Rapid Convergence of The Born Series

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Abstract

Contents

Chapter 1

Introduction

In this write-up we are concerned with the theoretical analysis of scattering experiments. The basic principle of scattering for classical particles is simple - we start with any number of particles (two in the simplest case) which are far apart in some sense. This means that we can assume that the particles don't interact with eachother in any way. After the passage of some time these particles "collide" or interact locally in some sense and after some time they are far apart again. From the initial and final properties (position, velocity, etc.) we can infer the details of the interaction.

In quantum scattering, however, matters are slightly more complicated. The very notion of a "path" with a definite velocity is meaningless. We instead need to calculate the probability of a particle to deviate or "scatter" through a given angle. This quantity is known as the differential cross-section. Although it is the fundamental quantity of interest in scattering theory, our focus in this write-up will be on a tool that is indirectly related to it - the Born series. We note that quantum scattering theory can be further divided into nonrelativistic and relativistic cases. In this write-up we are only concerned with the former case.

The Born series is a perturbation expansion that enables us to calculate the Scattering operator to a desired order. The Scattering operator calculates the final state given a specific initial state. This can then be used to compute the cross-section. The objects of interest that can be studied using this method are the Green's function and the T operator.

Chapter 2

Scattering Theory

This section is based on the textbook, [3] and the first part of the lecture notes, [4]. We will present the basic principles of quantum scattering and the use of the Born series. As an example, we use the problem of the scattering of a single particle off a general potential. It can be shown that this problem is equivalent to that of two-particle scattering. We define the Hamiltonian operator as,

$$H = H_0 + V \tag{2.1}$$

Where, H_0 is the free Hamiltonian given by,

$$H_0 = -\frac{\Delta}{2} \tag{2.2}$$

Δ is the Laplace operator and V corresponds to the potential. For convenience, we work in units where, $\hbar^2/m = 1$. Here, m is the mass of the particle.

2.1 Spectrum of The Hamiltonian

H_0 and H are self-adjoint operators on a Hilbert space $\mathcal{H}$. In general, the spectrum of a self-adjoint operator has two components,

- Discrete - corresponding to the bound states

- Continuous - corresponding to the scattering states

The continuous part of the spectrum can be further divided into into an *absolutely continuous* and a *singular continuous* part. This results in a corresponding decomposition of the Hilbert space into three invariant subspaces.

$$\mathcal{H} = \mathcal{H}^{pp} \oplus \mathcal{H}^{ac} \oplus \mathcal{H}^{sc} \tag{2.3}$$

Where, $\mathcal{H}^{pp}$ is the part of the Hilbert space corresponding to the discrete (pure point) part of the spectrum. For most systems of interest, the singular continous part is absent. Scattering theory is essentially perturbation theory applied on the absolutely continous part of the spectrum.

The spectrum of H_0 coincides with its absolutely continuous part - the discrete and singular parts are empty. In principle, the spectrum of H_0 is the

entire complex plane, but we are only interested in the positive real axis including zero ($\mathbb{R}^+ \cup \{0\}$). These correspond to free particles. We denote these eigenstates of H_0 in $3D$ as $|\mathbf{k}\rangle$, where $\mathbf{k} \in \mathbb{R}^3$. The eigenvalue corresponding to these eigenstates is $E = |\mathbf{k}|^2/2$, . These eigenstates are improper, i.e., they are not normalisable,

$$\langle \mathbf{k}'|\mathbf{k}\rangle = \delta\left(\mathbf{k}' - \mathbf{k}\right) \tag{2.4}$$

Where δ is the Dirac delta function. The reason for the notation is that, the wavefunction corresponding this eigenstate is given by,

$$\langle \mathbf{x}|\mathbf{k}\rangle = e^{i\mathbf{k}.\mathbf{x}} \tag{2.5}$$

viz., the plane-wave with wave vector $\mathbf{k}$.

Bound States

The eigenstates corresponding to the discrete part of the spectrum are called *bound* states and those of the continuous part are called the *scattering* states. The potentials we will be dealing with support at least one negative energy bound state. The divergence of the Born series at low energies is due to the presence of bound states close to 0. We will later see that the scattering states asymptotically (in terms of time-evolution) look like free-eigenstates while the bound states don't.

