6. Exercise on QFT for many-body systems

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14. 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

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

In the first QFT 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 $D(\epsilon)$ for $\boldsymbol{d = 1}$ explicitly and determine the interval $[\epsilon_1, \epsilon_2]$ on which $D(\epsilon) \neq 0$. Moreover, identify the values ϵ^* where D diverges, i.e. where $D(\epsilon^*) = \infty$. From which points $\mathbf{k}^*$ in the dispersion relation do these divergences originate? 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 singular points up to second order.)*

b) For $\boldsymbol{d = 2}$ one can show that $D(\epsilon)$ is essentially given by a complete elliptic integral of the first kind. In this exercise, however, only the singular contributions to $D(\epsilon)$ should be analyzed. Similarly 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 $D(\epsilon)$ 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 $\mathbf{d \geq 3}$.

d) Finally, consider the limit $\boldsymbol{d \to \infty}$. 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 $D_\infty(\epsilon)$ is proportional to a Gauss distribution.

15. Magnetic susceptibilities in d dimensions *1.5+1.5+1*+1+1*=5+2* points*

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 $T \to 0$ in $\boldsymbol{d=2}$ 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).* Which properties of the DOS and of the Fermi Surfaces are mostly responsible for the ferromagnetic and the antiferromagnetic results?

c) Discuss how the results of **b)** are modified in $\mathbf{d} \geq \mathbf{3}$ dimensions.

d) Consider the same electronic system for $\mathbf{d}=\mathbf{2}$, 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 particle-hole channel. On the basis of your RPA calculations, make your final considerations about the tendency of the system towards a given magnetic order at $T = 0$.

e) How do the results of **15d)** change in the attractive case ($U < 0$)? Why?

* Bonus points

Viel Spaß!