8.322: Quantum Theory II

Problem Set #1 Solutions
February 16, 2007

1. **The Schrödinger Equation in a Central Potential**

(a) The derivatives of the radial wavefunction $\phi_{El}(r) \equiv r f_{El}(r)$ are

$$\frac{d}{dr}\phi_{El} = f_{El} + r f'_{El}$$
$$\frac{d^2}{dr^2}\phi_{El} = 2f'_{El} + r f''_{El}.$$

Using these, we can rewrite the first term of (1):

$$-\frac{1}{2m}\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr}\right) f_{El} = -\frac{1}{2mr}(r f''_{El} + 2f'_{El}) = -\frac{1}{2mr}\frac{d^2\phi_{El}}{dr^2}.$$

Hence, the Schrödinger equation becomes

$$-\frac{1}{2m}\phi''_{El} + \left(V + \frac{l(l+1)}{2mr^2}\right)\phi_{El} = E\phi_{El}$$

$$\Rightarrow V_{\text{eff},l} = V(r) + \frac{l(l+1)}{2mr^2}.$$

(b) The radial equation is a second order ordinary differential equation. Thus, there exist two linearly independent solutions for given E and l.

(c) As $r \to 0$, the $V(r)$ potential can be neglected. In this limit we obtain

$$-\frac{1}{2m}\phi''_{El} + \left(\frac{l(l+1)}{2mr^2} - E\right)\phi_{El} = 0$$

In order for ψ_{Elm} to be normalizable, ϕ_{El} can be no more singular than $r^{-\frac{1}{2}}$ at the origin. Hence, we can expand the wavefunction $\phi_{El} \propto r^p$ for some p. Then the Schrödinger equation is

$$-\frac{1}{2m}p(p-1)\frac{1}{r^2}r^p + \frac{l(l+1)}{2mr^2}r^p = Er^p \to 0$$

Hence we require

$$p(p-1) = l(l+1)$$
$$\Rightarrow \quad p = \begin{cases} -l \\ l+1 \end{cases}$$

Normalizable wavefunction ⇒ only $p = l + 1$ is acceptable.

For the case of $l = 0$ it seems like $p = 0$ and $p = 1$ are both acceptable from the condition of normalizability; however, it is clear that $p = 0$ is not a solution to the Schroödinger equation.

(d) Setting $V(r) \propto \frac{1}{r}$ as $r \to 0$ does not change anything if $l > 0$.

For $l = 0$ in the $r \to 0$ limit we have

$$V_{\text{eff},l} - E \to \frac{c}{r}$$

Then we obtain the following equation for the radial wavefunction

$$-\frac{1}{2m}\phi''_{El} + \frac{c}{r}\phi_{El} = 0$$

The solution has the form

$$\phi(r) \propto r \cdot e^{-r/a_0}$$

For $r \to 0$, $\phi(r) \to r$, and thus our previous calculation still holds.

(e) As $r \to 0$, the Schrödinger equation is

$$\phi''_{El} = -2mE\phi_{El} = 2m|E|\phi_{El}$$

The solution is

$$\phi_{El} \propto e^{\pm\sqrt{2m|E|}r}$$

Only the one with negative sign is normalizable.

Even though this solution is valid for any $E < 0$, the function must also satisfy the Schrödinger equation for finite r which imposes conditions that must match up with the solution as $r \to \infty$. These conditions together lead to the quantization of E.

2. **Solutions to the Free Schrödinger Equation in 3 Dimensions — Spherical Bessel Functions**

Starting with (2), we have

$$z^2\frac{d^2}{dz^2}f_l(z)+2z\frac{d}{dz}f_l(z)+(z^2-l(l+1))f_l(z)=0$$

Putting $z=kr$, we recover (1) with $V(r)=0$ and $k^2=2mE$.

(a) As $z\to\infty$,

$$\begin{aligned}j_l(z)&\sim\frac{\sin(z-\frac{l\pi}{2})}{z}\\ y_l(z)&\sim-\frac{\cos(z-\frac{l\pi}{2})}{z}.\end{aligned}$$

(b) The potential is $V(r)=0$ for $r\le R$ and $V(r)\to\infty$ for $r>R$. We know therefore that the wavefunction must be zero at $r=0$ and at $r>R$. Inside the region $r<R$ the solution will just be the spherical Bessel functions. Because of the condition at the origin we are restricted to spherical Bessel functions of the first kind. The boundary condtion at $r=R$ will force that we choose l and k such that

$$j_l(kR)=0.$$

Thus

$$kR=j_{l,s}\Rightarrow E=\frac{\hbar^2 j_{l,s}^2}{2mR^2}$$

restoring the factors of $\hbar$.

