5. Exercise on QFT for many-body systems

Sommersemester 2023

TUTORIUM: Friday, 16.06.2023.

10. Van Hove singularities

2+2+1+2=5+2* points*

Consider the dispersion relation (single-particle energy states) for electrons on a simple hyper-cubic 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 $\boldsymbol{d=1}$ 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 $\boldsymbol{d=2}$ 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 $d \geq 3$.

d) (Bonus points) 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 $N_\infty(\epsilon)$ is proportional to a Gaußdistribution.

11. Magnetic susceptibilities in d dimensions *1.5+1.5+1+1=5 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 **10 b)**.

Hints: (1) For finding the $T\to 0$ behavior in the regular parts of the DOS, one can perform a Sommerfeld-like expansion. (2) For the antiferromagnetic case it is easier to consider the derivative of the susceptibility with respect to β and from that to conclude how the susceptibility itself behaves.

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

d) Consider now non-interacting electrons on a one-dimensional lattice with dispersion $\epsilon_k = -2t\cos(ka)$ at half-filling ($\mu = 0$). Is there a Q-point in the Brillouin zone, $Q \in [0, 2\pi]$, for which $\epsilon_{k+Q} = -\epsilon_k = 0$? What is the signature of this "nesting" property in the free (bubble) susceptibility $\chi_0(Q,\omega = 0)$ (calculated in Exercise 2, Problem 4c) at $T = 0$? Remember that the sum over k, $\sum_k$, can be replaced by $\int d\epsilon \mathcal{N}(\epsilon)$ with the density of states $\mathcal{N}(\epsilon)$ from Exercise 1.