The Dirac Equation and the Prediction of Antimatter

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Throughout the history of physics, there may be no scientist quite so genuinely *strange* as Paul Allen Maurice Dirac. In fact, his enigma so permeated all facets of his life that his own first name, shortened to P.A.M, was somewhat of an accidental mystery for years. Countless anecdotes of his socially awkward, detached, bizarre, and borderline autistic behavior are still recounted today. In one such story Dirac was said to be giving a lecture on his work on quantum mechanics. During the question period a member of the audience remarked that he did not understand how Dirac had derived a certain equation. After nearly 30 seconds of silence, the moderator prompted for a reply and Dirac merely responded, “That was not a question, it was a comment.” [4] Behavior like this can be seen to be the result of his broken family led by his cold father, but also showcases Dirac's incredible literalism and provides hints to fundamental characteristics that made him a great physicist. Brilliance, it seems, can be born from severe hardship.

Paul Dirac is perhaps most comparable with Isaac Newton as a physicist. While characters such as Einstein or Feynman relied more heavily upon their physical intuition, and both admitted a relative weakness in mathematics in comparison, Dirac and Newton showed a much greater appreciation for fundamental mathematics. For Dirac, this can be owed to his having received a degree in mathematics, not physics, from the University of Bristol. It was this mathematical approach to problems of quantum theory that would afford him success in combining equations of special relativity and quantum mechanics. This relativistic quantum theory was both complicated and elegant, and would win Dirac the Nobel Prize in Physics in 1933. It would also lead him to one of the most important and daring predictions in the history of science.

To understand such an important prediction, one must first know a bit about the theory that gave rise to it. In this case, the required theory relies upon fundamental principles of quantum mechanics, from the Schrödinger Equation to the Klein-Gordon Equation to the Dirac Equation in its totality. Proceeding with this progression in mind, one must first have a basic understanding of the Schrödinger Equation and where it came from. Before the advent of quantum theory, Newtonian mechanics dictated a direct approach to particles and motion. The basic function of Newtonian mechanics was to find the position of a particle at a given time, namely to derive the function for x(t) if only one direction is involved. Once this function is known, any dynamic variable can be calculated and as such its motion can be fully described and the physicist's job is done. To derive x(t), Newton gives his famous second law: $m\,d^2x/dt^2 = F$. If one knows the initial conditions, and perhaps potential energy function, this equation can yield the desired x(t).

This process seemed quite adequate until the beginning of the 20th century. It was around this time that not only was the special theory of relativity developed by Einstein, but also the need for quantum mechanics was first being seen. Experiments showing the discrete spectrum of the atom, the failure of kinetic theory relating to blackbody radiation, discretization of energy, and the photoelectric effect were all suggesting a need for a new theory of motion on the scale of the atom. In the everyday domain, when one is discussing cars or boxes moving, Newtonian mechanics could still dominate. It was seen that only when one starts to look at particles themselves does the need for quantum mechanics arise. This new quantum theory was developed throughout the early 1900's, and was really solidified in the years 1925 and 1926. It was during these years that Werner Heisenberg first introduced his abstract matrix formulation of quantum mechanics, extending the phenomenological Bohr model of the atom. Just one year later Erwin Schrödinger introduced his own formulation involving wave mechanics and a mysterious wavefunction. Both of these formulations were later proven to be mathematically equivalent, and various other formulations would show up in the form of Richard Feynman's sum over integral approach and David Bohm's ontological approach.

The Dirac Equation itself is based upon Schrödinger's formulation of quantum mechanics, and as such this is the only formulation that will be discussed from here forward. In this approach, the goal is much as in Newtonian mechanics. Instead of trying to find x(t), however, the desired function is $\Psi(x,y,z,t)$ (the particle's wavefunction). This wavefunction encodes all of the information that one would need to analyze the particle. To find this wavefunction, Schrödinger introduced a fundamental equation analogous to Newton's second law in quantum theory, given as:

$$i\hbar\frac{\partial\Psi}{\partial t}=\frac{-\hbar^2}{2\mathrm{m}}\nabla^2\Psi+V\Psi \tag{1}$$

