Thesis Draft 1

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Abstract

0.1 Scattering Theory

0.1.1 Formal Scattering Theory

The spectrum of any

We define the Hamiltonian operator as,

$$H = H_0 + V \tag{1}$$

Where, H_0 is the free Hamiltonian given by,

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

V is the potential.
The Green's function is formally defined as,

$$G\left(E + i\epsilon\right) = \left(E + i\epsilon - H\right)^{-1} \tag{3}$$

$$G_0\left(E + i\epsilon\right) = \left(E + i\epsilon - H_0\right)^{-1} \tag{4}$$

The Lippmann-Schwinger equation for the Green's function is given by,

$$G = G_0 + G_0 V G \tag{5}$$

Subsequently, the Born series for G is obtained by recursively substituting the $(n-1)^{th}$ order approximation for G in the R.H.S of (5) to get the n^{th} order term. The 0^{th} order approximation is the free Green's function G_0, the 1^{st} order approximation (the Born approximation) is given by,

$$G = G_0 + G_0 V G_0 \tag{6}$$

The Born series can thus be written as,

$$G = G_0 + G_0 V G_0 + G_0 V G_0 V G_0 + \ldots \tag{7}$$

Or more compactly,

$$G = \sum_{n=0}^{\infty} G_0 \left(V G_0\right)^n \tag{8}$$

0.2 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,

$$\psi(\mathbf{x}) \simeq \widetilde{\psi}(\mathbf{x}) = \sum_{n}^{N} c_n \phi_n(\mathbf{x}) \tag{9}$$

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,

$$S_{nm} = \int d^3x \phi_n(\mathbf{x})\phi_m(\mathbf{x}) \tag{10}$$

We also define the matrix,

$$B_{nm} = \int d^3x \nabla\phi_n(\mathbf{x}).\nabla\phi_m(\mathbf{x}) \tag{11}$$

0.2.1 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 $\partial\Omega$.

Dirichlet Boundary Condition

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

$$\psi(\mathbf{x}) = f(\mathbf{x}),\ \forall \mathbf{x} \in \partial\Omega \tag{12}$$

Where, f is a known function on Ω.

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,

$$\frac{\partial\psi(\mathbf{x})}{\partial\mathbf{n}} \equiv \nabla\psi(\mathbf{x}).\mathbf{n} = f(\mathbf{x}),\ \forall \mathbf{x} \in \partial\Omega \tag{13}$$

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 ($\partial\Omega_N$).

0.2.2 Python Implementation

0.3 FEM Formulation of Quantum Mechanics

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

$$-\frac{\Delta}{2}\psi + V(\mathbf{x})\psi = E\psi \tag{14}$$

Using the FEM approximation defined in (9),

$$-\frac{\Delta}{2}\sum_n^N c_n\phi_n(\mathbf{x}) + \sum_n^N c_n V(\mathbf{x})\phi_n(\mathbf{x}) = E\sum_n^N c_n\phi_n(\mathbf{x}) \tag{15}$$

We get the weak formulation of the problem by multiplying both sides by $\phi_m(\mathbf{x})$ and integrating over. After integrating by parts, the kinetic term gives us the following matrix element,

$$\int d^3x \phi_m(\mathbf{x}) \Delta \phi_n(\mathbf{x}) = -\int d^3x \nabla \phi_m(\mathbf{x}).\nabla \phi_n(\mathbf{x}) = -B_{mn} \tag{16}$$

The potential term is calculated from the known functions ϕ_n and is defined as,

$$\int d^3x V(\mathbf{x}) \phi_m(\mathbf{x}) \phi_n(\mathbf{x}) = V_{mn} \tag{17}$$

Finally, the R.H.S is given by,

$$E \int d^3x \phi_m(\mathbf{x}) \phi_n(\mathbf{x}) = E S_{mn} \tag{18}$$

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

$$H\underline{\mathbf{c}} = ES\underline{\mathbf{c}} \tag{19}$$

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

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

$$\begin{aligned} \int d^3x \chi^*(\mathbf{x}) \psi(\mathbf{x}) &= \sum_{m,n}^{N} c_m d_n \int d^3x \phi_m(\mathbf{x}) \phi_n(\mathbf{x}) && (20) \\ &= \mathbf{c}^\dagger S \mathbf{d} && (21) \end{aligned}$$

Where, $\mathbf{c}^\dagger = (\mathbf{c}^*)^T$.

0.3.1 Momentum Eigenstates

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

$$|\mathbf{k}\rangle = exp(-i\mathbf{k}.\mathbf{x}) + exp(i\mathbf{k}.\mathbf{x}) \tag{22}$$

These can be obtained by "solving" the free Schrödinger equation on a grid with open boundaries, i.e., by solving the eigenvalue problem,

$$H_0 \psi = \lambda S \psi \tag{23}$$

for ψ.

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

$$\begin{aligned} \langle \mathbf{k}|S|\mathbf{k}\rangle &= \int_\Omega d^3x && (24) \\ \langle \mathbf{k}'|S|\mathbf{k}\rangle &\simeq 0 && (25) \end{aligned}$$

Here, $\int_\Omega d^3x$ is the volume of the solution space.

