Physics 581 **Quantum Mechanics II** P. M. Goldbart, 3135 ESB

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1) Klein's paradox – optional: In this question we shall explore a striking difficulty with the Dirac equation as a proposal for one-particle quantum mechanics known as the Klein paradox. Consider the Dirac equation in one space dimension z for a particle of mass m moving in the presence of a potential $V\theta(z)$, where V is a positive constant and θ is the usual Heaviside step function. You may find it useful to choose units in which $\hbar$ and c are both unity. (They can always be restored using dimensional analysis.)

a) Find a complete set of plane-wave spinor solutions of the Dirac equation in the absence of the potential.

Now reinstate the potential and focus on the regime $V > E$.

b) For the region $z < 0$, write down a spinor $\psi_{\rm inc}$ describing a positive-energy plane wave incident from the negative z direction having spin up and momentum k.

Assume that the reflected wave is a positive-energy spin-up spinor with amplitude a:

$$\psi_{\rm ref}(z) = a \begin{pmatrix} 1 \\ 0 \\ -k/(E+m) \\ 0 \end{pmatrix} {\rm e}^{-ikz}, \quad \text{for} \quad z \le 0,$$

where $k \equiv +\sqrt{E^2 - m^2}$. Further assume that the transmitted wave has a similar form:

$$\psi_{\rm tra}(z) = c \begin{pmatrix} 1 \\ 0 \\ q/(E-V+m) \\ 0 \end{pmatrix} {\rm e}^{iqz}, \quad \text{for} \quad z \ge 0,$$

where $q \equiv +\sqrt{(E-V)^2 - m^2}$.

c) By making use of continuity across $z = 0$, establish the following matching conditions:

$$1 + a = c, \quad \text{and} \quad 1 - a = rc, \quad \text{where } r \equiv \frac{q}{k}\frac{E+m}{E-V+m}.$$

d) Show that the corresponding currents $\{j_{\rm inc}, j_{\rm ref}, j_{\rm tra}\}$ obey

$$\frac{j_{\rm tra}}{j_{\rm inc}} = \frac{4r}{(1+r)^2}, \quad \frac{j_{\rm ref}}{j_{\rm inc}} = \left(\frac{1-r}{1+r}\right)^2.$$

Notice that the conservation of probabilities does appear to be obeyed: $j_{\rm inc} = j_{\rm tra} + j_{\rm ref}$.

e) Observe that for $V - E < m$ the "wave-length" q is imaginary, so that the transmitted wave decays exponentially with increasing z. By reinstating the dimensionful parameters, give an order-of-magnitude estimate for the decay length for potential step strengths V in the vicinity of the threshold $V - E = m$.

Now contemplate increasing V to try to localize the particle even more sharply under the barrier. Observe that, for $V - E > m$, q is real, so the transmitted wave is oscillatory!

f) Show that for such values of V the ratio r is negative. Show that this suggests that the unphysical result that the reflected flux is larger than the incident one.

The Klein paradox is, at its root, a consequence of the breakdown of one-particle relativistic quantum mechanics in situations in which particles are localized on length-scales comparable to or shorter than their Compton wave-length. For particles of mass m, localization on a scale λ implies momenta on the scale $\hbar/\lambda$ and energies on a scale $\hbar^2/2m\lambda^2$. One-particle physics breaks down when this energy-scale becomes comparable to or greater than the energy-scale for relativistic particle production, mc^2, *i.e.*, for λ comparable to or greater than $\hbar/mc$, *i.e.*, the Compton wave-length.

2) Maxwell's and Dirac's equations – optional: The aim of this question to to show that the Dirac equation can be expressed in a form similar to that of the two Maxwell equations involving the *curl*. They are Faraday's law $\boldsymbol{\nabla} \times \mathbf{E} = -\partial_t \mathbf{B}$, and (the inhomogeneous version of) the Ampère-Maxwell law $\boldsymbol{\nabla} \times \mathbf{B} = \partial_t \mathbf{E}$.

To see this, first note that these laws an be expressed as

$$i\partial_t \mathbf{E} = -i\,(\mathbf{S}\cdot\boldsymbol{\nabla})\,i\mathbf{B}, \quad i\partial_t\, i\mathbf{B} = -i\,(\mathbf{S}\cdot\boldsymbol{\nabla})\,\mathbf{E},$$

where the three matrices $(S^j)_{kl}$ (for $j = 1, 2, 3$) are given by $-i\epsilon_{jkl}$ and, as we shall see, play the same role for the (spin-1) electromagnetic field as the Pauli matrices do for spin-1/2 and the pair of fields $(\mathbf{E}, i\mathbf{B})$.

