6. Exercise on QFT for many-body systems

Sommersemester 2018

TUTORIUM: Friday, 22.06.2018.

12. Van Hove singularities

 $2+2+1+2^*=5+2^*$ points

Consider the dispersion relation (single-particle energy states) for electrons on a simple hypercubic lattice in d dimensions, with only nearest-neighbor hopping:

$$\varepsilon_{\mathbf{k}} = -2t \sum_{i=1}^{d} \cos k_i,\tag{1}$$

with the hopping amplitude t and the lattice constant a = 1. The density of single-particle states in this system is then given by

$$N(\epsilon) = \frac{1}{(2\pi)^d} \int_{-\pi}^{\pi} d^d k \, \delta\left(\epsilon - \varepsilon_{\mathbf{k}}\right). \tag{2}$$

In the first exercise you have calculated numerically and then plotted these densities of states for d = 1, 2, 3. Here, the singular structures (divergences, cusps) of these functions should be analyzed analytically.

- a) Calculate $N(\epsilon)$ for d = 1 explicitly and determine the interval $[\epsilon_1, \epsilon_2]$ on which $N(\epsilon) \neq 0$. Moreover, identify the values ϵ^* where D diverges, i.e. where $N(\epsilon^*) = \infty$. From which points \mathbf{k}^* in the dispersion relation originate these divergences? Show that the divergences can be reproduced by taking into account only the contributions from these \mathbf{k}^* -points. (*Hint:* Replace $\varepsilon_{\mathbf{k}}$ in Eq. (2) by a corresponding Taylor-expansion around these points up to second order.)
- b) For d=2 one can show that $N(\epsilon)$ is essentially given by a complete elliptic integral of the first kind. Here, however, only the singular contributions to $N(\epsilon)$ should be analyzed. As in the one-dimensional case a singular contribution originates from stationary points in the dispersion relation. Determine the kind of stationary point (i.e., maximum, minimum or saddle point) which generates this so-called Van Hove singularity in the the two-dimensional DOS and determine the singular contribution to $N(\epsilon)$ by expanding $\varepsilon_{\mathbf{k}}$ around corresponding stationary point in Eq. (2) as for the one-dimensional case in **a**).
- c) Try to predict how the singular behavior of the DOS evolves with the dimensions of the system for $d \ge 3$.
- d) Finally, consider the limit $d \to \infty$. In this case, one has to rescale the hopping amplitude as $t \to \frac{t}{\sqrt{d}}$, in order to render the total energy of the system as well as the second moment (standard deviation) of the density of state finite. Show that $N_{\infty}(\epsilon)$ is proportional to a Gaußdistribution.

13. Magnetic susceptibilities in d dimensions

Consider a system of non-interacting electrons on a (hyper)cubic lattice whose energy dispersion is given by Eq. (1).

- a) Compute the magnetic susceptibility, i.e. the Fourier transform of the spin-spin response function $\langle T_{\tau}S_z(\mathbf{r}_i,\tau)S_z(0,0)\rangle$, for the frequency $\Omega_m = 0$ (static susceptibility), and for the two momenta $\mathbf{Q} = (0, 0, 0, \cdots)$ (ferromagnetic susceptibility) and $\mathbf{Q} = (\pi, \pi, \pi, \cdots)$ (antiferromagnetic susceptibility).
- b) Determine the leading divergences of the ferromagnetic and the antiferromagnetic susceptibilities for $T \rightarrow 0$ in d=2 dimensions. To this end write the total density of states as a sum of a singular and a regular contribution as calculated in 14 b). (Hint: Consider the derivative of the antiferromagnetic susceptibilities with respect to β and perform a Sommerfeld-like expansion for the regular part of the DOS.)
- c) Discuss how the results of b) are modified in $d \ge 3$ dimensions.
- d) Consider the same electronic system for d = 2, but now in presence of a local (repulsive) Hubbard interaction U > 0, and calculate within the random-phase approximation (RPA) the two (ferromagnetic and antiferromagnetic) susceptibilities in the corresponding particlehole channel. On the basis of your RPA calculations, make your final considerations about the tendency of the system towards a given magnetic order at T = 0.