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Strongly Correlated Electrons
7. Übung

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1. Specific heat of a d-wave BCS superconductor **2 points**

The electronic specific heat of a superconductor is given by

$$C_S = T\frac{\partial S}{\partial T} = \sum_{\mathbf{k}\,\sigma} E_{\mathbf{k}} \frac{\partial f_{\mathbf{k}}}{\partial T} \tag{1}$$

with the Fermi-Dirac distribution $f_{\mathbf{k}} = 1/(\exp(E_{\mathbf{k}}/T)+1)$,[1] where we used units such that $k_B = 1$, and where the second equality follows from the fact that the entropy for a Fermi gas can be written as $S = -\sum_{\mathbf{k}\,\sigma}[(1-f_{\mathbf{k}})\ln(1-f_{\mathbf{k}}) + f_{\mathbf{k}}\ln f_{\mathbf{k}}]$.

Let us now consider a d-wave BCS theory in a 2D square lattice. In this case, the energy of the elementary excitations is given by $E_{\mathbf{k}} = \sqrt{\xi_{\mathbf{k}}^2 + \Delta_{\mathbf{k}}^2}$ with $\xi_{\mathbf{k}} = -2t(\cos k_x + \cos k_y) - \mu$ and $\Delta_{\mathbf{k}} = 2\Delta_0(\cos k_x - \cos k_y)$. The important contributions to the specific heat (namely the ones determining the low temperature scaling) come from the momentum space region close to so-called nodal points at which the gap closes. Expanding the energy close to these points, one can approximate Eq. (1) as a simple integral. Use this to show that $C_S \sim T^2$ in the limit $T \to 0$.

2. A hole in a 2D antiferromagnetic background **6 points**

Let us consider the t-J model in a 2D square lattice with N sites. The Hamiltonian can be written as

$$\begin{aligned}
\hat{H} &= \hat{H}_0 + \hat{H}_1, \\
\hat{H}_0 &= -t\sum_{\langle ij\rangle\,\sigma}(\tilde{c}^\dagger_{i\,\sigma}\tilde{c}_{j\,\sigma} + \text{h.c.}) + J\sum_{\langle i,j\rangle}\left(S_i^Z S_j^Z - \frac{\hat{n}_i\hat{n}_j}{4}\right), \\
\hat{H}_1 &= \frac{J}{2}\sum_{\langle i,j\rangle}\left(S_i^+S_j^- + S_i^-S_j^+\right).
\end{aligned} \tag{2}$$

Here, $\tilde{c}_{i\,\sigma}$ stands for $c_{i\,\sigma}(1-n_{i\,-\sigma})$, $c^\dagger_{i\,\sigma}$ ($c_{i\,\sigma}$) creates (annihilates) an electron with spin $\sigma =\uparrow,\downarrow$ on a lattice site i, $\hat{n}_{i\,\sigma} = c^\dagger_{i\,\sigma}c_{i\,\sigma}$ is the electron density operator, and $\mathbf{S}$ is the electron spin operator. J is an antiferromagnetic exchange coupling, while t is the hopping energy. Assume that we have $N-1$ electrons, such that there is one mobile hole in the system. (Note that this exercise uses units such that $\hbar = 1$).

a) **1 point**

Let us first consider only $\hat{H}_0$. Assume that the hole is initially at site j. Show that, as the hole moves, a string of frustrated bonds is generated in the system. Show that for each frustrated bond, the energy of the system increases by $J/2$. You may use the schematic pictures as illustrated in Fig. 1.

b) **1 point**

Let us make the above discussion more quantitative. Consider the state $|j,\nu,p\rangle$, which corresponds to a hole that was initially at site j and has made ν hops. p is a label which denotes the geometry of the hole path. Consider only the Ising part of $\hat{H}_0$ and show that the following approximation holds

$$\hat{H}_{Ising}|j,\nu,p\rangle = \frac{J}{2}((z-2)\nu + 1 - \delta_{\nu,0})|j,\nu,p\rangle, \tag{3}$$

[1] Notice that, in the derivation of the second equality, we neglected the fact that $\Delta = \Delta(T)$. This procedure is justified in the limit of low T because the T-dependence of the gap provides subleading corrections to the specific heat in this case. Note that in the BCS theory $\Delta(T) - \Delta(T=0) \sim T^2$.

