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Class: Math 693B - Advanced Computational PDE **Date**: May 8, 2019

One-Dimensional Dirac Equation with Zero at Infinity

The Dirac Equation is one of the most elegant equations in all of mathematics and physics. This is a bold statement and needs little to no justification. Paul A. M. Dirac was an English mathematical physicist from the 20th century who made significant contributions to the development of atomic theory, in which he was awarded a Nobel Prize along with Erwin Schrödinger; also, Dirac made contributions to the field of general relativity, in an attempt to reconcile it with quantum mechanics. [1][2][3]

The goal of this paper is to apply a finite difference scheme (FDS) to approximate the one dimensional Dirac equation and explore the implications. I will apply the Leapfrog scheme (LFS) FDS to the system of equations generated by,

$$i\hbar\gamma^{\mu}\partial_{\mu}\Psi - mc\Psi = 0, \tag{1}$$

where $\Psi = \left[\psi_{E_+}, \psi_{E_-}\right]^T$ is the 'bi-spinor' wave function and ψ_{E_+}, ψ_{E_-} are the positive and negative energy spinors, respectively.

We will come to see that the positive and negative energy states of the particle being describes give rise to anti-matter; specifically, in the event that the particle being described is an electron, the positive energy state describes an electron and the negative energy state describes a positron.

Derivation

Dirac initially sought to reconcile quantum mechanics with special relativity. He approached this problem in a clever way by simply analyzing what the energy for a relativistic would be. The reason for this is that the Schrödinger equation,

$$i\hbar\frac{\partial}{\partial t}\psi = \frac{-\hbar^2}{2m}\nabla^2\psi + V\psi, \tag{2}$$

should either be symmetric in time, or symmetric in space. We shall inspect this equation to determine if either is the case. Our goal is to obtain a Lorentz invariant system which obeys the principles of special relativity and can be properly quantized. We will begin by starting with the relativistic expression for the energy of a particle,

$$E = \sqrt{p^2c^2 + m^2c^4}. \tag{3}$$

If we attempt to apply the quantization operators,

$$\hat{E} \to i\hbar\partial_t, \ \hat{p} \to -i\hbar\nabla, \tag{4}$$

to this expression then we can obtain the equation,

$$i\hbar\partial_t\psi = \sqrt{-(\hbar c)^2\nabla^2 + m^2c^4}\psi. \tag{5}$$

There is a serious problem. We do not know what it means to take the square root of the Laplacian, ∇^2. Perhaps, we can square both sides to obtain,

$$E^2 = p^2c^2 + m^2c^4. \tag{6}$$

If we were to substitute operators and apply a wave function to both sides then we arrive at the Klein-Gordon equation,

$$-\hbar^2\partial_t^2\psi = -\hbar^2c^2\nabla^2\psi + m^2c^4\psi. \tag{7}$$

The problem here is that this will not apply to the electron, in fact the Klein-Gordon equation only applies to spin 0 particles. Note that it is on equal footing with regards to the temporal and spatial derivative. Another issue is that only the positive energy states are allowed for the Klein-Gordon equation and that, in order for this equation to properly adhere to quantum mechanics it must obey the transformation,

$$i\hbar\frac{\partial|\psi\rangle}{\partial t} = \hat{H}|\psi\rangle, \tag{8}$$

which is *linear* in ∂_t and not of order 2. This is due, in part, to the Heisenberg Uncertainty Principle because we cannot simultaneously describe position and velocity.

$$\Delta x\Delta p \geq \frac{\hbar}{2} \tag{9}$$

Furthermore, we can disclude the Klein-Gordon equation by demonstrating that the wave function does not satisfy the continuity equation,

$$\frac{\partial\rho}{\partial t} + \nabla\cdot\vec{j} = 0. \tag{10}$$

For the remainder of the derivation, natural units will be used to simplify matters; this amounts to setting $\hbar = c = 1$. This is common practice among physicists and reduces our energy equation to,

$$E = \sqrt{p^2 + m^2}. \tag{11}$$

Our goal now is to obtain an equation that is linear in ∂_t, so that we might satisfy the quantum mechanical eigenvalue problem. We wish to express the energy as some linear combination of momenta and mass such that,

$$E = \sqrt{p^2 + c^2} = \alpha_x p_x + \alpha_x p_x + \alpha_x p_x + \beta m \tag{12}$$

$$E^2 = p^2 + m^2 \stackrel{?}{=} (\alpha_x p_x + \alpha_x p_x + \alpha_x p_x + \beta m)(\alpha_x p_x + \alpha_x p_x + \alpha_x p_x + \beta m). \tag{13}$$

If we compute the products on the right hand side then we obtain the 4 pure terms and 12 cross terms. We want to keep the four pure terms and have the cross terms cancel. This gives us a set of conditions that will help us determine what the α_i are.

$$\alpha_i^2 = 1,\ i = x, y, z \tag{14}$$
$$\alpha_i\alpha_j + \alpha_j\alpha_i = 2\delta_{ij} \tag{15}$$
$$\alpha_i\beta + \beta\alpha_i = 0,\ \forall i \neq j \tag{16}$$

The commutation relations, $[\hat{p}_i, \hat{p}_j] = 0,\ \forall i \neq j$, imply that α_i must be zero, but we must have $\alpha_i^2 = 1$, and thus the α_i is a matrix. The α matrices are 4×4 block matrices with the Pauli matrices taking on the off-diagonal block terms. The β matrix is simply 2 2×2 on-diagonal identity matrices, where the 2nd diagonal block matrix is the negation of the identity matrix. These are the simplest non-trivial matrices that satisfy this relationship,

$$\alpha_x = \begin{bmatrix} 0 & \sigma_x \\ \sigma_x & 0 \end{bmatrix},\ \alpha_y = \begin{bmatrix} 0 & \sigma_y \\ \sigma_y & 0 \end{bmatrix},\ \alpha_z = \begin{bmatrix} 0 & \sigma_z \\ \sigma_z & 0 \end{bmatrix},\ \beta = \begin{bmatrix} \mathbb{1} & 0 \\ 0 & -\mathbb{1} \end{bmatrix}$$
$$\text{where, } \sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix},\ \sigma_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix},\ \sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}.$$