This is known as Schrödinger's Equation, and can be solved to find the desired wavefunction. Perhaps just as fundamental, it was found that when one squares this wavefunction, a statistical law seems to hold. This is called Born's statistical interpretation, and is a way of defining this mysterious wavefunction. It says that this wavefunction squared gives the probability of finding the particle at the specified point at a certain time. One can then integrate this wavefunction, more really a probability density, to get the probability of finding the particle between two points. This is given by:

$$\int_a^b |\Psi(x,y,z,t)|^2\, dxdydz \tag{2}$$

It is important at this point to briefly discuss the merits of this wavefunction and its statistical interpretation. This wavefunction can be shown to be linear in $\partial/\partial t$, meaning that the wavefunction at one time determines the wavefunction at any other time. It also must be normalized, such that the integral over all space of the wavefunction squared be equal to one (as the particle must exist somewhere in space). The Schrödinger Equation then must certainly preserve this normalization of the wavefunction, otherwise the statistical interpretation is unphysical. This preservation of normalization can indeed be shown to be a feature of the Schrödinger Equation [5].

These features are crucial in the importance and relevance of the Schrödinger Equation to quantum theory. If either of these features is broken, the theory would be unphysical and would not make sense. As great as this formulation is in elucidating the indeterminacy of quantum mechanics, and giving us means to calculate observables, it has one major flaw: it is not Lorentz invariant. This breaking of Lorentz invariance means that it is not entirely tenable to the verified special theory of relativity. To note the initial problem that the Schrödinger Equation had, one must examine its origins a bit more carefully. The real fundamental form of the equation is actually given by:

$$i\hbar\frac{\partial\Psi}{\partial t}=\hat{H}\Psi$$

Here, this $\hat{H}$ is the Hamiltonian operator. For the Schrödinger Equation, the Hamiltonian used is the nonrelativistic classical Hamiltonian of $p^2/2\mathrm{m}+V$. The momentum is then taken to an operator in quantum mechanics, given by $\hat{p}=-i\hbar\nabla$, and one gets back equation 1. The problem here, of course, is that relativistic mechanics dictates explicitly the use of of the *relativistic* version of the Hamiltonian. This Hamiltonian is given, squared for convenience, by $H^2=p^2c^2+m^2c^4$.

It is certain that Schrödinger realized that his theory was not Lorentz invariant because of his use of the nonrelativistic Hamiltonian. He still decided to introduce only the nonrelativistic version, because of certain flaws which presented themselves in using the relativistic Hamiltonian. As such, the next step in getting to a correct relativistic version of the Schrödinger Equation is understanding these flaws. When one uses the relativistic Hamiltonian, squared now out of necessity, one gets the so called Klein-Gordon Equation (for a free particle):

$$\frac{\partial^2\Psi}{\partial t^2}=c^2\nabla^2\Psi-\frac{m^2c^4}{\hbar^2}\Psi \qquad (3)$$

Upon solving this system, the wavefunction has a plane wave form as before. The energy, however, has now become an irreversibly different quantity altogether. This stems from the fact that the relativistic Hamiltonian has to be squared before it can be used in the Schrödinger Equation. If we use the relativistic Hamiltonian as it stands, there is a square root in the expression and the differential operator would have no way of being evaluated. It also has the problem of being nonlocal as it stands [6].

Now that the need to square the relativistic Hamiltonian has been shown, we can look at the results. This Klein-Gordon Equation now yields two energies, because of this squaring of the Hamiltonian. These energies are given by $E_A = \sqrt{p^2 c^2 + m^2 c^4}$ and $E_B = -\sqrt{p^2 c^2 + m^2 c^4}$. Before, with the Schrödinger Equation, only one energy was present and everything seemed very physical. Now, two entirely different solutions for energy are present, and our first problem appears to arise. In classical relativistic mechanics this same problem of two energy solutions for a single particle exists, but the negative energy solution can be simply ignored on the grounds of being unphysical. It is not so easy to do that in the quantum domain. The whole of quantum theory is built upon complete sets of eigenfunctions, and one cannot merely drop the negative energy eigenstate in this construction. The full set of eigenstates is necessary here, because even an arbitrary wavefunction of the positive energy solution would, in general, evolve in time to have projections on the negative energy eigenstate. It also turns out that the Klein-Gordon Equation was seen to be flawed in that the statistical interpretation of the wavefunction was not physical. The integral of the square of the wavefunction was not a constant, and even suggested negative probabilities. There was, however, a value for which this preservation occurred, and it was given as $\rho = \Psi^* \dot{\Psi} - \dot{\Psi} \Psi^*$. This value also can take negative values unfortunately, and the problem persists.