0.3.2 Born Series - FEM Formulation

We calculate the FEM representation of the Greens Function using (19). We require that,

$$G_{fem}(z)\psi = (z - E_0)^{-1} S\psi \tag{26}$$

Where, ψ is an eigenstate of H of energy E_0. Thus, we define the Green's function as,

$$G_{fem}(z) = \left(z\mathbf{I} - HS^{-1}\right)^{-1} S \tag{27}$$

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, $\langle \mathbf{k}|G_{fem}(z)|\mathbf{k}\rangle$. For later convenience, the potential matrix is also suitably modified as,

$$V_{fem} = S^{-1} V S^{-1} \tag{28}$$

0.3.3 Modification of the Hamiltonian

In this section we use the techniques outlined in [1]. It this paper, the Born series is 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,

$$\Gamma = \lambda \sum_a |\psi_a\rangle\langle\psi_a| \tag{29}$$

The rate of convergence of the Born series is controlled by the parameter λ.

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

$$\widetilde{H} = H + \Gamma \tag{30}$$

$$\widetilde{H}_0 = H_0 + \Gamma \tag{31}$$

The modified Greens functions $\widetilde{G}$ and $\widetilde{G}_0$ are defined similarly as in (3). The modified Born Series for $\widetilde{G}$ is given by,

$$\widetilde{G} = \sum_{n=0}^{\infty} \widetilde{G}_0 \left(V\widetilde{G}_0\right)^n \tag{32}$$

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

0.4 Toy 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 function by inverting the appropriate matrix according the formal definition given in (3). 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 $n = 400$ discretization points, of order 40 and with open boundaries. This means that the axis is divided into 400 parts and each part 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.

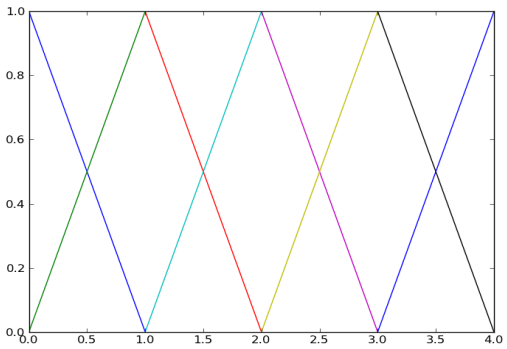

Figure 1: FEM axis. n=4, order=1

The different elements are distinguished by colour.

The "cosine eigenvectors" are computed using (22) and (23). The energies of the free wavefunctions are $E_n = n^2\pi^2/200$ for $n = 0, \ldots, 19$. The factor of 200 is a result of the discretization. The Green's function, $G(z)$ is calculated for $z = E_n + i\epsilon$, where, ϵ is a small positive number defined based on the problem. The purpose of epsilon is to avoid the singularity on the positive real axis.

0.4.1 First Case

In the first case, we define the potential as a finite well of strength 0.1 with support in $4 \leq x \leq 6$,

$$V = \begin{cases} -0.1 & 4 \leq x \leq 6 \\ 0 & \text{otherwise} \end{cases} \tag{33}$$

The Born Series is calculated for 15 iterations. The Hamiltonian is modified using the operator defined in (29) with $\lambda = 1$. We also set $\epsilon = 0.1$.

We see that the Born Series converges to the exact value in both cases but that the modified case converges in fewer iterations.

0.4.2 Second Case

In the second case, we define the potential as,

$$V = -200\texttt{exp}(-(x - 3.5)^2/0.5) - 200\texttt{exp}(-(x - 6.5)^2/0.5) \tag{34}$$

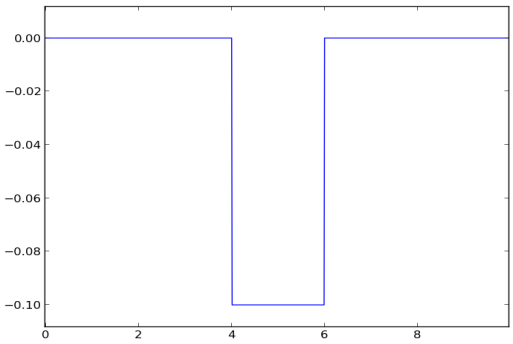

Figure 2: Test Potential 1

The born series is calculated for 15 iterations. We choose $\lambda = 700$ and $\epsilon = 10^{-8}$.

We see that the Born Series in the modified case converges to the exact value but diverges in the original case.

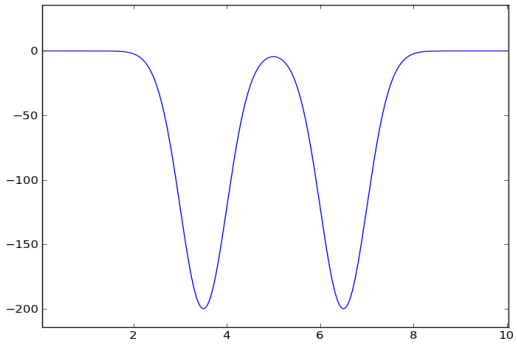

Figure 3: Test Potential 2

Bibliography

[1] V. I. Kukulin and Pomerantsev V. N. 1976.