WHAT IS...

the Dirac Equation?

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In the early part of the 20th century huge advances were made in theoretical physics that have led to vast mathematical developments and exciting open problems. Einstein's development of relativistic theory in the first decade was followed by Schrödinger's quantum mechanical theory in 1925. Einstein's theory could be used to describe bodies moving at great speeds, while Schrödinger's theory described the evolution of very small particles. Both models break down when attempting to describe the evolution of small particles moving at great speeds. In 1927, Paul Dirac sought to reconcile these theories and introduced the Dirac equation to describe relativistic quantum mechanics.

Dirac's formulation of a hyperbolic system of partial differential equations has provided fundamental models and insights in a variety of fields from particle physics and quantum field theory to more recent applications to nanotechnology, specifically the study of graphene.

Dirac equation. To formulate the Dirac equation consistent with a quantum mechanical interpretation, the wave function at time $t = 0$ should determine the wave function at all times, and hence the model needs to be first order in time [Tha92]. In addition, it should conserve the L^2 norm of solutions. Dirac combined the quantum mechanical notions of energy and momentum operators $E = i\hbar\partial_t$, $p = -i\hbar\nabla_x$ with the relativistic Pythagorean energy relation $E^2 = (cp)^2 + (E_0)^2$, where $E_0 = mc^2$ is the rest energy.

Inserting the energy and momentum operators into the energy relation leads to a Klein–Gordon equation

$$-\hbar^2\psi_{tt} = (-\hbar^2\Delta_x + m^2c^4)\psi.$$

The Klein–Gordon equation is second order, and does not have an L^2-conservation law. To remedy these shortcomings, Dirac sought to develop an operator[1]

$$D_m = -ic\hbar\alpha_1\partial_{x_1} - ic\hbar\alpha_2\partial_{x_2} - ic\hbar\alpha_3\partial_{x_3} + mc^2\beta$$

which could formally act as a square root of the Klein–Gordon operator, that is, satisfy $D_m^2 = -c^2\hbar^2\Delta + m^2c^4$. This is possible if the coefficients α_j, β are 4×4 matrices satisfying $\alpha_j^2 = \beta^2 = I$ and the anticommutation relationship (for $j \neq k$)

$$\alpha_j\alpha_k = -\alpha_k\alpha_j, \qquad \alpha_j\beta = -\beta\alpha_j.$$

Typically the Pauli matrices,

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

are used to formulate the Dirac system

$$i\hbar\psi_t(x,t) = \Big(-ic\hbar \sum_{k=1}^{3} \alpha_k\partial_{x_k} + mc^2\beta \Big)\psi(x,t), \qquad (1)$$

where

$$\beta = \begin{bmatrix} I_{\mathbb{C}^2} & 0 \\ 0 & -I_{\mathbb{C}^2} \end{bmatrix}, \ \alpha_i = \begin{bmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{bmatrix}.$$

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[1] *For concreteness, we only consider the case of three spatial dimensions, that is, when* $x \in \mathbb{R}^3$.

For notational convenience we choose physical units $c = \hbar = 1$, and denote $\sum_{k=1}^{3} \alpha_k \partial_{x_k} = \alpha \cdot \nabla$, to write the equation as

$$i\psi_t(x,t) = (-i\alpha \cdot \nabla + m\beta)\psi(x,t). \tag{2}$$

By the representation (2), it is clear that the Dirac operator does not act on a complex-valued wave function as the Schrödinger operator does, but rather acts on spinor fields. That is, the solution to (2) is a $\mathbb{C}^4$-valued function.

In contrast to the Schrödinger model, in which the free operator $H_0 = -\Delta$ is nonnegative, the free Dirac operator $D_m = -i\alpha \cdot \nabla + m\beta$ is unbounded both above and below. In particular, the spectrum is $\sigma(D_m) = (-\infty, -m] \cup [m, \infty)$.

These peculiarities lead to an ambiguity in the physical interpretation of the solution ψ. One interpretation is that the solution couples the evolution of a quantum particle with its antiparticle, namely coupling the evolution of electrons and positrons [Tha92]. This interpretation predicted the existence of the positron before its discovery in 1932.