Looking at the table of the zeros of the spherical Bessel functions the first six energy levels are thus (in units of $\frac{\hbar^2}{2mR^2}$)

$n=1$	9.8696	$l=0$
$n=2$	20.1907	$l=1$
$n=3$	33.2175	$l=2$
$n=4$	39.4784	$l=0$
$n=5$	48.8312	$l=3$
$n=6$	59.6795	$l=1$

(c) We now take a linear combination of $j_l(kr)$ and $y_l(kr)$. In order to match the boundary conditions imposed by the hard sphere, we need

$$\alpha j_l(kR)+\beta y_l(kR)=0.$$

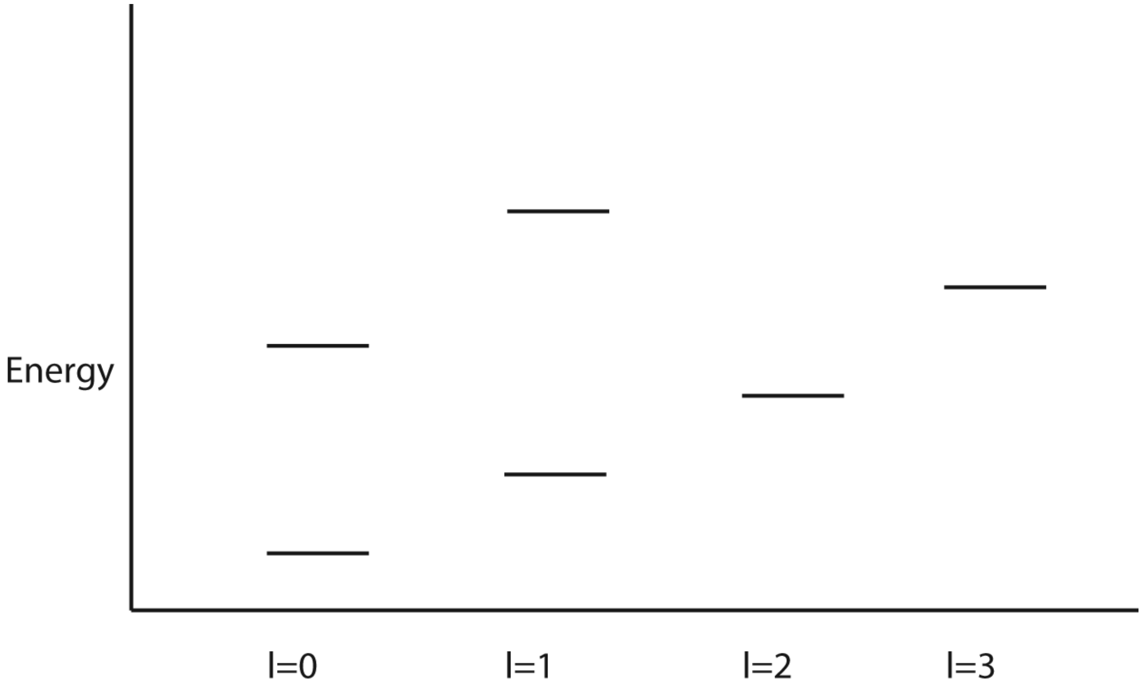

Figure 1: Energy Spectrum

Thus up to a constant

$$f_l(r) \sim y_l(kR)j_l(kr) - j_l(kR)y_l(kr).$$

Because we must take a particular linear combination of the two types of spherical Bessel functions the solution is unique up to a multiplicative constant. As $r \to \infty$

$$f_l(r) \to \frac{1}{kr}\left[y_l(kR)\sin(kr - \frac{l\pi}{2}) + j_l(kR)\cos(kr - \frac{l\pi}{2})\right]$$

If $R = 0$, the solutions would be Bessel functions of the first kind thus we write

$$f_l(r) \sim C\sin(kr + \delta_l(E) - \frac{l\pi}{2})$$

which gives

$$\delta_l(E) = \arctan(\frac{j_l(kR)}{y_l(kR)}).$$

3. **Qualitative Features of the Radial Wavefunction**

(a) From the Schrödinger equation we obtain

$$\frac{\phi''}{\phi} = 2m(V_{eff} - E)$$

In the allowed (forbidden) region this gives oscillation (exponential behavior). Figure 2 shows ϕ'' in the different regions.

