A Fundamental Form of the Schrödinger Equation in 1D

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Abstract

We propose a first order equation from which the Schrödinger equation can be derived in 1D. Matrices that obey certain properties are introduced for this purpose. We construct the solutions of this equation and solve the problem of an electron scattering from a step potential in 1D. We show that, with this approach, the Klein Paradox does not arise. We also show that the sum of the spin up and down, reflection and transmission coefficients, is equal to the quantum mechanical results for this problem.

\[1\]

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1 Introduction

Paul Dirac proposed his well known equation to describe a covariant theory for relativistic fermions [1]. A motivation for proposing this equation was to address the problem of negative probabilities that arise from the Klein Gordon equation. The problem of negative probability density was resolved while the negative energy solutions were interpreted as antiparticles. In addition, the Dirac equation also predicts the correct gyromagnetic ratio for the electron ($g_e = 2$) which is yet another triumph of this theory.

The Klein paradox [2] arises when the Dirac equation is used to study problems such as the scattering of an electron from a potential step, particularly when the barrier height $V_0 > 2mc^2$. For this problem the reflected current turns out to be larger than the incident current. This paradox can be resolved by assuming the production of particle-antiparticle pairs at the barrier. Other methods have also been proposed in literature to resolve this paradox (see, for example, the list of references [3]).

In this paper we discuss an approach with which the Klein Paradox does not arise. We first show that the Schrodinger equation can be derived from a fundamental first order equation in 1D. We construct the solutions to these equations and calculate the reflection and transmission coefficients for this process. We show that combining the results for spin up and down electrons leads to the quantum mechanical result for the reflection and transmission coefficients. Our analyses makes specific predictions about the manner in which spin up electrons can scatter off a step potential.

The paper is organized as follows: In section 2 we present a fundamental form of the Schrodinger equation in 1D and discuss the probability and current densities. We further discuss the plane wave solutions to this equation. We show that combining the results for spin up and down electrons leads to the quantum mechanical result for the reflection and transmission coefficients. Our analyses makes specific predictions about the manner in which spin up electrons can scatter off a step potential.

2 An Equation Underlying The Schrodinger Equation in 1D

In this section we present an equation that, even in the non-relativistic limit, can be seen as an underlying equation to the Schrodinger equation. The Schrodinger equation can be derived from this equation similar to the manner in which the Klein Gordon equation can be obtained from the Dirac equation. We restrict ourselves to a single spatial dimension (say, $z$) in this and the following sections. We will briefly discuss the problem involved in extending the equation to 3D in section 4. Our conclusions are presented in section 5.

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Here $\eta$ and $\eta^\dagger$ are matrices that obey certain relations described below. Using iteration the above equation leads to the following

$$(-i\partial_z)^2 \psi = (i\eta\partial_t)^2 \psi + i m \{\eta, \eta^\dagger\} \partial_t \psi + (\eta^\dagger)^2 m^2 \psi \quad (2)$$

In order to obtain the Schrodinger equation the matrices $\eta$ and $\eta^\dagger$ should satisfy the following properties

$$\eta^2 = 0 \quad (3)$$
$$\eta^\dagger_2 = 0 \quad (4)$$
$$\{\eta, \eta^\dagger\} = 2I \quad (5)$$

We find that the minimum dimension for the matrices $\eta$ that satisfy the relations above is four. Therefore, the matrices $\eta$ are $4\times4$ nilpotent matrices and the only eigenvalue of these matrices is 0. Furthermore, the trace and determinant of these matrices are also zero. The wave function $\psi$ in equation (1) is therefore a column matrix with four components. There are several possible representations of the matrix $\eta$. For instance, two possible representations of this matrix are as follows

$$\eta = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & -i & 0 & -1 \\ -i & 0 & 1 & 0 \\ 0 & 1 & 0 & -i \\ -1 & 0 & -i & 0 \end{pmatrix} = \frac{-i}{\sqrt{2}} \begin{pmatrix} \sigma_1 & \sigma_2 \\ -\sigma_2 & \sigma_1 \end{pmatrix} \quad (6)$$

and

$$\eta = \frac{i}{\sqrt{2}} \begin{pmatrix} 0 & I + \sigma_2 \\ I - \sigma_2 & 0 \end{pmatrix} \quad (7)$$

where $\sigma_i$ are the Pauli matrices. The matrix $\eta$ is symmetric ($\eta^T = \eta$) but not hermitian, therefore, $\eta^\dagger = \eta^\dagger \neq \eta$. For our analysis herein, we choose the representation in equation (6). The choice of this representation is primarily because the eigenstates corresponding to this representation are more relevant for the analysis in the following sections.