Now turn to the Dirac equation, and express the four-component spinor ψ as $\begin{pmatrix}\phi\\ \chi\end{pmatrix}$ in terms of two two-component spinors ϕ and χ. Show that, in terms of ϕ and χ, the Dirac equation can be expressed in a form analogous to Maxwell's equations, *i.e.*,

$$i\partial_t\,\phi = +m\phi - i\boldsymbol{\sigma}\cdot\boldsymbol{\nabla}\chi, \quad i\partial_t\,\chi = -m\phi - i\boldsymbol{\sigma}\cdot\boldsymbol{\nabla}\phi.$$

3) Noether's theorem for the O(3) vector model – optional: Consider the O(3) vector model for the triplet of real fields $\{\phi_1, \phi_2, \phi_3\}$, with Lagrange density

$$\mathcal{L} = \frac{1}{2}|\dot{\boldsymbol{\phi}}|^2 - \frac{c^2}{2}|\nabla\boldsymbol{\phi}|^2 - V\left(|\boldsymbol{\phi}|^2\right),$$

where $|\boldsymbol{\phi}|^2 \equiv \sum_{a=1}^3 \phi_a\phi_a$, $|\dot{\boldsymbol{\phi}}|^2 \equiv \sum_{a=1}^3 \dot{\phi}_a\dot{\phi}_a$, and $|\nabla\boldsymbol{\phi}|^2 \equiv \sum_{a=1}^3 \nabla\phi_a\cdot\nabla\phi_a$, and V depends only on the magnitude of $\boldsymbol{\phi}$. Observe the invariance of $\mathcal{L}$ under the global rotation transformation $\boldsymbol{\phi} \to \boldsymbol{\phi} + \boldsymbol{\theta}\times\boldsymbol{\phi}$, *i.e.*, $\phi_a \to \phi_a + \epsilon_{abc}\theta_b\phi_c$.

a) Derive the Noether charge densities and charge currents associated with this invariance.

b) By making explicit use of the classical equations of motion obeyed by $\boldsymbol{\phi}$, show that these densities and currents obey continuity equations.

4) Dirac equation via an action principle – optional: Consider the Lagrange density

$$\mathcal{L} = \hbar c\,\bar{\psi}\left(\gamma^{\mu} i\partial_{\mu} - \frac{mc}{\hbar}\right)\psi,$$

where m is a mass, $\hbar$ is Planck's constant and c is the speed of light *in vacuo*. ψ is a complex-valued four-component function of position and time, a *Dirac spinor*, and $\bar{\psi}$ is its adjoint $\psi^{\dagger}$ multiplied by the Dirac gamma-matrix γ^0.

a) By regarding ψ and $\bar{\psi}$ as independent functions, show that stationarity of $\mathcal{L}$ leads to the Dirac equation. Note the unusual property that if ψ is a solution of the Dirac equation then the action vanishes.

Interaction of the Dirac particle with electromagnetic fields is achieved via *minimal coupling*:

$$\mathcal{L} = \hbar c\,\bar{\psi}\left(\gamma^{\mu}\left(i\partial_{\mu} - \frac{e}{\hbar c}A_{\mu}\right) - \frac{mc}{\hbar}\right)\psi,$$

where e, the charge, measures the strength of this coupling and the (four-)vector potential A_{μ} determines the electromagnetic field.

b) By proceeding as in part (a), obtain the Dirac equation in the presence of an electromagnetic field.

c) The charge current is defined as $-c$ times the coefficient of the vector potential in a functional expansion of the Lagrangian in powers of the vector potential. Equivalently, it is defined via the functional derivative of the Lagrangian with respect to $-(1/c)A_{\mu}$. Show that the charge current density is given by $ec\bar{\psi}\gamma^{\mu}\psi$. Give the simplest expression for the charge density.

d) Show that if ψ obeys the Dirac equation then the charge current density is conserved, *i.e.*, $\partial_{\mu} j^{\mu} = 0$.

e) Show that the Dirac equation retains its form under the local U(1) gauge transformation

$$\psi \to \mathrm{e}^{-ie\Lambda/\hbar c}\,\psi, \qquad \psi \to \mathrm{e}^{-ie\Lambda/\hbar c}\,\psi, \qquad A_{\mu} \to A_{\mu} + \partial_{\mu}\Lambda,$$

where the gauge parameter Λ is an arbitrary function of position and time. The equation is said to be *form-invariant* or *covariant* with respect to gauge transformations. The Dirac equation can also be shown to be form-invariant under Poincaré transformations, and therefore consistent with the requirements of special relativity.