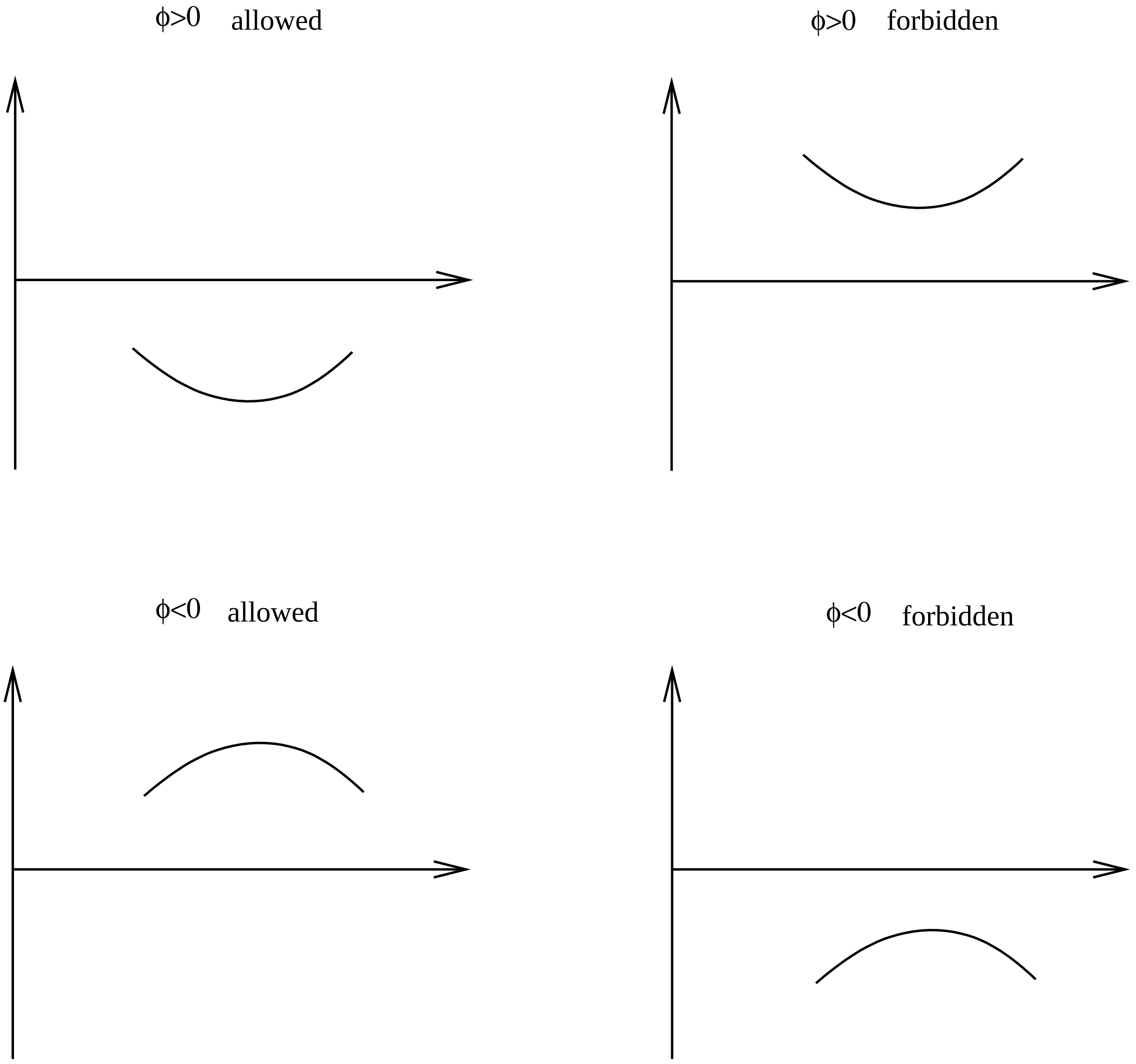

Figure 2: Behavior of ϕ'' in different regions.