We are now able to construct the Dirac equation by inserting the indicated operators and matrices into (10) and applying the wave function to both sides. Thus, we arrive at the Dirac equation for a free electron,

$$i\partial_t\Psi = -i\alpha_x\Psi_x - i\alpha_y\Psi_y - i\alpha_z\Psi_z + m\beta\Psi. \tag{17}$$

This equation can be written more succinctly as,

$$(i\not{\partial} - m)\Psi = 0, \tag{18}$$

where Ψ is the 4-component "bi-spinor" and $\not{\partial} \equiv \gamma^\mu\partial_\mu$. This is extremely elegant and compact with extremely rich dynamics, as we shall come to see. This equation is critical to the development of Quantum Field Theory and Quantum Electrodynamics; the 'crown jewel' of physics. [4]

Dirac Equation in One Dimension

The numerical analysis of the Dirac equation shall begin in the simplest sense possible, a free particle in one dimension.

$$\begin{cases} \psi_{1t} = -i\psi_1 - \psi_{4x} \\ \psi_{4t} = i\psi_4 - \psi_{1x} \end{cases} \tag{19}$$

We shall apply the LFS utilizing the stencil and define $\psi_1 = u$ and $\psi_2 = v$ for the spatial-temporal discretization yielding

$$\begin{cases} u_t + v_x = -iu \\ v_t + u_x = iv \end{cases}, \tag{20}$$

where u describes the spin up electron and v describes the spin down positron.

The spatial domain shall be discretized so that,

$$x_m = x_{\min} + m\delta x, \text{ for } m = 0, \ldots, M \tag{21}$$

and the temporal will be discretized so that $\delta t = \lambda \delta x$. This gives the discretization of time as,

$$t_n = t_{\min} + n\delta t, \text{ for } n = 0, \ldots, N. \tag{22}$$

After applying the LFS to (19) we arrive at the update formulas for u, v as

$$u_m^n = u_m^{n-2} - \lambda(v_{m+1}^{n-1} - v_{m-1}^{n-1}) - i\,\delta t\, u_m^{n-1} \tag{23}$$
$$v_m^n = v_m^{n-2} - \lambda(u_{m+1}^{n-1} - u_{m-1}^{n-1}) - i\,\delta t\, v_m^{n-1}. \tag{24}$$

The probability density and current can be computed from Eq. (9) by the definitions,

$$P(x,t) = |\psi_1|^2 + |\psi_4|^2 \tag{25}$$
$$J(x,t) = \overline{\psi}_1\psi_4 + \overline{\psi}_4\psi_1 \tag{26}$$

Initial Conditions

The first initial condition to be used will be a real valued Gaussian wave for the electron and zero for the positron. Thus,

$$\psi_1(x,0) = e^{-\sigma^2 x^2/2} \tag{27}$$
$$\psi_4(x,0) = 0, \tag{28}$$

where $x \in [-50, 50]$ with $\delta x = 0.1, \lambda = 0.1, \delta t = 0.01, \sigma = 0.2$. This will result in a wide wave packet which will exhibit distinct dynamics. This can be seen in Fig. 2.

The second initial condition will be similar to the first but with $\sigma = 2$ to display distinctly different behavior. We will use the same system as before but with parameters $x \in [-25, 25], \delta x = 0.1, \lambda = 0.1, \delta t = 0.01, \sigma = 2$. As seen in Figure 3, the wave packet is

The reason for different x intervals is simply a matter of convenience. The dynamics have no influence at the boundaries if we set our boundary conditions to be zero at infinity. The effective boundary conditions are placed 'very far away' since infinity does not exist numerically. This is a more practical approach which is easier to implement.

Analysis

First Condition

The wave packet is distributed in a nice smooth Gaussian function. This is closely related to the probability of finding the particle in a given space time region. Since the Gaussian is wide then we are not entirely sure 'where' the particle is. The dynamics that result are a smooth oscillatory diffusing behavior that are slow in nature. This is in accordance with Eq. (26) because if the uncertainty in the position is 'small' then the uncertainty in the momentum is 'large', in comparison. Fig. [2-5]

The probability density and current plot reflects this as a slow diffusion. The amplitude of the probability density function slowly decays in an oscillatory fashion as the wave packet spreads out over time. The current function is initially zero and then oscillates with respected to the origin to maintain a net zero current. The oscillations spread over time but always maintain symmetry. Fig. [6-10]

Second Condition

The second wave packet has a very sharp peak implying that the electron is *localized*. The uncertainty in the position is 'small', so the uncertainty in the momentum is 'large'. This is reflected in the evolution of the system. The wave function for the electron quickly decays into two separate wave functions traveling in opposite directions. Fig. [11-15]

The wave functions move very fast away from each other and this is in accordance with Eq. (26). There is a high degree of symmetry which should be noted. Initially, the positron has no presence but the wave function takes on a nonzero value rather quickly. The density function exhibits similar behavior and collapses quickly into two separate wave packets traveling in opposite directions. Fig. [16-20]

GitHub

Animated gifs of the motion described above can be found on my GitHub, even though a few snapshots can be found in the Figures section. This work should be able to be easily replicated and extended; as well as improved upon computationally. With regards to computational speed up, I would recommend improving upon the for loops by turning them into vectorized operations either via the Python package Numba or using the vectorized operations with Numpy. This would not be terribly difficult to complete.

Boundary Conditions

Initially, I had planned on using periodic boundary conditions but I had opted to simply set the boundary conditions to be zero 'at infinity'. If the boundary conditions are 'very far away' then they will have no influence on the dynamics or adversely affect the numerical approximation. The reason that this boundary condition was used is two-fold. First, modern laptops can handle the computation in a reasonable manner even though the meshgrid is 'relatively' large.

Secondly, I had accidentally set the left boundary condition at $x_{\min}$ to be zero and the right end point to be equal to the left endpoint. This clearly caused some rather erroneous errors in the approximation. This is reflected in Fig. 4 & 5. As the wave function interacts with the boundary then errors appear on both sides of the domain and persist for the remainder of the computation. This is undesirable and nonphysical. Fig. [21-22]

In practice it would seem best to maintain the boundary condition of zero at infinity. This seems reasonable from in an ontological sense; as well as empirically. Modern computers can handle this rather well and within a reasonable amount of time.

Conclusion

The LFS, with boundary conditions of zero at infinity, provided an exploratory methodology for analyzing the implications of the Dirac equation. We were able to correlate the dynamics of the system to the Uncertainy Principle, exhibit different types of dynamics given similar initial conditions, and observe the dynamics of the probability distribution.