As promising as the Klein-Gordon Equation was to creating a relativistic version of quantum theory, it fell short in these areas and was generally disregarded as flawed. A final nail in the coffin was that it did not allow for spin states, which were proven to be necessary in describing most particles. Dirac, however, knew that the Schrödinger Equation needed to be made Lorentz invariant if it was to be correct, and believed that modifying the Klein-Gordon Equation was the best way to go about that. It was known that the real reason that the Klein-Gordon Equation did not allow a positive definite conserved probability density was due to the second-order time derivative, and it therefore became necessary to begin with a first-order time derivative in any theory with a statistical interpretation. This was necessary so that one would not get negative probability densities. Dirac began by imposing this constraint and making the Klein-Gordon Equation linear in $\partial / \partial t$ (as well as in space derivative so that it would be covariant). Dirac's equation would then need to begin in the form:

$$i\hbar \frac{\partial \Psi}{\partial t} = (\alpha_1 c\, \hat{p}_x + \alpha_2 c\, \hat{p}_y + \alpha_3 c\, \hat{p}_z + \beta mc^2)\Psi$$

Here these alphas and the beta are the unknown quantities needed to make this equation consistent with the Klein-Gordon Equation, while still being linear in time and space derivative. In order to set these variables, one must operate twice on each side to get an equation which is of the form of the Klein-Gordon Equation. This yields the result:

$$-\hbar^2 \frac{\partial^2 \Psi}{\partial t^2} = (\alpha_1 c\, \hat{p}_x + \alpha_2 c\, \hat{p}_y + \alpha_3 c\, \hat{p}_z + \beta mc^2)^2 \Psi \tag{4}$$

The required next step then would be to set alpha and beta such that this equation is compatible with the Klein-Gordon Equation.

Dirac's great insight into this problem was that alpha and beta could not be simple scalar quantities to achieve such a feat, but the whole theory could work if they were matrices. Indeed, this fit in well with his previous work in the foundations of Heisenberg's matrix formulation. Instead of the proposed 2x2 matrices of the Pauli theory, or the singular component in the Schrödinger formulation, the wavefunction must really be made up of at least four components. The required alphas and beta can then be seen to be [8]:

$$\alpha_i = \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix} \text{ and } \beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

with σ_i as the standard 2x2 Pauli matrices given by:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \text{ and } \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \text{ and } \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

With these new 4x4 variables, the modified Klein-Gordon Equation becomes the Dirac Equation. This equation is now linear in time and space derivative, and therefore it is guaranteed to have a positive probability density. This probability density, however, was still not entirely constant and the constant quantity ρ from before was still allowed to be negative. In 1934, Pauli and Weisskopf would show that because the relativistic quantum mechanical equation had to allow creation and annihilation of particles, the probability density did not actually have to be kept constant and this was not a problem of the theory at all. The conserved quantity ρ was also shown to be the charge density, which is certainly allowed to be negative.

The final Dirac equation can be written in various forms, but the simplest seems to use γ_α matrices [6]. In this form it is given as:

$$\left(i\hbar\gamma_\alpha\frac{\partial}{\partial x_\alpha}-mc^2\right)\Psi=0 \quad \text{with} \quad \gamma_i=\begin{pmatrix}0 & \sigma_i\\ -\sigma_i & 0\end{pmatrix} \quad \text{and} \quad \gamma_0=\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$$

