PHY 215C, MidTerm Exam #2

Due: May 25, 2017

May 27, 2017

1. **Dirac Free Particle.** 40 points.
The Dirac state for a free electron has the space-time dependence and spinor form

$$\Psi(\vec{r},t) = \phi(k)e^{i\vec{k}\cdot\vec{r}-iE_kt/\hbar} = N_k^{-1/2}\begin{bmatrix} 1 \\ 0 \\ \frac{\gamma_k}{1\pm\sqrt{1+\gamma_k^2}} \\ 0 \end{bmatrix} e^{i\vec{k}\cdot\vec{r}-iE_kt/\hbar},$$

where $\vec{k}$ is the wavevector of the electron, and spinor $\phi(k)$ (commonly comprised of spinors χ and Φ) is independent of $\vec{r}$ and t. N_k is the "square" of the displayed bispinor, *i.e.* $N_k^{-1/2}$ normalizes the spinor. We use the shorthand $\gamma_k = \frac{\hbar k}{mc}$. Show all work in the following parts. Use the spin degeneracy to simplify all of the following (four solutions become two).

(i) Obtain the eigenvectors and eigenvalues from the t-independent Dirac equation

$$H_D\Psi = E\Psi; \quad H_D = c\vec{\alpha}\cdot\vec{P} + \beta mc^2.$$

Note: this is a 4×4 equation, so there are four eigenvalues and eigenvectors. The correct spin-up eigenvectors are provided above so some little goof will not mess up the following subproblems. However, show the steps to solution in detail.

Solution. Without loss of generality, let the motion be along the $\hat{z}$ direction $\vec{k} = k\hat{z}$. Eliminating $\Phi = c\vec{\sigma}\cdot\vec{P}/(E+mc^2)\chi$ in favor of χ and using $(\vec{\sigma}\cdot\vec{P})^2 = \vec{P}^2$, leads to a scalar (diagonal) equation

$$[E^2 - m^2c^4 - \hbar^2k^2c^2]\chi = 0$$

for the eigenvalues $E_k = \pm\sqrt{\hbar^2k^2c^2 + m^2c^4}$. χ is undetermined, a normalized choice is $\chi^\dagger$=[1,0], spin up. [An aside: this actually corresponds to spin in the $\hat{z}$ direction *in real space*; already at this level the spin is coupled to real space (the orbital) in Dirac theory.] The spin-down solutions give nothing new, the zeroes in χ and Φ are interchanged with the non-zero elements.. The ± sign in each eigenspinor corresponds to the corresponding eigenvalues $E_k = \pm\sqrt{\hbar^2k^2c^2 + m^2c^4}$.

(ii) Expand the eigenvalues in powers of $\hbar k/mc = k/\kappa_c \equiv \gamma_k$ to zero-th, first, and second order, and interpret the result at each level.
Solution.

$$|E_k| = mc^2[1+\gamma_k^2]^{1/2}] = mc^2[1 + \frac{1}{2}\gamma_k^2 - \frac{1}{8}\gamma_k^4 + ...] \approx mc^2 + \frac{\hbar^2k^2}{2m} - \frac{\gamma_k^2}{4}\frac{\hbar^2k^2}{2m} + ...$$

The zero-th term is the rest mass energy, the next term is $\frac{\hbar^2k^2}{2m}$ is simply the non-relativistic kinetic energy we are very familiar with. The next term can be written in a few ways, here it is given the interpretation of a correction -$\gamma_k^2/4$ to the non-relativistic kinetic energy.

(iii) Expand the eigenvalues in the *large* γ_k regime, again to lowest, and next lowest, order in γ_k^{-1}. Try to explain what is up.

Solution. For large γ_k in the (far) relativistic regime, we can write the expansion as $\gamma_k(1+\frac{1}{2}\gamma_k^{-2}+...)$. The main term is $\pm\hbar kc$, which is the dispersion relation for a *massless* particle (photon), only the next correction involves the mass. Expansion in this regime is questionable because this is in the highly relativistic regime of kinetic energy greater than the rest mass, where we now know that electron-positron creation can and does occur.

(iv) Expand the eigenvectors to first order in γ_k to compare the relative sizes of χ and Φ, for both the positive energy and negative energy eigenstates. Compare the results for the two independent states.

Solution. The non-trivial term in the eigenvectors is the denominator $1 \pm \sqrt{1+\gamma_k^2}$. For the positive energy solution, this is just 2 (to lowest order), so the non-zero component of Φ is $\gamma_k/2$. For the negative energy solution, we get (expanding) $1-[1+\gamma_k^2+....] = -\gamma_k/2$. This being in the denominator, the component of Φ is $-2/\gamma_k$.

If γ_k is small as usual, this looks disastrous. However, we need to recall that the normalization factor becomes, for the negative energy bispinor, $N_k = 1+(\gamma_k/[-2/\gamma_k^2])^2 \rightarrow 1+(-\gamma_k/2)^2 \approx \gamma_k^2/4$. Including this factor, the component of Φ becomes $-\gamma_k/2$, the same magnitude but the opposite sign compared to the positive energy solution.