The unboundedness in both directions creates challenges in the analysis of perturbations. For nonlinear perturbations, the concentration-compactness method fails for Dirac as it relies on the operator being bounded below. Moreover, one cannot define the Friedrichs extension for symmetric perturbations of Dirac operators since they are not bounded below [RS79].

The Dirac equation as a dispersive PDE. The Dirac equation is an example of a dispersive partial differential equation. By dispersive, we mean equations for which different frequency components of the initial data (wave) propagate with different velocities. We can envision the solution as being made up of *wave packets*, where the frequency of vibration is directly related to the speed at which the wave packet moves.

A model dispersive PDE is the free Schrödinger equation:

$$i\psi_t = -\Delta\psi. \tag{3}$$

A plane wave of the form $\psi(x,t) = \exp(ik \cdot x - i\omega t)$ formally solves the equation provided that the "dispersion relation," $\omega = |k|^2$, holds. Writing $\exp(ik \cdot x - i\omega t) = \exp(ik \cdot (x - kt))$, this relationship may be interpreted as saying the speed of the wave is equal to the frequency of vibration.

Using Fourier transform techniques, we can represent the initial data $\psi(x,0) = f(x)$ as a superposition of plane waves $\exp(ik \cdot x)$ for a broad class of initial data. Now, the dispersion relation dictates that higher frequency ($|k|$ large) portions of the solution move more quickly than lower frequency portions of the solution. A by-product is that a concentrated initial profile $f(x)$ will spread out, becoming smaller and smoother in some sense. The smoothing effect is more subtle compared to parabolic equations such as the heat equation since the linear evolution preserves the L^2-based Sobolev norms. Various quantifications of this decay and smoothing for linear equations are useful in the study of nonlinear counterparts. Heuristically, for equations with power nonlinearities the nonlinear terms become smaller compared to the linear terms due to the decay.

The best way to measure this spread is to use the Fourier transform techniques to represent the solution of (3) as a convolution integral. For $x \in \mathbb{R}^n$,

$$\psi(x,t) = (-4\pi it)^{-\frac{n}{2}} \int_{\mathbb{R}^n} e^{i|x-y|^2/4t} f(y)\, dy. \tag{4}$$

Using (4), one can see the global dispersive estimate

$$\|e^{it\Delta} f\|_{L^\infty_x} \leq C_n |t|^{-\frac{n}{2}} \|f\|_{L^1_x}.$$

This $L^1 \to L^\infty$ bound reflects the dispersion present in the Schrödinger equation, since the sup norm decays in time as the waves of varying frequencies spread out in space. These estimates can be used to obtain Strichartz estimates of the form

$$\|e^{it\Delta} f\|_{L^q_t L^r_x} \leq C \|f\|_{L^2_x}$$

for admissible exponents $q, r \geq 2$, $(q,r,n) \neq (2,\infty,2)$, with $\frac{2}{q} = n(\frac{1}{2} - \frac{1}{r})$.

Strichartz estimates were first obtained by Strichartz via Fourier restriction theory of Stein. Later, it was established that they can be obtained using $L^1 \to L^\infty$ estimates. These mixed space-time estimates provide another way to quantify the dispersive nature of the equation, and are ubiquitous in the study of nonlinear equations.

One can also measure the dispersion via smoothing estimates. Since a wave packet with frequency k moves with speed $\sim |k|$ it spends at most $\sim |k|^{-1}$ units of time on a ball of radius one. Averaging in time implies the Kato smoothing estimate

$$\|\langle x \rangle^{-\frac{1}{2}-\epsilon} (-\Delta)^{\frac{1}{4}} e^{it\Delta} f\|_{L^2_{t,x}} \leq C \|f\|_{L^2_x}.$$

This estimate can be interpreted to say that on average the solution is half a derivative smoother than the initial data.

The dispersion in the Dirac equation is weaker than that in the Schrödinger due to the hyperbolic nature of the equation. Since the square of the free Dirac operator $D_m^2 = -\Delta + m^2$ is a diagonal system of Klein–Gordon operators, there is finite speed of propagation and the large frequency behavior of solutions does not travel arbitrarily fast as in the Schrödinger evolution. This leads to weaker time decay and loss of derivatives in dispersive estimates.

