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Strongly Correlated Electrons
5. Übung

Sommersemester 2015

1. The Hubbard model in $d = \infty$ **6 points**

In this exercise, we will discuss the properties of the Hubbard model [see Eq.(2), second exercise sheet] in higher spatial dimensions d.

a) **1 point**

Let us consider the Hubbard model on a d-dimensional simple cubic lattice with unit lattice spacing. The dispersion of tight-binding electrons with hopping of strength t only between nearest neighbor on this lattice reads

$$\epsilon_{\mathbf{k}} = -2t \sum_{n=1}^{d} \cos(k_n), \tag{1}$$

where the d-dimensional momentum vector reads $\mathbf{k} = (k_1, k_2, ..., k_d)$ with $-\pi < k_n \leq \pi$ and t is the hopping energy. The density of states is given by

$$D_d(\epsilon) = \int_{BZ} \frac{d^d k}{(2\pi)^d} \delta(\epsilon - \epsilon_{\mathbf{k}}) \equiv \langle \delta(\epsilon - \epsilon_{\mathbf{k}}) \rangle_{BZ}. \tag{2}$$

Notice that Eq. (2) can also be seen as the average of $\delta(\epsilon - \epsilon_{\mathbf{k}})$ over the first Brillouin zone (BZ).

Calculate the averages of $\epsilon_{\mathbf{k}}$ and $\epsilon_{\mathbf{k}}^2$ over the first Brillouin zone. Use the central limit theorem [see note at the end of the exercise sheet] and calculate the density of states. Show that one obtains a finite quantity in the limit $d = \infty$ if the hopping term is rescaled by $t \to t/\sqrt{z}$, where $z = 2d$ is the coordination number of the d-dimensional cubic lattice. Compare $D_\infty(\epsilon)$ with $D_d(\epsilon)$ $(d = 1, 2, 3)$.

b) **1 point**

Consider now a Hubbard model with the rescaled hopping $t/\sqrt{2d}$. For some randomly chosen $\mathbf{k}$, the kinetic energy scales as

$$\frac{\epsilon_{\mathbf{k}}}{t} \propto \mathcal{O}(\sqrt{d}), \quad \text{for } d \to \infty. \tag{3}$$

Certainly, this is not the case for special values of $\mathbf{k}$ as for example $\mathbf{k} = (0, 0, \cdots)$. Nevertheless, for the cubic lattice in infinite dimensions the average kinetic energy of the electrons is a finite quantity since under the integral the singular points in momentum space have zero measure. For general lattices one may introduce an artificial finite bandwidth and work with a bounded density of states. We can also calculate the average kinetic energy from the zero-temperature Green's function formalism as

$$\langle \epsilon_{\mathbf{k}} \rangle_{BZ} = t \sum_{<i,j>} \sum_{\sigma} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi i} G_\sigma(i, j; \omega) e^{i\omega 0^+}, \tag{4}$$

where the first sum runs over all nearest neighbor sites.

From the fact that the average kinetic energy is finite for $d \to \infty$ deduce the scaling of the Green's function $G_\sigma(i, i+1; \omega)$ with d. Generalize the result to arbitrary neighbors $G_\sigma(i, j; \omega)$.

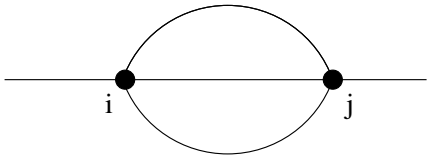
c) **1 point**

Let us now consider the on-site interaction term $U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$. If one treats this term perturbatively, it is possible to show that remarkable simplifications occur in the many-body diagrammatics in the limit