(b) The Schrödinger equation for energy E and $E + dE$

$$-\phi''_E + (V - E)\phi_E = 0$$
$$-\phi''_{E+dE} + (V - E - dE)\phi_{E+dE} = 0$$

Then,

$$\phi''_{E+dE}\phi_E - \phi''_E\phi_{E+dE} = -\phi_{E+dE}\phi_E \cdot dE$$
$$\frac{\partial}{\partial r}(\phi'_{E+dE}\phi_E - \phi'_E\phi_{E+dE}) = -\phi_{E+dE}\phi_E \cdot dE$$
$$\frac{\partial}{\partial r}\left(\left(\frac{\partial}{\partial E}\phi'_E\right)\phi_E - \phi'_E\left(\frac{\partial}{\partial E}\phi_E\right)\right) \cdot dE = -\phi_{E+dE}\phi_E \cdot dE.$$

Thus,

$$\frac{\partial}{\partial r}(\dot{\phi}'\phi - \phi'\dot{\phi}) = -\phi^2$$

Now

$$\frac{\partial}{\partial E}\left(\frac{\phi'}{\phi}\right) = \frac{\dot{\phi}'}{\phi} - \frac{\phi'\dot{\phi}}{\phi^2}$$
$$\frac{\partial}{\partial r}\left(\dot{\phi}'\phi - \phi'\dot{\phi}\right) = \frac{\partial}{\partial r}\left(\phi^2\frac{\partial}{\partial E}\left(\frac{\phi'}{\phi}\right)\right) = \phi^2$$

Hence

$$\phi^2\frac{\partial}{\partial E}\left(\frac{\phi'}{\phi}\right) = -\int \phi^2 dr$$
$$\frac{\partial}{\partial E}\left(\frac{\phi'}{\phi}\right) = -\frac{1}{\phi^2}\int \phi^2 dr < 0 \quad \text{for any r.}$$

(c) Since $\frac{\partial}{\partial E}\left(\frac{\phi'}{\phi}\right) < 0$ for all r, we have

$$\phi\,\dot{\phi}' - \phi'\dot{\phi} < 0.$$

Let $a(E)$ be the position of a node of ϕ. Thus $\phi(a(E), E) = 0$. If $\phi = 0$ at some point (r, E) then at that point ϕ' and $\dot{\phi}$ have the same sign. We then consider

$$\frac{d\phi}{dE} = 0,$$

which gives

$$\phi'\frac{da}{dE} = -\dot{\phi}.$$

Thus

$$\frac{da}{dE} < 0$$

and hence the nodes move toward the origin.

(d) We know that for arbitarily negative E, the wavefunction vanishes at the origin and has positive curvature everywhere. Thus it has no other nodes than the one at the origin. From our result in part (c), it is true that as E decreases the position of the node a strictly increases. Thus the node will move to ∞ for low enough energy. Since the wavefunction will fall of exponentially at large r and has a node at 0 it will be normalizable.