The Dirac Equation is fundamental to the development of Quantum Electrodynamics and Quantum Field Theory. Its importance to the understanding of the fundamental structure of reality and there is nothing more important than our understanding of the world around us. The implications of the Dirac Equation are far reaching and this is just beginning to scratch the surface.

Next Steps

The natural progression of the work here would be to evaluate the associated error and order of accuracy. Also, it would be important to improve upon the order by implementing the Crank-Nicolson scheme. I have gone ahead and found the updating system of equations but

was unable to implement them.

$$\left(1+i\frac{k}{2}\right)u_m^{n+1}+\frac{\lambda}{4}\left(v_{m+1}^{n+1}-v_{m-1}^{n+1}\right)=\left(1-i\frac{k}{2}\right)u_m^n+\frac{\lambda}{4}\left(v_{m-1}^n-v_{m+1}^n\right) \tag{29}$$

$$\frac{\lambda}{4}\left(u_{m+1}^{n+1}-u_{m-1}^{n+1}\right)+\left(1-i\frac{k}{2}\right)v_m^{n+1}=\left(1+i\frac{k}{2}\right)v_m^n+\frac{\lambda}{4}\left(u_{m-1}^n-u_{m+1}^n\right) \tag{30}$$

Also, it would be appropriate to do an improved error analysis *post factum*. Next, the physical phenomena Zitterbewegung should be demonstrated. This will showcase the 'jittery motion' behavior. Finally, the hydrogen orbitals should be reconstructed under this framework to analyze the fine structure of the hydrogen atom, examine the spin-orbit coupling and Darwin correction.

Figures

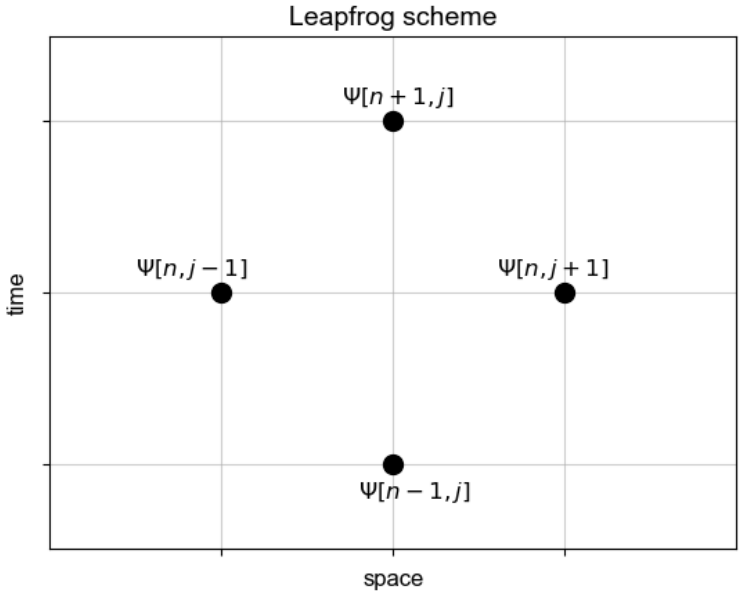

Figure 1. The spatial derivative is a central space difference for the LFS and the temporal derivative looks back two steps.

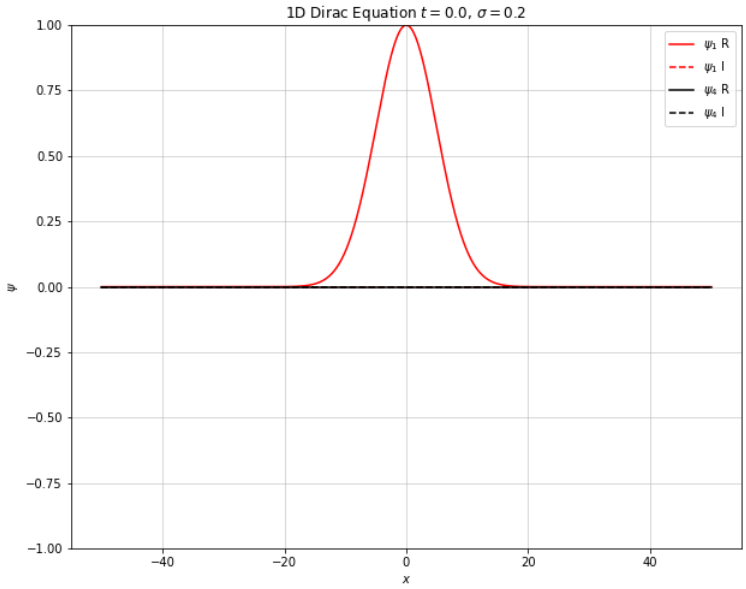

Figure 2. A plot of the initial condition for $\sigma = 0.2$. Notice that the wave packet is spread out.

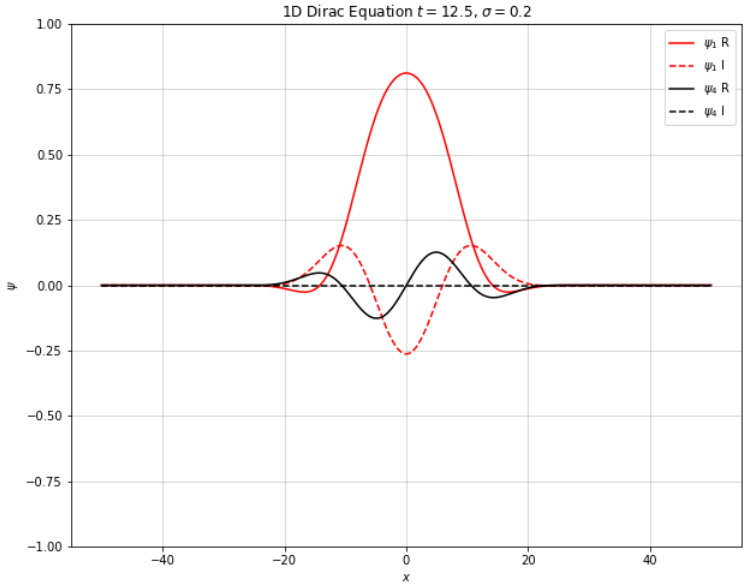

Figure 2. After only a bit of time the wave packet has barely diffused.

