langle f, H_{app} f\rangle = \int_{-\infty}^{\infty} |f'(x)|^2 dx + \sum_{k=1}^{N} M_k |f(x_k)|^2 \tag{1}$$

Since

$$\int_{-\infty}^{\infty} |f(x)|^2 V dx \approx \sum_{k=1}^{N} M_k |f(x_k)|^2 \tag{2}$$

for suitably chosen $M_1, M_2, ..., M_N$, $x_1, x_2, ..., x_N$ (consider the riemann sum),
this leads to the idea that $H = -\frac{d^2}{dx^2} + V$
can be approximated by operators of the form

$$H_{app} = -\frac{d^2}{dx^2} + \sum_{k=1}^{N} M_k \delta_{x_k}. \tag{3}$$

In fact, this was proven in cf.[1]. It states that:

- Theorem([1], theorem 3): Let $\mu_n, n \in N$, and μ be finite radon measures on $\mathbb{R}$. Supposse that $\mu_n \to \mu$ weakly. Then the operators $-\Delta + \mu_n$ converge to the operator $-\Delta + \mu$ in the norm resolvent sense.

3.2 Integrating The Theorem Proved By Brasche, Figari and Teta

It follows from the mentioned results by Brasche, Figari and Teta and by cf.[6], theorem viii.23, that for given V, one can choose families
$(x_{1(n)}, x_{2(n)}, ..., x_{N(n)})_{n=1}^{\infty}$ and
$(M_{1(n)}, M_{2(n)}, ..., M_{N(n)})_{n=1}^{\infty}$ such that,

$$E_j(-\frac{d^2}{dx^2} + V) = lim_{n\to\infty} E_j(-\frac{d^2}{dx^2} + \sum_{k=1}^{N(n)} M_{k(n)} \delta_{x_{k(n)}}). \tag{4}$$

where, $E_1(H) \leq E_2(H) \leq ..... \leq E_l(H) \leq 0$
are the negative eigenvalues of H.
Note that for every $V \in L^1(\mathbb{R})$ their exists measures μ_n of the form
$\mu_n = \sum_{k=1}^{N(n)} M_{k(n)} \delta_{x_k(n)}$ converging weakly to $V dx$.

4 Theoretical Problem

One may wonder why we dont use the positive eigenvalues.
Thus, in this section we want to show why we
choose only the negative eigenvalues.We have seen
that the approximate *schrödinger* operator is of the form:

$$H_{app} = -\frac{d^2}{dx^2} + \sum_{k=1}^{N} M_k \delta_{x_k} \tag{5}$$

for numbers $-\infty < x_1 < x_2 < ... < x_N < \infty$
and$M_1, M_2, ..., M_N$ given.
One can see from (5) that this is a *schrödinger* operator
where the potential is a finite Radon measure in $\mathbb{R}^1$.
We want to determine, for fixed E, the functions u, from $\mathbb{R} \to \mathbb{R}$, satisfying:

1. $-u''(x) = Eu(x)$ for $x \neq \{x_1, x_2, ..., x_N\}$.
2. u is continuous on $\mathbb{R}$.
3. $u'(x_k+) - u'(x_k-) = M_k u(x_k)$ for k=1,2,.....,N.
4. $\int_{-\infty}^{\infty} |u(x)|^2 dx < \infty$.

Note that E is an eigenvalue of H_{app} if and only if
u(satisfying 1-4) can be chosen such that u is not equal to zero.
We start off by doing a theoretical investigation
with very trivial mathematics so as to clearly understand.

Determine the solution with:

1. $-u''(x) = Eu(x)$ on $(-\infty, x_1)$.
   Working this out we get that the solution can only be
   $u(x) = C_0^+ e^{\sqrt{-E}x} + C_0^- e^{-\sqrt{-E}x}$
   which is the general solution with $C_0^{\pm}$ an element of the complex number set arbitrary, provided $E \neq 0$.

2. Now consider $\int_{-\infty}^{\infty} |u(x)|^2 dx < \infty$.
   We will determine the solution by varying E from $-\infty$ to $+\infty$.

   - when $E < 0$
     In this case $\sqrt{-E}$ is greater than 0 and therefore
     $e^{\sqrt{-E}x} \to 0$ as $x \to -\infty$ and $e^{-\sqrt{-E}x} \to \infty$ as $x \to \infty$.
     Thus we get that $u(x) = C_0^+ e^{\sqrt{-E}x}$ is the general solution satisfying
     $\int_{-\infty}^{x_1} |u(x)|^2 dx < \infty$, with $E < 0$.

4.1 Intervals

We will now determine the integral on each unique interval:
$(x_1, x_2), (x_2, x_3), ..., (x_n, \infty)$.
As earlier noted, the general solution of $-u''(x) = Eu(x)$ on (x_k, x_{k+1}) is given by
$u(x) = C_k^+ e^{\sqrt{-Ex}} + C_k^- e^{-\sqrt{-Ex}}$,
for k = 1,2,...., N-1, N where $x_{N+1} = \infty$.
We may put $C_0^+ = 1$.