$d = \infty$. In order to exemplify such a statement, let us consider a given diagram (in real space) for the self-energy [see Fig. below]. The solid lines correspond to free fermion propagators while i and j are lattice sites. Perform a power counting and show that for $i - j = 1$ the diagram is suppressed by a factor of order $d^{-\frac{3}{2}}$. For general lattice sites the diagram is suppressed by a factor of order $d^{-\frac{3}{2}R}$ for large d where $R = |i-j|$ is the distance between sites i and j. Consider now a diagram with two internal vertices which are connected by three or more independent paths which have no line in common. In this case one needs to sum over the internal lattice sites. Show that such a diagram is suppressed at least by a factor $d^{-(\frac{3}{2}-1)R}$. Which diagrams survive in the limit $d = \infty$? Explain why the single-particle propagator assumes the following form

$$G(\mathbf{k}, i\omega_n) = 1/\left(i\omega_n + \mu - \epsilon_{\mathbf{k}} - \Sigma(i\omega_n)\right), \tag{5}$$

where μ is the chemical potential.



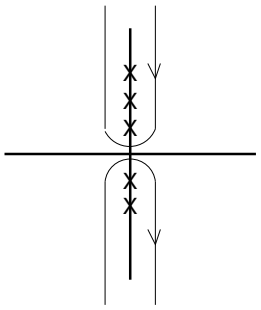
d) **1 point**

We now want to explore the consequences of Eq.(5) at zero temperature, and assuming that the self-energy $\Sigma(\omega)$ has Fermi-liquid properties. Let us start by looking at the renormalization of the Fermi surface due to the interactions. Calculate the particle density and show that

$$n = \frac{2}{\beta}\sum_{i\omega_n}\langle G(\mathbf{k}, i\omega_n)e^{i\omega_n 0^+}\rangle_{BZ} = 2\langle\Theta(\mu - \Sigma(0) - \epsilon_{\mathbf{k}})\rangle_{BZ}, \tag{6}$$

where $G(\mathbf{k}, i\omega_n)$ is given by Eq.(5), $\Theta(x)$ is the step function and the average $\langle\cdots\rangle_{BZ}$ is defined in Eq.(2). What can one conclude about the shape of the Fermi surface?

Hint.: perform the Matsubara summation in the usual way using the contour below. The identity $G(\mathbf{k}, \omega) = d(\ln(1/G(\mathbf{k}, \omega)))/d\omega + G(\mathbf{k}, \omega)d\Sigma/d\omega$ might be useful. Recall also that for a Fermi-liquid $\mathrm{Im}\Sigma(\omega) = \mathcal{O}(\omega^2)$ when $\omega \to 0$.



e) **1 point**

Consider now, with the same assumptions as in part d), the spectral density $\rho(\omega) = -\mathrm{Im}\langle G(\mathbf{k}, \omega + i\eta)\rangle_{BZ}/\pi$ for the interacting system. Write down the form of $\rho(\omega)$ and show that the density of states at the Fermi surface is not renormalized due to the interactions, i.e., $\rho(0) = \rho_0(0)$, where $\rho_0(\omega)$ is the density of states for non-interacting electrons.

Obs.: This is a strong implication of the fact that the self-energy is momentum-independent. Recall that a renormalization of $\rho(\omega)$ is related to a non-vanishing $d\Sigma/d\mathbf{k}$.

f) **1 point**

The fact that the self-energy is momentum-independent implies that the effective mass m^* of the quasi-particles is constant along the Fermi surface. The relation between m^* and the electronic mass m is given by the usual formula $Z^{-1} = m^*/m = 1 - (d\mathrm{Re}\Sigma/d\omega)_{\omega=0}$, where Z is the quasi-particle weight. Show that this renormalization implies that the slope of the density of states at the Fermi surface increases, i.e., $\rho'(0) = (m^*/m)\rho_0'(0)$.

Obs.: Notice that the results derived in items (c)-(e) are exact.

Note: The central limit theorem: let $x_1, x_2, ..., x_N$ be a set of N independent random variables which have an arbitrary probability distribution $P(x_1, ..., x_N)$ with mean μ_i and a *finite* variance σ_i^2. Then

$$X = \frac{\sum_{i=1}^{N} x_i - \sum_{i=1}^{N} \mu_i}{\sqrt{\sum_{i=1}^{N} \sigma_i^2}}$$

has a limiting cumulative distribution function which approaches a *normal distribution.*