Quantum Physics III (8.06) Spring 2008
Assignment 7

Apr 1, 2008 **Due Tuesday April 8, 2007**

- Please remember to put your name **and section time** at the top of your paper.
- This problem set is due in a week, as usual. The next problem set, Problem Set 8, will be available on Tuesday April 8 as usual but will be due on Friday April 18. You have a longer interval for Problem Set 8 because in the interim the first draft of your term paper is due.
- **The Final Exam will be on Monday May 19, 1:30 pm-4:30 pm, in Johnson Ice Rink.**
- If you want further problems, beyond those I assign below, with which to teach yourself about the variational method, prepare for the final exam, gain physics intuition and learn some new applications, you could try Griffiths' Problems 7.7, 7.15, 7.16, 7.17, 7.18, 7.19, 7.20.

Readings

The reading assignment for this problem set and the first part of the next one is:

- Griffiths Chapter 7.
- Cohen-Tannoudji Chapter XI, Complements E (scanned copy available at 8.06 website).
- Griffiths Chapter 8 and the Supplementary Notes on the Connection Formulae. (You do not need them for this problem set.)

Problem Set 7

1. **Variational bound on the ground state in a power-like potential (10 points)**

   Consider a particle of mass m moving in the one dimensional potential

   $$V(x) = \lambda x^4 \tag{1}$$

   We can obtain an upper bound on the energy of the ground state using the variational method. To find a trial wave function, we regard (1) as a harmonic oscillator potential with a space-dependent frequency, i.e. $V(x) = \frac{1}{2}m\omega^2(x)x^2$

with $\frac{1}{2}m\omega^2(x) = \lambda x^2$. This motivates us to choose the trial wave function to resemble the ground state of a harmonic oscillator potential, i.e.

$$\psi(x) = Ae^{-bx^2}$$

Find the value of b that minimizes $\langle\psi|H|\psi\rangle$ and obtain an upper bound on the ground state energy. (Hint: normalize ψ first to express A in terms of b.)

2. Variational bound on the excited states (15 points)

(a) Prove the following corollary to the variational principle: if $\langle\psi|\psi_{gs}\rangle = 0$, then $\langle\psi|H|\psi\rangle \geq E_{fe}$, where $|\psi_{gs}\rangle$ denotes the ground state wave function and E_{fe} is the energy of the first excited state.

In general it is difficult to be sure a state $|\psi\rangle$ is orthogonal to $|\psi_{gs}\rangle$ since the latter is generally not known exactly. However, if the potential $V(x)$ has some symmetry, it is often possible to realize $\langle\psi|\psi_{gs}\rangle = 0$. For example, if the potential $V(x)$ is an even function of x, then the ground state wave function should also be even in x and thus an odd trial function will be automatically orthogonal to ψ_{gs}.

(b) Choose a set of trial wave functions, specified by a single parameter to obtain an upper bound on the first excited state energy of the one-dimensional harmonic oscillator $V(x) = \frac{1}{2}m\omega^2x^2$.

(c) Give an example of a set of trial wave functions, specified by a single parameter, that could be used to obtain an upper bound on the first excited state energy of (1). Explain your reasoning for choosing the ansatz. But do not go further than writing down the ansatz.

3. Variational bound on the ground state in an exponential potential (20 points)

Unlike in one dimension, an attractive potential in three dimensions does not always have a bound state. A simple variational guess can give us an estimate of how strong a potential must be in order to have a bound state, even though the exact solution would require solving the Schrödinger equation numerically.

Consider a particle of mass m moving in three dimensions under a central force derived from an exponential potential,

$$V(r) = -\alpha e^{-2\mu r} \ ,$$

where α and μ are positive. Take a simple exponential variational *ansatz* for the ground state wavefunction:

$$\psi_\lambda(r) = Ce^{-\lambda r} \ . \qquad (2)$$

(a) Find the constant C by demanding that $\int d^3r|\psi_\lambda(r)|^2 = 1$.

(b) Compute the variational estimate of the energy of ψ, as a function of λ.

Hint: Once you have normalized the wave function, the variational estimate is given by

$$E(\lambda) = \int d^3r \left\{ \frac{\hbar^2}{2m} \left| \frac{d\psi_\lambda(r)}{dr} \right|^2 + V(r) \left|\psi_\lambda(r)\right|^2 \right\} \tag{3}$$

Hint: The only integral needed is $\int_0^\infty dx x^n e^{-x} = n!$.