4.1.1 First interval: connecting $(-\infty, x_1)$ and (x_1, x_2)

Connecting both intervals $(-\infty, x_1)$ and (x_1, x_2), we get that $u(x)$ should be continuous on $(-\infty, x_2)$.
$u(x_1-) = e^{\sqrt{-Ex_1}}$
$u(x_1+) = C_1^+ e^{\sqrt{-Ex_1}} + C_1^- e^{-\sqrt{-Ex_1}}$
which finally gives,
$C_1^+ e^{\sqrt{-Ex_1}} + C_1^- e^{-\sqrt{-Ex_1}} = e^{\sqrt{-Ex_1}}$
We also know that
$u'(x_1+) - u'(x_1-) = M_1 u(x_1)$
$u'(x_1-) = \sqrt{-E} e^{\sqrt{-Ex_1}}$
and,
$u'(x_1+) = \sqrt{-E} C_1^+ e^{\sqrt{-Ex_1}} - \sqrt{-E} C_1^- e^{-\sqrt{-}Ex_1}$
which finally gives,
$\sqrt{-E} C_1^+ e^{\sqrt{-Ex_1}} - \sqrt{-E} C_1^- e^{-\sqrt{-Ex_1}} - \sqrt{-E} e^{\sqrt{-}Ex_1} = M_1 e^{\sqrt{-Ex_1}}$.
Rewriting this in matrix form gives us

$$\begin{bmatrix} e^{\sqrt{-Ex_1}} & e^{-\sqrt{-Ex_1}} \\ \sqrt{-E} e^{\sqrt{-Ex_1}} & -\sqrt{-E} e^{-\sqrt{-Ex_1}} \end{bmatrix} \times \begin{bmatrix} C_1^+ \\ C_1^- \end{bmatrix} = \begin{bmatrix} e^{\sqrt{-Ex_1}} \\ M_1 e^{\sqrt{-Ex_1}} + \sqrt{-E} e^{\sqrt{-Ex_1}} \end{bmatrix}$$

4.1.2 Second interval: connecting (x_1, x_2) and (x_2, x_3)

Now we consider the interval (x_2, x_3).
The general solution for $-u''(x) = Eu(x)$ on (x_2, x_3) is,
$u(x) = C_2^+ e^{\sqrt{-Ex}} + C_2^- e^{-\sqrt{-Ex}}$.
Connecting the intervals (x_1, x_2) and (x_2, x_3) gives us:
$u(x_2, -) = C_1^+ e^{\sqrt{-Ex_2}} + C_1^- e^{-\sqrt{-Ex_2}}$
$u(x_2, +) = C_2^+ e^{\sqrt{-Ex_2}} + C_2^- e^{-\sqrt{-Ex_2}}$.
which finally gives,
$C_2^+ e^{\sqrt{-Ex_2}} + C_2^- e^{-\sqrt{-Ex_2}} = C_1^+ e^{\sqrt{-Ex_2}} + C_1^- e^{-\sqrt{-Ex_2}}$.
We also know that
$u'(x_2+) - u'(x_2-) = M_2 u(x_2)$
$u'(x_2-) = C_1^+ \sqrt{-E} e^{\sqrt{-Ex_2}} - C_1^- e^{-\sqrt{-Ex_2}}$
$u'(x_2+) = C_2^+ \sqrt{-E} e^{\sqrt{-Ex_2}} - C_2^- \sqrt{-E} e^{-\sqrt{-Ex_2}}$
which finally gives us,

$C_2^+\sqrt{-E}e^{\sqrt{-Ex_2}} - C_2^-\sqrt{-E}e^{-\sqrt{-Ex_2}} - C_1^+\sqrt{-E}e^{\sqrt{-Ex_2}} - C_1^-e^{-\sqrt{-Ex_2}}$
$= M_2(C_1^+e^{\sqrt{-Ex_2}} + C_1^-e^{-\sqrt{-Ex_2}})$
Rewriting this in matrix form gives us

$$\begin{bmatrix} e^{\sqrt{-Ex_2}} & e^{-\sqrt{-Ex_2}} \\ \sqrt{-E}e^{\sqrt{-Ex_2}} & -\sqrt{-E}e^{-\sqrt{-Ex_2}} \end{bmatrix} \times \begin{bmatrix} C_2^+ \\ C_2^- \end{bmatrix}$$

$$= \begin{bmatrix} C_1^+e^{\sqrt{-Ex_2}} + C_1^-e^{-\sqrt{-Ex_2}} \\ M_2(C_1^+e^{\sqrt{-Ex_2}} + C_1^-e^{-\sqrt{-Ex_2}}) - C_1^-e^{-\sqrt{-Ex_2}} + C_1^+\sqrt{-E}e^{\sqrt{-Ex_2}} \end{bmatrix}$$

4.1.3 Third interval: connecting (x_2, x_3) and (x_3, x_4)

Now we consider the interval (x_3, x_4).
The general solution for $-u''(x) = Eu(x)$ on (x_3, x_4) is,
$u(x) = C_3^+e^{\sqrt{-Ex}} + C_3^-e^{-\sqrt{-Ex}}$
Connecting the intervals(x_2, x_3) and (x_3, x_4) gives us:
$u(x_3, -) = C_2^+e^{\sqrt{-Ex_3}} + C_2^-e^{-\sqrt{-Ex_3}}$
$u(x_3, +) = C_3^+e^{\sqrt{-Ex_3}} + C_3^-e^{-\sqrt{-Ex_3}}$.
which finally gives,
$C_3^+e^{\sqrt{-Ex_3}} + C_3^-e^{-\sqrt{-Ex_3}} = C_2^+e^{\sqrt{-Ex_3}} + C_2^-e^{-\sqrt{-Ex_3}}$.
We also know that
$u'(x_3+) - u'(x_3-) = M_3u(x_3)$.
$u'(x_3-) = C_2^+\sqrt{-E}e^{\sqrt{-Ex_3}} - C_2^-e^{-\sqrt{-Ex_3}}$
$u'(x_3+) = C_3^+\sqrt{-E}e^{\sqrt{-Ex_3}} - C_3^-\sqrt{-E}e^{-\sqrt{-Ex_3}}$
which finally gives us,
$C_3^+\sqrt{-E}e^{\sqrt{-Ex_3}} - C_3^-\sqrt{-E}e^{-\sqrt{-Ex_3}} - C_2^+\sqrt{-E}e^{\sqrt{-Ex_3}}$
$-C_2^-e^{-\sqrt{-Ex_3}} = M_3(C_2^+e^{\sqrt{-Ex_3}} + C_2^-e^{-\sqrt{-Ex_3}})$
Rewriting this in matrix form gives us