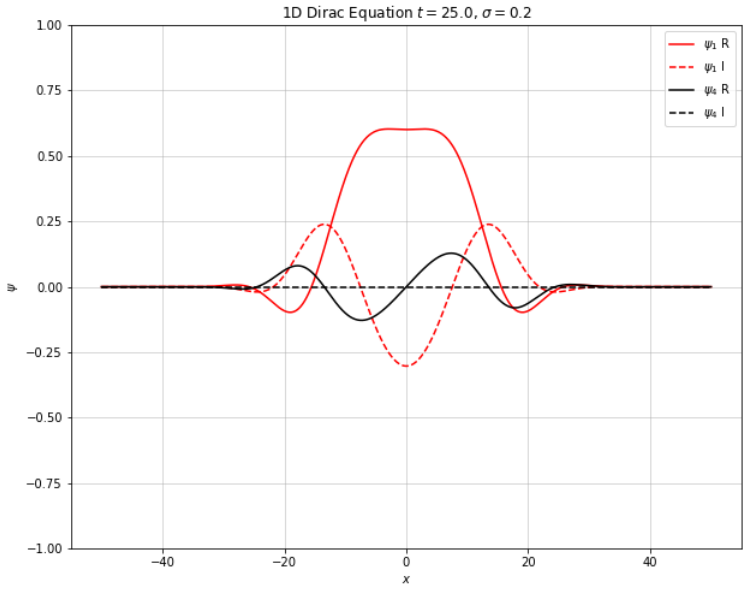

Figure 3. The wave packet continues to spread out in a smooth and slow manner.

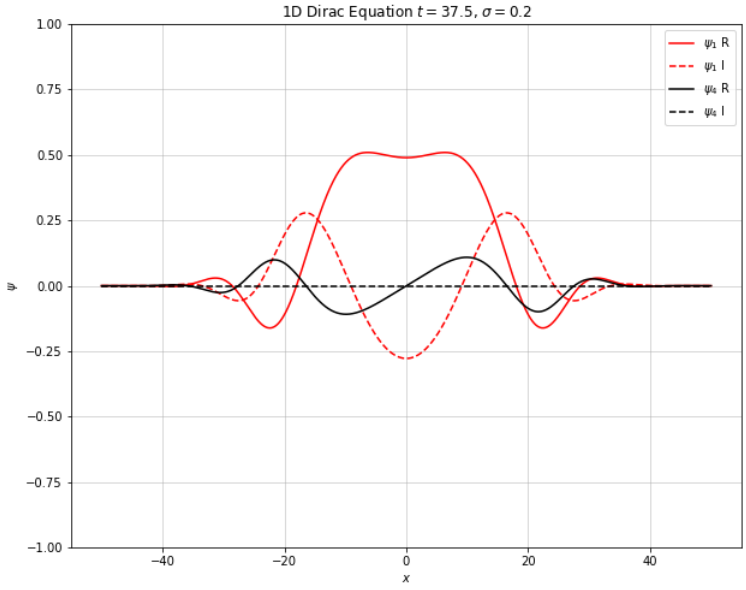

Figure 4. After some more time the same behavior persists as t increases.

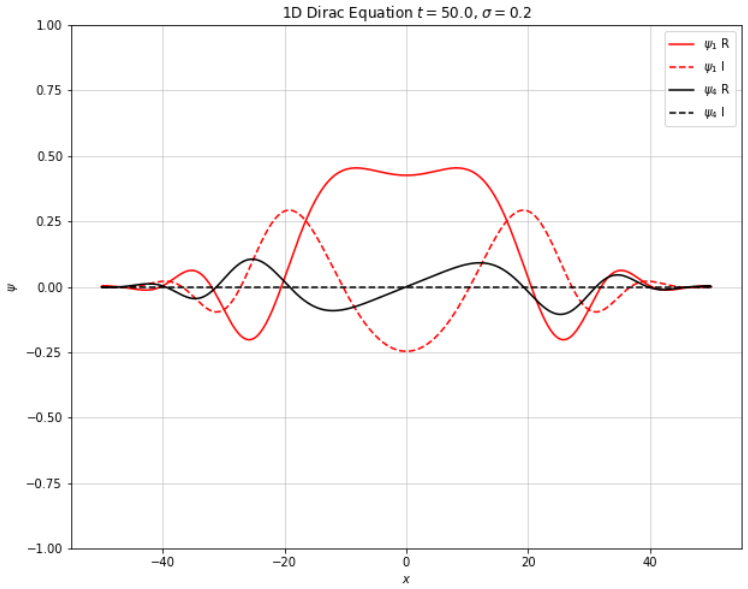

Figure 5. After some more time the same behavior persists as t increases.

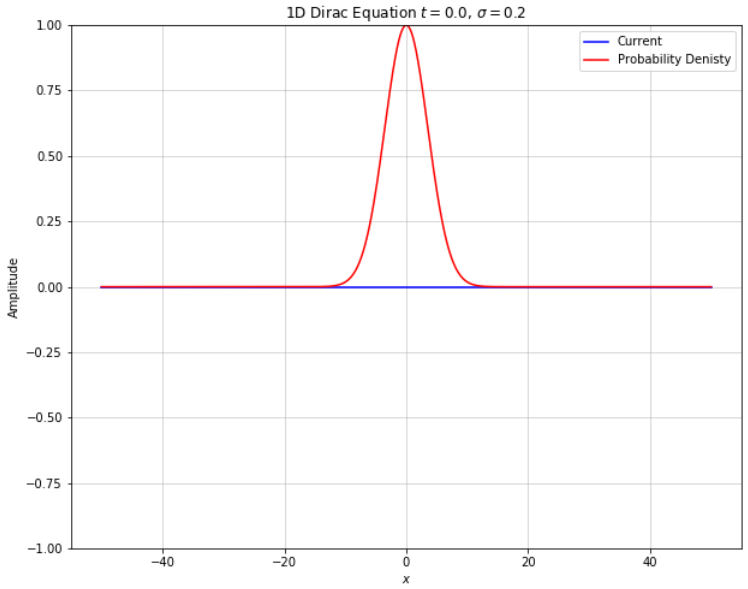

Figure 6. A plot of the probability density and current for $\sigma = 0.2$. The density function has a similar distribution as to the wave form.

