Final Homework – CH125A

100 points

This homework is intended to serve as a culmination of the material of this course. It's provided for you to test your conceptual understanding of quantum mechanics.

What system are we describing with each Hamiltonian below, in vector calculus notation?

1. $H = -\frac{\hbar^2}{2m}\nabla^2 + \frac{1}{2}kr^2$, where r is position and k is a constant.
2. $H = -\frac{\hbar^2}{2m}\nabla^2_{(r)} - \frac{e^2}{r} + \frac{L^2}{2mr^2}$, where L^2 is a scalar operator.
3. $H = -\frac{\hbar^2}{2m}\nabla^2 + \frac{1}{2}k_1 r^2 + \frac{1}{6}k_2 r^3 + B_1 J(J+1) + B_2 J^2 (J+1)^2$.

Let's now explore Hamiltonians written in second quantization (raising and lower operator) notation that are particularly useful in solid-state physics.

4. The Hubbard model describes two competing forces on electrons: (1) a kinetic term for tunneling to neighboring atoms and (2) a repulsive potential term (U) pushing it away from neighboring electrons. We can write the Hamiltonian as:

$$H = -t\sum a_i^+ a_j + U\sum n_{i\uparrow} n_{i\downarrow}$$

where a^+ and a are creation and annihilation operators for electrons at specific sites and n is the number operator at a given site. Explain how these two terms of the Hamiltonian lead to the described behavior for $t > 0$ and $U > 0$.

5. The t-J model is based on the Hubbard model, but contains an additional term to describe antiferromagnetism:

$$H = -t\sum a_i^+ a_j + U\sum n_{i\uparrow} n_{i\downarrow} + J\sum \left(S_i \cdot S_j - \frac{n_i n_j}{4}\right)$$

where J is the antiferromagnetic exchange coupling and S describes spin. Explain how the t-J model accounts for antiferromagnetism.

6. As another model Hamiltonian based on the Hubbard model, the Hubbard-Holstein Hamiltonian describes electron-phonon coupling. The Holstein Hamiltonian (for systems with no Coulomb repulsion; $U = 0$) is given by:

$$H = -t\sum a_i^+ a_j + \hbar\omega\sum b_i^+ b_i + \sum (b_i^+ + b_i) a_i^+ a_i$$

where a^+ and a are creation and annihilation operators for phonons.

a. What assumption are we making about the phonon potential?
b. How does the Holstein Hamiltonian describe electron-phonon coupling?