(v) The Dirac spin matrix $\vec{S}$ is the 4×4 matrix that has $\vec{\sigma}$ along the (2×2) diagonal. First, write the general expression for the expectation value $<\Psi|\vec{S}|\Psi>$ in terms of χ and Φ. Then evaluate the contribution to $<\Psi|S_y|\Psi>$ from the two components of χ.

Solution. In the 2×2 (super)space that χ and Φ live within, $\vec{S}$ is diagonal. So

$$<\vec{S}>=\frac{\hbar}{2}[\chi^\dagger\vec{\sigma}\chi+\Phi^\dagger\vec{\sigma}\Phi].$$

Now, $\chi^\dagger=[1,0]$, and multiplying $\chi^\dagger\sigma_y\chi$ gives the (1,1) component of σ_y, which is zero. Analogously, Φ will also pull out the (1,1) component of σ_y, also giving zero. So $<S_y>=0$. [Additional observation: σ_x also will give zero. This χ is pure spin in $\hat{z}$ direction.]

(vi) What will the eigenspinor(s) whose expectation value is $<\vec{S}>=\frac{\hbar}{2}(1,0,0)$?

Solution. For $\hat{x}$ spin, $\chi^\dagger=[1,1]/\sqrt{2}$ and Φ will also be proportional to this. This is a direct generalization of spinors we have studied earlier to the two-component χ and Φ spinors.

2. Dirac Electron in an Infinite Square Well. 10 points.
Consider a Dirac electron in one dimension in an infinite square well potential, $V = 0$ for $-a < x < +a$, $V = +\infty$ outside this well. The normal boundary condition applies, and recall that the free particle solution is already given for you above.

(i) Solve for the ground state energy. (We are only interested in the positive energy solutions).
Solution. Solution, involving the usual matching at boundaries, is provided on a separate sheet.

(ii) For what value of a, the well halfwidth, will the ground state energy be 10% of the (electron) rest mass energy?
Solution. This will also be given on the separate sheet.

3. **Scattering From of a Bound Dimer.** 30 points.

A scattering center consists of two heavy (i.e. fixed in position) δ-function potentials at $\vec{R}$ and $-\vec{R}$: $V(r) = r_o^3 V_o[\delta(\vec{r}-\vec{R}) + \delta(\vec{r}+\vec{R})]$. (The r_o^3 factor makes V_o have units of energy.) Note that this scatterer is not spherically symmetric.

(i) Calculate the scattering amplitude in the Born approximation.

Solution.

(i) The scattering amplitude is

$$f(\theta,\phi) = -\frac{\mu}{2\pi\hbar^2}\int e^{-i\vec{q}\cdot\vec{r}}V(\vec{r})d^3r = -\frac{\mu V_o r_o^3}{2\pi\hbar^2}(e^{-i\vec{q}\cdot\vec{R}} + e^{i\vec{q}\cdot\vec{R}}) = -\frac{2\mu V_o r_o^3}{2\pi\hbar^2}cos(\vec{q}\cdot\vec{R}).$$

Here $\vec{q} \equiv \vec{k}_f - \vec{k}_i$ with both initial and final wavevectors having length k. Then $|\vec{q}| = q = 2ksin(\theta/2)$.

(ii) Consider the two cases where the line separating the two scatterers lies (1) parallel to the incoming particle along the $\hat{z}$ axis, and (2) perpendicular, along the $\hat{x}$ axis. Which orientation leads to the largest forward scattering amplitude? Is this independent of energy?

Solution. For parallel alignment (1) $cos(\vec{q}\cdot\vec{R}) \rightarrow cos(q_z R)$, for perpendicular alignment (2) it is $cos(q_x R), R \equiv |\vec{R}|$. Recall that $\vec{q} = \vec{k}_f - \vec{k}_i$, with $\vec{k}_i = k\hat{z}$, and $\vec{k}_f = k(sin\theta cos\phi, sin\theta sin\phi, cos\theta)$, so $\vec{q} = k(sin\theta cos\phi, sin\theta sin\phi, cos\theta - 1)$. Then

(1) $cos(q_z R) = cos(kR\ [cos\theta - 1])$,

(2) $cos(q_x R) = cos(kR\ sin\theta sin\phi)$.

Forward scattering is $\theta = 0$, and in each case the argument of *cosine* is zero. The *amplitudes are equal* (and at the maximum value for any angle), and are *independent of energy* (k).

(ii) Consider scattering at $\theta = \pi/2$ and describe the differences in the magnitudes of the scattering amplitudes. A simple sketch might help.

Solution. For this case $\theta = \pi/2$ we have

(1) $cos(q_z R) = cos(kR\ [zero - 1]) = cos(kR)$,

(2) $cos(q_x R) = cos(kR\ sin\phi)$.