Linear perturbations. To account for particle interactions or external electromagnetic fields in three dimensions, one perturbs (1) with a 4×4 matrix-valued potential, i.e.,

$$i\psi_t = (D_m + V)\psi. \tag{5}$$

For simplicity, we will assume that V is Hermitian. Under mild decay and local singularity assumptions on V the perturbed Dirac operator $H := D_m + V$ is essentially self-adjoint, and $\sigma_{ess}(H) = \sigma(D_m)$ by Weyl's Theorem. In contrast to other dispersive equations, such perturbations can produce infinitely many eigenvalues in the spectral gap $(-m, m)$ [Tha92]. Faster decay of the potential ensures there are only finitely many eigenvalues [EGT19]. See [GM01] for a more thorough discussion of further spectral issues.

Dispersive estimates discussed in the previous section for (5) do not hold in general if the operator H has eigenvalues. One can project onto the continuous spectrum to recover dispersive estimates, though threshold eigenvalues or resonances (at energies $\lambda = \pm m$) are known to affect the time decay [EGT19].

One can study the perturbed evolution through a generalized eigenfunction expansion, or through the resolvent operators and functional calculus techniques. The free resolvent operators are defined by $\mathcal{R}_0(z) = (D_m - z)^{-1}$ for $z \in \mathbb{C} \setminus \sigma(D_m)$. Recalling that $D_m = -i\alpha \cdot \nabla + m\beta$, and the the anticommutation relations of the Pauli matrices, we see that $D_m^2 = -\Delta + m^2$, and

$$(D_m - \lambda)(D_m + \lambda) = -\Delta + m^2 - \lambda^2.$$

Formally, this leads us to the relationship

$$\mathcal{R}_0(\lambda) = (D_m + \lambda) R_0(\lambda^2 - m^2), \tag{6}$$

where $R_0(z) = (-\Delta - z)^{-1}$ is the Schrödinger resolvent. By Agmon's limiting absorption principle for Schrödinger operators, we can define the limiting operators as z approaches the essential spectrum from the upper and lower half plane.

In the massive case, when $m > 0$ for $|\lambda|$ close to m, the dominant contribution of the Dirac resolvent behaves like the Schrödinger resolvent. This leads to a generic time-decay rate of size $|t|^{-\frac{3}{2}}$ in three spatial dimensions. When λ is away from the threshold energies $\pm m$, solutions behave like solutions to a Klein–Gordon equation; hence smoothness of the initial data is required to obtain a time-decay. In the massless case, $m = 0$, the equation behaves like the wave equation which has decay rate $|t|^{-1}$ in $\mathbb{R}^3$.

Although the relationship between the resolvents, (6), leads one to expect that there should be analogous results for the dynamics of solutions to the Dirac equation to those known about the Schrödinger equation, at least at the linear level, the analysis of the Dirac equation presents many nontrivial technical challenges.

Perturbations of linear differential operators with the Coulomb potential appear naturally in many areas of physics. For the Dirac operator in $\mathbb{R}^3$ the Coulomb potential takes the form $V(x) = \frac{\gamma}{|x|} I_4$ models electric and/or gravitational interaction between the electron and proton in hydrogenic atoms. The gradient scales like $\frac{1}{|x|}$, so the Coloumb potential is critical for the Dirac operator. The coupling constant γ determines whether the corresponding operator is well-defined or not. In fact, $D_m + \frac{\gamma}{|x|} I_4$ is essentially self-adjoint if and only if $|\gamma| \leq \frac{\sqrt{3}}{2}$ [Tha92].