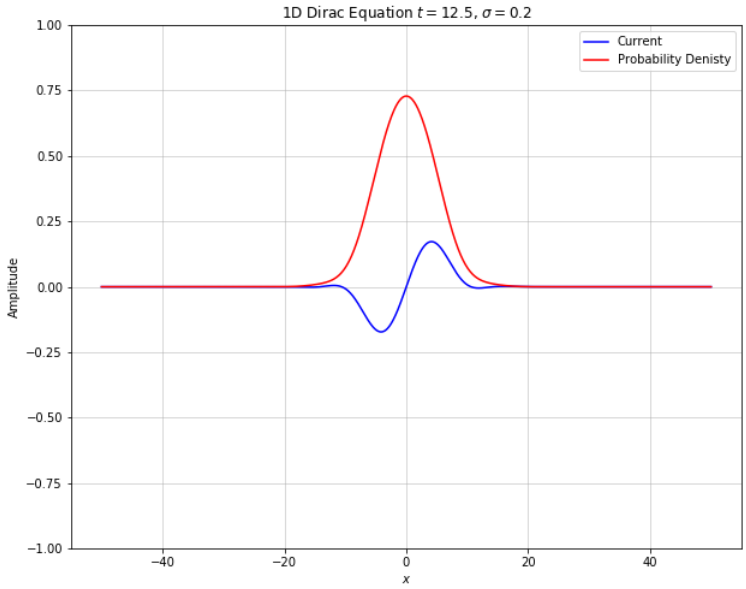

Figure 7. The density function decays in amplitude and the current function begins to oscillate.

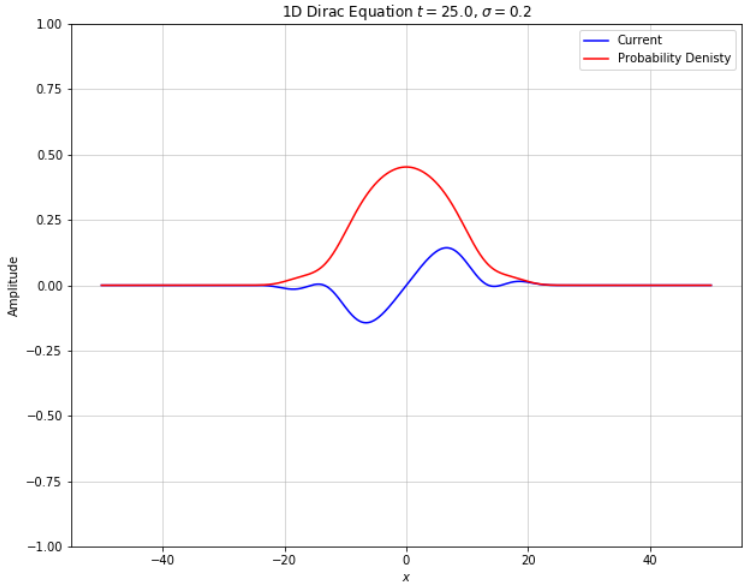

Figure 8. The same behavior persists as the density spreads out.

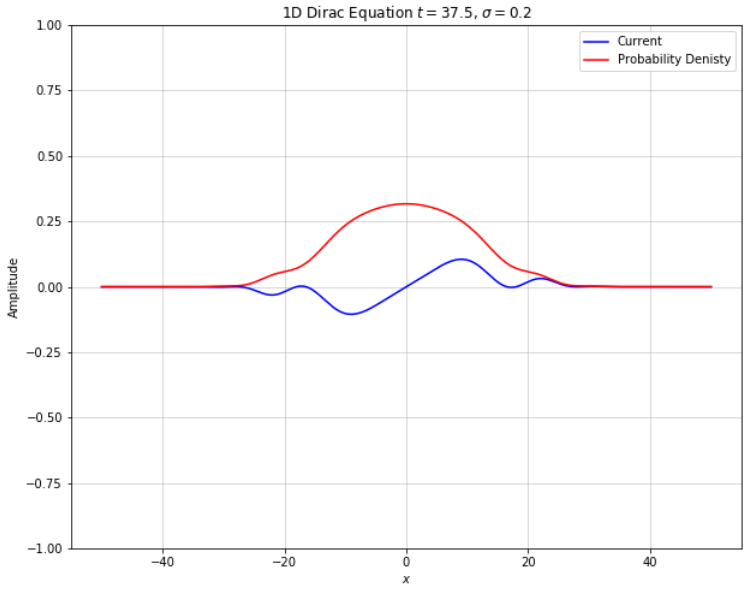

Figure 9. The density continues to smear out and the current plot oscillates and spreads out as well.

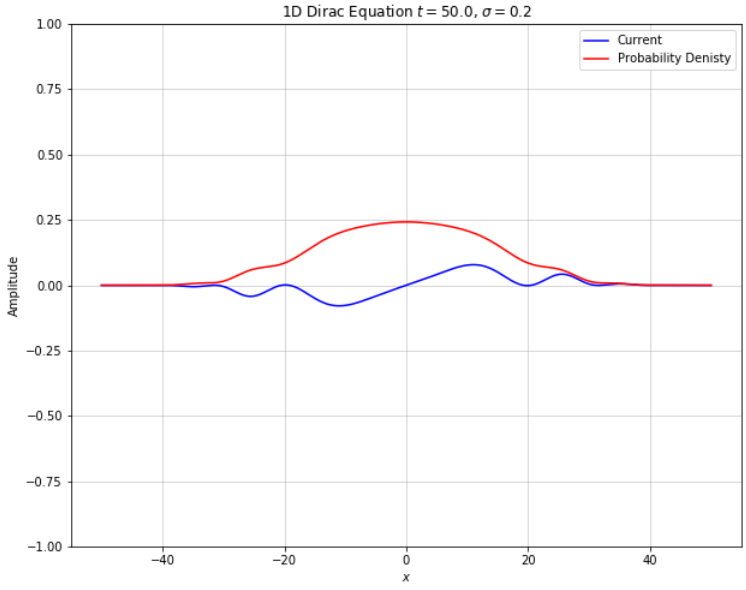

Figure 10. After awhile the probability density smears out over the whole space and the current continues to oscillate and spread out as well.

