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Strongly Correlated Electrons
2. Übung

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1. Kramers-Kronig relations **1 point**

Consider a complex function $F(z)$ assumed to have no singularities in the upper half plane, and that obeys $F(z) \sim 1/z$ for $|z| \to \infty$. Specialize to $\lim_{\delta \to 0} F(z = y + i\delta)$ with $y \in \mathbb{R}$, and derive the Kramers-Kronig relations

$$\begin{aligned} Re\, F(y) &= -\frac{1}{\pi}\mathcal{P}\int_{-\infty}^{\infty} \frac{Im\, F(x)}{y-x} dx, \\ Im\, F(y) &= \frac{1}{\pi}\mathcal{P}\int_{-\infty}^{\infty} \frac{Re\, F(x)}{y-x} dx. \end{aligned} \tag{1}$$

Hints:
$F(z)$ is analytical in the upper half plane, thus

$$F(z) = \frac{1}{2\pi i}\oint_{\gamma} du \frac{F(u)}{u-z}$$

if z and the path γ are in the upper half plane. Deform γ such that the path runs along the real axis from $-R$ to R and then closes along a semi-circle. Show that the semi-circle does not contribute in the limit $R \to \infty$. Also the Dirac identity

$$\lim_{\delta \to 0} \frac{1}{x \pm i\delta} = \mathcal{P}\frac{1}{x} \mp i\pi\delta(x),$$

might help.

2. From the Hubbard to the t-J model **8 points**

Let us consider the single-band Hubbard model

$$\hat{H} = \hat{T} + \hat{V} = -t \sum_{\langle i,j \rangle\, \sigma} \hat{c}^{\dagger}_{i\,\sigma} \hat{c}_{j\,\sigma} + U \sum_i \hat{n}_{i\,\uparrow} \hat{n}_{i\,\downarrow}, \tag{2}$$

where $\hat{c}^{\dagger}_{i\,\sigma}$ ($\hat{c}_{i\,\sigma}$) creates (annihilates) an electron with spin $\sigma =\uparrow, \downarrow$ on a lattice site i, $\hat{n}_{i\,\sigma} = \hat{c}^{\dagger}_{i\,\sigma}\hat{c}_{i\,\sigma}$ is the electron density operator, t is the hopping energy, and $U > 0$ is the on-site repulsion energy. Notice that U is the amount of energy that should be paid if two electrons are on the same lattice site. We want to study the model (2) in the limit $U \gg t$. An effective Hamiltonian ($\hat{H}_{eff}$), which describes the low-energy sector of the model (2), can be derived using second order perturbation theory which can be implemented via a canonical transformation. (This excercise uses units such that $\hbar = 1$).

a) **1 point**

The Hilbert space of the model (2) can be divided into two subspaces $\mathcal{S}$ and $\mathcal{D}$, where the former contains configurations in which there is either zero or one electron per lattice site, while the latter contains at least one doubly occupied lattice site. Show that the hopping term $\hat{T}$ can be written as $\hat{T} = \hat{T}_0 + \hat{T}_+ + \hat{T}_-$, where

$$\begin{aligned}
\hat{T}_0 &= -t \sum_{\langle i,j\rangle\,\sigma} (1-\hat{n}_{i\,-\sigma})\hat{c}^\dagger_{i\,\sigma}\hat{c}_{j\,\sigma}(1-\hat{n}_{j\,-\sigma}) + \hat{n}_{i\,-\sigma}\hat{c}^\dagger_{i\,\sigma}\hat{c}_{j\,\sigma}\hat{n}_{j\,-\sigma}, \\
\hat{T}_+ &= -t \sum_{\langle i,j\rangle\,\sigma} \hat{n}_{i\,-\sigma}\hat{c}^\dagger_{i\,\sigma}\hat{c}_{j\,\sigma}(1-\hat{n}_{j\,-\sigma}), \qquad (3) \\
\hat{T}_- &= -t \sum_{\langle i,j\rangle\,\sigma} (1-\hat{n}_{i\,-\sigma})\hat{c}^\dagger_{i\,\sigma}\hat{c}_{j\,\sigma}\hat{n}_{j\,-\sigma}.
\end{aligned}$$

