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3. CMS exercise:
The Random Phase Approximation for the 2D Hubbard model

Introduction

Despite its simple appearance, the Hubbard model

$$H = \sum_{k\sigma} \epsilon_k c^\dagger_{k\sigma} c_{k\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} \tag{1}$$

contains a rich variety of intriguing physical phenomena, not all of which are actually understood to date. While there exist exact solutions in one and infinite spatial dimensions, the most relevant cases of two and three dimensions have to be tackled with sophisticated numerical techniques.
Here, we will consider the Hubbard model in two spatial dimensions, which is for example advocated to be the minimal setup for the understanding of unconventional high-temperature superconductivity in the cuprate materials. We will focus on magnetic instabilities of the paramagnetic phase, that develop as divergences in the static spin susceptibility and signal the onset of an ordered state.

The setup

Consider a square lattice with a nearest neighbour hopping amplitude t. In two dimensions, the dispersion then is

$$\epsilon_k = -2t \sum_{\alpha=x,y} \cos(k_\alpha a). \tag{2}$$

In the following, we will set the lattice constant $a = 1$ and define our energy units by setting $4t = 1$. The momentum k lives in the Brillouin zone, i.e. $k_\alpha \in (-\pi, \pi]$.
We shall only deal with the particle-hole symmetric case (half-filling: one electron in total), which is achieved by setting the chemical potential $\mu = 0$.
As a reminder, the spin susceptibility of the non-interacting case ($U = 0$) is given by the following Lindhard function

$$\chi_0(q,\omega) = \frac{1}{N_k} \sum_k \frac{f(\epsilon_{k+q}) - f(\epsilon_k)}{\omega + \epsilon_k - \epsilon_{k+q} + i0^+} \tag{3}$$

where N_k is the number of k-points in the discretized Brillouin zone. The magnetic susceptibility of the interacting system ($U \neq 0$) in the random phase approximation is (see lecture notes)

$$\chi_{RPA}(q,\omega) = \frac{\chi_0(q,\omega)}{1 - U\chi_0(q,\omega)}. \tag{4}$$

A magnetic instability of the paramagnetic phase occurs if in the magnetic susceptibility a pole develops at zero energy cost, i.e. in the $\omega \to 0$ limit (the static χ_0 is real and we can omit the $i0^+$ in the denominator). As we shall see, the wavevector Q at which the pole appears defines the character of the magnetic ordering.

Exercises

1. Density of states

Compute the density of states (DOS)

$$D(\omega) = 2/N_k \sum_k \delta(\omega - \epsilon_k) \tag{5}$$

on a frequency grid by using a parametrization of the delta-distribution that has a finite width. The factor of two accounts for the summation over spins. Note that $D(\omega)$ is not continuous at $\omega = 0$, indeed one can show analytically that it is logarithmically divergent, i.e. for $|\omega| \ll 1$: $D(\omega) \sim \ln(t/|\omega|)$.

2. The non-interacting Fermi surface

The Fermi surface of a band-structure is defined by the intersections (Fermi vectors) k_F of ϵ_k with the chemical potential: $\epsilon_{k_F} - \mu \stackrel{!}{=} 0$. As we have chosen the case of half-filling ($\mu = 0$), we are looking for the zeros of the dispersion of Eq. 2 in the two-dimensional Brillouin zone k_x, k_y. How does the Fermi surface look like in this case?

3. Non-interacting susceptibility

(a) Write a program that computes the *static* susceptibility à la Eq. 3. Use a fine mesh ($\sim 100 \times 100$) for vectors k, with $k_\alpha \in (-\pi, \pi]$, and a coarser mesh ($\sim 10 \times 10$) for q, which can be limited to $q_\alpha \in [0, \pi]$. A few warnings are in order: We are looking for enhancements of χ_0. However, we have to distinguish between the approaching of a physical instability from numerical singularities. There are several problematic situations for Eq. 3 that we have to deal with:

- Evidently for $q = 0$, we would be dividing zero with zero in Eq. 3. In your program take care of this by using for $q = 0$ the $q \to 0$ limit expression of Eq. 3.
- There is a single vector $Q \neq 0$ that translates *every* Fermi vector k_F to another point on the Fermi surface: $\forall k_F$: $k_F + Q = k'_F$. Note that the Brillouin zone is repeated periodically. Identify the vector Q.
- There are other q-vectors that connect *individual* points of the Fermi surface. In the limit $N_k \to 0$, these contributions are negligible. For finite discretizations we have to take care of these:

Analytically, vectors k and q for which $\epsilon_k = \epsilon_{k+q}$ do not give a contribution because of the vanishing numerator. Numerically, however, we will be dividing small numbers. To numerically regularize Eq. 3 you should exclude contributions to Eq 3 for which $|\epsilon_k - \epsilon_{k+q}|$ is smaller than $|\epsilon_k - \epsilon_{k+q+dk}|$ where dk indicates the shifting to the nearest neighbours of $k + q$.

(i) Using an inverse temperature $\beta = 50/(4t)$ in the Fermi functions, towards which vector Q^* does χ_0 increase? Is this a special vector?

(ii) Follow the value of $\chi_0(Q^*)$ from low (~ 5) to high (~ 200) $4t\beta$ and plot it as a function of temperature, $1/\beta$.

(iii) For the magnetization in the presence of a perturbing magnetic field in linear response holds: $m(q) = \chi(q)B(q)$. If the static χ_0 diverges at Q^*, this points towards a *spontaneous* magnetization, i.e. a symmetry breaking in the absence of a perturbing field. What is the real-space structure of the magnetization corresponding to the vector Q^*?[1]

[1] Consider $m_i = \sum_q e^{iqR_i} m(q)$ with the only contribution stemming from $q = Q^*$. R_i indexes sites on the lattice.

(b) *Analytical* considerations for $\chi_0(Q^*)$ [optional]
Verify that for the dispersion at half-filling, Eq. 2, the following relation holds:

$$\epsilon_k = -\epsilon_{k+Q^*}. \tag{6}$$

This is the so-called *nesting* condition. The concept of nesting was pioneered by R. Peierls for explaining charge density wave states (an ordered state where the charge, not the spin exhibits long range order). If Eq. 6 holds for larger regions k of the Brillouin zone for a specific vector q, the corresponding parts of the Fermi surface have the same topology and are connected by a simple translation. Whenever this is the case, the system is prone to instabilities.

(i) using the property Eq. 6 rewrite Eq. 3: Show and use that $f(\epsilon_{k+Q^*}) - f(\epsilon_k) = \tanh(\beta\epsilon_k/2)$. Then substitute the k-summation with an integral over the density of states, Eq. 5.

(ii) show that $\chi_0(Q^*)$ is *finite* in the limit of large temperatures.

(iii) show that in the $T \to 0$ limit

$$\chi_0(Q^*, \omega = 0) = \int d\epsilon \frac{D(\epsilon)}{2|\epsilon|} \tag{7}$$

which diverges logarithmically if the DOS is finite at the Fermi level. In our case, the DOS is itself divergent at $\omega = 0$, thus enhancing the divergence at half-filling.

Note that up to now, we where dealing with the *non-interacting* susceptibility. This means that the tendency towards magnetic order with wave-vector Q^* is a pure band-structure effect!

4. The RPA susceptibility

Now compute the RPA magnetic susceptibility via Eq. 4.

(i) plot $\chi_{RPA}(q = 0)$ as a function of U at $\beta = 100/(4t)$. You will find a divergence above a critical value U_c of the interaction. The emergence of which kind of spin-ordering does the enhanced $q = 0$ magnetic susceptibility point to? Compare the value of U_c to that of the Stoner criterion.

(ii) for $U/(4t) = 0.5$, plot $\chi_{RPA}(q = 0)$ as a function of $1/\beta$ in the range $[0.0015 : 0.1]$. Interpret the result.

(iii) for $U > U_c$ as well as $T < T_c$, i.e. beyond the critical interaction and below the Curie temperature, the susceptibility is again finite. Why is this an unphysical result? Why can't we anymore interpret the susceptibility as the response function of the system?

Please hand in your source code and a pdf (or handwritten notes) with a discussion of the exercises!