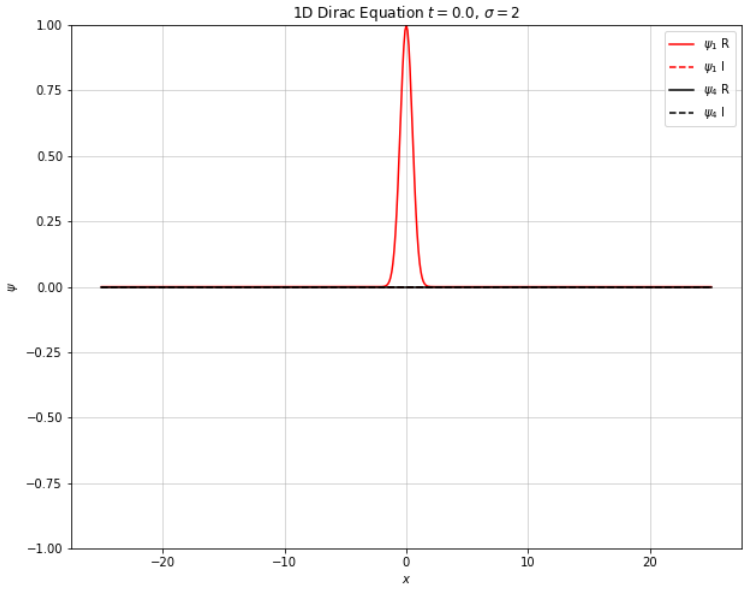

Figure 11. A plot of the initial condition for $\sigma = 2$. The wave packet is extremely narrow and localized.

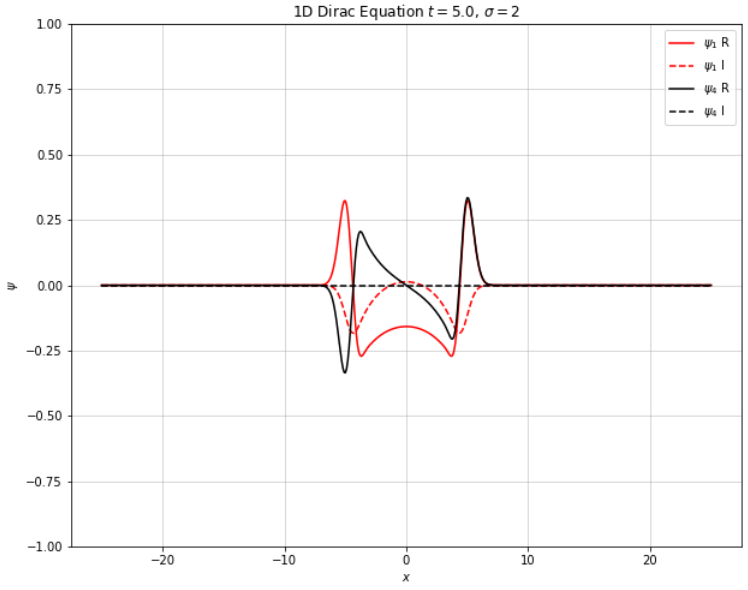

Figure 12. After only a small amount of time the wave form completely devolves from a sharp peak into two separate wacve packets.

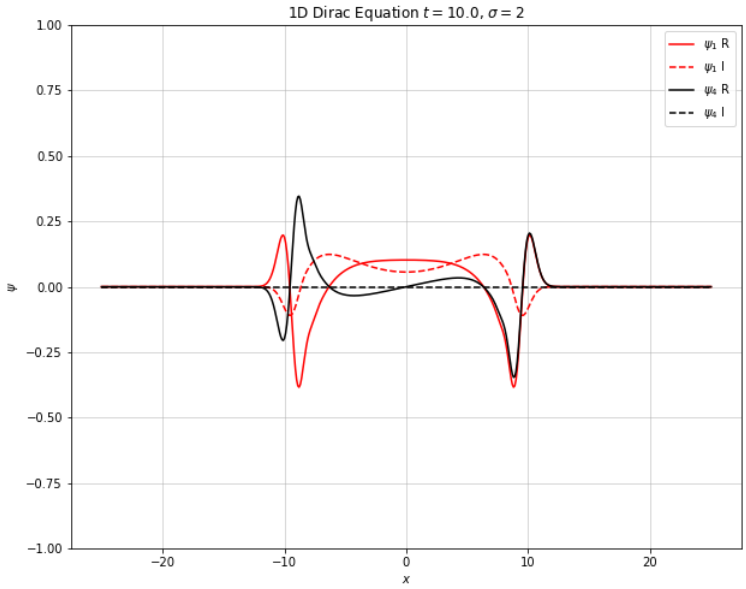

Figure 13. The wave packets move quickly away from each other and there is almost no remanence of the original wave form.

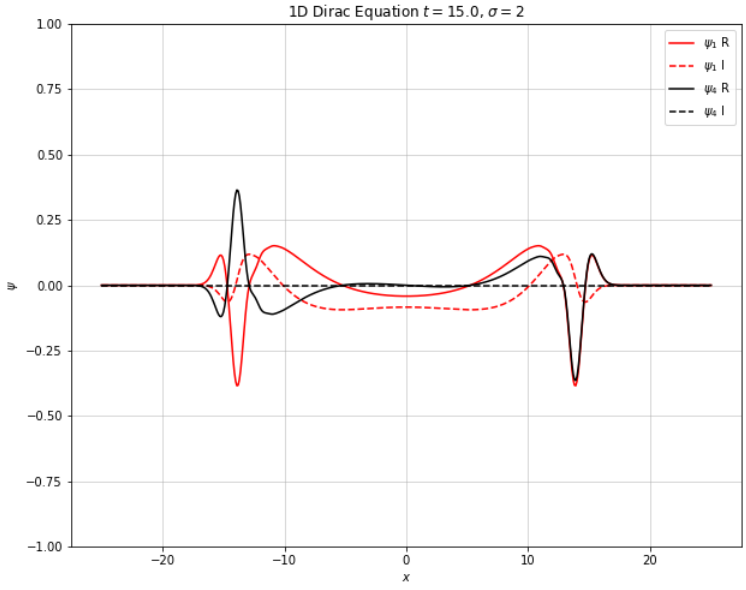

Figure 14. The momentum of the wave function can not be ignored and is reflected in the separation of the wave packets.

