Massachusetts Institute of Technology
Physics Department

Physics 8.322 **Spring 2007**
Quantum Theory II **February 7, 2007**

Assignment 1

DUE FEBRUARY 16, 2007, AT THE END OF THE DAY

Announcements

- Usually problem sets will be available on Mondays, nine days before they are due. This is an exception — a problem set intended to help you review properties of the Schrödinger wave function in central potentials.
- $\hbar = 1$ **in 8.322, unless otherwise noted.**
- Problem Sets can be downloaded from http://web.mit.edu/8.321/

Reading topics for this period

- Review: Schrödinger equation in three dimensions. Qualitative behavior of wave functions.
- Relativistic quantum mechanics and the Dirac equation

Reading Recommendations 1

- Qualitative behavior of wave functions

  These concepts can be found in any introductory book on quantum mechanics (*eg.* Griffiths, Gasiorowicz, Cohen-Tannoudji, ...) usually in the sections on the one-dimensional Schödinger equation, the radial equation, the variational principle, and/or scattering theory.
- Relativistic quantum mechanics: Bjorken and Drell *Relativistic Quantum Mechanics* §1, scanned material posted on the 8.322 website.

Problem Set 1

Topics covered in the problems

- Review of the Schrödinger equation in three dimensions. Those of you who took 8.321 will remember that we did almost no wave mechanics — solving the Schrödinger equation in coordinate space. That subject is usually well treated in undergraduate courses. In 8.322 I would like to assume that everyone is familiar with basic properties of Schrödinger wave functions. This problem set is intended as a review of those properties. If you are familiar with them, it should take only an hour or so... If not, please review the material in the reading references.

About calculations in 8.322

By the way, I don't care how you do integrals. You can do them by hand, use a symbolic manipulation program, or look them up in tables. However, I strongly recommend doing as much of the work analytically as possible. Please quote the results clearly, so the grader can understand your work. For example: after considerable work you may reduce a problem to the calculation of the integral $\int_0^1 \frac{dx}{\sqrt{1-x^4}}$, which you could then quote as $\sqrt{\pi}\Gamma(5/4)/\Gamma(3/4) = 1.31103....$

About sketches and plots in 8.322

I do have a preference about plots, however. When I ask you to sketch something, I prefer if you would do it free hand. View it as a challenge to your artistic ability: make as accurate a free hand sketch as you can. [I don't think you learn as much when the computer makes generates the sketch.] On the other hand, when I ask for a plot, you can use any method you like.

Problems

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

   A particle moves in a central potential, $V(r)$. Assume that the potential is *short range*,
   $$\lim_{r\to\infty} r^2 V(r) = 0$$
   and regular at the origin,
   $$\lim_{r\to 0} V(r) = \text{ constant}$$
   Energy and angular momentum are conserved, so the wave function of an energy eigenstate can be written
   $$\psi_{Elm}(\vec{x}) = f_{El}(r) Y_{lm}(\theta, \phi),$$

and $f_{El}(r)$ obeys,

$$-\frac{1}{2m}\left(\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}\right)f_{El}(r)+\left(V(r)+\frac{l(l+1)}{2mr^2}\right)f_{El}(r)=Ef_{El}(r) \qquad (1)$$

with $r \geq 0$.

(a) Define the *radial wavefunction*, $\phi_{El}(r) \equiv r f_{El}(r)$ and show that it obeys an effective one dimensional Schödinger equation in r, the *radial equation*, with an effective potential, $V_{\text{eff},l}(r) = V(r) + l(l+1)/2mr^2$.

(b) How many linearly independent solutions are there to the radial equation for a given E and l?

(c) Show that $\phi_{El}(r) \propto r^p$ as $r \to 0$. What are the values of p allowed by the differential equation? Which values of p are physically acceptible? Why?

(d) What changes if $V(r) \sim 1/r$ as $r \to 0$?

