

Physics 580: Quantum Mechanics I
Department of Physics, UIUC
Fall Semester 2006
Professor Eduardo Fradkin

Problem Set No. 6
Bound States and Scattering Theory
Due Date: November 13, 2006

1 Square Well in Three Dimensions

In this problem you will consider the quantum mechanics of a particle of mass M moving in three dimensions, in the field of the potential

$$U(\vec{r}) = \begin{cases} U_0 & \text{for } |\vec{r}| \leq r_0 \\ 0 & \text{otherwise} \end{cases}$$

with $U_0 < 0$.

1. List *all* the operators that commute with the Hamiltonian of this system. What is the largest set of these operators which can be diagonalized simultaneously with the Hamiltonian. What are the quantum numbers and the wave functions of these operators in spherical coordinates?
Here

$$\begin{aligned} x &= r \cos \phi \sin \theta \\ y &= r \sin \phi \sin \theta \\ z &= r \cos \theta \end{aligned}$$

2. Write the Schrödinger Equation in spherical coordinates (r, θ, ϕ) for this problem. Show that the wave functions of the eigenstates in these coordinates have the form

$$\psi(r, \theta, \phi) = R(r)F(\theta, \phi)$$

Justify why you can write the wave functions in this form. What is the form of the angular wave functions $F(\theta, \phi)$? Why?

3. Solve the radial Schrödinger equation for this problem for $E < 0$. Work out explicitly the boundary conditions that you need to impose at $r = 0$, $r = a$ and as $r \rightarrow \infty$. Justify your answers. What is the form of the wave functions for $r > r_0$? And for $r \leq r_0$?
4. Discuss how many s and p energy levels you find for different ranges of the parameters U_0 and r_0 . What is the degeneracy of the energy levels? Why? Is it the same as in the Hydrogen atom? Why? Why not?

- Construct explicitly the wave functions for the singlet bound states with quantum numbers $1s$ and $2s$, and for the triplet states $2p$. What do these numbers mean for this particular problem? For what range of the parameters U_0 and a do all of these states exist? Why? What is the degeneracy of these states?
- Find an expression for the *total* probability current

$$\vec{J} = \int d^3x \frac{\hbar}{2Mi} \left(\psi^*(\vec{r}) \vec{\nabla} \psi(\vec{r}) - \psi(\vec{r}) \vec{\nabla} \psi^*(\vec{r}) \right)$$

for the $1s$, $2s$ and $2p$ states. For what states is $\vec{J} \neq 0$? Why?

Hint: Work in spherical coordinates. The gradient operator in spherical coordinates is

$$\vec{\nabla} = \hat{e}_r \frac{\partial}{\partial r} + \hat{e}_\phi \frac{1}{r \sin \theta} \frac{\partial}{\partial \phi} + \hat{e}_\theta \frac{1}{r} \frac{\partial}{\partial \theta}$$

2 A diatomic molecule in 3D

A very crude model of a diatomic molecule moving in three-dimensional space consists of two particles of masses M_1 and M_2 coupled together by an elastic force with spring constant K , *i.e.* it obeys Hooke's Law. The position vectors of the particles are \vec{r}_1 and \vec{r}_2 respectively.

- Show that the Hamiltonian for this problem separates into center of mass and relative coordinate terms. Write the quantum mechanical Hamiltonian for the relative coordinate \vec{r} in spherical coordinates. Show that its eigenstates are also eigenstates of the relative angular momentum operators \hat{L}^2 and \hat{L}_z .
- Derive the form of the equation satisfied by $\chi(r) = rR(r)$ where r is the relative coordinate and $R(r)$ is the radial wave function for this problem. Scale the relative coordinate r and the energy E so as to make the equation dimensionless. What length and energy scales do these re-scalings define?
- Show that, as $r \rightarrow 0$, $\chi(r) \sim r^{\ell+1}$, and that, as $r \rightarrow \infty$, $\chi(r) \sim \exp(-\lambda r^2/2)$. Compute the constant λ .
- Find the differential equation satisfied by $w(r)$, where

$$\chi(r) = r^{\ell+1} e^{-\frac{\lambda}{2} r^2} w(\lambda r^2)$$

Show that it has the form of the confluent hypergeometric equation (discussed in class for the Hydrogen atom and in problem set 4 for the problem of a particle in a magnetic field)

$$zw''(z) + (\gamma - z)w'(z) - \alpha w(z) = 0$$

where $z = \lambda r^2$. Determine α and γ .

5. As we discussed in class, this equation has a solution that is regular at $r = 0$, the confluent hypergeometric function $F(\alpha, \gamma, z)$,

$$F(\alpha, \gamma, z) = 1 + \frac{\alpha z}{\gamma 1!} + \frac{\alpha(\alpha+1) z^2}{\gamma(\gamma+1) 2!} + \dots + \frac{\alpha(\alpha+1)\dots(\alpha+k) z^k}{\gamma(\gamma+1)\dots(\gamma+k) k!} + \dots$$

This solution behaves as $F(\alpha, \gamma, z) \sim e^z$ as $z \rightarrow \infty$. Use an argument similar to the one used in class to find the quantization of the energy levels for this problem, and show that the energy eigenvalues are given by the formula

$$E_{n,\ell,m} = \hbar\omega \left(\frac{3}{2} + 2n + \ell \right)$$

where $\ell = 0, 1, 2, \dots$ and $n = 0, 1, 2, \dots$. Find the quantum numbers and the degeneracies of the states in the lowest *four energy levels*. What is the form of their eigenfunctions in spherical coordinates?

