QUANTUM MECHANICS II

PHYS 517

Problem Set #1

Distributed March 30, 2011

Due April 6, 2011

Instructions: Answer each question correctly.

If you got a question completely correct in the Final you may submit that in lieu of rewriting your solution. This offer does not apply to problems 1b, 8 and 9, as they differ slightly from the form given on the Final.

1. Hydrogen Atom: 40 pts.

a. Draw an energy level diagram for the bound states of the nonrelativistic hydrogen atom. Show the energy scale (in eV), organize the energies in terms of the angular momentum values of the various levels, and identify the degeneracy of these levels, neglecting spin.

b. Write down the wave function for the hydrogen atom state with quantum numbers nlm, where the latter two are "saturated": that is, $m = l$ and $l = n - 1$. Write down this wave function explicitly in terms of the spherical coordinates r, θ, ϕ. Write down the integral expression for the normalization of this wavefunction. Compute the normalization by carrying out the elementary integral(s).

2. Scaling: 20 pts.

A muonium atom (μ^+-μ^- in a binding Coulomb potential) in a $2p$ bound state decays to the $1s$ ground state and emits a photon. What is the wavelength of the photon? **Useful datum:** the wavelength of a 1eV photon is 1.24×10^{-6} m. **Useful datum:** $m_\mu c^2/m_e c^2 \simeq 207$.

3. Molecules: 40 pts.

The linear triatomic molecule ABA oscillates in one dimension. The masses are $M_A = M,\ M_B = 16M$. The interaction is between only adjacent atoms and is represented by linear springs with spring constant k.

a. Describe the classical normal modes.

b. For each, what is the energy?

c. Quantize the vibrations of this molecule.

d. Write down the quantum mechanical hamiltonian in terms of the total momentum and the vibrational mode creation/annihilation operators.

4. Thermal Energy: 20 pts. $\langle (n+\frac{1}{2})\hbar\omega\rangle_T = ?$

5. Lattice Vibrations: 40 pts.

A one-dimensional lattice has N unit cells, each with one atom of mass m. The atoms interact with each other through NN (Nearest Neighbor) and NNN (Next Nearest Neighbor) interactions. The NN interactions are through a spring with spring constant k. The NNN interactions are through a spring with spring constant $\kappa = \frac{1}{2}k$. Assume cyclic boundary conditions.

a. Draw a picture.

b. Write down the secular equation for the oscillation frequencies.

c. Write down the expressions for the dispersion relation ($E(\epsilon)$ or $E(\phi) = \hbar\omega(\phi)$, with $\phi = 2\pi k/N$, $-N/2 \le k \le +N/2$ with $\epsilon = e^{i\phi}$). Use $\omega_0 = \sqrt{k/m}$.

d. Write down the quantum mechanical hamiltonian for this one-dimensional chain.

6. SU(3): 25 pts.

A three-dimensional harmonic oscillator has a hamiltonian with energy level spectrum

$$H = (n_1 + n_2 + n_3)mc^2 + [n_3 - (n_1 + n_2)]\,\Delta + (n_1 - n_2)\epsilon$$

with $mc^2 = 100, \Delta = 10, \epsilon = 1$. Sketch the spectrum for the states with $n_1 + n_2 + n_3 = N = 3$.

7. Numerical Diagonalization: 25 pts.

A particle of mass $m = 1$ is placed inside an infinitely deep one-dimensional potential well of length $L = 10$. Adopt units where $\hbar = 1$.

a. Compute the lowest 5 eigenstates and their energy eigenvalues by solving Schrödinger's differential equation. Normalize each eigenfunction.

b. Now discretize the Schrödinger equation for this problem by choosing steps of size $\Delta = 0.1$. What is the matrix that describes the kinetic energy operator? What are the eigenvectors of this matrix? What is the eigenvalue for each eigenvector?

c. Write down the lowest eigenvector.

d. Evaluate this eigenvector at $x = 5$ and compare this value with that of the ground state eigenvector computed in **a.**, evaluated at the same point.

e. How do you normalize the eigenvectors computed in **b.** so they can be compared with the analytically computed eigenvectors from part **a.**?

8. Approximation Methods: 40 pts.

Two electrons are tossed into the presence of a lithium nucleus ${}^6_3Li$.

a. When the "dust settles" what states do you expect the electrons to be in? Specify the orbital labels and the spins of these electrons.

b. Write down an approximate expression for the electrostatic potential as a function of r. This will be a superposition of the potential set up by the three positive charges in the lithium nucleus and the two screening electrons.

c. Compute and plot $Z(r)$ vs. r.

d. A third electron is now tossed into the pot. After the "dust settles" what state do you expect the electron to be in?

e. What (and why) do you expect the third electron wavefunction to be like asymptotically near the nucleus? ...

f. ... and far outside the two $1s$ electron orbitals? (and why?)

g. Suggest a way to parameterize the third electron's $2s$ wavefunction so that it might be a good, realistic approximation for what the electron really thinks it ought to look like. Write down such a parameterized wavefunction.

h. Explain how you would use this approximation to the wavefunction to estimate an upper bound on the ${}^{6}_{3}Li$ binding energy.

9. Perturbation Theory: 25 pts.

a. Compute the effect of a quadrupole perturbation $Q(3z^2-r^2) = \sqrt{\frac{16\pi}{5}} r^2 Y_0^2(\theta,\phi)$ on the $1s$ ground state of the hydrogen atom.

b. Carry out the sum.

c. Does this perturbation raise or lower the the ground state energy?

d. What happens if the sign of Q is reversed? Why?

The radial integral you are searching for is

$$\left| \int_0^\infty R_{n2}(r)\ r^2\ R_{10}(r)\ r^2\ dr \right|^2 = 2^{12} a_0^4 n^9 \frac{(n^2-2^2)}{(n^2-1^2)^7} \left(\frac{n-1}{n+1} \right)^{2n}$$

(N. Chair et al, J. Phys. A: Math. Theor. **44**, 095306 (2011), Eq. (14).

10. Time Dependence: 25 pts.

An electron of mass m in a harmonic potential with spring constant k finds itself in a linear combination of the first and second excited states with equal amplitudes: $\psi = \frac{1}{\sqrt{2}}(|1\rangle + |2\rangle)$ at $t=0$.

a. Write down its wavefunction at any future time.

b. Compute $\langle x \rangle$ as a function of time. Use $\langle 2|a^\dagger|1\rangle = \sqrt{2}$.

c. Compute $\langle p \rangle$ as a function of time.

d. Plot $\langle p \rangle$ vs. $\langle x \rangle$.

e. What is the periodicity? Relate this to the behavior of a classical particle in the same harmonic potential.