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Advanced Condensed Matter Theory — SS10

Exercise 10

Please return your solutions during the lecture on July 21, 2010
to be discussed on July 22, 2010

Presence exersice 1.1: Tight-Binding system: Interaction effects (10 points)

In the tight-binding system the interactions effects, due to the Coulomb repulsion between the electrons, can significantly influence the character of the ground state and affect the nature of quasi-particles. Comparable effects combined with interaction may drive the system towards a correlated magnetic state or an insulating phase. To understand how this happens, we express the Hamiltonian, describing the system, in field operators associated with the localized Wannier states, i. e.

$$H = \sum_{\sigma} \sum_{i,j} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + \sum_{\sigma,\tau} \sum_{i,i',j,j'} U_{ii'jj'} c^{\dagger}_{i\sigma} c^{\dagger}_{i'\tau} c_{j'\tau} c_{j\sigma}. \tag{1}$$

The first term describes the hopping of electrons from site i to site j with the associated transition amplitude t_{ij}. The second term is the Coulomb interaction in Wanier representation, where

$$U_{ii'jj'} = \frac{1}{2} \int \mathrm{d}^d x \int \mathrm{d}^d y \Psi^*_i(\mathbf{x}) \Psi^*_{i'}(\mathbf{y}) V_{\text{Coulomb}}(\mathbf{x}-\mathbf{y}) \Psi_{j'}(\mathbf{y}) \Psi_j(\mathbf{x}), \tag{2}$$

with Ψ_i as the Wanier states and V_{Coulomb} as the Coulomb interaction between the electrons. The Hamiltonian (1) is exact, apart from the neglect of the neighboring energy subbands.

a) In order to analyze the effects of the interaction, focused on the interaction part of the Hamiltonian (1), and show that the mayor contributions are

1. $\sum_i U_{iiii} n_{i\uparrow} n_{i\downarrow}$,
2. $\sum_{i\neq j} U_{ijij} \left(\sum_\sigma n_{i\sigma}\right) \cdot \left(\sum_\tau n_{j\tau}\right)$, and
3. $\sum_{i\neq j} U_{ijji} \sum_{\sigma,\tau} c^{\dagger}_{i\sigma} c^{\dagger}_{j\tau} c_{i\tau} c_{j\sigma}$.

Give an interpretation for first two contributions and explain why did you neglect the other terms with respect to these.

b) Now we want to study the third contribution above in more detail. With this purpose show next, that

$$\sum_{\sigma,\tau} c^{\dagger}_{i\sigma} c^{\dagger}_{j\tau} c_{i\tau} c_{j\sigma} = -2 \left(\mathbf{S}_i \cdot \mathbf{S}_j + \frac{1}{4} \left(\sum_\sigma n_{i\sigma} \right) \cdot \left(\sum_\tau n_{j\tau} \right) \right),$$

where $\mathbf{S}_i = \frac{1}{2} \sum_{\alpha,\beta} c^{\dagger}_{i\alpha} (\vec{\sigma}_i)_{\alpha\beta} c_{i\beta}$ with $\vec{\sigma}_i = (\sigma^x_i, \sigma^y_i, \sigma^z_i)$.

Hint: Use the Pauli matrix identity $\vec{\sigma}_{\alpha\beta} \cdot \vec{\sigma}_{\gamma\delta} = 2\delta_{\alpha\delta}\delta_{\beta\gamma} - \delta_{\alpha\beta}\delta_{\gamma\delta}$

c) Prove, that

$$J^F_{ij} \equiv U_{ijji} > 0,$$

and give an interpretion of the third contribution in a). Compare the present situation with the one in atomic physics, where is manifested as *Hund's rule*.

Homework 1.1: Antiferromagnetism - Spin wave Theory (15 points)

The simplest picture of an antiferromagnetic is that of two interpenetrating sub-lattices with $\uparrow$ spins on one and $\downarrow$ on the other (see Figure (1)).

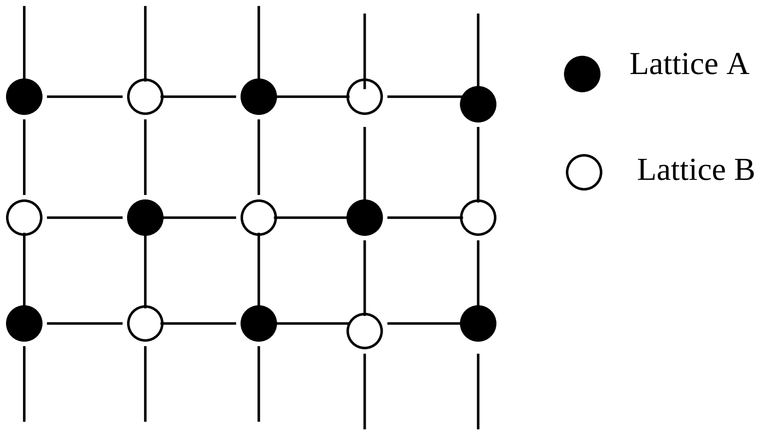

Figure 1: Bipartite lattice

This system can be described by the Heisenberg Hamiltonian

$$H_{AF} = J \sum_{\langle i,j \rangle} \mathbf{S}_i \mathbf{S}_j, \quad J > 0, \tag{3}$$

where $\langle \cdot, \cdot \rangle$ means that the sum is taken over nearest-neighbors.

