PHY 246 Quantum Mechanics

Additional Problems; Due April 18th 2005

These problems are more challenging than those assigned in the regular homework sets. You might attempt them if you find the other set too easy.

1. Determine the ground state energy of an atom (or ion) with two electrons using a variational ansatz.

The hamiltonian is (in dimensionless variables)

$$H = p_1^2 + p_2^2 - \frac{Z}{|x_1|} - \frac{Z}{|x_2|} + \frac{1}{|x_1 - x_2|} \tag{1}$$

where x_1, x_2 are the position vectors of the electrons and p_1, p_2 the momentum vectors. In the ground state,the electrons will have opposite spins and have a wavefunction $\psi(x_1, x_2)$ that is symmetric under the interchange of positions. Thus the problem is to find the symmetric function with as small a value as you can get for $\frac{<\psi|H|\psi>}{<\psi|\psi>}$.

Try the ansatz

$$\psi(x_1, x_2) = Ce^{-a|x_1|-a|x_2|}. \tag{2}$$

That is find the C for which $||\psi|| = 1$ and then find $< \psi|H|\psi >$ as a function of a; then minimize as a function of a. The hardest part will be to find the expectation of the last term in the hamiltonian (the repulsion energy). You will find it useful to use the integral formula for solving Poisson's equation in electrostatics. Shankar's book does something similar but in perturbation theory.

There is even a stable ground state of two electons bound to a nucleus of unit electric charge (negatively charged hydrogen ion). Can you determine its binding energy by some variational argument as above?

2. Find the eigenvalues of the rotational energies of a system with hamiltonian

$$H = \frac{L_1^2}{2I_1} + \frac{L_2^2}{2I_2} + \frac{L_3^2}{2I_3} \tag{3}$$

where $I_1 < I_2 < I_3$ for the values of total angular momentum $l = \frac{1}{2}, 1, \frac{3}{2}, 2 \cdots$. (Go as far as you can.. it gets quite difficult beyond $l = 4$, I will be happy if you can do up to $l = 2$.)

Landau and Lifshitz Vol III section 103 is the definitive reference.

3. Find the binding energy of the H_2^+ molecular ion; i.e, two protons at fixed positions bound to one electron which orbits them. The exact solution of this problem involves a peculiar co-ordinate system in which the Schrodinger equation separates. A good approximation is to use as variational ansatz the product of two wavefunctions centered at each of the nuclei:

$$\psi(x) = Ce^{-a|x-\frac{R}{2}|-a|x+\frac{R}{2}|} \tag{4}$$

where R is the vector connecting the positions of the protons. Find the best value of the ground state energy of the electron that this ansatz can produce by minimizing in a. The answer will depend on R.