Now that the Dirac Equation is known to be Lorentz invariant, it is appropriate to re-examine the prior problems with the Klein-Gordon Equation. As stated before, the second problem was eventually shown by Pauli and Weisskopf to be not a problem at all. The original problem of a negative energy solution still remains. As the Dirac Equation, up to this point, has afforded us such success, it is not unreasonable to begin to believe in its predictive powers. Solving this equation through for a particle at rest, one actually gets two states for the positive energy solution and two states for the negative energy solution as follows:

$$\Psi_A=e^{-imt}\begin{pmatrix}1\\0\end{pmatrix} \quad \text{and} \quad \Psi_A=e^{-imt}\begin{pmatrix}0\\1\end{pmatrix} \quad \text{(positive energy)}$$

$$\Psi_B=e^{imt}\begin{pmatrix}1\\0\end{pmatrix} \quad \text{and} \quad \Psi_B=e^{imt}\begin{pmatrix}0\\1\end{pmatrix} \quad \text{(negative energy)}$$

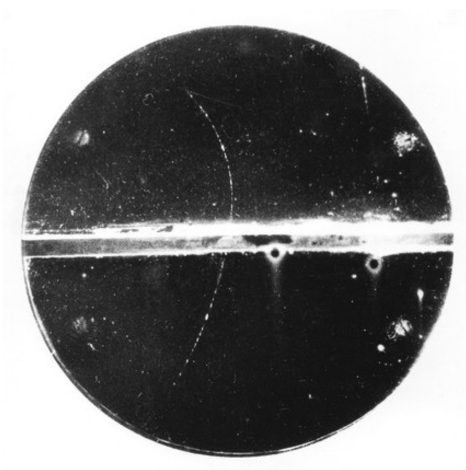
These two states per energy correspond to the two spin states of a spin-1/2 fermion, obey the Pauli Exclusion Principle, and give us further validation of the theory's usefulness. After serious deliberation, and with a certain amount of hesitance, Dirac declared his belief in the physical existence of these confusing negative energy states. While other theorists of the time were quite sure these solutions represented either a quirk of the theory, or a serious flaw in the equation, Dirac stood by his mathematics. This was met with some opposition, and at times blatant attacks on the very scientific character of Dirac himself. He was criticized by some for blindly following a mathematical construct over physical intuition. In fact Werner Heisenberg himself, a friend of Dirac, was quoted as saying, "The saddest chapter of modern physics is and remains the Dirac theory...I regard it as learned trash which no one can take seriously" [4].

To understand the hostility towards these negative energy solutions, it is useful to go a bit deeper into their theoretical flaws. If an electron occupying a negative energy state is possible, then an electron in a positive energy state should be able to emit a photon and jump down past zero to a negative energy state. This could then continue until the electron has emitted an infinite amount of energy, and would therefore be able to keep climbing down to a lower and lower energy state. This does not seem possible, and is certainly not a feature of electrons. To fix this, Dirac proposed that perhaps all of the negative energy solutions still exist, but are in fact all occupied. By the Pauli Exclusion Principle then, an electron in a positive energy state could not drop below zero and occupy one of these states because they are already filled. By virtue of his theory, all positive energies are greater than mc^2 and all negative energies are less than $-mc^2$ and an energy gap between the two is $2\mathrm{mc}^2$. It seems possible, then, that a negative energy electron could absorb a photon of energy greater than $2\mathrm{mc}^2$ and make a jump to a positive energy state. A hole is then left in the previously occupied negative energy "sea" of electrons. At first Dirac believed this hole to be a proton, but it was later shown that it would need to have all of the same properties of an electron but with positive charge. This proposed hole is then, in reality, what would be called a positron [3].

Dirac's prediction of a particle with these strange properties, which had never been observed before, was certainly bold. Problems and oddities still existed with his interpretation of an infinite sea of particles with negative energy. It seemed strange that there would exist an asymmetry in vacuum of negative and positive energy, especially considering the symmetries inherent in the Dirac Equation itself. In many ways this so-called Dirac Sea was more of a theoretical convenience than a true fitting view of reality. The development of quantum field theory would eventually make this odd construction unnecessary and even cumbersome, though perhaps not quite incorrect. It is very rarely referenced today, and in the history of quantum mechanics can be seen as more of a stepping stone rather than an extensive model. In any case, it was this view that would lead Dirac to make one of the most exciting and surprising theoretical discoveries of all time.