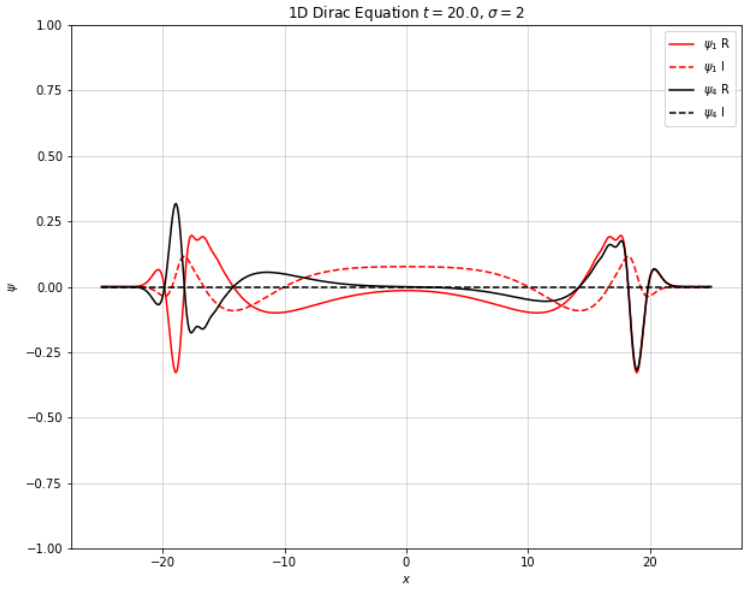

Figure 15. After some time there is no presence of the initial wave function as a consequence of the Heisenberg Uncertainty Principle.

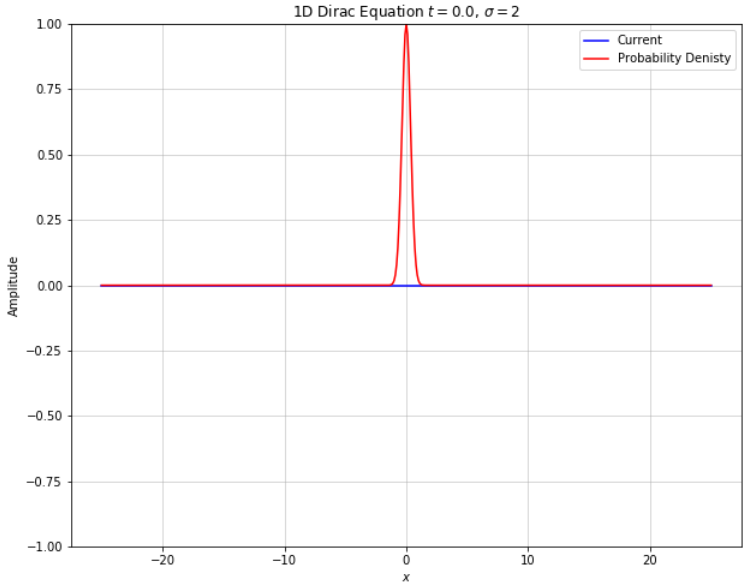

Figure 16. A plot of the probability density and current for $\sigma = 2$. The extreme localization is reflected in the density function.

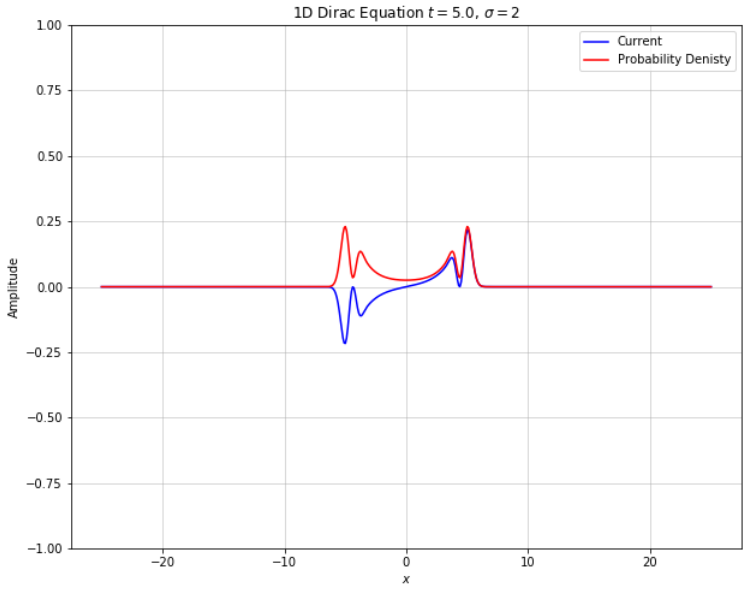

Figure 17. The density quickly spreads out and splits into two distinct density 'bumps'.

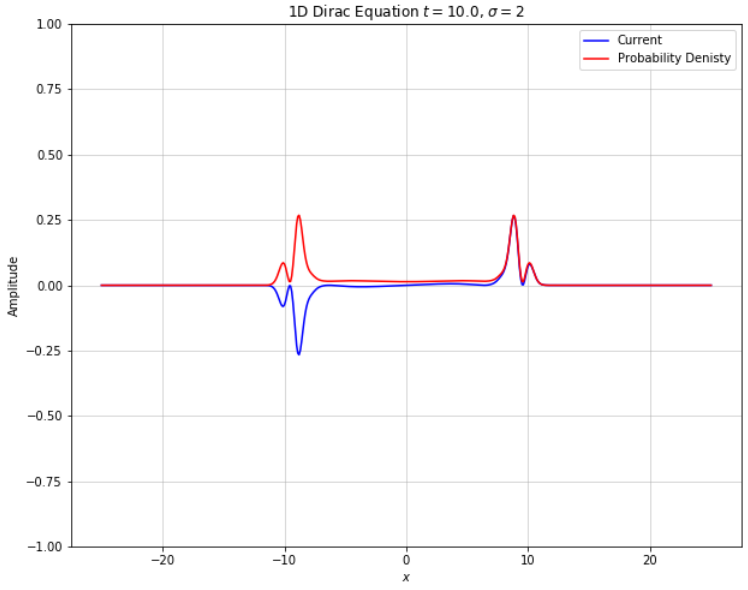

Figure 18. The behavior persists and the two density functions move away from each other symmetrically. The net current is zero.