**Probability Current**

Multiplying equation (1) with $\psi^\dagger(\eta + \eta^\dagger)$ from the left we obtain the following equation

$$-i \psi^\dagger(\eta + \eta^\dagger) \partial_z \psi = (i\psi^\dagger \eta^\dagger \eta \partial_t) \psi + m \psi^\dagger \eta^\dagger \psi \quad (8)$$

Similarly, taking the complex conjugate of equation (1) and multiplying by $(\eta + \eta^\dagger)\psi$ on the right we obtain the following equation

$$i \partial_z \psi^\dagger(\eta + \eta^\dagger) \psi = (-i \partial_t \psi^\dagger \eta^\dagger \eta) \psi + m \psi^\dagger \eta^\dagger \psi \quad (9)$$
Subtracting (8) from (9) we obtain the continuity equation

\[ i\partial_z[(\psi^\dagger(\eta + \eta^\dagger)\psi)] = -i\partial_t[\psi^\dagger\eta^\dagger\eta\psi] \]  

(10)

with the probability and current densities given as

\[ J = \psi^\dagger(\eta + \eta^\dagger)\psi \]  

(11)

\[ \rho = \psi^\dagger\eta^\dagger\eta\psi \]  

(12)

The probability and current densities are therefore hermitian. For the representation of \( \eta \) in (6), \( \eta + \eta^\dagger = -i\sqrt{2}\gamma_2 \) and \( \eta^\dagger\eta = I + i\gamma_3 \), where \( \gamma_i \) are the gamma matrices.

### 2.1 Plane Wave Solutions

We first consider motion along a single (z) direction and seek plane wave solutions of equation (1) of the form

\[ \psi = u(p)e^{-ipz} = u(p)e^{-i(E-t-pz)} \]  

(13)

where, \( E = p_z^2/2m \). Therefore, in momentum space equation (1) becomes

\[ p_z \psi = (E\eta + mn^\dagger)\psi \]  

(14)

The above equation is an eigenvalue equation with the momentum operator given as, \( \hat{P} = E\eta + \eta^\dagger m \), which is not hermitian. However, the eigenvalues of this operator are real. The eigenvectors of the matrix \( E\eta + mn^\dagger \) consists of two states with eigenvalues of momentum \( \pm \sqrt{2Em} = p_z \) and two other with states \( -\sqrt{2Em} = -p_z \). This is consistent with the energy momentum relationship of particles in quantum mechanics, \( E = p_z^2/2m \). Following are the eigenstates of the matrix \( E\eta + \eta^\dagger m \),

\[ u^{(1)} = \begin{pmatrix} 1 \\ 0 \\ i\alpha(E - m) \\ -\sqrt{2}\alpha p_z \end{pmatrix}, \quad u^{(2)} = \begin{pmatrix} 0 \\ 1 \\ \sqrt{2}\alpha p_z \\ -i\alpha(E - m) \end{pmatrix} \]  

(15)

\[ u^{(3)} = \begin{pmatrix} 1 \\ 0 \\ i\alpha(E - m) \\ \sqrt{2}\alpha p_z \end{pmatrix}, \quad u^{(4)} = \begin{pmatrix} 0 \\ 1 \\ -\sqrt{2}\alpha p_z \\ -i\alpha(E - m) \end{pmatrix} \]  

