Dirac Equation

in 1D with Periodic Boundary Conditions

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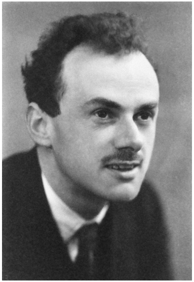
Background

The Dirac Equation is named after the great mathematical physicist Paul Dirac. He is best known for his seminal work in Quantum Mechanics and is considered the father of Quantum Electrodynamics. He was awarded the 1933 Nobel Prize in Physics for his foundational work of atomic theory, along with Erwin Schrödinger. The 'dirac' is a unit of one word per hour, which jokingly made fun of how often he spoke.



The Problem

For high kinetic energy levels the Schrödinger equation no longer provides an accurate description. In this regime special relativity can no longer be cast as negligible. Thus, the Dirac equation is a better description for the electron with high kinetic energy. [1,2,3]

Dirac Equation

The Dirac Equation can be expressed succinctly in natural units as,

$$(i\partial\!\!\!/ - m)\Psi = 0, \tag{1}$$

and is fundamental in the development of a relativistic theory for spin 1/2 massive particles, such as electrons or quarks. [4]

This representation is extremely elegant and simple but quite deceiving. Natural units are used with,

$$\hbar = c = 1,$$

and the Feynman slash notation is defined as,

$$\not{\partial} \equiv \gamma^{\mu} \partial_{\mu}$$

This gives the Dirac Equation a more practical representation of,

$$(i\hbar\gamma^{\mu}\partial_{\mu} - mc)\Psi = 0 \tag{2}$$

The Dirac equation utilizes the Einstein summation notation convention. Symbols with repeated indices in covariant (subscript) and contravariant (superscript) positions are summed over, *e.g.*

$$\gamma^\mu \partial_\mu = \sum_{i=0}^{3} \gamma^i \partial_i = \gamma^0 \partial_0 + \gamma^1 \partial_1 + \gamma^2 \partial_2 + \gamma^3 \partial_3.$$

The γ matrices are defined as,

$$\gamma^0 = \begin{bmatrix} \mathbb{1} & 0 \\ 0 & -\mathbb{1} \end{bmatrix},\ \gamma^i = \begin{bmatrix} \sigma_i & 0 \\ 0 & \sigma_i \end{bmatrix},\ i = 1, 2, 3$$

$$\text{where,}\ \ \sigma_1 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix},\ \sigma_2 = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix},\ \sigma_3 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}.$$

Spinor Theory

Dirac utilized spinors to handle the intrinsic spin property of these fundamental particles. This results in Ψ being a "bi-spinor", $\Psi = [\Psi_{E>0}, \Psi_{E<0}]^T$, where $\Psi_{E>0} = [|\uparrow\rangle, |\downarrow\rangle]^T$ and $\Psi_{E<0} = [|\uparrow\rangle, |\downarrow\rangle]^T$.

These vector quantities do not transform like a normal 4-vector and require a bit more care, as to conform to the Pauli Exclusion Principle. We will come to see that this describes an electron and its anti-particle; the positron.

Dirac Equation in One-Dimension

Consider the Dirac Equation in 1D with normal units,

$$(i\gamma^0\partial_t + i\gamma^1\partial_x - m)\Psi = 0.$$

Carrying out the matrix multiplication reduces to the system,

$$\begin{cases} \psi_{1t} + \psi_{1x} = -i\psi_1 \\ \psi_{4t} + \psi_{1x} = i\psi_4. \end{cases}$$

Thus, we can see that in 1D, $\Psi(t, \vec{x}) = [\psi_1, 0, 0, \psi_4]^T$. We shall set $m = 1$ for simplicity.