Answer: $E(\lambda) = \frac{\hbar^2\lambda^2}{2m} - \alpha(\frac{\lambda}{\mu+\lambda})^3$.

(c) Show that for small α, the minimum value of $E(\lambda)$ is zero and is obtained for $\lambda = 0$. Interpret this result (for example, where is the particle found when $\lambda = 0$?).

(d) Lets scale out some of the dimensionful parameters to make this problem easier to analyze. Consider $\mathcal{E} = \frac{mE}{\mu^2}$. Show that $\mathcal{E}$ can be written as a function of $x = \lambda/\mu$ and a scaled strength of the potential, $\kappa = \alpha m/\mu^2$. Rewrite the result of part (b) as $\mathcal{E}(\kappa, x)$. Analyze this equation graphically or numerically and find the minimum value of κ for which a bound state exists. What is the value of x at this value of κ.

(e) Does the result of the previous section give you a minimum value of α (for fixed m and μ) required for a bound state, or a maximum, or neither? Explain.

4. **Helium atom (15 points)**

The Hamiltonian for a Helium atom can be written as

$$H = -\frac{\hbar^2}{2m}(\nabla_1^2 + \nabla_2^2) - \frac{2e^2}{r_1} - \frac{2e^2}{r_2} + \frac{e^2}{|\vec{r}_1 - \vec{r}_2|} \tag{4}$$

where $r_1 = |\vec{r}_1|$ and $r_2 = |\vec{r}_2|$. Since H is spin-independent, we can take energy eigenfunctions to have the form

$$\psi(1,2) = \Phi(\vec{r}_1, \vec{r}_2)\,\chi(1,2) \tag{5}$$

where $\Phi(\vec{r}_1, \vec{r}_2)$ denotes the spatial part and $\chi(1,2)$ denotes the spin part of the wave function.

(a) Show that $\Phi(\vec{r}_1, \vec{r}_2)$ can be taken to be either symmetric or anti-symmetric under the exchange of 1 and 2.

(b) Write down the spin part of the wave function for Φ being symmetric and anti-symmetric (under exchange of 1 and 2) respectively.

(c) Now consider finding (5) using perturbation theory with

$$H = H_0 + H' \tag{6}$$

and

$$H_0 = -\frac{\hbar^2}{2m}(\nabla_1^2 + \nabla_2^2) - \frac{2e^2}{r_1} - \frac{2e^2}{r_2} \ , \tag{7}$$

$$H' = \frac{e^2}{|\vec{r}_1 - \vec{r}_2|} \ . \tag{8}$$

Since H_0 is the sum of two separate Hamiltonians for each electron, a zero-th order wave functions can only be one of the following three types:

(1) Both electrons are in ground state of the individual Hamiltonian;

(2) One electron is in ground state and the other is in an excited state;

(3) Both electrons are in excited states.

Argue that (to first order in perturbation theory) an energy eigenstate of H corresponding to a third type of state (i.e. both electrons are in excited states) always has a higher energy than the ground state of a He^+ ion plus a free electron. Thus a Helium atom in such a state will quickly ionize into a He^+ ion plus a free electron.

(d) Now suppose we would like to do perturbation theory for the second type of states in (c) (i.e. one electron is in ground state and the other is in an excited state). For simplicity let us treat two electrons as distinguishable, say 1 is in ground state and 2 is in an excited state. Then there is in fact a better way to separate the Hamiltonian H into a free part and a perturbation than (6), by appropriately choosing V_1 and V_2 in the following decomposition

$$H = \tilde{H}_0 + \tilde{H}' \tag{9}$$

with

$$\tilde{H}_0 = -\frac{\hbar^2}{2m}(\nabla_1^2 + \nabla_2^2) + V_1(r_1) + V_2(r_2) \ , \tag{10}$$

$$\tilde{H}' = -\frac{2e^2}{r_1} - V_1(r_1) - \frac{2e^2}{r_2} - V_2(r_2) + \frac{e^2}{|\vec{r}_1 - \vec{r}_2|} \ . \tag{11}$$

How would you like to choose V_1 and V_2? Explain your reasoning.

[Hint: The choice of $V_1(r_1)$ and $V_2(r_2)$ should reflect the screening effect. Note that since we are doing perturbation theory rather than variational method, there is no free parameter in V_1 and V_2.]