4. **Sketching Wavefunctions**

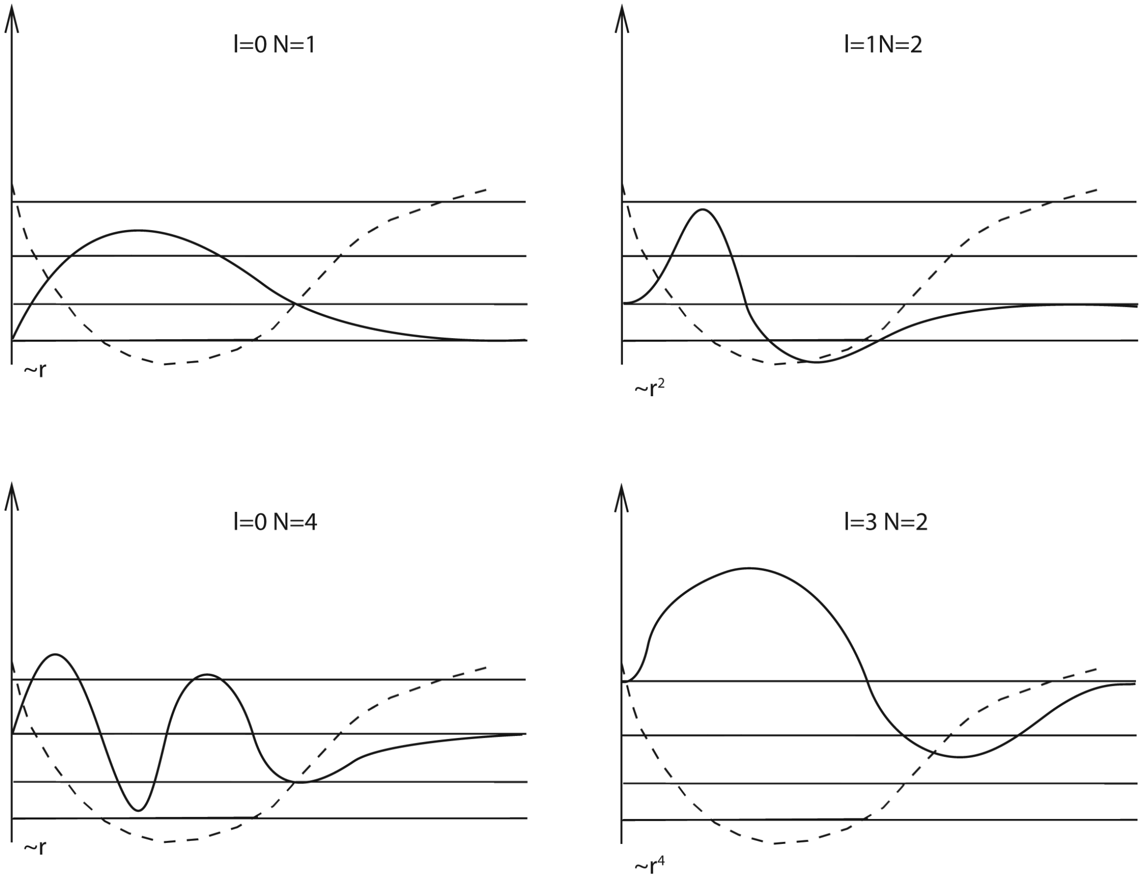

Figure 3: Central potential. Case one.