2.2 Time Evolution and The Asymptotic Condition

In the Schrödinger picture, the time evolution of a state $|\psi_t\rangle$ is given by,

$$i\frac{d}{dt}|\psi_t\rangle = H|\psi_t\rangle \tag{2.6}$$

Given an initial state $|\psi\rangle$, the formal solution of (2.6) given by,

$$|\psi_t\rangle = U(t)|\psi\rangle \tag{2.7}$$

Where, $U(t) = e^{-iHt}$. Since H is self-adjoint, $U(t)$ is a unitary operator on $\mathcal{H}$, i.e., it is a linear operator that maps the whole of the Hilbert space onto itself and preserves the norm. Put more precisely,

$$\mathcal{D}\left(U(t)\right) = \mathcal{R}\left(U(t)\right) = \mathcal{H}$$

And, $\|\Omega\psi\| = \|\psi\|$. As a consequence, we are led a useful property of unitary operators,

$$U^\dagger(t)U(t) = U(t)U^\dagger(t) = \mathbb{I} \tag{2.8}$$

The essence of scattering theory is that (2.7) describes the evolution of some scattering wavefunction such that,

$$U(t)|\psi\rangle \xrightarrow[t\to-\infty]{} U^0(t)|\psi_{in}\rangle \tag{2.9}$$

$$U(t)|\psi\rangle \xrightarrow[t\to+\infty]{} U^0(t)|\psi_{out}\rangle \tag{2.10}$$

Where, $U^0(t) = e^{-iH_0 t}$ is the free evolution operator and $|\psi_{in}\rangle$ and $|\psi_{out}\rangle$ are the in and out states. To be precise, the in and out states describe the behaviour of the system a long time before and after the interaction respectively. The in and out states behave like free wave-packets - i.e., their time evolution is governed by the free Hamiltonian.

The asymptotic condition states that for every $|\psi_{in}\rangle$ in $\mathcal{H}$ there is a $|\psi\rangle$ such that (2.9).

2.2.1 Time-Independent Scattering Theory

2.3 Green's Operator

The Green's operator is formally defined as,

$$G\left(E \pm i0\right) = \left(E \pm i0 - H\right)^{-1} \tag{2.11}$$

$$G_0\left(E \pm i0\right) = \left(E \pm i0 - H_0\right)^{-1} \tag{2.12}$$

Where, $G\left(E \pm i0\right) = \lim_{\epsilon \to 0} G(E \pm i\epsilon)$. The sign of $i\epsilon$ indicates the direction of time (positive for forward scattering). The Lippmann-Schwinger equation for the Green's operator is given by,

$$G = G_0 + G_0 V G \tag{2.13}$$

The above equation can be derived by using the matrix identity,

$$A^{-1} = B^{-1} + A^{-1}\left(B - A\right)B^{-1} \tag{2.14}$$

Subsequently, an operator-series expansion for G is obtained by iteratively substituting the $(n-1)^{th}$ order approximation for G in the R.H.S of (2.13) to get the nth order term. The 0th order approximation is the free Green's operator G_0, the 1st order approximation (the Born approximation) is given by,

$$G = G_0 + G_0 V G_0 \tag{2.15}$$

The Born series for the Green's operator can thus be written as,

$$G = G_0 + G_0 V G_0 + G_0 V G_0 V G_0 + \ldots \tag{2.16}$$

Or more compactly,

$$G = \sum_{n=0}^{\infty} G_0 \left(V G_0\right)^n \tag{2.17}$$

2.4 T-Operator

As described in [3], it is convenient to define the T-operator,

$$T = V + V G V \tag{2.18}$$

Multiplying both sides by G_0 we get and using (2.13), we get,

$$G_0 T = G V \tag{2.19}$$

Substituting this relation back in (2.18) we get a Lippmann-Schwinger equation for the T-Operator,

$$T = V + VG_0T \tag{2.20}$$

And correspondingly, through iteration, a Born Series,

$$T = \sum_{n=0}^{\infty} V (G_0V)^n \tag{2.21}$$

The Born approximation in this case is, $T \simeq V$.

