Homework 14

Due in class Dec. 9

1. Consider an infinite square well with a barrier:



- (a) Take b = a/2 and $\beta = \sqrt{2mV_0/\hbar^2}a = 0.7\pi$. Find the exact ground and first excited state energies by solving (numerically) the transcendental equation resulting from matching.
- (b) Find an approximate ground state energy using the variational principle. A single parameter trial function is sufficient for this exercise, but pick a trial function that is easy to differentiate and integrate, satisfies the boundary conditions, and has the symmetry you expect of the ground state. Do not choose a trial function that has the same functional form as the exact solution — we want to see the variational principle at work.
- (c) Find an approximate first excited state energy using the variational principle. Use the same guidelines as in (b).
- (d) Compare your approximate energies with the exact energies. Suggest improvements to your trial wave function for both states.

2. Use the variational principle to find an approximation to the ground state energy of He (*i.e.* the $1s^2$ ¹S state). Use a hydrogenic trial function for each electron, but take the charge in the function to be an effective charge, $Z_{\rm eff}$, which will be the variational parameter. In this way, the variational procedure takes into account the screening of the nucleus by the other electron. (You may find it useful to work in atomic units: $\hbar = m_e = e = 1$.)

(a) Write down the ground singlet trial function (make sure it is properly symmetrized and is an angular momentum eigenstate!).

- (b) Find the optimal Z_{eff} and thus the approximate ground state energy for He. Compare with the exact result.
- (c) Repeat (b) for the H⁻ ion. Is H⁻ stable in this approximation, or is it more favorable to break up into H+e? That is, which of these channels (configurations) has the lower energy?
- (d) Are your variational energies better than the perturbative ones from HW 13? Discuss the comparison physically.

3. The effect of magnetic fields on atoms is typically weak, such that it can be considered a perturbation on the fine structure levels. The effects of magnetic fields on atoms or molecules are collectively called the Zeeman effect.

We will assume that the magnetic field is $\mathbf{B} = B_0 \hat{z}$, and the perturbation is written as

$$H' = \frac{\mu_B}{\hbar} (\mathbf{L} + 2\mathbf{S}) \cdot \mathbf{B}$$

where μ_B is the Bohr mageton. Physically, this perturbation describes the interaction of a magnetic dipole with the field $(-\mu \cdot \mathbf{B})$.

- (a) Why did we choose **B** to be along the z-axis? Physically, does it matter?
- (b) Take the unperturbed Hamiltonian to be

$$H_0 = -\frac{\hbar^2}{2m} \nabla^2 - \frac{Ze^2}{4\pi\epsilon_0 r} + \xi(r) \mathbf{L} \cdot \mathbf{S}.$$

The last term is the spin-orbit interaction you worked with on HW 13. Calculate the energy level shifts due to the presence of the magnetic field using perturbation theory. NOTE: It is *not* necessary to know the unperturbed energies to calculate the shifts; it is only necessary to know whether there are degeneracies and which states are degenerate.

- (c) For what values of B_0 is the Zeeman effect truly perturbative? Are these large magnetic fields (*i.e.* are they accessible in the lab)?
- (d) Plot the total energies of the $1s_{\frac{1}{2}}, 2s_{\frac{1}{2}}, 2p_{\frac{1}{2}}$, and $2p_{\frac{3}{2}}$ levels as a function of B_0 . You'll probably have to plot them on different scales. Identify in your plot where perturbation theory breaks down.