3. CMS exercise: Random Phase Approximation applied to the 2d Hubbard Model

Introduction

The two-dimensional Hubbard model displays, at low-temperatures, some of the most intriguing (and heatedly debated!) physics of condensed matter. For instance, it is considered the basic model for describing the unconventional high-temperature superconductivity of the cuprates, in the slightly hole-doped regime away from half-filling. Depending on the filling level, however, a very rich phase diagram with competing instabilities is found. In this CMS exercise, we will concentrate to analyze, using the RPA, the tendency towards charge and spin (magnetic) instabilities at half-filling (particle-hole symmetric case).

The definition of the RPA susceptibility $\chi^{RPA}_{C/S}(\vec{q},\omega)$ and the non-interacting susceptibility $\chi_0(\vec{q},\omega)$ has been given in the lecture

$$[\chi^{RPA}_{C/S}(\vec{q},\omega=0)]^{-1} = [\chi_0(\vec{q},\omega=0)]^{-1} \pm U \tag{1}$$

where the "$+/-$"signs on the l.h.s. of the equation correspond to the charge (C) and spin (S) susceptibility, respectively, and

$$\chi_0(\vec{q},\omega=0) = \chi_0(\vec{q}) = -\frac{1}{(\#k)}\sum_{\vec{k}} \frac{f(\epsilon_{\vec{k}+\vec{q}}) - f(\epsilon_{\vec{k}})}{\epsilon_{\vec{k}+\vec{q}} - \epsilon_{\vec{k}}} \tag{2}$$

where $f(x) = (\mathrm{e}^{\beta x}+1)^{-1}$ is the Fermi-Dirac distribution function, and $\beta = 1/T$ is the inverse temperature.

Purpose of the exercise

The aim of the exercise is to write a program "from scratch" capable of calculating the $\vec{q}$-dependent (but, static, i.e., $\omega = 0$) charge and spin susceptibilities for the half-filled 2d Hubbard Model using the RPA. The half-filled 2d Hubbard Model is given by the Hamiltonian

$$H_{\text{Hub}} = \sum_{\vec{k},\sigma} \epsilon_{\vec{k}}\, c^{\dagger}_{\vec{k},\sigma} c_{\vec{k},\sigma} + U \sum_i n_{i\uparrow} n_{i,\downarrow} \tag{3}$$

where $\epsilon_{\vec{k}} = -2t[\cos(k_x) + \cos(k_y)]$, $k_x, k_y \in]-\pi,\pi]$. Typically one sets $4t = D = 1$ and $U > 0$. You may use any programming language of your choice (but Fortran is suggested to ensure a "uniformity" among the source files). The program will then be used to investigate the tendencies towards charge and magnetic instabilities of the system with focus on the asymptotic temperature regions.

Tasks

1. Calculate numerically $\chi_0(\vec{q})$ for $\beta = 0.5, 1, 10, 100, 1000$ for a sparse q-grid in the (irreducible)[1] Brillouin zone (BZ). Identify the point $\vec{Q}_*$ where $\chi_0(\vec{q})$ display its maximal

[1] For the q-grid, you might, alternatively, consider the reduced, but not fully irreducible BZ, such as $q_x, q_y \in [0,\pi]$ Note that the k-summation has to be performed, instead, on a fine mesh over the whole BZ.

value. Is there a connection between $\vec{Q}^*$ and the Fermi surface (of your half-filled case), i.e., the k-points where $\epsilon(\vec{k}) = 0$ in the Brillouin zone? If yes, which one?

2. Calculate $[\chi_S^{RPA}(\vec{Q}^*)]^{-1}$ and $[\chi_C^{RPA}(\vec{Q}^*)]^{-1}$ for $U = 0.005, 0.0075, 0.01, 0.02, 0.1, 0.2$ and plot them versus the temperature $T = 1/\beta \in [0.001, 1]$. Make sure that the k-point integral is converged. *Hint*: Calculate $\chi_0(\vec{Q}^*)$ first and then make a loop over U. Which susceptibility diverges ($\chi_{RPA}^{-1} \to 0$) and which is suppressed? Give a physical interpretation of the effect of U in RPA. Extract the critical temperature T_* for each U from your data.

3. By rotating the coordinate system and using the symmetries of the system one can show that
$$\chi_0(\vec{Q}^*) \propto \int_0^{\frac{\pi}{2}} \int_0^{\frac{\pi}{2}} \frac{\tanh(\beta \cos(u)\cos(v))}{\cos(u)\cos(v)} \mathrm{d}u \mathrm{d}v. \tag{4}$$
Find the proportionality constant (either analytically or numerically). What is the asymptotic form of $\chi_0(\vec{Q}^*)$ for $\beta \ll 1$ (to first order)? For $\beta \gg 1$ $\tanh(\beta x)$ will mainly act as low energy cut off, that is
$$\chi_0(\vec{Q}^*) \propto \int_0^{\mathrm{acos}(\Lambda/\beta)} \int_0^{\mathrm{acos}(\Lambda/\beta)} \frac{1}{\cos(u)\cos(v)} \mathrm{d}u \mathrm{d}v, \tag{5}$$
for a suitable Λ. What is the asymptotic form of $\chi_0(\vec{Q}^*)$ for $\beta \gg 1$ (to first order)? *Hint*: sec(x)=1/cos(x) can be found in a 'list of integrals of trigonometric functions'.

4. Give an expression for the critical temperature T_* as a function of U in the region $T_* \ll 1$ and in the region $T_* \gg 1$, using the asymptotic forms of $\chi_0(\vec{Q}^*)$. Fit Λ in the expression for $T_* \ll 1$ to the critical temperature for $U = 0.005$. Plot the two expressions and the previously calculated critical temperatures in a single graph (T_* v.s. U).

5. Try to relate the observed behavior of χ_0 at low-T with the generic properties of the two-dimensional model at half-filling. *Hint*: Express the k-sum defining $\chi_0(\vec{Q}^*)$ as an integral over the density of states $N(E)$, and identify the contribution from each factor in the integral. Elaborate on the physical origin of each contribution.

6. How would your results for $\chi_C^{RPA}(\vec{q})$ and $\chi_S^{RPA}(\vec{q})$ change, if you instead had considered the half-filled **but** attractive (i.e., $U < 0$) Hubbard model?

Please write a small report (in a **single** .pdf file) and send it in per e-mail with your source file(s) attached.

Viel Spaß ... und Erfolg!