Homework 1

Due September 6, beginning of class

This homework should be almost completely review, but should serve to get you thinking about quantum mechanics again.

From Bransden and Joachain (B&J): 2.3, 2.8, 2.17, 2.22, 2.23, 3.4

1. In the Bohr model of the hydrogen atom, how do the following scale with mass, charge, and the principal quantum number n?

(a) Orbital period T

(b) Energy E

(c) Velocity v

(d) Radius r

(e) Do these scalings work for the real hydrogen atom? Quantify your answer as much as possible. Explain any failings.

2. Atomic units are defined by setting $\hbar$=m_e=e=1 and form a very convenient set of units for atomic and molecular problems. Most quantities are defined from the Bohr model of the hydrogen atom with the above definitions.

(a) How is the atomic unit of length defined and what is its value in SI units?

(b) How is the atomic unit of energy defined and what is its value in SI units? in eV? in cm^{-1}? in K (Kelvin)?

(c) How is the atomic unit of time defined and what is its value in SI units? in fs?

(d) What is the speed of light in atomic units?

(e) Write down the time-dependent Schrödinger equation for a hydrogen-like atom in atomic units.

3. Apply the variational principle to find the low-lying spectrum of

$$V(x) = \begin{cases} \infty & |x| > a \\ 10\frac{\hbar^2}{ma^2}\frac{x}{a} & |x| \le a \end{cases} .$$

In particular, use the expansion

$$\psi(x) = \sum_{n=1}^{N} a_n \phi_n(x)$$

where $\{\phi_n(x)\}$ are the infinite square well eigenstates, and answer the following questions:

(a) First, sketch a picture of the potential with what you expect the ground state to look like. Add the infinite square well energy levels to your sketch.

(b) Carry out the variational calculation for N=1,2,3,4 and report your energies for the lowest three states.

(c) Estimate the error in your best ground state energy from (b). When you compare the energies you obtained, do they follow the pattern you expect for variational approximations (*i.e.*, do they look like Fig. 2.10)?

(d) Plot your best ground state wave function. Does it make sense? Which infinite square well states contribute the most to it? Does this make sense?

(e) Treat the above potential in first order perturbation theory (for the ground state only) and compare to your results from (b). Explain whether your results make sense.

(f) What is the smallest N that gives the ground state energy accurate to four digits? the first excited state energy to four digits?

4. Given $\ell_1 = 1$ and $\ell_2 = 4$ (note that you may calculate any Clebsch-Gordan coefficients by whatever method you like):

(a) Calculate the possible values of the total angular momentum $\mathbf{L} = \mathbf{L_1} + \mathbf{L_2}$.

(b) Write down the explicit expressions in terms of $|\ell_1 m_1\rangle|\ell_2 m_2\rangle$ for the states

(*i*) $|(14)3-3\rangle$

(*ii*) $|(14)4-3\rangle$

(*iii*) $|(14)5-5\rangle$

(*iv*) $|(14)54\rangle$.

(c) Turn the expansion around and write the state $|11\rangle|4-3\rangle$ as an expansion on eigenstates of total angular momentum.

5. Calculate the transformation matrix between the spherical and parabolic eigenstates for the n=2 manifold. Be explicit if you use any shortcuts and tell me what shortcut you're using. Discuss whether your results make sense (you will probably want to talk about symmetry).