Approach

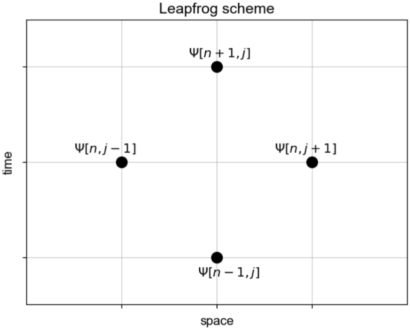
The Leapfrog Scheme (LFS) is implemented with a periodic boundary conditions.

The (t, x) plane is discretized into a mesh grid of dimensions $N \times M$ where N and M are the lengths of the t and x arrays; respectively.

$$t = t_0 + n\delta t, \;\; n = 0, ..., N$$
$$x = x_0 + j\delta x, \;\; j = 0, ..., M$$

Stencil

LFS implemented for the numeric solution is based upon the scheme that was used for the one-way wave equation and was adapted from Strikwerda. [5]



The Leapfrog scheme looks backwards two time steps for the temporal derivative and only one time step backwards for a central spatial derivative.

Implementation

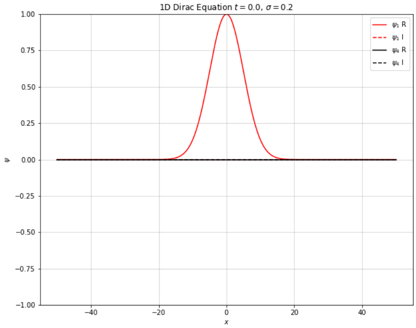
After applying the LFS to the 1D Dirac Equation, we obtain the update formulas,

$$
\begin{aligned}
u_j^n &= u_j^{n-2} - \lambda(v_{j+1}^{n-1} - v_{j-1}^{n-1}) - i\,\delta t\, u_j^{n-1} \\
v_j^n &= v_j^{n-2} - \lambda(u_{j+1}^{n-1} - u_{j-1}^{n-1}) - i\,\delta t\, v_j^{n-1}.
\end{aligned}
$$

Initial Condition

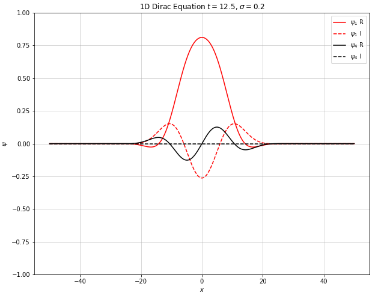
For $x \in [-50, 50]$ at $t = 0$ with $\delta x = 0.1, \delta t = 0.01$, $\sigma = 0.2$, we have a wide wave packet.

$$\Psi(0, x) = e^{-\sigma^2 x^2/2} \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

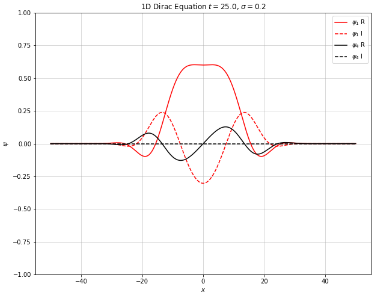


Initially, there is just an electron with spin up and positive energy. The negative energy wave function is not present and has an amplitude of zero.

As we evolve time we can see that the wave function for the positron becomes nonzero and influences the electron's wave function; as expected.

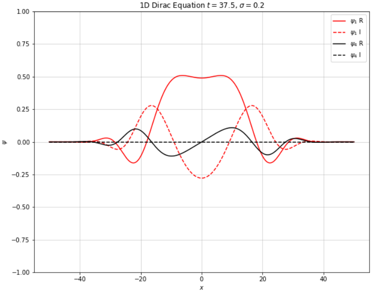


The positron waveform slowly grows while the electron wave function decreases in amplitude.

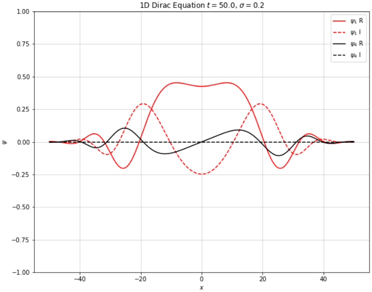


The waveforms oscillate and diffuse in a slow Smooth manner.