The momentum space matrix elements of the T-matrix are given by,

$$t (\mathbf{k}' \leftarrow \mathbf{k}) = \langle \mathbf{k}'|T|\mathbf{k}\rangle \tag{2.22}$$

2.5 Scattering Operator

We first define the Møller operators, $\Omega_\pm$ as,

$$\Omega_\pm = \lim_{t \to \mp\infty} U(t)^\dagger U^0(t) \tag{2.23}$$

These operators act on the in and out states to give,

$$|\psi\rangle = \Omega_+|\psi_{in}\rangle \tag{2.24}$$

$$|\psi\rangle = \Omega_-|\psi_{out}\rangle \tag{2.25}$$

The Møller wave operators acting on an in or out state give the corresponding scattering state for the Hamiltonian. These operators are isometric, i.e., they are defined on all of $\mathcal{H}$ and preserve the norm. They differ from unitary operators in that, $\mathcal{R}(\Omega_\pm) \neq \mathcal{H}$. Unlike the property (2.8) for unitary operators, we have $\Omega_\pm^\dagger \Omega_\pm = \mathbb{I}$, but in general, $\Omega_\pm \Omega_\pm^\dagger \neq \mathbb{I}$. We also note that all Unitary operators are isometric.We can now define the scattering operator,

$$\mathcal{S} = \Omega_-^\dagger \Omega_+ \tag{2.26}$$

The scattering operator has the property that,

$$|\psi_{out}\rangle = \mathcal{S}|\psi_{in}\rangle \tag{2.27}$$

i.e., given an in state, the scattering operator gives the corresponding out state. An important property of the $\mathcal{S}$ operator is that, unlike the Møller operators, it is unitary. As a consequence of this, every $|\psi_{in}\rangle$ is mapped to a unique $|\psi_{out}\rangle$ in $\mathcal{H}$.

In practice, only the asymptotic free motion is observable. Therefore, the operator $\mathcal{S}$ contains all the information of experimental interest. For a scattering process, $|\psi_{in}\rangle \to |\psi_{out}\rangle$, the probability is given by,

$$\mathbf{w}(|\psi_{out}\rangle \leftarrow |\psi_{in}\rangle) = |\langle \psi_{out}|\mathcal{S}|\psi_{in}\rangle|^2 \tag{2.28}$$

The momentum space matrix elements of the scattering operator are related to (2.22) as,

$$\langle \mathbf{k}'|\mathcal{S}|\mathbf{k}\rangle = \delta_3(\mathbf{k}' - \mathbf{k}) - 2\pi i \delta (E_{p'} - E_p) t (\mathbf{k}' \leftarrow \mathbf{k}) \tag{2.29}$$

The physical interpretation of the above expression is that, given an incoming plane wave, after the interaction the outgoing wave is given by the incoming wave plus a component which a consequence of the interaction. The T operator in a sense contains all the information about the interaction. Thus we see that, given a good approximation to the Green's operator or the T-operator, we can directly calculate the S operator and thereby the cross-sections.

Chapter 3

Finite Element Method

The Finite Element Method (FEM) is a numerical technique used to solve differential equations. The method exploits the locality of the differential operator. The solution space is divided into subspaces. These subspaces take the form of a mesh, i.e., a collection of simplices - triangles in 2D, tetrahedra in 3D, etc. The function is then approximated using smooth basis functions with support in these subspaces. These basis functions with finite support are referred to as finite elements.

Let ψ be a solution to a differential equation. We denote the basis functions by ϕ_n,

$$\psi(\mathbf{x}) \simeq \widetilde{\psi}(\mathbf{x}) = \sum_n^N c_n \phi_n(\mathbf{x}) \tag{3.1}$$

A feature of FEM is that the basis functions have a finite overlap i.e., they are not orthogonal. The overlap matrix in general has a block-diagonal form. The overlap matrix is denoted by,

$$S_{nm} = \int J(\mathbf{x}) d^n x \phi_n(\mathbf{x}) \phi_m(\mathbf{x}) \tag{3.2}$$

We also define the matrix,

$$B_{nm} = \int J(\mathbf{x}) d^n x \nabla \phi_n(\mathbf{x}).\nabla \phi_m(\mathbf{x}) \tag{3.3}$$

Here, $J(\mathbf{x})$ is the Jacobian for the chosen coordinate system.

3.1 Boundary Conditions

In order to solve the differential equations we must also specify appropriate boundary conditions. Let Ω be the solution space. We denote its boundary by $\partial\Omega$.

3.1.1 Dirichlet Boundary Condition

The Dirichlet boundary condition requires that the function has a known value on the boundary.

$$\psi(\mathbf{x}) = f(\mathbf{x}), \ \forall \mathbf{x} \in \partial\Omega \tag{3.4}$$

Where, f is a known function on Ω.