5) Dirac equation and quantum field theory – optional: The Dirac equation was introduced as an attempt to cure a difficulty possessed by relativistic quantum mechanics in the form of the Klein-Gordon equation, the latter equation allowing negative values of the particle number. Although it fails to provide a cure, it does furnish us with several vital structural ingredients for formulating a quantum field theory for many-fermion systems. Such a theory—one allowing for processes in which the particle number changes—is mandatory if ones wishes to build a theory consistent with both quantum mechanics and special relativity. From the higher ground of quantum field theory, in which states containing electrons are regarded as excited states of a quantum field—the Dirac field—in a way that is similar to our view of photons as being excited states of the Maxwell field.

Let us warm up by considering the more familiar world of nonrelativistic quantum mechanics, in the occupation number representation. Consider a system of many spinless identical bosons of mass m whose dynamics is governed by the Hamiltonian

$$\mathcal{H} = -\frac{\hbar^2}{2m}\int d^3r\,\psi^\dagger(\mathbf{r})\nabla^2\psi(\mathbf{r}) + \int d^3r\,\psi^\dagger(\mathbf{r})\,U(\mathbf{r})\,\psi(\mathbf{r})\,,$$

where $\psi(\mathbf{r})$ and $\psi^\dagger(\mathbf{r})$ are field operators obeying boson commutation relations and $U(\mathbf{r})$ is a single-particle potential. Let the state of the system in the Heisenberg picture be denoted by $|\Phi\rangle$.

a) Derive an equation of motion for the amplitude $\langle\Gamma|\psi(\mathbf{r},t)|\Phi\rangle$ for finding the system to be in the state consisting of the ground state $|\Gamma\rangle$ to which a single particle has been added at the location $\mathbf{r}$ at time t. $\psi(\mathbf{r},t)$ is $\psi(\mathbf{r})$ in the Heisenberg picture, and similarly for $\psi^\dagger(\mathbf{r},t)$.

b) Do you arrive at a closed (and familiar!) system of equations?

c) Now augment the Hamiltonian with a term that introduces two-body interactions $V(\mathbf{r}_1,\mathbf{r}_2)$ between the particles,

$$\frac{1}{2}\int d^3r_1\,d^3r_2\,\psi^\dagger(\mathbf{r}_1)\,\psi^\dagger(\mathbf{r}_2)\,V(\mathbf{r}_1,\mathbf{r}_2)\,\psi(\mathbf{r}_2)\,\psi(\mathbf{r}_1)\,,$$

and seek an equation of motion for the amplitude $\langle\Gamma|\psi(\mathbf{r},t)|\Phi\rangle$. Do you find a closed system?

Now let us return to the relativistic world of Dirac particles. The connection between the quantized Dirac field and the Dirac equation comes from considering the general state of the quantum field $|\Phi\rangle$ and studying the amplitude for the system to be in the one-particle state $\psi^\dagger(\mathbf{r},t)|0\rangle$, where $|0\rangle$ is the vacuum state and $\psi^\dagger(\mathbf{r},t)|0\rangle$ is the vacuum state with a Dirac particle added at the position $\mathbf{r}$ at time t. Here, ψ and $\psi^\dagger$ are field operators for Dirac particles and obey fermion *anticommutation* relations.

d) Show that if the dynamics of the Dirac field is governed by the Hamiltonian $\mathcal{H} = -i\hbar c\boldsymbol{\alpha}\cdot\nabla + \boldsymbol{\beta}mc^2$, the amplitude of single-particle quantum states $|\Phi_1\rangle$ evolves according to the Dirac equation.

Note that if the Hamiltonian were augmented by interparticle interactions (either direct or mediated by another field) then, generically, the state would not remain wholly within the one-particle sector of states. This would show up via the appearance, in the equation of motion, of amplitudes for the system to be in other sectors of states.