Homework 12 Due in class Dec. 12

These problems are in addition to those from HW 11 which will also be due Dec. 12.

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 $1s^{2} {}^{1}S$ state). Use a hydrogenic trial function for each electron, but take the charge in the function to be an effective charge, Z_{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 $Z_{\rm eff}$ 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?