3.1.2 Neumann Boundary Condition

The Neumann boundary condition requires that the gradient of the function normal to the boundary is fixed to a known function. That is,

$$\frac{\partial \psi(\mathbf{x})}{\partial \mathbf{n}} \equiv \nabla \psi(\mathbf{x}).\mathbf{n} = f(\mathbf{x}), \ \forall \mathbf{x} \in \partial \Omega \tag{3.5}$$

3.1.3 Mixed Boundary Condition

It is also possible to have a boundary such that the function has a Dirichlet boundary condition on one part (denoted by $\partial \Omega_D$) and a Neumann boundary condition on the other ($\partial \Omega_N$).

Continuity

The function is further constrained to be continuous at the boundaries of the finite element.

Note

We will be working in 1-dimension with a Jacobian, $J(x) = 1$. We should also mention here that, a $2D$ problem in polar coordinates with azimuthal symmetry reduces to a $1D$ problem with a Jacobian, $J(x) = x$ and similarly, a $3D$ problem in spherical coordinates with symmetry in both angular direction reduces to a $1D$ problem with a Jacobian, $J(x) = x^2$. The python implementation is discussed in Appendix A.

Chapter 4

FEM in Quantum Mechanics

The Schrödinger equation for a wave function ψ is given by,

$$-\frac{\Delta}{2}\psi + V(\mathbf{x})\psi = E\psi \tag{4.1}$$

Using the FEM approximation defined in (3.1),

$$-\frac{\Delta}{2}\sum_n^N c_n\phi_n(\mathbf{x}) + \sum_n^N c_n V(\mathbf{x})\phi_n(\mathbf{x}) = E\sum_n^N c_n\phi_n(\mathbf{x}) \tag{4.2}$$

Now, we get the weak formulation of the problem by multiplying both sides by $\phi_m(\mathbf{x})$ and integrating over. We now integrate by parts and use the finite support of the basis functions to set the boundary terms to zero. We have to note here that the integration is over all space not just the "box" of our problem. Even if the wavefunction has a non-zero value on the boundary of the box, the finite element basis functions go to zero as $|\mathbf{x}| \to \infty$

Now we use the definition in (3.3), to get the following matrix element,

$$B_{mn} = -\int d^3x \phi_m(\mathbf{x})\Delta\phi_n(\mathbf{x}) = \int d^3x \nabla\phi_m(\mathbf{x}).\nabla\phi_n(\mathbf{x}) \tag{4.3}$$

This is the FEM representation of the kinetic term. The potential term is calculated from the known functions ϕ_n and is defined as,

$$V_{mn} = \int d^3x V(\mathbf{x})\phi_m(\mathbf{x})\phi_n(\mathbf{x}) \tag{4.4}$$

Finally, using the definition of the overlap matrix in (3.2), the R.H.S is given by,

$$ES_{mn} = E\int d^3x \phi_m(\mathbf{x})\phi_n(\mathbf{x}) \tag{4.5}$$

Finally, we define the coefficient vector, $\underline{\mathbf{c}} = [c_1, c_2, \ldots, c_N]^T$. The Schrödinger equation thus reduces to the following generalized eigenvalue problem,

$$H\underline{\mathbf{c}} = ES\underline{\mathbf{c}} \tag{4.6}$$

Where, $H = \left(\frac{B}{2} + V\right)$

Inner Products

The inner product of two wavefunctions ϕ and χ is given by,

$$\int d^3x \chi^*(\mathbf{x})\psi(\mathbf{x}) = \sum_{m,n}^{N} c_m^* d_n \int d^3x \phi_m(\mathbf{x})\phi_n(\mathbf{x})$$
$$= \mathbf{c}^\dagger S \mathbf{d} \tag{4.7}$$

Where, $\mathbf{c}^\dagger = (\mathbf{c}^*)^T$ and we used the definition of the overlap matrix in (4.5).

4.1   Momentum Eigenstates

We now want to find an FEM representation for free eigenstate of momentum $\mathbf{k}$ (energy, $E_k = |\mathbf{k}|^2/2$). These are the improper eigenstates of the operator $H_0 = B/2$. It is most convenient to do so by defining a "cosine eigenvector",

$$|\mathbf{k}_c\rangle = exp(-i\mathbf{k}.\mathbf{x}) + exp(i\mathbf{k}.\mathbf{x}) \tag{4.8}$$

These can be obtained by "solving" the free Schrödinger equation on a grid with open boundaries, i.e., by solving (4.6) with $H = H_0$, i.e.,

$$H_0\psi = E_k S\psi \tag{4.9}$$

for ψ.