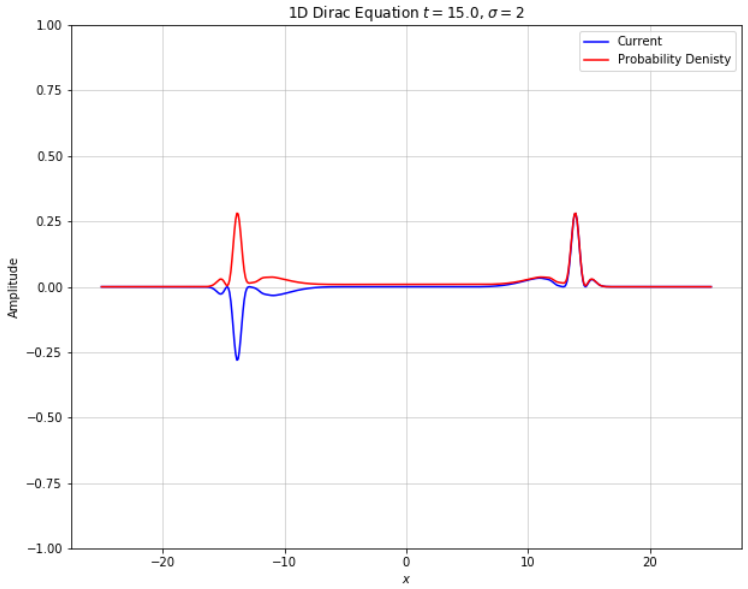

Figure 19. As more time passes the initial electron is not found anywhere near its original location. There are distinct currents of equal and opposite magnitude.

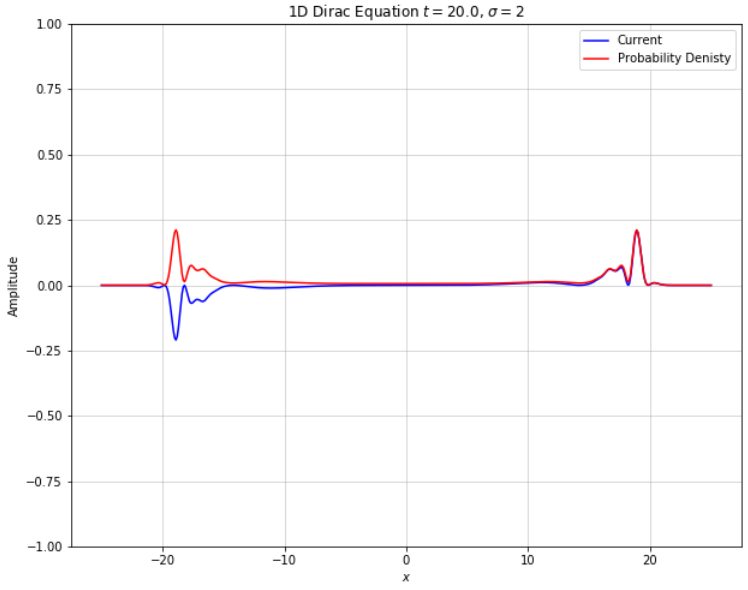

Figure 20. The original density function has completely collapsed and split into two symmetric distributions and the current indicates that the elrctron moved to the left and the positron to the right.

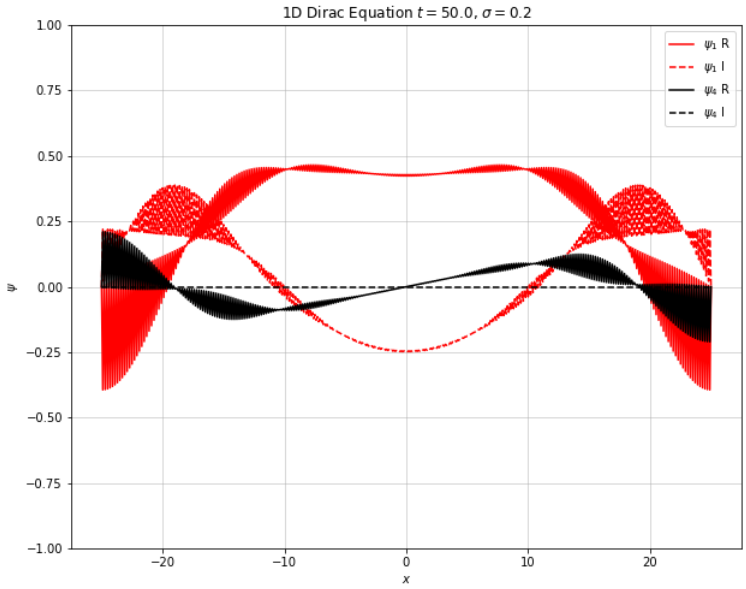

Figure 21. An example of the first initial conditions plotted with periodic boundary conditions. As time passes the wave function interacts with the boundary and an error propagates throughout the entire space.

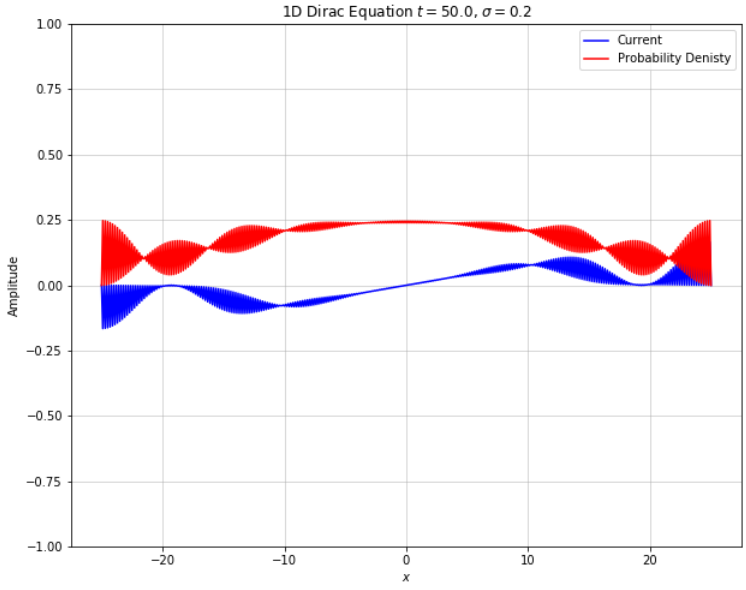

Figure 22. A probability density and current plot of the first initial condition with periodic boundary conditions. Similar to before, the errors propagates throughout the space.

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GitHub: github.com/BryceWayne