(16)

where \( \alpha = 1/(E + m) \) and \( p_z = \sqrt{2Em} \). The eigenstates \( u^{(1)} \) corresponds to a spin up particle with positive momentum and \( u^{(2)} \) corresponds to spin down particle with the same momentum. The eigenstates \( u^{(3)} \) and \( u^{(4)} \) correspond to particles with negative momentum, i.e.,
moving in the negative $z$ direction. The eigenstates are related as $u^{(1)}(p_z) = u^{(3)}(-p_z)$ and $u^{(2)}(p_z) = u^{(4)}(-p_z)$. We will employ these eigenstates in the following section when we study the scattering problem. The normalization condition for the eigenstates are

$$u^{(1)*}u^{(1)} = 2$$  \hspace{1cm} (17)  \\
$$u^{(1)*}u^{(2)} = 0$$  \hspace{1cm} (18)

and similarly for $u^{(3)}$ and $u^{(4)}$. Since the energy momentum relationship of these states does not follow the relativistic expression, it is not relevant to discuss how these states transform under Lorentz transformations.

3 Potential Step problem

The potential step problem is one of the foundational examples in quantum mechanics (Figure 1). As described earlier, solving this problem with the Dirac equation leads to the Klein paradox. In this section we analyze this problem for electron scattering from a potential step in 1 dimension using the solutions presented in previous sections. We will show that the resulting transmission and reflection coefficients for spin up and down particles are related to the ones in quantum mechanics. For regions $I$ and $II$, equation (14) is given by

$$p_1 \psi = (E\eta + m\eta^\dagger) \psi$$  \hspace{1cm} (19)  \\
$$p_2 \psi = ((E - V_0)\eta + m\eta^\dagger) \psi$$  \hspace{1cm} (20)
3.1 Case I: $E > V_0$

We first consider the case of a spin up electron incident on a potential step with energy $E > V_0$. The incident and reflected electron waves in region $I$ are given by

$$
\psi_I = A \begin{pmatrix} 1 \\ 0 \\ i\alpha(E - m) \\ -\sqrt{2}\alpha p_1 \end{pmatrix} e^{ip_1 z} \tag{21}
$$

$$
\psi_I' = B \begin{pmatrix} 1 \\ 0 \\ i\alpha(E - m) \\ \sqrt{2}\alpha p_1 \end{pmatrix} e^{-ip_1 z} + B' \begin{pmatrix} 0 \\ 1 \\ \sqrt{2}\beta p_2 \\ -i\beta(E - V_0 - m) \end{pmatrix} e^{-ip_2 z} \tag{22}
$$

Similarly for region $II$ we have

$$
\psi_{II} = C \begin{pmatrix} 1 \\ 0 \\ i\beta(E - V_0 - m) \\ -\sqrt{2}\beta p_2 \end{pmatrix} e^{ip_{2z}} + C' \begin{pmatrix} 0 \\ 1 \\ \sqrt{2}\beta p_2 \\ -i\beta(E - V_0 - m) \end{pmatrix} e^{ip_{2z}} \tag{23}
$$

where $\alpha = 1/(E + m)$, $\beta = 1/(E - V_0 + m)$, $p_1 = \sqrt{2Em}$ and $p_2 = \sqrt{2(E - V_0)m}$. At $z = 0$ the continuity of the wave function implies

$$
\psi_I(z = 0) + \psi_I'(z = 0) = \psi_{II}(z = 0) \tag{24}
$$

From this condition the coefficients are found to be

$$
\frac{B}{A} = \frac{(-E + m)V_0}{(E + m)(2E + 2\sqrt{E(E - V_0)} - V_0)} \tag{25}
$$

$$
B' = C' \tag{26}
$$

$$
\frac{C}{A} = \frac{-2E^2 - 2m\sqrt{E(E - V_0)} + 2E(m + \sqrt{E(E - V_0)} + V_0)}{(E + m)V_0} \tag{27}
$$