$$\begin{bmatrix} e^{\sqrt{-Ex_3}} & e^{-\sqrt{-Ex_3}} \\ \sqrt{-E}e^{\sqrt{-Ex_3}} & -\sqrt{-E}e^{-\sqrt{-Ex_3}} \end{bmatrix} \times \begin{bmatrix} C_3^+ \\ C_3^- \end{bmatrix}$$

$$= \begin{bmatrix} C_2^+e^{\sqrt{-Ex_3}} + C_2^-e^{-\sqrt{-Ex_3}} \\ M_3(C_2^+e^{\sqrt{-Ex_3}} + C_2^-e^{-\sqrt{-Ex_3}} - C_2^-e^{-\sqrt{-Ex_3}} + C_2^+\sqrt{-E}e^{\sqrt{-Ex_3}} \end{bmatrix}$$

We continue in this way and arrive eventually at the,

4.1.4 Last interval

As we continue from interval to interval, we realise the recurrence of the matrices and can thus predict the final interval (x_N, ∞) to be:

$$\begin{bmatrix} e^{\sqrt{-Ex_N}} & e^{-\sqrt{-Ex_N}} \\ \sqrt{-E}e^{\sqrt{-Ex_N}} & -\sqrt{-E}e^{-\sqrt{-Ex_N}} \end{bmatrix} \times \begin{bmatrix} C_N^+ \\ C_N^- \end{bmatrix}$$

$$= \begin{bmatrix} C_{N-1}^+e^{\sqrt{-Ex_N}} + C_{N-1}^-e^{-\sqrt{-Ex_N}} \\ M_N(C_{N-1}^+e^{\sqrt{-Ex_N}} + C_{N-1}^-e^{-\sqrt{-Ex_N}}) - C_{N-1}^-e^{-\sqrt{-Ex_N}} + C_{N-1}^+\sqrt{-E}e^{\sqrt{-Ex_N}} \end{bmatrix}$$

Since $u(x) = C_N^+ e^{\sqrt{-Ex}} + C_N^- e^{-\sqrt{-Ex}}$ for $x_N < x < \infty$ the condition(4) is satisfied if and only if $C_N^+ = 0$.Thus$E < 0$ is an eigenvalue of H_{app} if and only if $C_N^+ = 0$ (note that the numbers $C_k^\pm$ depend on E, $C_k^\pm(E)$. For notational purposes, we have surpressed this dependence). With the help of MATLAB, we will solve the matrix

$$C = \begin{bmatrix} C_N^+ \\ C_N^- \end{bmatrix} \tag{6}$$

- when $E = 0$
  In this case, $u(x) = C_0^+ + C_0^- x$ is the general solution, where $C_0^\pm$ are constants.
  So we see that $\int_{-\infty}^{x_1} |u(x)|^2 dx < \infty$ is satisfied if and only if $C_0^+ = 0 = C_0^-$.
  By mimicking the reasoning for$E < 0$, we get that $C_k^\pm = 0$ for all k. Thus $u(x) = 0$ and $E = 0$ is not an eigenvalue.
- when $E > 0$
  In this case $\sqrt{-E} = i\sqrt{E}$.
  Thus we get $u(x) = C_0^+ e^{i\sqrt{Ex}} + C_0^- e^{-i\sqrt{Ex}}$.
  Again,$\int_{-\infty}^{x_1} |u(x)|^2 dx < \infty$ implies that $C_0^+ = 0 = C_0^-$. As before, if we follow the reasoning for $E < 0$, we get that $E > 0$ is not an eigenvalue.

Proving that we can only work with negative eigenvalues.

5 Particle In A Box

Imagine that a very small, particle like an electron is trapped in a box. The principles of quantum mechanics tell us that the total energy of the particle in this box must change in fixed, discrete (quantum!) leaps.

Assume that the boundaries of the box are perfectly reflecting and that there are no forces acting on the particle. The motion of the particle is described by the time-dependent *schrödinger* equation supplemented with the boundary condition that the wave function at the edge of the rectangular area is zero. The wave describing the quantum particle is reflected at the boundaries, a phenomenon analogous to the reflection of light by a mirror.
In this case one gets infinitely many eigenvalues.

The situation we are looking at is different. This is when the box has only finite depth. Here,[4]theorem 3.5 mentioned earlier, tells us that there are only finitely many eigenvalues. We are now going to describe how to calculate them.
The box potential $V(x)$ for $a, h > 0$, is expressed as:

$$V(x) = \begin{cases} -h, & \text{if } 0 < x < a\ ; \\ 0, & \text{otherwise.} \end{cases} \tag{7}$$

which is the expression for the potential of the particle-in-a-box, where a is the width of the box and h the depth of the box.

The domain of H is,

$$D(H) = \begin{cases} f \in L^2 : f \in \mathbb{C}^1(\mathbb{R}), \quad f' \text{ absolutely continuous;} \\ f, f', f'' \in L^2. \end{cases}$$

and, Hf = -f"(x) +V(x).
Let, Hf = Ef ie ,
Hf = -f"(x) +V(x)f(x) = Ef .
Here, remember that E¡0.

