Advanced Quantum Theory (WS 21/22)

Homework no. 12 (January 10, 2022)

Please hand in your solution by Monday, January 17!

1 Hubbard Model

This problem is an application of the formalism developed in chapters 6.3 and 6.4.

Consider a cubical lattice, where electrons sit at locations $\vec{R}_i = \vec{n}_i a$, where a is the lattice constant (i.e., the distance between neighboring lattice sites), and $\vec{n}_i = (n_{x,i}, n_{y,i}, n_{z,i})$, $n_{(x,y,z),i}$ being integers. The Hamiltonian is assumed to be the sum of kinetic energy and a two–particle interaction,

$$\hat{H} = \sum_{i,j} \sum_{s} t_{ij} \hat{b}^\dagger_{i,s} \hat{b}_{j,s} + \frac{1}{2} \sum_{i,j,k,l} \sum_{s,s'} V_{ijkl} \hat{b}^\dagger_{i,s} \hat{b}^\dagger_{j,s'} \hat{b}_{l,s'} \hat{b}_{k,s} . \tag{1}$$

Here i, j, k, l label the lattice sites, and $s, s' \in \{-1/2, 1/2\}$ determine the $z-$component of the electron spin. Hence $\hat{b}^\dagger_{i,s}$ creates an electron with spin $S_z = \hbar s$ at the $i.-$th lattice site.

In the Hubbard model one assumes that the electrons are quite localized, with one–particle states described by

$$\varphi_{i,s}(\vec{x}) = \chi_s \phi(\vec{x} - \vec{R}_i) , \tag{2}$$

where χ_s describes the spin state, and the spatial part is taken to be a Gaussian,

$$\phi(\vec{x}) = \frac{1}{\Delta^{3/2} \pi^{3/4}} \mathrm{e}^{-\vec{x}^2/(2\Delta^2)} . \tag{3}$$

1. Compute the diagonal contributions t_{ii} to the kinetic energy. *Hint:* They are, of course, independent of i; from dimensional arguments it follows that $t_{ii} \equiv t \propto \hbar^2/(m\Delta^2)$. Keep in mind that one is working in three dimensions! **[4P]**

2. Show that the contribution from nearest neighbors to the kinetic energy is suppressed by a factor $\mathrm{e}^{-a^2/(4\Delta^2)}$, relative to t computed above. *Hint:* You can assume $\vec{R}_j = \vec{R}_i + a\vec{e}_x$, $\vec{e}_x$ being the unit vector in $x-$direction, since a cubical lattice is invariant under exchanges of the three unit vectors of Cartesian coordinates. **[4P]**

3. Due to the strong localization of the electrons, the interaction term can to good approximation be written as $V_{ijkl} = V_{ij} \delta_{il} \delta_{jk}$. Compute the diagonal contribution V_{ii} and the contribution from nearest neighbors, and show that the latter is suppressed by a factor $\mathrm{e}^{-a^2/(2\Delta^2)}$ relative to the former. *Hint:* Use

   $$V_{ij} = \int d^3x \int d^3y \left| \phi(\vec{x} - \vec{R}_i) \right|^2 V(\vec{x}, \vec{y}) \left| \phi(\vec{y} - \vec{R}_j) \right|^2 ,$$

   using a simple contact interaction,

   $$V(\vec{x}, \vec{y}) = \lambda \delta^3(\vec{x} - \vec{y}) .$$

   [5P]

4. Finally, explicitly write down the leading terms in the Hamiltonian (1) in the limit $\Delta \ll a$, i.e. for strong localization. Use the properties of the fermionic creation and annihilation operators to collapse the double sum over spins in the interactions to a single sum. **[3P]**