A similar situation occurs for the Schrödinger operator with inverse square potential, $-\Delta + \frac{\beta}{|x|^2}$. This operator is essentially self-adjoint in $\mathbb{R}^3$ if $\beta \geq \frac{3}{4}$ [RS79]. For $-\frac{1}{4} \leq \beta < \frac{3}{4}$, one can define Friedrichs extension since $-\Delta + \frac{\beta}{|x|^2}$ remains a positive operator. Since the Dirac operator is unbounded below, the Friedrichs extension can not be defined. There are infinitely many self-adjoint extensions if $|\gamma| > \frac{\sqrt{3}}{2}$. However, when $\frac{\sqrt{3}}{2} < |\gamma| < 1$, there is a unique distinguished self-adjoint extension analogous to the Friedrichs extension; see, e.g., [Gal17].

Nonlinear models. Often a nonlinear Schrödinger equation is formed by adding a nonlinear term:

$$iu_t = -\Delta u \pm f(u)u,$$

typically of the form $f(\tau) = |\tau|^\gamma$. There are more choices for how to create the nonlinearity out of the $\mathbb{C}^4$-valued spinor. The Soler model from quantum field theory is

$$i\psi_t = D_m\psi - f(\psi^*\beta\psi)\psi, \tag{7}$$

with f real-valued satisfying $f(0) = 0$, $\psi^* = \overline{\psi^T}$, and β is the matrix used in defining the Dirac operator. One-dimensional analogues of this model include the Gross–Neveu and massive Thirring equations for scalar and vector self-interaction, respectively. The Soler model is well-posed provided the initial data has enough Sobolev regularity, $\psi(x, 0) \in H^s(\mathbb{R}^n)$ for $s > \frac{n}{2}$ [BC19]. The Thirring and Soler (with $f(\tau) = \tau$) nonlinearities are Lorentz covariant and exhibit a null-structure, comparable to other geometric nonlinear wave equations.

Scattering results, that is, the series of conclusions that large-time behavior of solutions approaches that of a free wave, are known for (7) with $f(\tau) = \tau$ in low dimensions provided the initial data is small in an appropriate Sobolev norm [BH15].

A solitary wave is a solution of (7) of the form

$$\psi(x, t) = \phi(x)e^{-i\omega t},$$

where ω is a real-valued parameter and ϕ solves a stationary nonlinear Dirac equation. Such solitary waves are known to exist for broad classes of nonlinearities, but the stability results are less developed. Linearizing about such stationary solutions leads to linear equations of the form considered in (5). Spectral stability is known for classes of nonlinearity f that are polynomial-like [BC19]. Stronger stability results, such as orbital and asymptotic stability of

these solutions for general f is thus far incomplete and less developed than other dispersive equations [Dod19]. One cannot use the concentration-compactness arguments that are standard for other dispersive equations [NS11], among other challenges. Although, somehow unexpectedly, there seems to be a lack of blow-up phenomenon in nonlinear Dirac equations which commonly occurs in other dispersive nonlinear models [BC19].

Honeycomb potentials. Finally, we briefly note the appearance of a two-dimensional Dirac equation in the study of waves in periodic structures inspired by the study of graphene, a material with layers of hexagonal lattices of carbon atoms. The evolution of waves in graphene is modeled by a two-dimensional Schrödinger equation $-\Delta + V$ with a periodic "honeycomb" potential, i.e., V is periodic, even, and invariant under $2\pi/3$ rotations. In contrast to the previous discussion, V does not decay as $|x| \to \infty$.

When decomposing the solution of the Schrödinger equation into Floquet-Bloch states there are Dirac points of the honeycomb structure, where the dispersion surfaces intersect. This leads to an intersection of successive spectral energy bands at some energy μ and the time-independent operator $-\Delta + V - \mu$ has a two-dimensional nullspace spanned by $\Phi_1(x), \Phi_2(x)$. A wave-packet spectrally localized at this energy is of the form (with δ a small parameter)

$$\psi(x,t) \approx e^{i\mu t} \sum_{j=1}^{2} \delta\alpha_j(\delta x, \delta t)\Phi_j(x),$$

where α_j are the amplitudes. Writing $\alpha = (\alpha_1, \alpha_2) \in \mathbb{C}^2$, the evolution of α is governed by a two-dimensional Dirac equation with zero mass. The dynamics of such wave packets is believed to be responsible for the remarkable properties of graphene [FW14].

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