Now substituting V(x), we get :

$$Hf = -f''(x) - hf(x) = Ef \quad \text{on} \quad [0, a]. \tag{8}$$

$$Hf = -f''(x) = Ef \quad \text{on} \quad (-\infty, 0) \cap (a, \infty). \tag{9}$$

The eigenvalues E can be determined by solving for (9), which gives us

$$f(x) = e^{\sqrt{-Ex}} \quad \text{on} \quad (-\infty, 0). \tag{10}$$

$$f(x) = Ce^{-\sqrt{-Ex}} \quad \text{on} \quad (a, \infty). \tag{11}$$

We now compute the solution to equation(8), the bounded region [0,a], which is:
$f_1^E = e^{\sqrt{-(h+E)x}}$ and $f_2^E = e^{-\sqrt{-(h+E)x}}$
giving us the general solution as:

$$f = C_1 f_1^E + C_2 f_2^E \quad \text{on} \quad [0, a] \tag{12}$$

We now want to get the constants C_1 and C_2.
We know that f must be continuous and so is f'.
So we check, for given E, whether the constants $C_1$and C_2 can be chosen
such that(10),(11)and (12) describe a continuously differentiable function.
This means that the following conditions are met:
i) $e^{\sqrt{-Ex}}{}_{x=0} = C_1 f_1^E(0) + C_2 f_2^E(0)$ and,
ii) $\frac{d}{dx} e^{\sqrt{-Ex}}{}_{x=0} = \frac{d}{dx}[C_1 f_1^E(0) + C_2 f_2^E]_{x=0}$

The solution of this is
$C_1^E = 1 - \frac{\sqrt{-E}}{\sqrt{-(h+E)}}$ while $C_2^E = 1 + \frac{\sqrt{-(E)}}{\sqrt{-(h+E)}}$.

Thus,E is an eigenvalue if and only if we can choose a "c" such that :
i) $C_1^E f_1^E(a) + C_2^E f_2^E(a) = ce^{-\sqrt{-E(x-a)}}$, and
ii) $\frac{d}{dx}(C_1^E f_1^E + C_2^E f_2^E)_{x=a} = \frac{d}{dx} ce^{\sqrt{-E(x-a)}}{}_{x=a}$.

You will notice again, that there are finitely many eigenvalues $E_1, E_2, ..., E_N < 0$.

6 Numerical Solution

We now use mathematical modelling. This is by creating a program that directly gives us the position of the eigenvalues. We continue to assume that the particle is moving in a potential described by(7).

The first Matlab file we formulate, is one to help us find ALL the eigenvalues (solve (6)).We seek to interprete our results into a language understandable by the computer. Thus, we note that,

$H = -\frac{d^2}{dx^2} - h \cdot 1_{[0,a]}$,

$1_{[0,a]}(x) = \begin{cases} 1 & \text{if } 0 < x < a; \\ 0 & \text{otherwise .} \end{cases}$

h$\cdot 1_{[0,a]} \approx h \cdot \sum_{j=1}^{N} \frac{a}{N} \delta_{\frac{ja}{N}} = \sum_{j=1}^{N} \frac{ah}{N} \delta_{\frac{ja}{N}}$

and therefore,

$H \approx -\frac{d^2}{dx^2} - \sum_{j=1}^{N} \frac{ah}{N} \delta_{\frac{ja}{N}}$