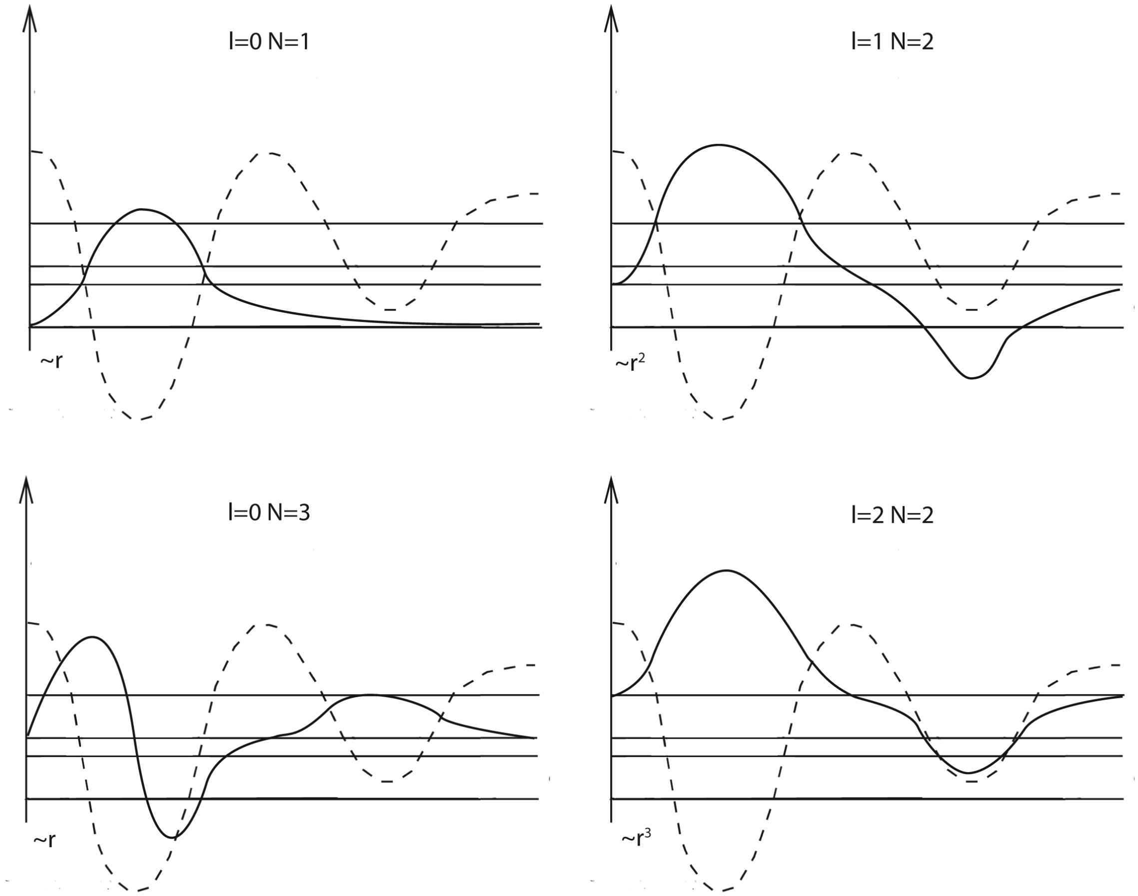

Figure 4: Case two.

5. **The Feynman–Hellman Theorem**

   (a)

$$\begin{aligned}
E(\lambda) &= \langle\psi(\lambda)|H(\lambda)|\psi(\lambda)\rangle \\
\frac{d}{d\lambda}E(\lambda) &= \langle\frac{\partial}{\partial\lambda}\psi(\lambda)|H(\lambda)|\psi(\lambda)\rangle + \text{h.c.} + \langle\psi(\lambda)|\frac{\partial}{\partial\lambda}H(\lambda)|\psi(\lambda)\rangle \\
&= E(\lambda)\left(\langle\frac{\partial}{\partial\lambda}\psi(\lambda)|\psi(\lambda)\rangle + \text{h.c.}\right) + \langle\psi(\lambda)|\frac{\partial}{\partial\lambda}H(\lambda)|\psi(\lambda)\rangle \\
&= E(\lambda)\frac{\partial}{\partial\lambda}\langle\psi(\lambda)|\psi(\lambda)\rangle + \langle\psi(\lambda)|\frac{\partial}{\partial\lambda}H(\lambda)|\psi(\lambda)\rangle \\
&= \langle\psi(\lambda)|\frac{\partial}{\partial\lambda}H(\lambda)|\psi(\lambda)\rangle
\end{aligned}$$

(b) Try $\lambda = e$. Then,

$$\begin{aligned} H &= -\frac{1}{2m}\nabla^2 + \frac{e^2}{r} \\ \frac{\partial E}{\partial e} &= \frac{4}{e}E \quad \text{as} \quad E \propto e^4 \\ \frac{\partial H}{\partial e} &= \frac{2}{e}V \quad \text{as} \quad V \propto e^2. \end{aligned}$$

Hence we obtain the virial theorem

$$2E(N) = \langle N|\frac{-e^2}{r}|N\rangle.$$

6. **Feshbach-Villars Formalism for the Klein Gordon Equation**

(a) From the Klein-Gordon equation and its conjugate we find

$$\begin{aligned} \psi^* \left[(i\partial_\mu - \frac{e}{\hbar c}A_\mu)^2\psi - \kappa^2\psi\right] &= 0 \\ \psi \left[(-i\partial_\mu - \frac{e}{\hbar c}A_\mu)^2\psi^* - \kappa^2\psi*\right] &= 0. \end{aligned}$$

Subtratcing these two equations gives

$$\begin{aligned} -\psi^*\partial_\mu\partial^\mu\psi + \psi\partial_\mu\partial^\mu\psi^* - \frac{2ie}{\hbar c}\left[A_\mu\psi^*\partial^\mu\psi + A_\mu\psi\partial^\mu\psi^*\right] &= 0 \\ \partial_\mu\left[(-\psi^*\partial^\mu\psi - \psi\partial^\mu\psi^*) - \frac{2ie}{\hbar c}A^\mu\psi^*\psi\right] &= 0. \end{aligned}$$

Thus

$$j_\mu = \frac{i\hbar}{mc}(\psi^*\partial_\mu\psi - \psi\partial_\mu\psi^*) - \frac{2e}{mc^2}\psi^*\psi A_\mu$$

is conserved.