6. You could have also solved this problem in cartesian coordinates. What is the analog of the energy level formula in cartesian coordinates? What are the quantum numbers? Show how to relate these quantum numbers for the states in the lowest four energy levels you found above. Show how the wave functions in both coordinates are related for the first excited states.

3 Scattering from a Short Range Potential

In this problem you will consider a particle of mass M interacting with a fixed scatterer, located at the origin of the coordinate system. At time t_0 , in the remote past (namely before the particle reached the field of the scatterer), the particle is in the state $\psi_{\vec{k}_0}(\vec{r})$ which is a plane wave state with wave vector \vec{k}_0 , velocity $\hbar\vec{k}_0/M$, and energy $E_{\vec{k}_0} = \frac{\hbar^2 k_0^2}{2M}$.

1. Show that, for a general short range scattering potential $U(\vec{r})$, the exact eigenstates of the Schrödinger equation $\psi_{\vec{k}}(\vec{r})$ in the continuum part of the spectrum ($E > 0$), satisfy the integral equation

$$\psi_{\vec{k}}(\vec{r}) = e^{i\vec{k} \cdot \vec{r}} - \frac{M}{2\pi\hbar^2} \int d^3r' \frac{e^{ik|\vec{r}' - \vec{r}|}}{|\vec{r}' - \vec{r}|} U(\vec{r}') \psi_{\vec{k}}(\vec{r}')$$

where $k = |\vec{k}|$. Show that $\psi_{\vec{k}}(\vec{r})$ satisfies the boundary conditions for a scattering state, *i. e.* it is a linear combination of an incoming plane wave and an outgoing spherical wave.

2. Use this result to show that far from the scatterer, *i. e.* for $|\vec{r}| \gg |\vec{r}'|$, this equation reduces to

$$\psi_{\vec{k}}(\vec{r}) = e^{i\vec{k} \cdot \vec{r}} + \frac{e^{ikr}}{r} f_{\vec{k}}(\hat{r})$$

where $\hat{r} = \frac{\vec{r}}{|\vec{r}|}$ is a unit vector along the direction \vec{r} .

$$f_{\vec{k}}(\hat{r}) = -\frac{M}{2\pi\hbar^2} \int d^3r' e^{-ik\hat{r}\cdot\vec{r}'} U(\vec{r}') \psi_{\vec{k}}(\vec{r}')$$

is the scattering amplitude.

3. Show that in general the differential cross section for scattering from an initial plane wave state with wave vector \vec{k}_0 to a point along the direction \hat{r} is given by

$$\frac{d\sigma}{d\Omega} = |f_{\vec{k}_0}(\hat{r})|^2$$

4. Show that for a short range *rotationally invariant* scattering potential $U(r)$, the scattering amplitude depends only on the colatitude θ , and that it has the partial wave expansion

$$f(\theta) = \frac{1}{k} \sum_{\ell=0}^{\infty} (2\ell+1) P_{\ell}(\cos\theta) e^{i\delta_{\ell}} \sin\delta_{\ell}$$

where δ_{ℓ} is the *phase shift*. Give a definition of the phase shift for a short ranged potential.

5. Show that the total cross section σ has the partial wave decomposition

$$\sigma = \frac{4\pi}{k^2} \sum_{\ell=0}^{\infty} (2\ell+1) \sin^2\delta_{\ell}$$

6. Use the Born Approximation for the phase shifts

$$\delta_{\ell} = -\frac{2Mk}{\hbar^2} \int_0^{\infty} dr r^2 U(r) (j_{\ell}(kr))^2$$

to compute the phase shifts for

- (a) an attractive spherical potential well of radius r_0 and depth $U_0 < 0$.
 (b) for the Yukawa potential

$$U(r) = \frac{U_0}{\kappa r} e^{-\kappa r}$$

where $U_0 > 0$ is an energy, and κ is the inverse range.

What do these result tell you about the total cross section?
 You may have to use these integrals:

$$\int_0^a dx x [J_{\ell+1/2}(x)]^2 = \frac{1}{2} [J_{\ell+3/2}(a)]^2$$

$$\int_0^{\infty} dx e^{-ax} [J_{\ell+1/2}(x)]^2 = \frac{1}{\pi} P_{\ell}(1+a^2/2)$$

7. Use the Born Approximation for the scattering amplitude

$$f_{\vec{k}}(\hat{r}) = -\frac{M}{2\pi\hbar^2} \int d^3r' e^{i(\vec{k}-\vec{k}')\cdot r'} U(|\vec{r}'|)$$

where $\vec{k}' = k\hat{r}$, to compute the differential cross section for the Yukawa potential. Find the form of the differential cross section in the limit $\kappa \rightarrow 0$. Discuss the connection between this limit and a repulsive Coulomb scatterer. Compare your answer with the classical Rutherford formula. Hint: do the Fourier transform in spherical coordinates. After doing the angular integrals, you will encounter an integral of the form:

$$\int_0^\infty dr' e^{-\kappa r'} \sin(qr') = \text{Im} \int_0^\infty dr' e^{-\kappa r' + iqr'} = \frac{\kappa}{\kappa^2 + q^2}$$