As time evolves even more the waveforms spread out and become nonlocalized. In particular, the diffusion is rather slow for a wide wave packet.



The waves spreads slowly outwards towards infinity in a symmetric fashion.



Nonlocalization of the waveform is a process which is quite similar to diffusion.

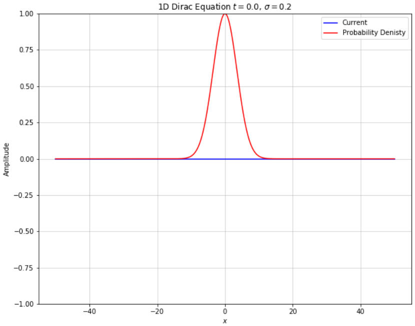
Probability Density and Current

The probability density of finding an electron at any given point in a space time region is given by,

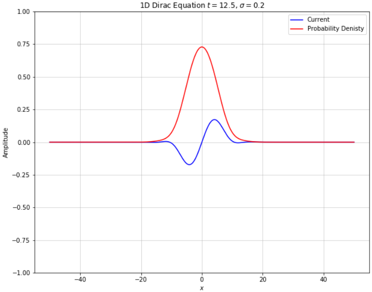
$$P(t, x) = |\psi_1|^2 + |\psi_4|^2 \tag{3}$$

$$J(t, x) = \overline{\psi}_1 \psi_4 + \overline{\psi}_4 \psi_1. \tag{4}$$

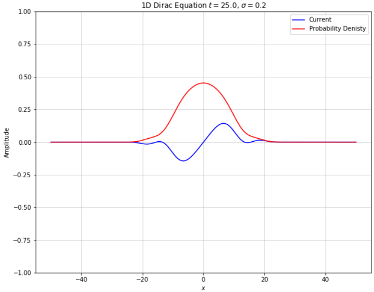
$$\text{where } P_t + J_x = 0 \tag{5}$$



As the system evolves the probability density decays; very much like the diffusion that occurs in the heat equation.

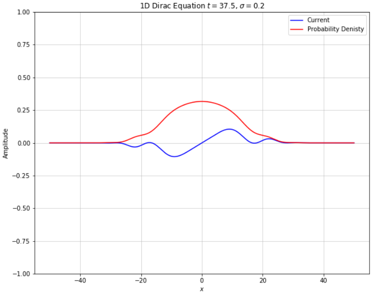


The positron waveform slowly grows while the electron decreases in amplitude.

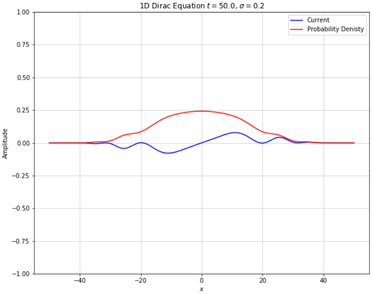


The probability density exhibits diffusive behavior while the current is symmetric with respect to the origin.

The diffusion of the probability density function becomes more apparent over time and the current maintains a net zero distribution.



The diffusive behavior persists and the current spreads.

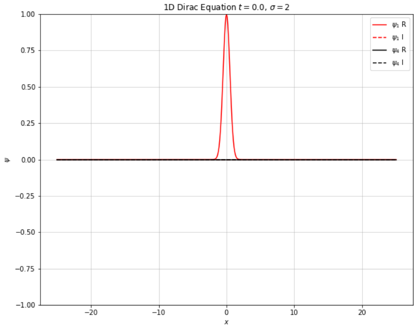


As t goes to infinity we would expect to observe the electron anywhere in space equally as a consequence of diffusion.