Because of all of the mentioned problems and confusions related to the Dirac Equation and the Dirac Sea, it is not surprising that it wasn't universally accepted right away. It did have the bonus of being immediately falsifiable, and the search for the positron was quickly underway. It would only take until 1932, a mere four years after Dirac's first proposition of the Dirac Equation, for it to be experimentally verified. This verification took place in a popular device of the time known as a cloud chamber, which is a particle detector consisting of a supersaturated vapor. When a type of ionizing radiation passes through this vapor, it is ionized and these ions form a mist. This ion mist creates a trail, which can in turn be photographed and analyzed. Different particles with different properties will form distinctive track shapes. Even better, if a uniform magnetic field is applied across this vapor, the particles will curve in opposite directions due to the Lorentz force law. It is precisely this fact that made the recognition of the positron so simple and obvious.

Carl D. Anderson was the first scientist to report a sighting of the positron in a cloud chamber [2]. A rather young physicist working at Caltech, Anderson was analyzing cosmic ray tracks when he came upon something peculiar. He noticed that one particle seemed to make precisely the track of an electron, but its path curvature suggested that it had a positive charge. It quickly became obvious to him that this particle was indeed the positron predicted by Dirac's calculations. He published his results, and was actually the man who coined the name “positron”. He would later win the Nobel Prize in physics in 1936 for his discovery and subsequent publishing. It is speculated that others before Anderson had actually seen the positron as well, but disregarded it as an anomaly and believed their work to be inconclusive [4]. Below is a photograph of the positron that Anderson saw, along with a photograph of him working in his lab at Caltech. One can see the curved track near the middle of the photograph which shows a particle moving upwards and passing through a lead plate in the middle. Due to the applied magnetic field it was calculated that this curvature was precisely opposite of what one would expect for an electron.



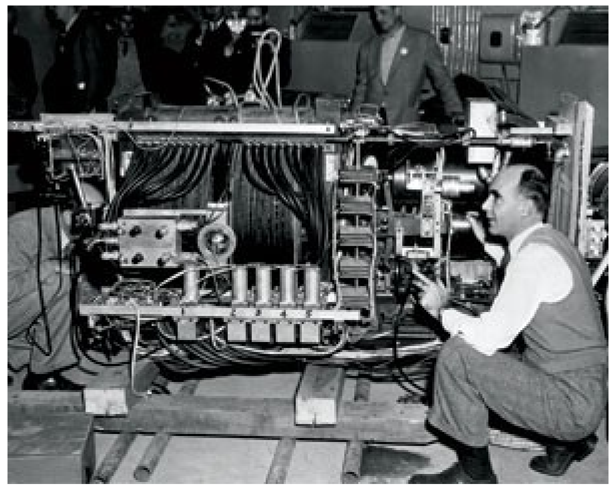


Figure 1: The First Recorded Picture of a Positron/ Carl Anderson at Caltech [1]

After this great discovery, Dirac's equation was seen to be verified and the importance of his work realized. Throughout the years other antiparticles were observed, and Dirac was fully vindicated. Much of his work would lead to revolutions in quantum electrodynamics, which to this day explains a large amount of physics to incredible precision. Richard Feynman, a pioneer in this field and legendary physicist in his own right, would refer to Dirac in an almost reverential manner. Referring to his own Nobel Prize winning work he is quoted as saying, “I don't what all the fuss is about – Dirac did it all before me.” [4] It is slightly ironic, then, that Dirac, who contributed so much to such a useful field, was more than wary of its inception. He certainly believed in his theories, but he was noted to have disliked the work being done in QED. His own theories in this field would result in troubling infinities, and the modern approach was to introduce a concept of renormalization of the wavefunction. Dirac despised this approach all of his life, and although it was and is accepted in modern science, he saw it as arbitrary and even ignorant. The story plays out much the same way that Einstein's did a few decades before: a brilliant mind inspires a new field of science, yet is later found to vehemently oppose its direction and interpretation. Regardless, Dirac will always be remembered for his taciturn nature, his revolutionary work on quantum mechanics, and his precise mathematical elegance.

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