$|\mathbf{k}_c\rangle$ has the following properties,

$$\langle \mathbf{k}_c|S|\mathbf{k}_c\rangle = \int_\Omega d^3x = V_\Omega \tag{4.10}$$

$$\langle \mathbf{k}_c'|S|\mathbf{k}_c\rangle \simeq 0 \tag{4.11}$$

Here, V_Ω is the volume of the solution space.

4.2   Born Series - FEM Formulation

We now use the definition of the Greens function in (2.11) and the FEM formulation of the Schrödinger equation, (4.6) to calculate the FEM representation of the Greens Function. We require that,

$$G_{fem}(z)\psi = (z - E_0)^{-1}S\psi \tag{4.12}$$

Where, ψ is an eigenstate of H of energy E_0 and $z \neq E_0$ is a complex number. Thus, we define the Green's operator as,

$$G_{fem}(z) = \left(z\mathbf{I} - HS^{-1}\right)^{-1} S \tag{4.13}$$

Where, $\mathbf{I}$ is the identity matrix. The free Greens function is defined similarly by setting $H = B/2$. We will ultimately be testing the convergence of the matrix element, $\langle \mathbf{k}|G_{fem}(z)|\mathbf{k}\rangle$. For later convenience, the potential matrix is also suitably modified as,

$$V_{fem} = S^{-1}VS^{-1} \tag{4.14}$$

Chapter 5

Orthogonal Projection Method

In this section we use the techniques introduced in [1] and elaborated in [2]. In this paper, it is suggested that the Born series can be rearranged by using orthogonally projecting pseudopotentials (OPP). It is then proved that the rearranged Born series converges for all negative and small positive energies even if the system contains bound states.

Let the bound states (indexed by a) of the Hamiltonian H be denoted by $|\psi_a\rangle$. The potential is modified by the operator Γ given by,

$$\Gamma = \lambda \sum_a |\psi_a\rangle\langle\psi_a| \tag{5.1}$$

The rate of convergence of the Born series is controlled by the parameter λ. It is seen that for weak potentials, λ has very little influence on the convergence while for stronger potentials which support several bound states, λ seems to have an optimal range for convergence.

The modified Hamiltonian and the modified free Hamiltonian are denoted by,

$$\widetilde{H} = H + \Gamma \tag{5.2}$$

$$\widetilde{H}_0 = H_0 + \Gamma \tag{5.3}$$

The modified Greens functions $\widetilde{G}$ and $\widetilde{G}_0$ are defined similarly as in (2.11). The modified Born Series for $\widetilde{G}$ is given by,

$$\widetilde{G} = \sum_{n=0}^{\infty} \widetilde{G}_0 \left(V \widetilde{G}_0 \right)^n \tag{5.4}$$

Physically, this means that the modified Hamiltonian has the same continuous spectrum but the discrete spectrum has been shifted by λ.

5.1 Example Problem - Scattering in 1D

We now use the above methods in an example with scattering off a potential in 1D. Due to the simplicity of the problem, it is possible to explicitly calculate

the exact Green's operator by inverting the appropriate matrix according the formal definition given in (2.11). We will examine the problem in two cases:

- In the first case, we have convergence with both the modified and unmodified Hamiltonian but at a faster rate with the modification.

- In the second case, the modified hamiltonian gives a convergent Born series whereas the unmodified one diverges.

Our box is defined as an FEM axis from $x = 0$ to $x = 10$ with $N = 200$ discretization points, of order 40 and with open boundaries. This means that the axis is divided into 200 segments and each segment has functions (elements) upto order 40. Order 1 being a straight line. As an example, we show an axis, $0 \leq x \leq 4$ with $N = 4$ discretization points, open boundaries and order 1.
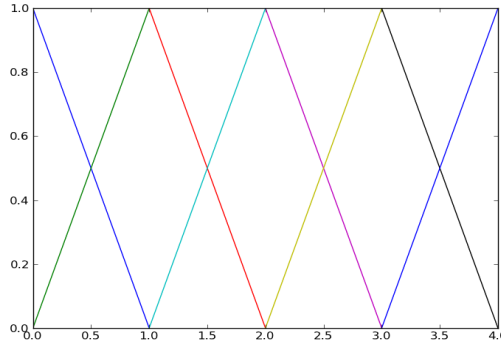