For the computer, this gives,

$M_j = \frac{ah}{N}, j = 1, 2, ..., N$

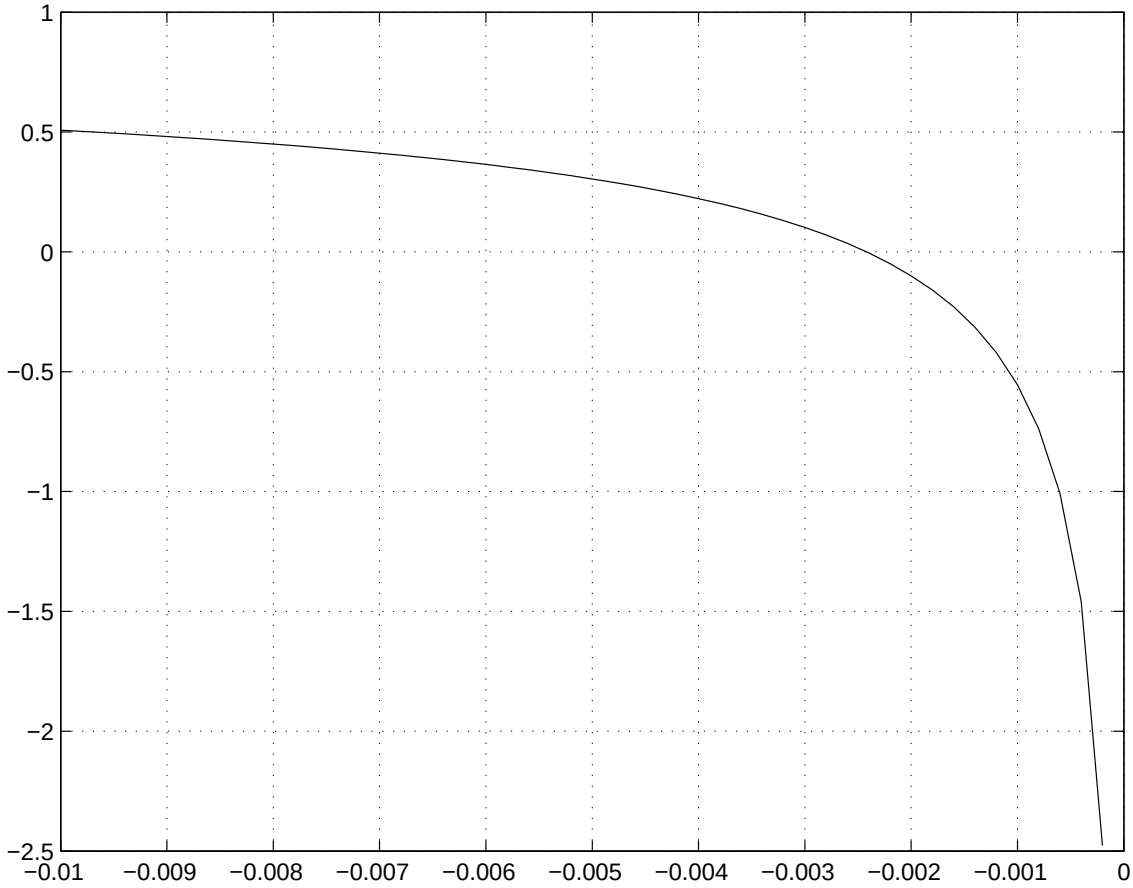
$x_j = \frac{ja}{N}$

With all this in view, we create an m-file with the following input data:

```
and
clear
fc=(0);
a=1; width of the box
h=0.1; depth of the box
N=2^7;
M=(-h*a)/N; mass of particle
X=0:a/N:a; position of particle
for E=-.01:.0002:-.00009
    c=[1;0];
     for j=1:N
      A=[exp(sqrt(-E)*X(j)) exp(-sqrt(-E)*X(j));sqrt(-E)*exp(sqrt(-E)*X(j))
         -sqrt(-E)*exp(-sqrt(-E)*X(j))];
      B=[c(1)*exp(sqrt(-E)*X(j))+c(2)*exp(-sqrt(-E)*X(j));M*(c(1)
         *exp(sqrt(-E)*X(j))+c(2)*exp(-sqrt(-E)*X(j)))+c(1)*sqrt(-E)
         *exp(sqrt(-E)*X(j))-c(2 *sqrt(-E)*exp(-sqrt(-E)*X(j))];
      c=A\B;
    end
    fc=[fc,c(1)];
end
fc=fc(2:length(fc));
plot(-.01:.0002:-.00009,fc)
grid
and
```

If we run this program, it gives an interesting curve with the values of E at the x-axis and the fc at the y-axis, where fc is the matrix of all the c^+'s which we call c1. Our main interest however, is to get the exact values of E when the $fc = 0$.

Figure 1: The curve with a=1 and h=0.1



By just looking at the figure, we see that there is an eigenvalue between -0.003 and -0.002 but it is impossible to determine the exact value.

This brings us to a point where we have to create another program to help us solve this problem.This is not an easy task and so we employ a couple of mathematical facts :

Remark From the theory,

- The smallest $E \geq -\frac{ha}{2}$.
  Where E is the energy eigenvalues

- By [4]theorem 3.5, the number of E's is less than $1 + \frac{ha^2}{2}$

- For negative μ, there exists at least one negative eigenvalue.
  Thus,

- to get exactly one eigenvalue,
  it is sufficient that $a = 1$ and $h \leq 2$.

Our matlab file to determine the negative eigenvalues, looks like this

```
 and
E1=(-h*a)/2;E2=-0.00009;
a=1;
h=0.1;
N=2^7;
M=(-h*a)/(N+1);
X=0:a/N:a;
E=E2;c=[1;0];
    for j=1:N+1
      A=[exp(sqrt(-E)*X(j)) exp(-sqrt(-E)*X(j));sqrt(-E)*exp(sqrt(-E)*X(j))
         -sqrt(-E)*exp(-sqrt(-E)*X(j))];
      B=[c(1)*exp(sqrt(-E)*X(j))+c(2)*exp(-sqrt(-E)*X(j));M*(c(1)
         *exp(sqrt(-E)*X(j))+c(2)*exp(-sqrt(-E)*X(j)))+c(1)*sqrt(-E)
         *exp(sqrt(-E)*X(j))-c(2)*sqrt(-E)*exp(-sqrt(-E)*X(j))];
      c=A\B;
    end
      c2=c(1);

for m=1:10
    E=(E1+E2)/2;c=[1;0];
 for j=1:N+1
      A=[exp(sqrt(-E)*X(j)) exp(-sqrt(-E)*X(j));sqrt(-E)*exp(sqrt(-E)*X(j))
          -sqrt(-E)*exp(-sqrt(-E)*X(j))];
      B=[c(1)*exp(sqrt(-E)*X(j))+c(2)*exp(-sqrt(-E)*X(j));M*(c(1)
         *exp(sqrt(-E)*X(j))+c(2)*exp(-sqrt(-E)*X(j)))+c(1)*sqrt(-E)
         *exp(sqrt(-E)*X(j))-c(2)*sqrt(-E)*exp(-sqrt(-E)*X(j))];
      c=A\B;
    end
      c1=c(1);
if c1*c2<0
    E1=E;
else
E2=E;c2=c1;
end
end
E
and
```

Where we set $E1 = (-h * a)/2$ because this is the smallest E possible. We could also use this in the former program as the lower bound for E.
If we run the program as it is, we get that there is only one eigenvalue existing. The value of this is given as E = -0.0025 which is not possible to determine by just looking at the figure.
We will now take different examples in order to test our programs.