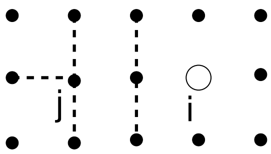

Figure 1: Schematic representation of the state $|j, 2, p\rangle$. The dashed lines stand for frustrated bonds while the empty circle for the hole.

where z is the number of nearest-neighbor sites. What kind of processes are neglected in Eq. (3)?

c) **1 point**

Consider now the following ansatz wavefunction

$$|\phi_j\rangle = \sum_{\nu \geq 0,\, p} \alpha_\nu |j, \nu, p\rangle, \tag{4}$$

which describes a hole bound (confined) to the site j. Demand that Eq. (4) is an eigenvector of $\hat{H}_0$ with eigenvalue E_B, and derive the following set of difference equations

$$-zt\alpha_1 = E_B \alpha_0,$$

$$-t\left[(z-1)\alpha_{\nu+1} + \alpha_{\nu-1}\right] = \left[E_B - J(\nu(z-2)+1)/2\right]\alpha_\nu. \tag{5}$$

Notice that the second equation above is a one-dimensional Schrödinger equation with a linearly increasing (confining) potential.

d) **1 point**

Let us now consider the spin-flip term $\hat{H}_1$. It is possible to show that $\hat{H}_1$ connects two different states $|\phi_i\rangle$ and $|\phi_j\rangle$. Apply $\hat{H}_1$ to the state $|j, 2, p\rangle$ illustrated in Fig. 1, and show that its leading effect is to reduce the length of the string by 2 sites. Show that $\langle\phi_i|H|\phi_j\rangle = (J/2)\alpha_0\alpha_2$ for this particular case.

e) **1 point**

The observation of the previous item indicates that the confined hole can tunnel from site j to site i. Therefore, the motion of the hole can be described by an effective tight-binding model. More precisely, we can consider the ansatz wavefunction for the hole $|\mathbf{k}\rangle = N^{-1/2}\sum_j \exp(-i\mathbf{k}\cdot\mathbf{R}_j)|\phi_j\rangle$, where $\mathbf{R}_j$ denotes a lattice site. The dispersion relation is simply given by $E(\mathbf{k}) = \langle\mathbf{k}|H|\mathbf{k}\rangle/\langle\mathbf{k}|\mathbf{k}\rangle$. In order to calculate $E(\mathbf{k})$, it is necessary to determine $\langle\phi_i|H|\phi_j\rangle$.

Generalize the arguments of item (d) for the case $\nu > 2$ and show that the effective tight-binding model is characterized by two hopping matrix elements $\tau_{0,2}$ and $\tau_{1,1}$, which correspond respectively to hops to the second, and third nearest neighbor. Show that $\tau_{1,1} = 2\tau_{0,2}$ and

$$\tau_{0,2} = J\sum_{\nu \geq 0}(z-1)^\nu \alpha_\nu \alpha_{\nu+2}. \tag{6}$$

Recall that the coefficients α_ν are given by the solutions of Eqs. (5).

f) **1 point**

Diagonalize the effective tight-binding model for a square lattice (with a unity lattice constant), and show that

$$E(\mathbf{k}) = 4\tau_{0,2}\left(\cos(k_x) + \cos(k_y)\right)^2 + \text{const.} \tag{7}$$

Notice that the bandwidth is given by the exchange constant J, and not by the original hopping energy t. The effective mass of the hole is strongly renormalized due to the interactions. Eq. (7) has a minimum along the lines $|k_x| + |k_y| = \pi$. It is possible to show that by including the process neglected in item (b), the degeneracy is lifted and Eq. (7) has only four minima at $\mathbf{k} = (\pm\pi/2, \pm\pi/2)$.