(e) Consider $E < 0$. What are the linearly independent solutions of the radial equation as $r \to \infty$, $\{\phi_i, i = 1, 2\}$? Which one is physically acceptable? If one of the solutions as $r \to \infty$ is acceptable for any $E < 0$, why are the allowed values of the energy quantized for bound states?

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

The differential equation that defines spherical Bessel functions, $f_\ell(z)$, is

$$z^2 f_\ell''(z) + 2z f_\ell'(z) + (z^2 - \ell(\ell+1))f_\ell(z) = 0 \qquad (2)$$

Clearly $f_\ell(kr)$ is a solution to the eq. (1) with $V(r) = 0$. What is k in terms of the parameters in eq. (1)?

The solutions to eq. (2) that are *regular* at the origin are spherical Bessel functions of the first kind, $j_\ell(z)$. The solutions that are irregular at the origin are spherical Neumann functions, or spherical Bessel functions of the second kind, $y_\ell(z)$ (sometimes denoted $n_\ell(z)$). Some important properties of j_ℓ and y_ℓ are summarized on the pages copied from Abramowicz and Stegun *Handbook of Mathematical Functions*, appended to this problem set. Note that these functions are simply power series in $\frac{1}{z}$ multiplying sines and cosines of z. Note also the series expansions at small z, **10.1.2** and **10.1.3**.

(a) Using the representation by elementary functions, **10.1.8** and **10.1.9**, find the asymptotic behavior of $j_\ell(z)$ and $y_\ell(z)$ as $z \to \infty$.

(b) Find the spectrum of the infinite potential hole ($V(r) = 0$ for $r \leq R$ and $V(r) \to \infty$ for $r > R$) in three dimensions. Express your answer in terms of the s^{th} zero of $j_\ell(z)$, denoted $j_{\ell,s}$. What are the energies (in units of $\hbar^2/2mR^2$), and angular momenta of the first six energy levels in this potential? Make a sketch of the spectrum to this order. [You can find the zeros of spherical Bessel functions on the fourth page of the attached section of J&S, on the web, or can compute them using Mathematica, Matlab, ...]

(c) Now consider the Schrödinger equation outside a hard sphere, $r > R$. Aside from the boundary condition $f(R) = 0$, there is no interaction. What is the Schrödinger wavefunction with energy E? Is it unique (up to a multiplicative constant)? Express its asymptotic form (as $r \to \infty$) in terms of a phase $\delta_\ell(E)$ relative to the case $R = 0$.

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

Some very simple properties of the Schrödinger equation provide a qualitative guide to the behavior of energy eigenfunctions. This problem explores some of these properties for the *radial wavefunction*, $\phi(r)$, defined in Problem 1 a). However some of the properties are quite subtle and have far reaching consequences.

(a) The *classically allowed* (*forbidden*) region is the range of r where $E > V_{\text{eff},l}(r)$ ($E < V_{\text{eff},l}(r)$). How does $\phi''_{El}(r)/\phi_{El}(r)$ behave in each of these regions? Sketch $\phi''_{El}(r)$ for $\phi_{El}(r) > 0$ and $\phi_{El}(r) < 0$ in classically allowed and forbidden regions.

Often the solutions to the Schrödinger equation are obtained by starting at $r = 0$ with the regular solution (the one with the r dependence you found in Problem 1), and integrating out to increasing r. This is a good way to find bound states, for example: you integrate out to large r and adjust the energy E so the solution at large r *falls* exponentially with r. Considerations like this make it interesting to know the variation of the radial wavefunction, $\phi(r, E)$ with E, which is established in the next part.

(b) Show that

$$\frac{d}{dE}\left(\frac{\phi'(r,E)}{\phi(r,E)}\right) < 0 \quad \text{for any } r$$

The "Hint" includes the entire material in brackets

[Hint: Write the Schrödinger equation for energy E and again for energy $E+dE$. Follow steps similar to the derivation of the Wronskian identity to obtain

$$\frac{d}{dr}\left(\dot{\phi}'\phi - \phi'\dot{\phi}\right) = -\phi^2$$

where $\dot{\phi} \equiv d\phi/dE$ (I've set $\hbar^2/2m = 1$.).]