Different Behavior

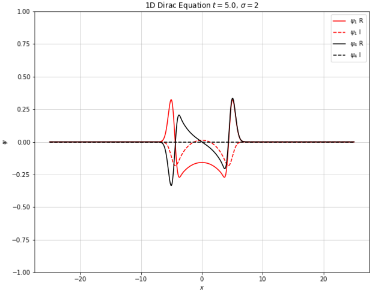
For $x \in [-25, 25]$ at $t = 0$ with $\delta x = 0.1, \delta t = 0.01$, $\sigma = 2$, we have a narrow wave packet.

$$\Psi(0, x) = e^{-\sigma^2 x^2/2} \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

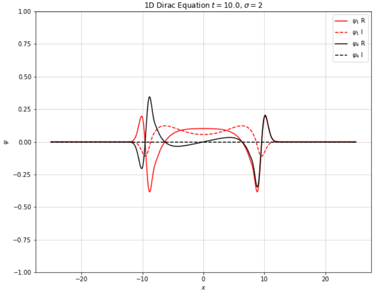


Initially, there is just an electron with spin up and positive energy. The negative energy wave function is not present and has an amplitude of zero.

As we evolve time we can see that the wave functions behave quite differently than before.

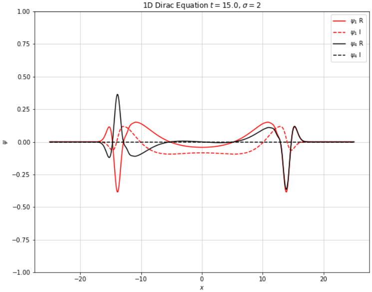


The waveforms style display a symmetric type of behavior but quickly part ways.

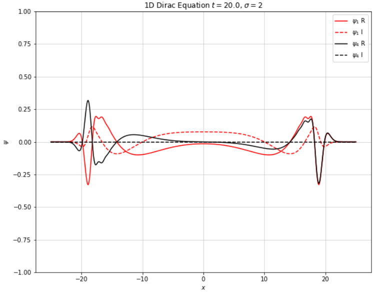


This split in the wave functions is a result of localization.

The wave functions have separated quickly and, as we will see if the probability density plot, that we would not expect to observe the particle again in its starting location.



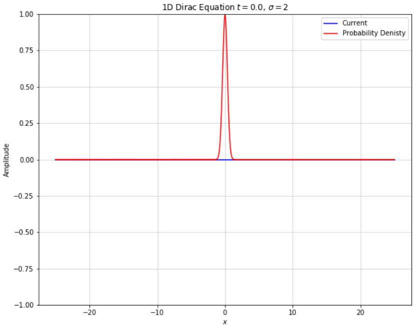
The particles have separated even more and are traveling away from each other.



The same behavior persists as t increases.

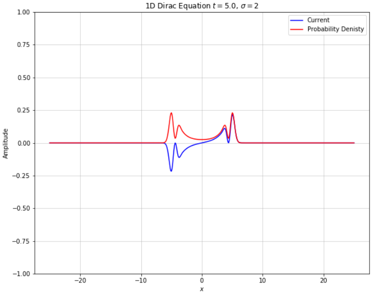
Probability Density and Current

The probability density function is a sharp spike for the narrow initial wave packet.

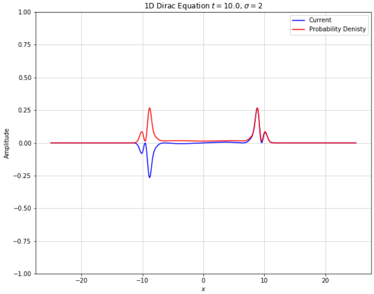


The Heisenberg Uncertainty Principle suggests that if we are quite sure of the position then we are rather unsure of the momentum.