Here $-\sigma =\uparrow$ if $\sigma =\downarrow$ and vice-versa. What kind of process does each of the three terms in Eq. (3) describe? Why can we treat $\hat{H}_1 = \hat{T}_+ + \hat{T}_-$ as a perturbation to $\hat{H}_0 = \hat{T}_0 + \hat{V}$ in the limit $U \gg t$?

b) **2 points**

In order to calculate the effective Hamiltonian $\hat{H}_{eff}$ described above, we perform the following canonical transformation

$$\begin{aligned}
\hat{H}_{eff} = e^{\hat{S}}\hat{H}e^{-\hat{S}} &= \hat{H} + [\hat{S},\hat{H}] + \frac{1}{2!}[\hat{S},[\hat{S},\hat{H}]] + \dots \\
&= \hat{H}_0 + \hat{H}_1 + [\hat{S},\hat{H}_0] + [\hat{S},\hat{H}_1] + \frac{1}{2!}[\hat{S},[\hat{S},\hat{H}_0]] + \dots, \qquad (4)
\end{aligned}$$

where the operator $\hat{S}$ is determined by imposing that the term linear in t in Eq. (4) vanishes, i.e.,

$$\hat{H}_1 + [\hat{S},\hat{H}_0] = 0, \qquad (5)$$

The effective Hamiltonian then reads

$$\hat{H}_{eff} = \hat{H}_0 + \frac{1}{2}[\hat{S},\hat{H}_1] + \mathcal{O}(t^3). \qquad (6)$$

Show that the condition (5) is fullfiled in first order in t/U if we choose

$$\hat{S} = \frac{1}{U}\left(a^+\hat{T}_+ + a^-\hat{T}_-\right). \qquad (7)$$

Calculate the constants a^+ and a^-. Verify that $\hat{S}$ is anti-hermitian.

c) **1 point**

Before we continue, prove the following identity

$$\sum_{\sigma,\sigma'} \hat{c}^\dagger_{i\,\sigma}\hat{c}^\dagger_{j\,\sigma'}\hat{c}_{i\,\sigma'}\hat{c}_{j\,\sigma} = -\frac{1}{2}\left(\hat{n}_i\hat{n}_j + 4\hat{\mathbf{S}}_i\cdot\hat{\mathbf{S}}_j\right), \qquad i \neq j \qquad (8)$$

where the spin operator is defined as

$$\hat{\mathbf{S}}_i = \frac{1}{2}\sum_{\sigma,\sigma'} \hat{c}^\dagger_{i\,\sigma}\hat{\tau}_{\sigma,\sigma'}\hat{c}_{i\,\sigma'} \qquad (9)$$

with $\hat{\tau} = (\tau_x, \tau_y, \tau_z)$ a vector of Pauli matrices.

d) **3 points**

Suppose that we are at half-filling, i.e., $\langle \hat{n}_i\rangle = \langle \hat{n}_{i\uparrow} + \hat{n}_{i\downarrow}\rangle = 1$. Using the results of excercise 4b), calculate $\hat{H}_{eff}$. Project the resulting Hamiltonian into the subspace $\mathcal{S}$ and explain why some terms drop out after the projection. Use the identity (8) and show that $\hat{H}_{eff}$ can be written as

$$\hat{H}_{eff} = J\sum_{\overline{\langle i,j\rangle}} \left(\hat{\mathbf{S}}_i\cdot\hat{\mathbf{S}}_j - \frac{1}{4}\right), \qquad (10)$$

where the exchange constant $J = 4t^2/U$, and where $\overline{\langle i,j\rangle}$ denotes pairs of sites i,j.

e) **1 point**

Suppose we now move away from half-filling by introducing some holes in the system. In this case, Eq. (10) should be modified, i.e., some extras terms should be added to it. The final result is the so-called t-J model, which is relevant for the description of the high-T$_c$ superconductors. Using the previous results, derive the Hamiltonian of the t-J model.