LMU München
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Lehrstuhl für Theoretische Nanophysik
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4. Exercise Sheet TA1: Theoretical Solid State Physics

To be discussed on Friday, November 18, 2016.

Exercise 1: Sommerfeld expansion

Let us suppose that we have an integral of the form:

$$\int_{-\infty}^{\infty} d\epsilon\, H(\epsilon) f(\epsilon),$$

where the Fermi distribution is:

$$f(\epsilon) = \frac{1}{e^{(\epsilon-\mu)/k_B T} + 1},$$

and where $H(\epsilon)$ is a generic function that vanishes as $\epsilon \to -\infty$ and diverges no more rapidly than some power of ϵ as $\epsilon \to \infty$. Also we assume the $H(\epsilon)$ is smooth close to the chemical potential μ.

We want to derive the Sommerfeld expansion:

$$\int_{-\infty}^{\infty} d\epsilon\, H(\epsilon) f(\epsilon) = \int_{-\infty}^{\mu} d\epsilon\, H(\epsilon) + \sum_{n=1}^{\infty} (k_B T)^{2n}\, a_n \frac{d^{2n-1}}{d\epsilon^{2n-1}} H(\epsilon)|_{\epsilon=\mu}, \tag{1}$$

where the a_n are dimensionless numbers.

Proceed as follows:

a. Taking $K(E) = \int_{-\infty}^{\epsilon} d\epsilon'\, H(\epsilon')$, show that

$$\int_{-\infty}^{\infty} d\epsilon\, H(\epsilon) f(\epsilon) = \int_{-\infty}^{\infty} d\epsilon\, K(\epsilon) \left(-\frac{\partial f}{\partial \epsilon}\right).$$

b. Expand the function $K(\epsilon)$ in a Taylor series around $\epsilon = \mu$. Using that $\partial f/\partial\epsilon$ is an even function of ϵ, show that

$$\int_{-\infty}^{\infty} d\epsilon\, H(\epsilon) f(\epsilon) = \int_{-\infty}^{\mu} d\epsilon\, H(\epsilon) + \sum_{n=1}^{\infty} \int_{-\infty}^{\infty} d\epsilon\, \frac{(\epsilon-\mu)^{2n}}{(2n)!} \left(-\frac{\partial f}{\partial \epsilon}\right) \frac{d^{2n-1}}{d\epsilon^{2n-1}} H(\epsilon)|_{\epsilon=\mu}.$$

c. With the substitution $x = (\epsilon - \mu)/k_B T$ you should obtain the Sommerfeld expansion Eq. (1) and find an expression for the dimensionless coefficients a_n for all n.

Exercise 2: Free gas in 2D

We consider a gas of N free and independent electrons, in two dimension in a box of linear dimensions L_x and L_y.

a. What is the relationship between n and k_F in two dimension ?

b. Prove that in two dimension, the free electron density of states $g(\epsilon)$ is a constant independent of ϵ for $\epsilon \geq 0$ and for $\epsilon < 0$. Calculate the constants.

c. Show that, as $g(\epsilon)$ is constant, every term in the Sommerfeld expansion for n vanishes, except the $T = 0$ term. Consider that this expansion is exact, and deduce that $\mu = \epsilon_F$ at any temperature.

d. Using that $n = \int_{-\infty}^{\infty} d\epsilon\, g(\epsilon) f(\epsilon)$, deduce that when $g(\epsilon)$ is constant as in (c) then:

$$\epsilon_F = \mu + k_B T \ln\left(1 + e^{-\mu/k_B T}\right).$$

e. Using the last equation, estimate the amount by which μ differs from ϵ_F. Comment on the numerical significance of this 'failure' of the Sommerfeld expansion and on the mathematical reason for the failure.

Exercise 3: Geometrical structure factor

X-Rays scattered by a crystal show special patterns which can be used to infer the structure of the lattice. For certain sharply defined wavelengths and incident directions, intense peaks of scattered radiation can be observed. These peaks occur when rays scattered from each primitive cell interfere constructively. If the crystal structure is that of a monatomic lattice with an n-atom basis (n atoms placed at positions $\boldsymbol{d}_1, \ldots, \boldsymbol{d}_n$ within the primitive cell), then the intensity of the peaks will depend on the extent to which the rays scattered from these basis sites interfere with one another. The overall amplitude of a peak then contains the structure factor:

$$S_{\boldsymbol{K}} = \sum_{j=1}^{n} \mathrm{e}^{i\boldsymbol{K}\boldsymbol{d}_j}. \tag{2}$$

a. Show that the structure factor [Eq. (2)] for a monatomic hexagonal close-packed crystal structure can take on any of the six values $1 + \mathrm{e}^{in\frac{\pi}{3}}$, $n = 1, \ldots 6$, as $\boldsymbol{K}$ ranges through the points of the simple hexagonal reciprocal lattice.

b. Show that all reciprocal lattice points have nonvanishing structure factor in the plane perpendicular to the z-axis containing $\boldsymbol{K} = \boldsymbol{0}$.

c. Show that points of zero structure factor are found in alternating planes in the family of lattice planes perpendicular to the z-axis.

d. Show that in such a plane the point that is displaced from $\boldsymbol{K} = \boldsymbol{0}$ by a vector parallel to the z-axis has zero structure factor.

e. Show that the removal of all points of zero structure factor from such a plane reduces the triangular network of reciprocal lattice points to a honeycomb array.