(b) Using,

$$\theta \equiv \frac{i}{\kappa}\left(\frac{1}{c}\frac{\partial}{\partial t} + \frac{ie\Phi}{\hbar c}\right)\psi$$

the Klein-Gordon equation gives

$$\begin{aligned} \left(\frac{i}{c}\frac{\partial}{\partial t} - \frac{e}{\hbar c}\Phi\right)^2\psi - \left(i\nabla - \frac{e}{\hbar c}\mathbf{A}\right)^2\psi &= \kappa^2\psi \\ \kappa\left(\frac{i}{c}\frac{\partial}{\partial t} - \frac{e}{\hbar c}\Phi\right)\theta - \left(i\nabla - \frac{e}{\hbar c}\mathbf{A}\right)^2\psi &= \kappa^2\psi. \end{aligned}$$

Using $\psi = \frac{1}{\sqrt{2}}(\chi + \xi)$ and $\theta = \frac{1}{\sqrt{2}}(\chi - \xi)$ and plugging this into the defenition of θ and the Klein-Gordon equation, we use these two equations to solve for $\dot{\xi}$ and $\dot{\chi}$

$$\begin{aligned} i\hbar\dot{\chi} &= mc^2\chi + e\Phi\chi + \frac{\hbar^2}{2m}\left(i\nabla - \frac{e}{\hbar c}\mathbf{A}\right)^2(\chi + \xi) \\ i\hbar\dot{\xi} &= -mc^2\xi + e\Phi\xi - \frac{\hbar^2}{2m}\left(i\nabla - \frac{e}{\hbar c}\mathbf{A}\right)^2(\chi + \xi) \end{aligned}$$

Looking at the form of the Pauli matrices, we see that we thus have

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

where Ψ and H are given by (7) and (8) respectively.

(c) The charge density $\rho = j^0$.

$$\begin{aligned} \Psi^\dagger\tau_3\Psi &= \chi^*\chi - \xi^*\xi \\ &= \psi^*\theta + \theta^*\psi \\ &= \frac{i}{\kappa}\psi^*\left(\frac{1}{c}\frac{\partial}{\partial t} + \frac{ie}{\hbar c}\Phi\right)\psi + \text{c.c.} \\ &= \frac{i\hbar}{mc}\left(\psi^*\dot{\psi} - \dot{\psi}^*\psi\right) - \frac{2e}{mc^2}\psi^*\psi\Phi \\ &= j^0. \end{aligned}$$

(d) If $A_\mu = 0$,

$$H = -(\tau_3 + i\tau_2)\frac{\hbar^2}{2m}\nabla^2 + mc^2\tau_3.$$

We now try the solution

$$\Psi = e^{-ik_0t + i\mathbf{k}\cdot\mathbf{x}}\begin{pmatrix}\chi_0 \\ \xi_0\end{pmatrix},$$

which gives the eigenvalue equation

$$\begin{pmatrix} mc^2 + \frac{\hbar^2k^2}{2m} - \hbar k_0 & \frac{\hbar^2k^2}{2m} \\ -\frac{\hbar^2k^2}{2m} & -mc^2 - \frac{\hbar^2k^2}{2m} - \hbar k_0 \end{pmatrix}\begin{pmatrix}\chi_0 \\ \xi_0\end{pmatrix} = 0.$$

Solutions only exist if the determinant is zero thus,

$$\hbar k_0 = \pm\sqrt{m^2c^4 + \hbar^2k^2c^2}.$$

Plugging this solution into

$$\xi_0 = \frac{2m}{\hbar^2k^2}(mc^2 + \frac{\hbar^2k^2}{2m} - \hbar k_0)\chi_0$$

gives

$$\frac{\xi_0}{\chi_0} = \frac{\hbar k_0 - mc^2}{\hbar k_0 + mc^2}$$

so for $E > 0$

$$\Psi = \begin{pmatrix} 1 \\ \frac{E-mc^2}{E+mc^2} \end{pmatrix} e^{(-iEt+i\mathbf{p}\cdot\mathbf{x})/\hbar}$$

and for $E < 0$

$$\Psi = \begin{pmatrix} \frac{E+mc^2}{E-mc^2} \\ 1 \end{pmatrix} e^{(-iEt+i\mathbf{p}\cdot\mathbf{x})/\hbar}$$

where $\mathbf{p} = \hbar\mathbf{k}$ and $E = \hbar k_0$.

(e)

$$Q = \int d^3x \Psi^\dagger \tau_3 \Psi \sim \begin{pmatrix} \chi_0(p) & \xi_0(p) \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} \chi_0(p) \\ x_0(p) \end{pmatrix}$$

Thus for $E > 0$

$$Q \sim 1 - \frac{E - mc^2}{E + mc^2} = \frac{2mc^2}{E + mc^2} > 0$$

and for $E < 0$

$$Q \sim \frac{E + mc^2}{E - mc^2} - 1 = \frac{2mc^2}{E - mc^2} < 0.$$