Physics 726: Assignment 2

(to be submitted by Tuesday, February 9, 2016)

1. A system of independent electrons is described by the purely bilinear Hamiltonian

$$\hat{H} = \sum_{\alpha} \int d^3r\, \hat{\psi}_\alpha(\boldsymbol{r})^\dagger T(\boldsymbol{r}) \hat{\psi}_\alpha(\boldsymbol{r}).$$

   Here, T is some differential operator, not necessarily $-\hbar^2\nabla^2/2m$, and α ranges over the two spin projections. For concreteness, suppose that the Hamiltonian describes electrons bound to a diatomic molecule.

   (a) Consider a single-particle basis $\{\phi_1, \phi_2\}$ consisting of two states that are not eigenfunctions of T. We'll think of $\phi_1(\boldsymbol{r})$ as a wave function localized on atom 1 and $\phi_2(\boldsymbol{r})$ as a wave function localized on atom 2. Use the field operator expansion

$$\hat{\psi}_\alpha(\boldsymbol{r}) = \sum_{j=1,2} \phi_j(\boldsymbol{r}) \chi_\alpha c_{j,\alpha}$$

   to show that

$$\hat{H} = \sum_{\alpha} \begin{pmatrix} c_{1,\alpha}^\dagger & c_{2,\alpha}^\dagger \end{pmatrix} \begin{pmatrix} \varepsilon_1 & -t \\ -t^* & \varepsilon_2 \end{pmatrix} \begin{pmatrix} c_{1,\alpha} \\ c_{2,\alpha} \end{pmatrix},$$

   where

$$\varepsilon_j = \int d^3r\, \phi_j(\boldsymbol{r})^* T(\boldsymbol{r}) \phi_j(\boldsymbol{r}) \text{ and } -t = \int d^3r\, \phi_1(\boldsymbol{r})^* T(\boldsymbol{r}) \phi_2(\boldsymbol{r}).$$

   (b) For the case of a homonuclear atom ($\varepsilon_1 = \varepsilon_2 \equiv \varepsilon$), solve for the one- and two-particle ground states.

   (c) Now consider the case where the atoms in the molecule are different ($\varepsilon_1 = \varepsilon - \Delta$ and $\varepsilon_2 = \varepsilon + \Delta$). What is the average number of electrons on atom 1 and on atom 2 in the one-particle ground state?

2. The Hamiltonian

$$\hat{H} = \varepsilon a^\dagger a + \frac{\Delta}{2}\left[a^2 + (a^\dagger)^2\right]$$

   is built from bosonic creation and annihilation operators, $a^\dagger$ and a.

   (a) Show that there is an operator $\hat{A} \sim a + \lambda a^\dagger$ that obeys the bosonic commutation relation $[\hat{A}, \hat{A}^\dagger] = 1$. Determine the constant of proportionality.

   (b) Show that, up to a constant, $\hat{H} = \tilde{\varepsilon}\hat{A}^\dagger\hat{A}$, so long as you can find values $\tilde{\varepsilon}$ and λ such that

$$\varepsilon = \frac{\tilde{\varepsilon}(1+\lambda^2)}{1-\lambda^2} \text{ and } \Delta = \frac{2\tilde{\varepsilon}\lambda}{1-\lambda^2}.$$

   (c) Explicitly construct the ground state and first three excited states. *Hint:* consider repeated applications of $\hat{A}^\dagger$ on the bosonic vacuum.