$$
\frac{C'}{A} = \frac{2i\sqrt{Em}V_0}{(E + m)(2E + 2\sqrt{E(E - V_0)} - V_0)} \tag{28}
$$
Figure 2: The plot shows the transmission and reflection coefficients for spin up and down electrons given in equations (A-1), (A-2), (A-3) and (A-4). The red lines show the coefficients of spin up electron and the blue lines correspond to spin down electron. The value of the potential step is chosen to be \( V_0 = 100 \) eV. For \( E \approx V_0 \) there is no transmission and the electron is completely reflected with its spin up. For \( E \) slightly greater than \( V_0 \), the transmission of spin up and down electron occurs with nearly equal probabilities. For \( E/V_0 \gtrsim 1.05 \) the transmitted electron is dominantly spin up. The lower panel shows the reflection coefficients. We can see that there is a very small probability that the reflected electron has its spin flipped. The reflection coefficient for spin down is small but non-zero. As the energy increases the barrier appears more and more transparent to the electron and the transmission coefficient of the spin up electron becomes large. For \( E \approx 3V_0 \) the barrier is nearly transparent to the electron.
Figure 3: Plot shows the reflection coefficients (A-3) and (A-4) for $V_0 = 100$ keV and $V_0 = 1$ MeV. The red lines correspond to spin up electrons whereas the blue lines are for spin down electron. The plot of the transmission coefficients for these cases are similar to the one shown in Figure 2. We can observe that the reflection coefficient changes notably as the height of the barrier is increased. For $V_0 = 100$ keV, the probability of the spin up electron being reflected as a spin up or down electron is nearly equal. For $V_0 = 1$ MeV, the electron is dominantly reflected with its spin flipped.
The transmission and reflection coefficients \( T_1, T_2, R_1 \) and \( R_2 \) are given by

\[
T_1 = \frac{(E + m)(E - V_0)^{1/2}}{(E - V_0 + m)^{1/2}} \left| \frac{C}{A} \right|^2, \quad T_2 = \frac{(E + m)(E - V_0)^{1/2}}{(E - V_0 + m)^{1/2}} \left| \frac{C'}{A} \right|^2
\] (29)

\[
R_1 = \left| \frac{B}{A} \right|^2, \quad R_2 = \left| \frac{B'}{A} \right|^2
\] (30)

The complete expression for these coefficients are presented in the appendix in equations (A-1), (A-2), (A-3) and (A-4). The sum of these coefficient is always equal to 1, i.e.,

\[
(T_1 + T_2) + (R_1 + R_2) = 1
\] (31)

The quantum mechanical transmission and reflection coefficients are related to these coefficients as

\[
T_{QM} = T_1 + T_2 = \frac{4E^{3/2}\sqrt{E - V_0}}{(\sqrt{E} + \sqrt{E - V_0})^2}
\] (32)

\[
R_{QM} = R_1 + R_2 = \left( \frac{\sqrt{E} - \sqrt{E - V_0}}{\sqrt{E} + \sqrt{E - V_0}} \right)^2
\] (33)

We can see that although the reflection and transmission coefficients \( T_1, T_2, R_1 \) and \( R_2 \) depend on the mass of the incident particle, the sum, which is the quantum mechanical result, is independent of it. The current densities for the incident, reflected and transmitted spin up and down particle are given by

\[
J^\uparrow_I = \psi_1^\dagger(\eta + \eta^\dagger)\psi_I = \frac{4|A|^2p_1}{E + m}
\] (34)

\[
J^\uparrow_r = \psi_r^\dagger(\eta + \eta^\dagger)\psi_r = -\frac{4p_1|B|^2}{E + m}
\] (35)

\[
J^\uparrow_r = \psi_r^\dagger(\eta + \eta^\dagger)\psi_r = -\frac{4p_1|B'|^2}{E + m}
\] (36)

\[
J^\uparrow_T = \psi_T^\dagger(\eta + \eta^\dagger)\psi_T = \frac{4p_2|C|^2}{E + m - V_0}
\] (37)

\[
J^\uparrow_T = \psi_T^\dagger(\eta + \eta^\dagger)\psi_T = \frac{4p_2|C'|^2}{E + m - V_0}
\] (38)