Figure 5.1: FEM axis. N=4, order=1

The "cosine eigenvectors" are computed using (4.8) and (4.9). The energies of the free wavefunctions are $E_n = n^2\pi^2/2L^2$ for $n = 0, \ldots, N$ and $L = 10$. The Green's operator, $G(z)$ is calculated for $z = E_n + i\epsilon$, where ϵ is a small positive number. The purpose of ϵ is to avoid the singularity of the Green's operator on the positive real axis. We first encountered it in (2.11) where we originally took $\epsilon \to 0$. In the numerical example, however, epsilon is fixed to be a small number which is larger than the energy spacing between the bound states close to the origin.

5.1.1 First Case

In the first case, we define the potential as a finite well of strength 0.01 with support in $4.5 \leq x \leq 5.5$,

$$V = \begin{cases} -0.01 & 4.5 \leq x \leq 5.5 \\ 0 & \text{otherwise} \end{cases} \tag{5.5}$$

The Born Series is calculated for 15 iterations. The Hamiltonian is modified using the operator defined in (5.1) with $\lambda = 1$. We also set $\epsilon = 10^{-3}$.

We now plot the elements of the Born Series against the number of iterations. In order to compare the modified and unmodified cases, we plot them side by
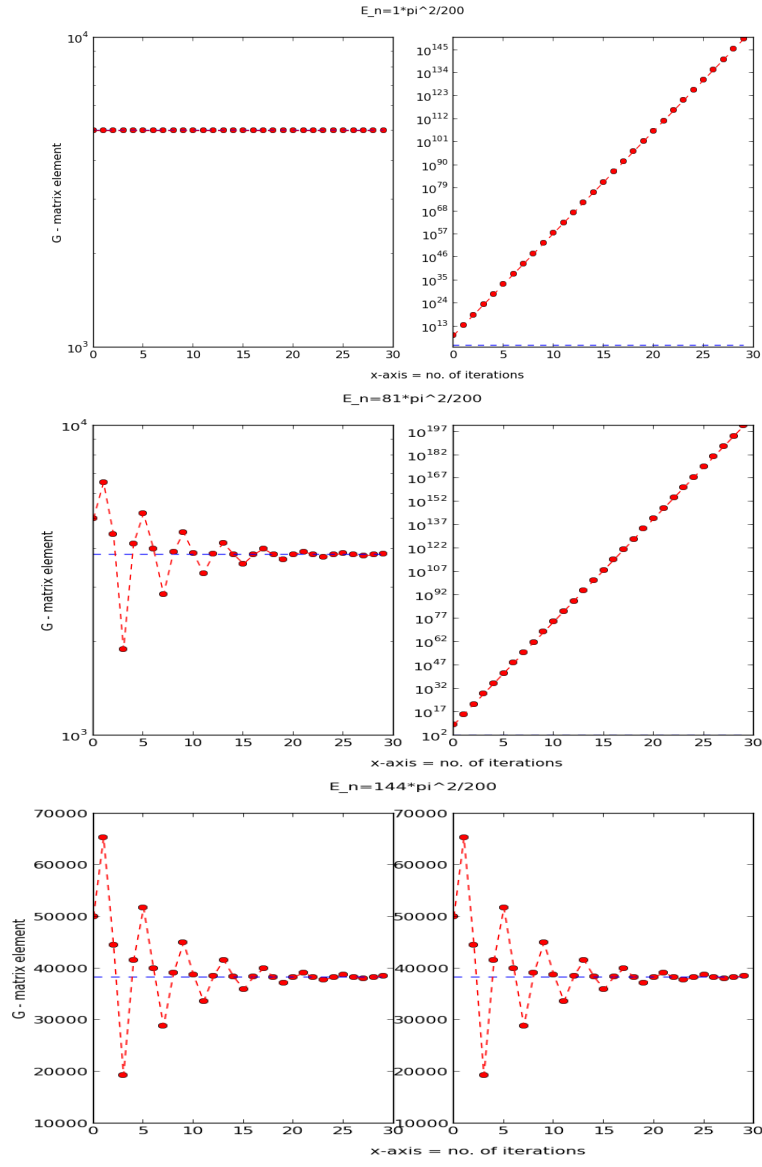
Figure 5.2: First Case - Weak Finite Well

side with the modified case on the left and the unmodified one on the right. We follow this convention in the other next case as well.