(c) Consider the solution of the radial equation that is regular at the origin *as a function of the energy* E. Except at the eigenvalues of H these are not normalizable and therefore not acceptable quantum states of the system. Nevertheless we can study them as functions of r and E. Show that the nodes in $\phi(r, E)$ always move to the left (*ie.* toward smaller r) as E increases.

(d) Use the results derived in the previous parts of this problem to show the following: If a potential, $V(r)$, has bound states, then the wavefunction of the bound state with the lowest energy has no nodes except the ones required at $r = 0$ and as $r \to \infty$.

4. **Sketching Wavefunctions**

   Consider the potentials shown in the Figure. Some of the energy eigenvalues are marked by the horizonal lines. The angular momentum and the order of excitation ($N = 1$ is the lowest state with this value of l, $N = 2$ next, *etc.*) of the corresponding to the eigenvalue are shown. For each potential, make a sketch — as accurately as you can — of the radial wavefunction associated with each state. For regions where you know the functional dependence on r, indicate it.

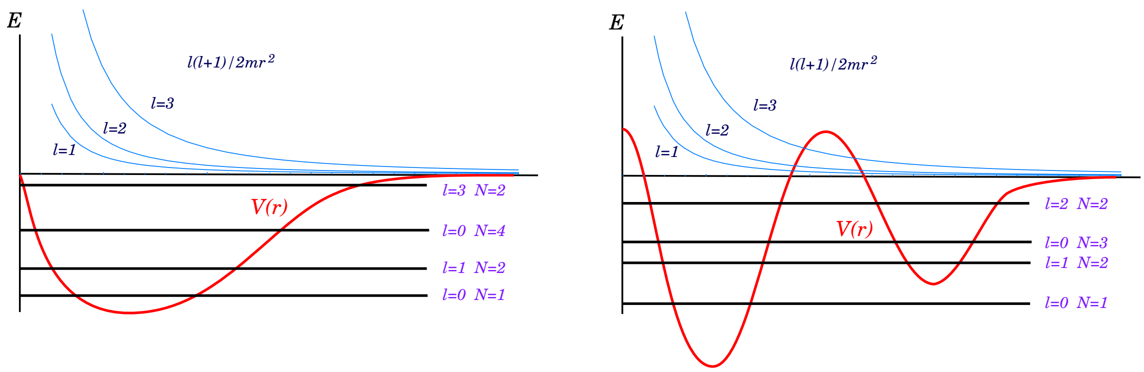

Figure 1: Two potentials, $V(r)$, shown in red. The angular momentum "barrier", $l(l+1)/2mr^2$ is shown in blue. The energies of various bound states are shown as horizontal lines labeled with the value of l and the level of excitation, N, which begins with $N = 0$.

5. **The Feynman–Hellman theorem**

   This theorem can be found in Richard Feynman's MIT Senior Thesis. The literature citations are R. P. Feynman, Phys. Rev. **56** 340 (1939) and H. Hellmann, *Einfuhrung die Quantunchemie* (Deutike, Leipzig, 1937).

   Suppose the Hamiltonian of a system depends on a paramter λ, $H \equiv H(\lambda)$. Note the dependence does not have to be linear. Of course the eigenvalues and eigenfunctions of H will also depend on λ, so we denote them $E(\lambda)$ and $|\psi(\lambda)\rangle$.

   (a) Prove the theorem:

$$\frac{dE(\lambda)}{d\lambda} = \langle\psi(\lambda)|\frac{\partial H}{\partial\lambda}|\psi(\lambda)\rangle \tag{3}$$

   Hint: Write $E(\lambda) = \langle\psi(\lambda)|H(\lambda)|\psi(\lambda)\rangle$, differentiate w.r.t. λ and use standard properties of energy eigenstates.