So, these factors differ by having axial anisotropy for the $\hat{x}$-directed pair. It is maximum $\phi = 0$ or π, i.e. maximum q_x. At $\phi = \pm\pi/2$, $f(\theta,\phi)$ is the same as for the $\hat{z}$-directed pair – they are, after all, symmetrically oriented in this case of scattering in the $\pm\hat{y}$ directions. The scattering strength oscillates with energy (k), oscillating faster with larger separation R.

(iv) Considering again the same two cases as in part (ii), which falls off the fastest as θ increases from zero? Interpret briefly.

Solution.

The angular factors for small θ are

$$\begin{aligned} (1)\ \ cos(kR[cos\theta - 1]) &\approx cos(\frac{1}{2}\theta^2 kR) \approx 1 - \frac{1}{4}\theta^4(kR)^2, \\ (2)\ \ cos(kR\theta sin\phi) &\approx 1 - \frac{1}{2}\theta^2(kR)^2. \end{aligned} \tag{1}$$

The variation of case (1) is much slower (θ^4) than for the perpendicular alignment (2). The dependence on energy is the same. Interpret? It is a matter of phase interference, but that is what this problem is all about – with the mathematics doing everything for us. One thing this result does point out is that the angular dependence of scattering can be used to learn some things about the internal workings of the scattering center.

4. **The Relativistic H Atom.** 20 points.

The eigenvalues for the Dirac hydrogen atom are given by

$$E_{n,j}/mc^2 = [1 + (\frac{\alpha}{n - (j+\frac{1}{2}) + [(j+\frac{1}{2})^2 - \alpha^2)]^{1/2}})^2]^{-1/2}.$$

Here n is the principal quantum number and j is the value of the total angular momentum $J = L + S$ of the state, and $\alpha = e^2/\hbar c$ is the fine structure constant.

(i) Find the difference in energy between the $2p_{1/2}$ and $2p_{3/2}$ states to lowest non-vanishing order in α^2. Express this difference in a convenient atomic scale unit (eV, meV, Ry, mRy, etc.), i.e. not just as a fraction of the rest mass energy.

Solution. The two states in question are the n=2, j=1/2 and 3/2 states. The rest is largely a practice in expanding in the (very) small parameter α^2. The zero-th order result will be just the rest mass energy. The first order (in α^2) result will be the usual (non-relativistic) result $E_n = 1Ry/n^2$. So the expansion must be to second order, i.e. to include α^4 terms. Might as well begin expanding at the "innermost" layer of the expression to order α^2. Notation: let $J \equiv j + \frac{1}{2}$. Then

$$[J^2 - \alpha^2)]^{1/2} = J(1 - \frac{\alpha^2}{J^2})^{1/2} \approx J(1 - \frac{1}{2}\frac{\alpha^2}{J^2})$$

so the denominator is

$$n - J + [J^2 - \alpha^2)]^{1/2} \approx n - J + (J - \frac{1}{2}\frac{\alpha^2}{J}) = n(1 - \frac{1}{2}\frac{\alpha^2}{nJ}).$$

Inverting this keeping the α^2 term (which will be multiplied by the α^2 already in the numerator, we obtain

$$\begin{aligned} E_{nj}/mc^2 &\approx (1 + \frac{\alpha^2}{n^2}[1 - \frac{1}{2}\frac{\alpha^2}{nJ}]^{-2})^{-1/2} \\ &\approx (1 + \frac{\alpha^2}{n^2}[1 + \frac{\alpha^2}{nJ}])^{-1/2} \\ &= (1 + \frac{\alpha^2}{n^2} + \frac{\alpha^4}{n^3 J}])^{-1/2} \\ &\approx (1 - \frac{1}{2}\frac{\alpha^2}{n^2} + \frac{3}{8}\frac{\alpha^4}{n^4} - \frac{1}{2}\frac{\alpha^4}{n^3 J}] \\ &= 1 + \frac{1}{2}\frac{\alpha^2}{n^2} - \frac{1}{2}\frac{\alpha^4}{n^4}(\frac{n}{J} - \frac{3}{4}) \end{aligned} \tag{2}$$

with $J \equiv j+1$. Observe: the coefficient in the α^2 term is correct, giving the non-relativistic eigenvalues of $(1Ha/2)/n^2 = 1Ry/n^2$.

The question is the difference between the $2p_{1/2}$ and $2p_{3/2}$ energies. The first minus the second is simply from the last term involving $n/J = n/(j + [1/2])$ with n=2:

$$\Delta E = -mc^2\frac{1}{2}\frac{\alpha^4}{n^4}(\frac{n}{2} - \frac{n}{1}) = -\frac{1}{2}\frac{mc^2\alpha^4}{n^4}[-1] = 2Ry\frac{1}{2}\frac{\alpha^2}{16} = \frac{\alpha^2}{16}Ry.$$

This is 3.3×10^{-6} Ry = 4.5 $\times10^{-5}$ eV = 45 μeV, with the $2p_{3/2}$ level higher in energy.