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Übungen zur Festkörpertheorie II — SS04

1. Übungsblatt

1. Hubbard Model - Mean Field Approximation

In solids with narrow conduction electron bands a simple description, including the on-site electron-electron interaction is given by the Hubbard Hamiltonian

$$H = \sum_{i,j,\sigma} t_{ij}\ a^{\dagger}_{i\sigma} a_{j\sigma} + U \sum_{i\sigma} n_{i\ \sigma} n_{i\ -\sigma} - h \sum_{i\sigma} \sigma\ n_{i\ \sigma} \tag{1}$$

with an additional external magnetic field h, acting on the local spin states.

a) The Hamiltonian Eq.1 is given in the *Wannier*-basis, instead of the usual Bloch representation. The Wannier states can be obtained be a Fourier transform of the Bloch wave function with respect to the lattice vectors $\vec{R}_i$.

$$a^{\dagger}_{i\sigma} = \frac{1}{\sqrt{N}} \sum_k e^{-i\vec{k}\vec{R}_i} c^{\dagger}_{k\sigma} \qquad a_{i\sigma} = \frac{1}{\sqrt{N}} \sum_k e^{i\vec{k}\vec{R}_i} c_{k\sigma} \tag{2}$$

From $H_0 = \sum_{i,j,\sigma} t_{ij}\ a^{\dagger}_{i\sigma} a_{j\sigma} = \sum_{k\sigma} \epsilon_k\ c^{\dagger}_{k\sigma} c_{k\sigma}$ one can derive the equation for the hopping intergral t_{ij}. Additionally it has to be shown that $\sum_i n_{i\sigma} = \sum_k n_{k\sigma}$.

b) Mean field approximation: In the following the fluctuations or the number operator $n_{i\sigma}$ around its mean value $< n\sigma >$ will be neglected ($n_{i\sigma} - < n_\sigma >= 0$).
An approximation for the operator product $n_{i\sigma} n_{i-\sigma}$ can be derived.

c) Using the above assumption transform the Hamiltonian Eq.1 to the k-momentum space. Write down the resulting Green's function.

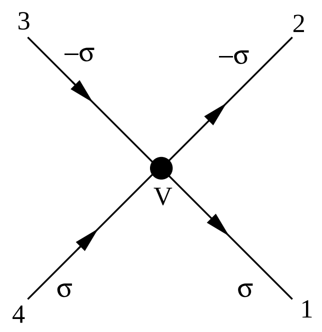

Figure 1: An elementary vertex appearing in Eq.3.

2. Hartree-Fock Approximation - 1st Order Perturbation Theory

Using the relations of Eqn.2 the Hamiltonian Eq.1 can be transformed to k-space. Writing H in the general two particle interaction form

$$H = \sum_{k\sigma} E_{h\sigma}(k)\; c^{\dagger}_{k\sigma} c_{k\sigma} + \sum_{k_1 \ldots k_4} v(k_1 k_2\;, k_3 k_4)\; c^{\dagger}_{k_1} c^{\dagger}_{k_2} c_{k_3} c_{k_4} \tag{3}$$

with $k_i = (\vec{k}_i, \sigma_i)$. The c-operators are ordered concerning the vertex figure 1.

Derive the Matsubara self-energy in 1st order perturbation theory and compare the result for the Green's function to the previous results.

3. Spectral Theorem

In the following there will be no external field applied (h=0). From the Green's function as derived above one can determine the spectral function $A_{k\sigma}(\omega)$. Using the relation

$$G^{<}_{k\sigma}(\omega) = -2\pi i \cdot A_{k\sigma}(\omega) f(\omega) \tag{4}$$

one can derive an equation for the mean occupation number per k-state $< n_{k\sigma} >$. Finally one gets an implicit equation for the mean spin state density $< n_{\sigma} >$. Solving this equation one can show that above a temperature T_c there exists no spontaneous magnetization m. For T $\rightarrow$ 0 a finite m occurs when $1 \leq U\rho_0(\epsilon_F)$ (Stoner-Criterion).