The conservation of probability density implies

\[
\frac{|J^\uparrow_I|}{|J^\dagger_I|} + \frac{|J^\uparrow_r|}{|J^\dagger_r|} + \frac{|J^\uparrow_T|}{|J^\dagger_T|} + \frac{|J^\uparrow_T|}{|J^\dagger_T|} = 1
\] (39)
\[
\frac{|B|^2}{|A|^2} \frac{(E + m)(E - V_0)^{1/2}}{(E - V_0 + m)E^{1/2}} \frac{|C|^2}{|A|^2} + \frac{|B'|^2}{|A|^2} \frac{(E + m)(E - V_0)^{1/2}}{(E - V_0 + m)E^{1/2}} |C'|^2 = 1 \quad (40)
\]

which agrees with the calculations of the transmission and reflection coefficient. Figure 2 shows the plot of the transmission and reflection coefficients. We can see from this Figure that when the energy of the incident electron is close to the height of the barrier the electron is completely reflected. As the energy of the electron increases relative to the barrier the reflection coefficient falls sharply and the electron is mostly transmitted as spin up. There is however a small probability that the transmitted electron flips its spin as well. This can be seen from the blue line in the upper panel of Figure 2. We show the reflection coefficients for \( V_0 = 100 \text{ keV} \) and \( 1 \text{ MeV} \) in Figure 3. We can see that the spin of the reflected electron depends on the height of the potential barrier. For \( V_0 < m_e \) the reflected electron is dominantly spin up (Figure 2) whereas for \( V_0 = 1 \text{ MeV} > m_e \), the electron is mostly reflected with spin down. The upper panel of Figure 3 shows an intermediate situation when the probabilities of reflection of electron as spin up and down are comparable.

### 3.2 Case II: \( E < V_0 \)

We next analyze the case when the energy of the incident electron is less than the height of the barrier. The equations for incident and reflected electron in region \( I \) remain the same as equations (19) and (20). For the transmitted electron in region \( II \), however, the equation is now given by

\[
\begin{align*}
ip_2' \psi &= [-(V_0 - E)i\eta + m_\eta^\dagger] \psi \\
(II)
\end{align*}
\]

The operator \( \hat{P} = -(V_0 - E)i\eta + m\eta^\dagger \) has eigenvalues \( \pm i\sqrt{2(V_0 - E)m} = \pm ip_2' \). We choose the eigenvalue \( ip_2' \) which imply a decaying wave (\( \psi = u(p)e^{-ip.z} = u(p)e^{-iE't}e^{-p.z} \)) within the barrier. We choose the eigenvectors corresponding to eigenvalue \( ip_2' \) for spin up and down electrons in region \( II \). The wave function in region \( II \) is therefore given by

\[
\psi''_I = D \begin{pmatrix}
1 \\
i\rho(V_0 - E + m) \\
\sqrt{2i\rho \ p_2'}
\end{pmatrix} e^{-p_2'z} + D' \begin{pmatrix}
0 \\
1 \\
-\sqrt{2i\rho \ p_2'}
\end{pmatrix} e^{-p_2'z} \quad (42)
\]

where \( \rho = 1/(V_0 - E - m) \) and \( p_2' = \sqrt{2m(E - V_0)} \). From the continuity condition (24) we find the coefficients for this case as well. These are presented in equations (A-5), (A-6) and (A-7) and (A-8) of the Appendix. The reflection coefficients \( R'_1 = |B/A|^2 \) and \( R'_2 = |B'/A|^2 \) coefficients are given by

\[
R'_1 = \frac{(E - m)^2}{(E + m)^2} \quad (43)
\]

\[
R'_2 = \frac{4Em}{(E + m)^2} \quad (44)
\]
Figure 4: Figure shows the plot of the reflection coefficients for the case when energy of the incident electron is less than the height of the barrier, $E < V_0$. The coefficients are given in equations (43) and (44). For very small values of energy the incident spin up electron is reflected without a change in its spin. As the energy of the incident electron increases the probability that it flips its spin upon reflection increases considerably.

The sum of these coefficients is always equal to one. The current densities for the transmitted wave ($J_↑^T$ and $J_↓^T$) is zero in this case and therefore there is essentially no wave transmitted in the barrier. Moreover, the reflection coefficients are independent of the height of the barrier for $E < V_0$. The probability of the reflection of spin up and down electrons is shown Figure 4. We can see that for very small energies the incident spin up electron is reflected with the same spin. As the energy of the electron increases, the probability that it is reflected with the spin flipped increases considerably.