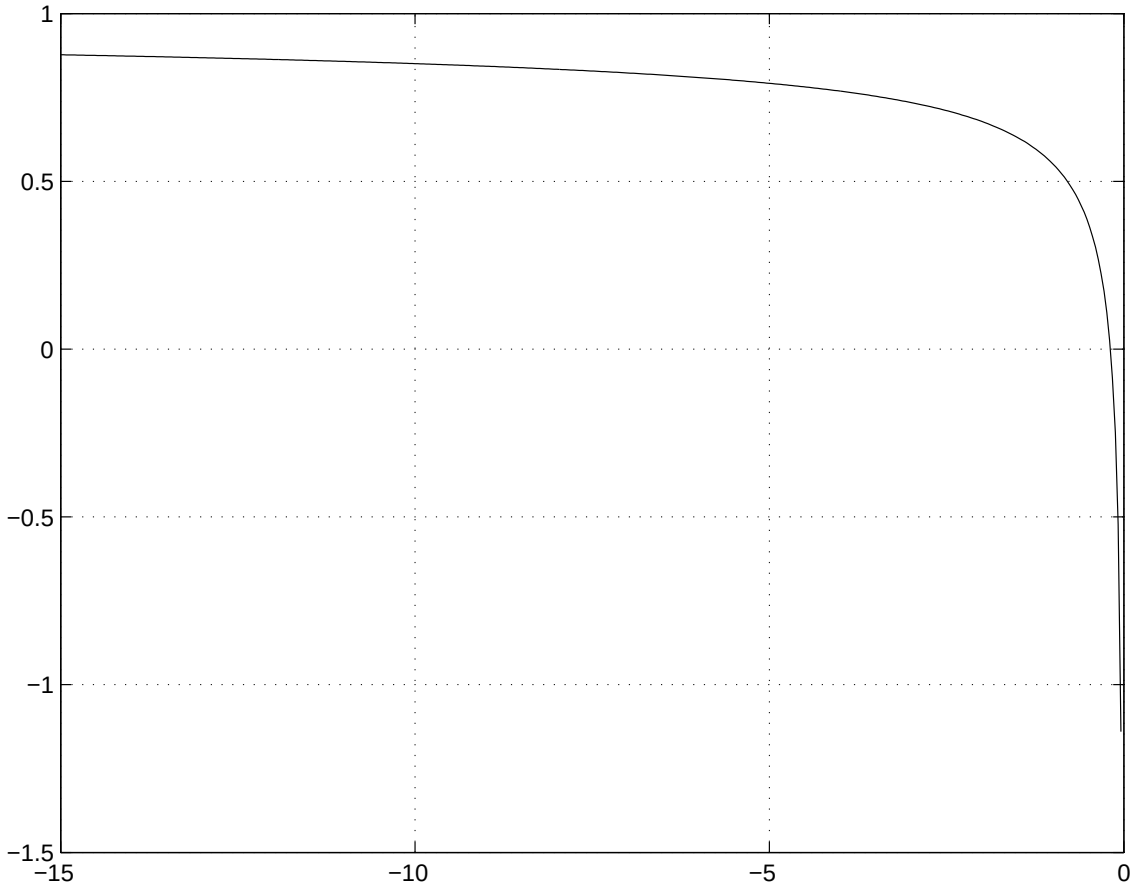
6.1 Further Examples

We want to find out the number of eigenvalues we get when we vary the parameters and also to figure out if the facts, discussed earlier on, concur with our results.
We start off by:

6.1.1 varying h

Our first choice is a value of $h \leq 2$ with $a = 1$. We choose $h = 0.1$, which gives us the curve in the previous page.We see from the figure that only one eigenvalue exists.
Taking another example, we choose our $h = 1$, which gives us:

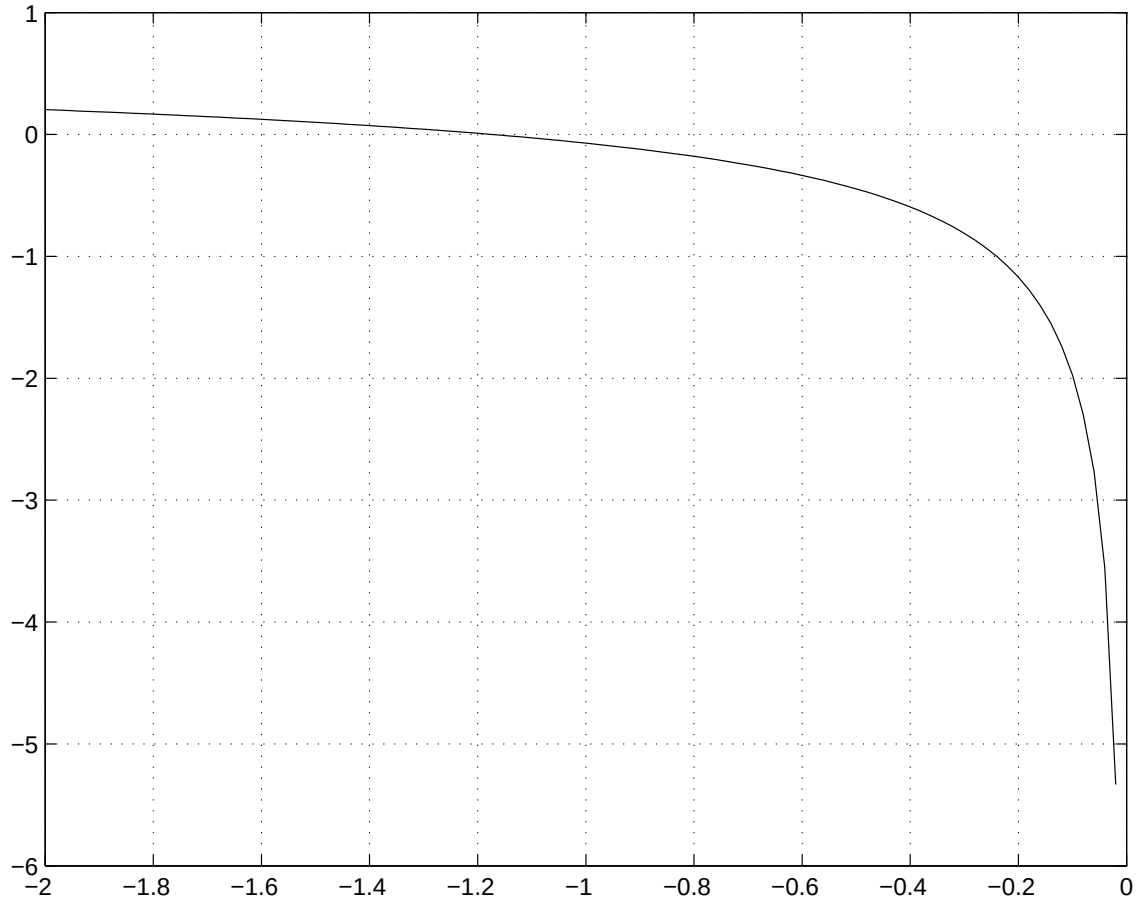
Figure 2: The curve showing the eigenvalue with a=1 and h=1



This also gives us only one eigenvalue E = -0.0500.