a) Use the *Holstein-Primakoff transformation*

$$S_i^{(\ell)\,+} = \sqrt{2S - c_i^{(\ell)\,\dagger} c_i^{(\ell)}}\, c_i^{(\ell)}, \quad S_i^{(\ell)\,-} = c_i^{(\ell)\,\dagger} \sqrt{2S - c_i^{(\ell)\,\dagger} c_i^{(\ell)}}, \quad S_i^{(\ell)\,z} = S - c_i^{(\ell)\,\dagger} c_i^{(\ell)} \tag{4}$$

where c_i^ℓ is the annihilation operator referring to the ith atom on the sublattice $\ell \in \{A, B\}$, and prove that

$$\begin{aligned} H_{AF} &= -JS^2NZ + JSZ \left(\sum_i c_i^{(A)\,\dagger} c_i^{(A)} + \sum_j c_j^{(B)\,\dagger} c_j^{(B)} \right) \\ &\quad + SJ \sum_{\langle i,j \rangle} \left(c_i^{(A)\,\dagger} c_j^{(B)\,\dagger} + c_i^{(A)} c_j^{(B)} \right) + \mathcal{O}\left(\frac{1}{S} \right) + \mathcal{O}\left(n^{(A)} \cdot n^{(B)} \right) \end{aligned}$$

with Z as the number of nearest-neighbors.

b) Perform a Fourier transformation of the creation and annihilation operators $c_{\mathbf{k}}^{(\ell)} = N^{1/2} \sum_j e^{-i\mathbf{k}\mathbf{R}_j} c_i^{(\ell)}$ and obtain

$$H_{AF} = -JS^2NZ + JZS \sum_{\mathbf{k}} \left[\gamma_{\mathbf{k}} \left(c_{\mathbf{k}}^{(A)\dagger} c_{\mathbf{k}}^{(B)\dagger} + c_{\mathbf{k}}^{(A)} c_{\mathbf{k}}^{(B)} \right) + \left(c_{\mathbf{k}}^{(A)\dagger} c_{\mathbf{k}}^{(A)} + c_{\mathbf{k}}^{(B)\dagger} c_{\mathbf{k}}^{(B)} \right) \right] . \tag{5}$$

Give $\gamma_{\mathbf{k}}$ and use that with center symmetry $\gamma_{\mathbf{k}} = \gamma_{-\mathbf{k}}$ holds.

c) Unlike the ferromagnon case (see lecture), we cannot solve this trivially: we must diagonalize the Hamiltonian (5). Consider the *Bogoliubov transformation*, which involves the bosonic operators $\alpha_{\mathbf{k}}$ and $\beta_{\mathbf{k}}$

$$\alpha_{\mathbf{k}} = u_{\mathbf{k}} c_{\mathbf{k}}^{(A)} - v_{\mathbf{k}} c_{\mathbf{k}}^{(B)\dagger}, \quad \beta_{\mathbf{k}} = u_{\mathbf{k}} c_{\mathbf{k}}^{(B)} - v_{\mathbf{k}} c_{\mathbf{k}}^{(A)\dagger} \tag{6}$$

and show that $u_{\mathbf{k}}^2 - v_{\mathbf{k}}^2 = 1$.
Which functions satisty this equation?

Use the transformation (6) to diagonalize H_{AF} and obtain

$$H_{AF} = -NZJS(S+1) + \sum_{\mathbf{k}} \omega(\mathbf{k}) \left[\alpha_{\mathbf{k}}^\dagger \alpha_{\mathbf{k}} + \beta_{\mathbf{k}}^\dagger \beta_{\mathbf{k}} + 1 \right] \tag{7}$$

with the dispersion relation $\omega(\mathbf{k}) = JZS\sqrt{1-\gamma_{\mathbf{k}}^2}$.

In addition, show that long wavelength limit $ka \ll 1$, if we consider a simple cubic lattice, the dispersion vanishes as

$$\omega(\mathbf{k}) \sim ka .$$

d) Compute the magnetization of the sublattice A $M^{(A)} = \sum_i S_i^{(A)\,z}$, and show that it decreases as

$$\langle M^{(A)} \rangle \sim \left(\frac{T}{\theta_c} \right)^2$$

for low temperatures, θ_c being of the order of the critical or Neel temperature.