4 Extending to 3D

In the previous sections we saw how solutions of equation (1) leads to the transmission and reflection coefficients of the spin up and down electron scattering for the case of an electron scattering off a potential step. The analysis was performed in 1 dimension. For 2 and 3 dimensions the analysis is more subtle since equation (1) takes the following form in 3D

$$-i\sqrt{\Delta}\psi = (i\eta\hat{\partial}_t + \eta^\\dagger m)\psi$$

(45)

where $\Delta \equiv \partial^i\partial_i = \nabla_x^2 + \nabla_y^2 + \nabla_z^2$. Solving the above equation by iteration again leads to the Schrodinger equation in 3 dimensions. The matrices obey the same properties as before.
Problems are encountered when we write the above equation in the form of a continuity equation which appears problematic since it involves the square root of $\Delta$. The 1D analysis, however, can be applied to a wide variety of problems in quantum mechanics and needs to be further tested by applying it to other similar problems.

5 Conclusion

We proposed that the Schrodinger equation in 1D can be derived from a more fundamental equation given in (1). Nilpotent matrices that obey anti-commutation relation (5) were introduced for this purpose. We further constructed the solutions of this equation and employed these to solve the problem of a spin up electron scattering from a potential step. We show that issues such as the Klein paradox do not arise in this case and the quantum mechanical transmission and reflection coefficients are obtained as the sum of those for the spin up and down electron. Further investigation is required by applying this equation to other similar problems in quantum mechanics.

Appendix A

Transmission and Reflection Coefficients for $E > V_0$

\[
T_1 = \frac{(E + m)(E - V_0)^{1/2}}{(E - V_0 + m)E^{1/2}} \left| \frac{C}{A} \right|^2
\]

\[
= \frac{4\sqrt{1 - \frac{V_0}{E}} \left( E^2 + m\sqrt{E(E - V_0)} - E \left( m + \sqrt{E(E - V_0)} + V_0 \right) \right)^2}{(E + m)(E + m - V_0)V_0^2}
\]  \hfill (A-1)

\[
T_2 = \frac{(E + m)(E - V_0)^{1/2}}{(E - V_0 + m)E^{1/2}} \left| \frac{C'}{A} \right|^2
\]

\[
= \frac{4m\sqrt{E(E - V_0)V_0^2}}{(E + m)(E + m - V_0) \left( -2E - 2\sqrt{E(E - V_0)} + V_0 \right)^2}
\]  \hfill (A-2)
\[ R_1 = \left| \frac{B}{A} \right|^2 = \frac{(E - m)^2 V_0^2}{(E + m)^2 \left( -2E - 2 \sqrt{E(E - V_0)} + V_0 \right)^2} \]  
(A-3)

\[ R_2 = \left| \frac{B'}{A} \right|^2 = \frac{4EmV_0^2}{(E + m)^2 \left( -2E - 2 \sqrt{E(E - V_0)} + V_0 \right)^2} \]  
(A-4)

Coefficients for \( E < V_0 \)

\[ \frac{B}{A} = \frac{(-E + m)V_0}{(E + m) \left( 2E - V_0 + 2i \sqrt{E(-E + V_0)} \right)} \]  
(A-5)

\[ \frac{B'}{A} = \frac{2\sqrt{EmV_0}}{(E + m) \left( -2iE + iV_0 + 2\sqrt{E(-E + V_0)} \right)} \]  
(A-6)

\[ \frac{D}{A} = \frac{2 \left( E^2 + E(m - V_0) + i \left( m \sqrt{E(-E + V_0)} + \sqrt{E^3(-E + V_0)} \right) \right)}{(E + m) \left( 2E - V_0 + 2i \sqrt{E(-E + V_0)} \right)} \]  
(A-7)

\[ \frac{D'}{A} = \frac{2\sqrt{EmV_0}}{(E + m) \left( -2iE + iV_0 + 2\sqrt{E(-E + V_0)} \right)} \]  
(A-8)

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