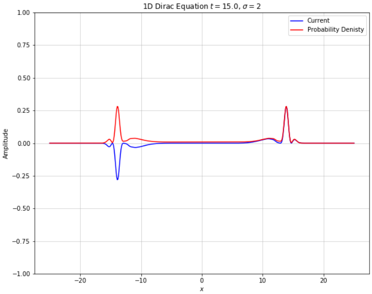
The probability density decays rapidly As the system evolves and splits into two separate distributions that travel in opposite directions.

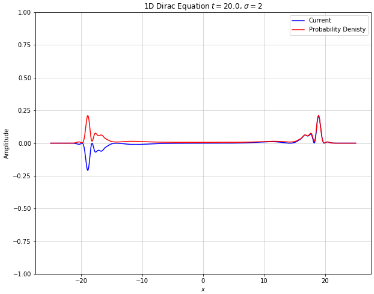


The current quickly grows in amplitude while the probability quickly decreases.



The two functions diffuse and spread. This is a result of extreme localization.



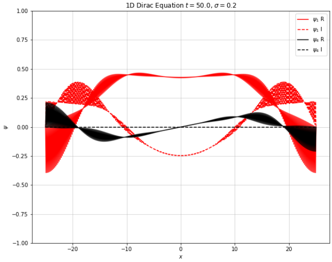


The seperation behavior persists and the wave forms disperses.

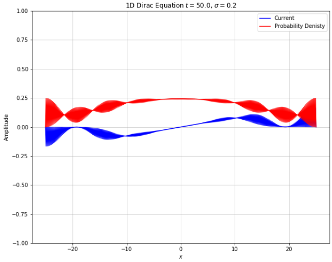
After some time, the wave functions ‘part ways’ and travel in opposite directions; far away from each other.

Drawbacks

The issue with the periodic boundary conditions arises when the wave function. This results in undesired physical behavior. This can be avoided by placing the boundaries ‘far away’.



The wave functions behave erratically when periodic boundary conditions were applied.



The probability density and current functions will have similar behavior.

Recap

We were able to observe that a positron was created through the time evolution of the Dirac equation and that there was a high level of symmetry in the system. The periodic boundary conditions imposed give rise to undesired behavior; something like noise that propagates. This can be avoided by establishing our boundaries ‘at infinity’.

Next Steps

- Implement Crank-Nicolson

$$\left(1+i\frac{k}{2}\right)u_m^{n+1}+\frac{\lambda}{4}\left(v_{m+1}^{n+1}-v_{m-1}^{n+1}\right)=\left(1-i\frac{k}{2}\right)u_m^{n}+\frac{\lambda}{4}\left(v_{m-1}^{n}-v_{m+1}^{n}\right)$$
$$\frac{\lambda}{4}\left(u_{m+1}^{n+1}-u_{m-1}^{n+1}\right)+\left(1-i\frac{k}{2}\right)v_m^{n+1}=\left(1+i\frac{k}{2}\right)v_m^{n}+\frac{\lambda}{4}\left(u_{m-1}^{n}-u_{m+1}^{n}\right)$$

- Error Analysis
- Demonstrate Zitterbewegung
- Reconstruct the Hydrogen Orbitals
  - Fine Structure
  - Spin-Orbit Coupling
  - Darwin Term

References

[1] Roig, Francesc. “Relativistic Quantum Mechanics.” Lecture Notes, UCSB CCS Physics, Santa Barbara, 2009.

[2] Bao, Weizhu, Yongyong Cai, Xiaowei Jia, and Qinglin Tang. ”Numerical Methods and Comparison for the Dirac Equation in the Nonrelativistic Limit Regime.” SpringerLink. January 18, 2017. Accessed May 02, 2019. JSci

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[4] Khruschov, and V. V. ”Some Examples of Uses of Dirac Equation and Its Generalizations in Particle Physics.” ArXiv.org. April 13, 2010. Accessed May 04, 2019. arXiv

[5] Strikwerda, John C. *Finite Difference Schemes and Partial Differential Equations.* Philadelphia, PA: SIAM, 2004.