Thesis Draft 1

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1 Scattering in 1D

1.1 Preliminaries

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,

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

1.2 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,

$$\Gamma = \lambda \sum_a |\psi_a\rangle\langle\psi_a| \tag{9}$$

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,

$$\widetilde{H} = H + \Gamma \tag{10}$$

$$\widetilde{H}_0 = H_0 + \Gamma \tag{11}$$

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,

$$\widetilde{G} = \sum_{n=0}^{\infty} \widetilde{G}_0 \left(V\widetilde{G}_0\right)^n \tag{12}$$

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,

$$\psi(\mathbf{x}) \simeq \widetilde{\psi}(\mathbf{x}) = \sum_n^N c_n \phi_n(\mathbf{x}) \tag{13}$$

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,

$$S_{nm} = \int d^3x \phi_n(\mathbf{x})\phi_m(\mathbf{x}) \tag{14}$$

We also define the matrix,

$$B_{nm} = \int d^3x \nabla\phi_n(\mathbf{x}).\nabla\phi_m(\mathbf{x}) \tag{15}$$

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 $\partial\Omega$.

3 FEM Formulation of Quantum Mechanics

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

$$-\frac{\Delta}{2}\psi + V(\mathbf{x})\psi = E\psi \tag{16}$$

Using the FEM approximation defined in (13),

$$-\frac{\Delta}{2}\sum_{n}^{N} c_n\phi_n(\mathbf{x}) + \sum_{n}^{N} c_n V(\mathbf{x})\phi_n(\mathbf{x}) = E\sum_{n}^{N} c_n\phi_n(\mathbf{x}) \tag{17}$$

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,

$$\int d^3x\phi_m(\mathbf{x})\Delta\phi_n(\mathbf{x}) = -\int d^3x\nabla\phi_m(\mathbf{x}).\nabla\phi_n(\mathbf{x}) = -B_{mn} \tag{18}$$

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

$$\int d^3x V(\mathbf{x})\phi_m(\mathbf{x})\phi_n(\mathbf{x}) = V_{mn} \tag{19}$$

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

$$E\int d^3x\phi_m(\mathbf{x})\phi_n(\mathbf{x}) = ES_{mn} \tag{20}$$

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,

$$H\underline{\mathbf{c}} = ES\underline{\mathbf{c}} \tag{21}$$

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

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

$$\int d^3x\chi^*(\mathbf{x})\psi(\mathbf{x}) = \sum_{m,n}^{N} c_m d_n \int d^3x\phi_m(\mathbf{x})\phi_n(\mathbf{x}) \tag{22}$$

$$= \mathbf{c}^\dagger S\mathbf{d} \tag{23}$$

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

3.1 Momentum Eigenstates

We now want to find an FEM representation for free eigenstate of momentum $\mathbf{k}$. It is most convenient to do so by defining a "cosine eigenvector",

$$|\mathbf{k}\rangle = exp(-i\mathbf{k}.\mathbf{x}) + exp(i\mathbf{k}.\mathbf{x}) \tag{24}$$

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

$$H_0\psi = \lambda S\psi \tag{25}$$

for ψ.

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

$$\langle \mathbf{k}|S|\mathbf{k}\rangle = \int_\Omega d^3x \tag{26}$$

$$\langle \mathbf{k}'|S|\mathbf{k}\rangle \simeq 0 \tag{27}$$

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

3.2 Born Series - FEM Formulation

We calculate the FEM representation of the Greens Function using (21). We require that,

$$G(z)\psi = (z - E_0)^{-1} S\psi \tag{28}$$

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

$$G(z) = \left(z\mathbf{I} - HS^{-1}\right)^{-1} S \tag{29}$$

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, $\langle \mathbf{k}|G(z)|\mathbf{k}\rangle$.

References

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