   (b) In 8.321 we proved a "virial theorem" for hydrogen bound states: $\langle\frac{e^2}{r}\rangle|_N = -2E(N)$, where $E(N) = -\frac{mc^2\alpha^2}{2N^2}$, $N = 1, 2, 3...$, is the total energy. Prove this result using the Feynman-Hellman Theorem.

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

It seems odd that the Klein-Gordon equation yields a Hamiltonian that is not local in coordinate space,

$$H = \pm\sqrt{-\hbar^2 c^2 \nabla^2 + m^2 c^4}$$

(note, $\hbar$ is not set equal to unity in this problem).

Years ago Herman Feshbach and Felix Villars (both MIT professors) showed how to define a local Hamiltonian to describe the relativistic wave mechanics of a spinless particle[1]. The trick is to introduce a *two component* wavefunction, leading to states of positive and negative energy with opposite electric charge, in contrast to the situation in the Dirac equation.

Consider the Klein Gordon equation with an external electromagnetic field, $A^\mu = (\Phi, \vec{A})$, obeying the Lorentz-gauge condition $\partial_\mu A^\mu = 0$,

$$\left(i\partial_\mu - \frac{e}{\hbar c}A_\mu\right)^2 \psi - \kappa^2 \psi = 0 \tag{4}$$

where $\kappa = mc/\hbar$.

(a) Show that

$$j_\mu = \frac{i\hbar}{mc}\left(\psi^* \partial_\mu \psi - \psi \partial_\mu \psi^*\right) - \frac{2e}{mc^2}\psi^* \psi A_\mu \tag{5}$$

is a conserved current: $\partial_\mu j^\mu = 0$.

Note that the time component, $\rho = j^0$ is not positive definite, so it is not possible to interpret ρ as a probability density. Instead we will try to interpret it as a charge density.

Now introduce a *two component* form for the Klein-Gordon wavefunction. Define

$$\begin{aligned}
\theta &\equiv \frac{i}{\kappa}\left(\frac{1}{c}\frac{\partial}{\partial t} + \frac{ie\Phi}{\hbar c}\right)\psi \\
\chi &\equiv \frac{1}{\sqrt{2}}(\psi + \theta) \\
\xi &\equiv \frac{1}{\sqrt{2}}(\psi - \theta)
\end{aligned} \tag{6}$$

(b) Show that the Klein-Gordon equation can be written

$$H\Psi = i\hbar \frac{\partial \Psi}{\partial t} \tag{7}$$

with

$$\Psi \equiv \begin{pmatrix} \chi \\ \xi \end{pmatrix}$$

[1] H. Feshbach and F. Villars, Rev. Mod. Phys. **30** 24 (1958).

and

$$H = (\tau_3 + i\tau_2)\frac{\hbar^2}{2m}\left(i\vec{\nabla} + \frac{e}{\hbar c}\vec{A}\right)^2 + mc^2\tau_3 + e\Phi \tag{8}$$

where $\{\tau_i, i = 1, 2, 3\}$ are the Pauli matrices.

(c) Show that the charge density, ρ, is simply $\Psi^\dagger \tau_3 \Psi$.

(d) Find the plane wave solutions to eq. (7) for $A_\mu = 0$, of the form

$$\Psi = \begin{pmatrix} \chi_0(p) \\ \xi_0(p) \end{pmatrix} \exp[-i(E(p)t + i\vec{p}\cdot\vec{x})/\hbar] \tag{9}$$

with positive and negative eigenvalues,

$$E(p) = \pm\sqrt{p^2c^2 + m^2c^4}$$

(e) Show that the positive and negative energy eigenstates of the previous section have opposite charge if charge is defined to be $Q = \int d^3x \Psi^\dagger \tau_3 \Psi$.

Thus the Klein-Gordon equation has positive and negative energy solutions with opposite charge. In comparison, the Dirac equation has positive and negative energy solutions with *the same charge.* This difference will eventually lead to the requirement that Dirac particles (spin-1/2) obey Fermi statistics) while KG particles obey Bose statistics.