5.1.2   Second Case

The potential is give by,

$$V = -100\exp(-(x-3.5)^2/0.5) - 100\exp(-(x-6.5)^2/0.5) \qquad (5.6)$$
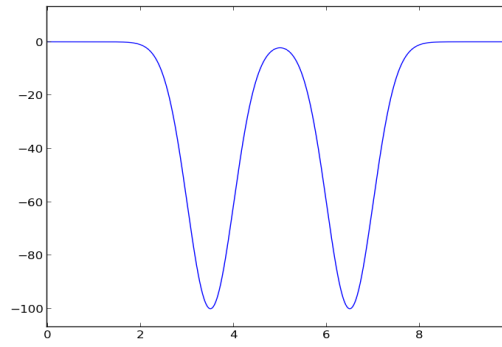
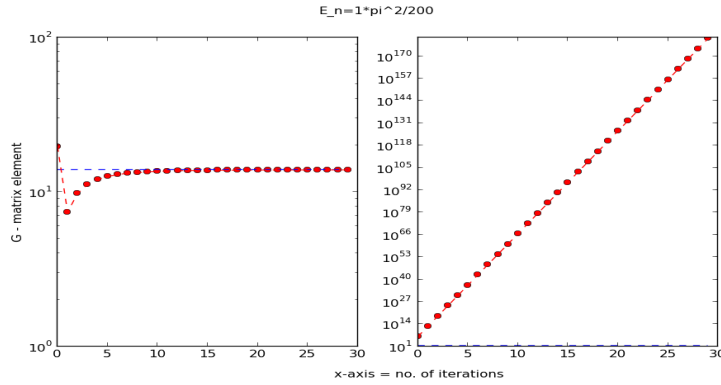We set $\epsilon = 10^{-6}$ and $\lambda = 100$.

Figure 5.3: Test Potential 2

We see that for some energies the Born Series in the modified case converges to the exact value but diverges in the original case. We also note that for certain energies, the Born Series diverges in both cases but the divergence in the unmodified case is slower.
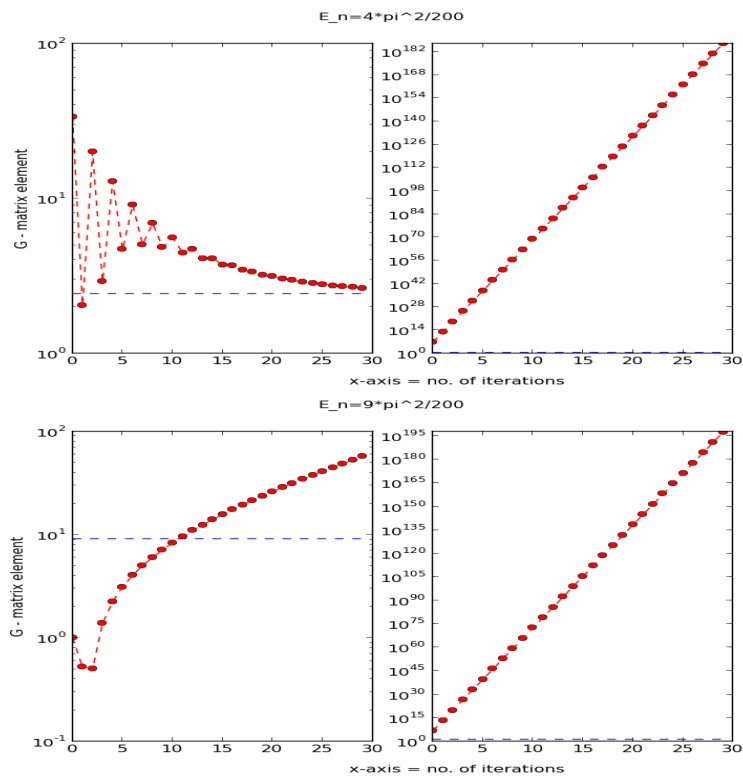
15

Figure 5.4: Gaussian Like Potential

Chapter 6

Conclusion

Appendix A

Python Implementation

The main object of interest is the `Axis` class, which is defined in the file `axis.py`.

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