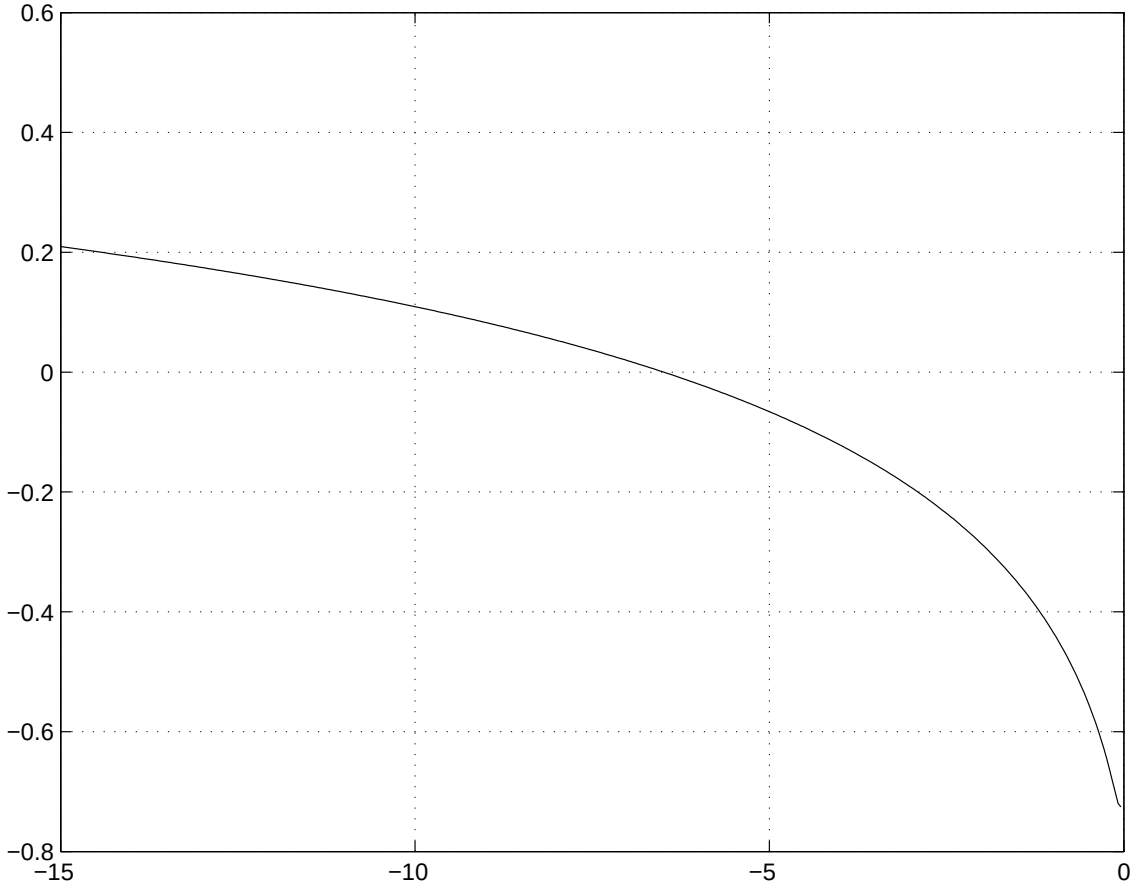
Now we try some examples with $h > 2$.
The first example will be to set $h = 3$. After running the programs,
we get that there is only one eigenvalue, -1.1704 .

Figure 3: The curve showing the eigenvalues with a=1 and h=3



In this example, we use a much larger h, $h = 10$, and notice that there is still only one eigenvalue.

Figure 4: The curve showing the eigenvalues with a=1 and h=10

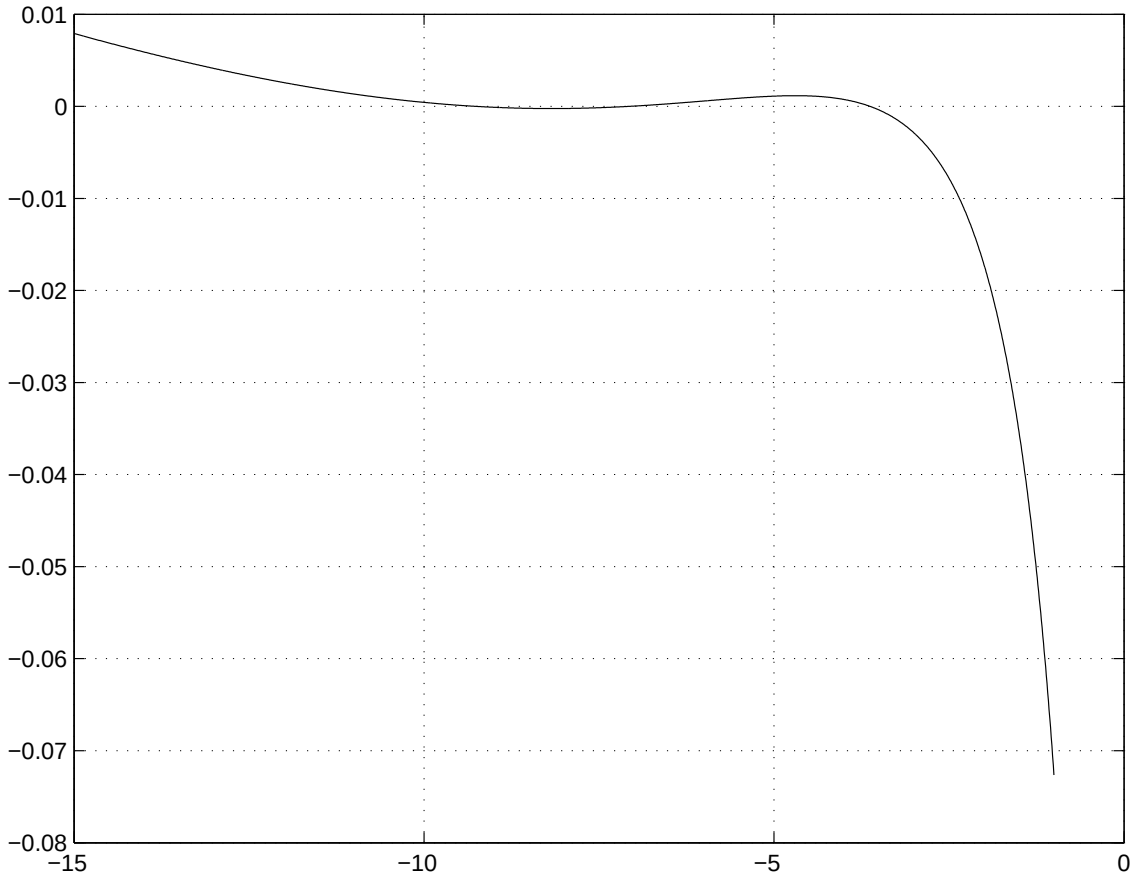


These examples clearly show that the conditions $a = 1$ and $h \leq 2$ are not necessary in order to get exactly one eigenvalue.
For sure, we can get one eigenvalue even with a much larger value of h.

6.1.2 varying a

We work with the same values of h and change the value of a. Starting with h=10 and a=3. Here, we see that there are 3 eigenvalues.The positions are -3.6415, -7.0295 and -9.1931.

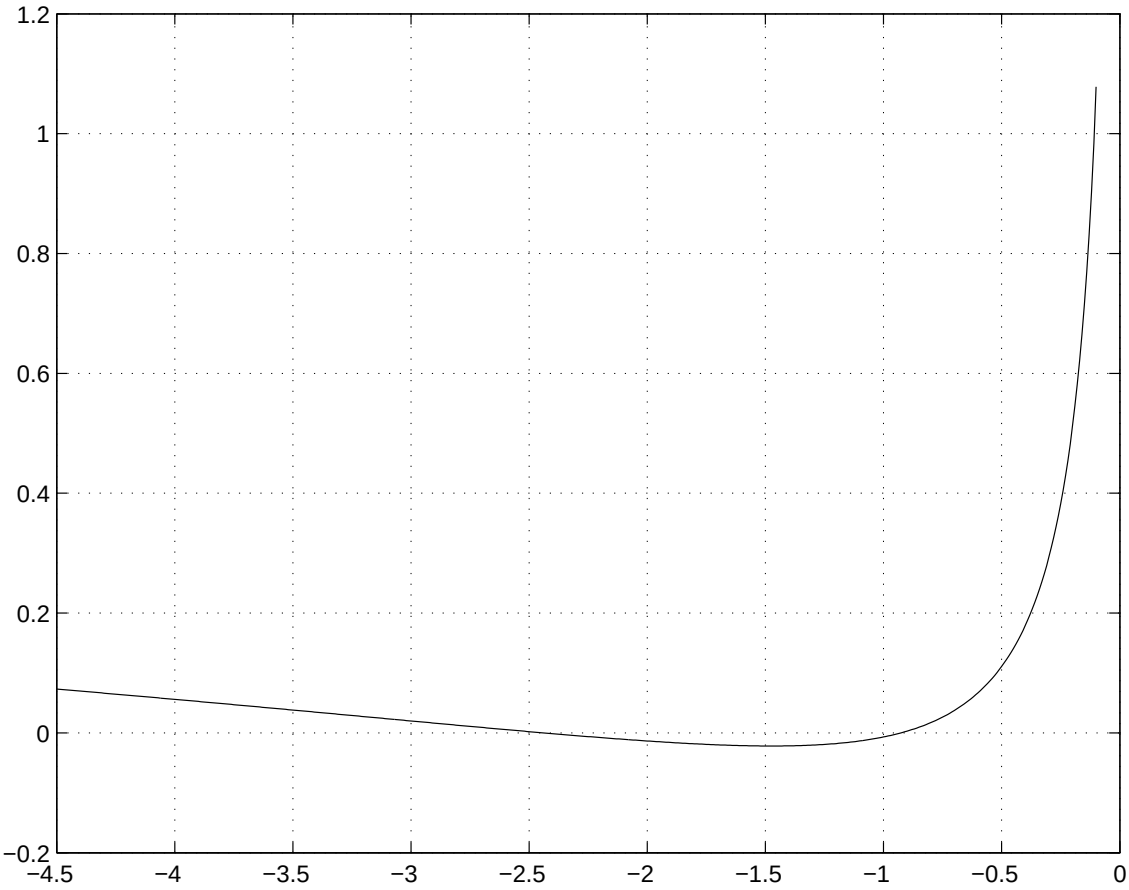
Figure 5: The curve showing the eigenvalues with a=3 and h=10



According to the second fact, there should be less than 46 eigenvalues, which is true. Also, according to the first fact, the smallest eigenvalue is greater than -15.
We have thus shown that the facts are all true.

Now we use h=3 and a=3 and it gives us another interesting curve

Figure 6: The curve showing the eigenvalue with a=3 and h=3



Here, we see that there are also 2 eigenvalues. One at -0.9302 and the other at -2.4258.

6.2 Limitations

We have seen how effective this programs are but we also realise that a number of errors can occur in the running of this program. Mostly , it is due to the choice of E1 and E2 since they are determined by the user of the program. It is possible to choose an E1 and E2 that lie on the same side of the curve before any change of sign happens.
This leads to a wrong formulation.

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