https://www2.physik.uni-muenchen.de/lehre/vorlesungen/wise_24_25/TA1_theoretical_condensed_matter/index.html

Problem set 9

Problem 1 Mastering the Sommerfeld expansion

The Sommerfeld expansion is a helpful tool to approximate integrals over fermionic single-particle states that appear when evaluating thermodynamic quantities. The basic idea is to exploit the fact that the typical electronic energy scale, e.g., the hopping amplitude, is much smaller then any practically relevant temperature such that the Fermi-Dirac distribution is basically a step function with only very small, symmetric deviations in the vicinity of the Fermi energy $\varepsilon_F \equiv \mu$. We denote by $H_w(\varepsilon)$ a function of the single-particle energies ε such that

$$\int_{-\infty}^{\infty} \mathrm{d}\varepsilon\, H_w(\varepsilon) f_\beta(\varepsilon - \mu) = w\,, \tag{1}$$

where w is the thermodynamic quantity we want to compute (particle number, internal energy,...) and $f_\beta(z) = [\mathrm{e}^{z\beta} + 1]^{-1}$ is the Fermi-Dirac distribution.

(1.a) Show that the derivative of $f_\beta(z)$ is an even function.

(1.b) We now define the auxiliary function

$$G_w(\varepsilon) = \int_{-\infty}^{\varepsilon} \mathrm{d}z\, H_w(z)\,. \tag{2}$$

Assuming $H_w(\varepsilon \to \infty) = 0$ as well as $H_w(\varepsilon \to \infty) \sim \mathcal{O}(\varepsilon^k)$ for some $k \in \mathbb{N}$, show that

$$w = \int_{-\infty}^{\infty} \mathrm{d}\varepsilon\, G_w(\varepsilon) \left(-\frac{\mathrm{d}f_\beta}{\mathrm{d}\varepsilon}\right)\,. \tag{3}$$

Sketch the integrand and give a motivation, why it could be a good idea to evaluate the integral only near $\varepsilon = \mu$.

(1.c) Now we explicitly expand $G_w(\varepsilon)$ around μ such that

$$w = \sum_{k=0}^{\infty} \frac{1}{k!} \left.\frac{\mathrm{d}^k G_w}{\mathrm{d}\varepsilon^k}\right|_{\varepsilon=\mu} \int_{-\infty}^{\infty} \mathrm{d}\varepsilon\, (\varepsilon - \mu)^k \left(-\frac{\mathrm{d}f_\beta}{\mathrm{d}\varepsilon}\right)\,. \tag{4}$$

Show that this expansion can be simplified to

$$w = \sum_{k=0}^{\infty} a_k \left.\frac{\mathrm{d}^{2k} G_w}{\mathrm{d}\varepsilon^{2k}}\right|_{\varepsilon=\mu} (k_\mathrm{B}T)^{2k}\,, \quad a_k = \frac{1}{(2k)!} \int_{-\infty}^{\infty} \mathrm{d}z\, z^{2k} \frac{\mathrm{e}^z}{(\mathrm{e}^z + 1)^2}\,. \tag{5}$$

Problem 2 S and P-orbitals, tightly bound

Consider a one-dimensional chain of alternating atoms of type S and P. The S atoms should have a single atomic s-orbital with energy ϵ_s, and the P atoms should have p_x, p_y, and p_z orbitals of energy ϵ_p. The nearest-neighbor overlap integrals in the tight-binding approximation between an S atom and its right neighboring P atom shall be given by J_x, J_y, J_z.

(2.a) Determine the overlap integrals between the S atom and its left neighboring P atom and specify, which integrals must be zero by symmetry.

(2.b) Compute the band structure and sketch the energy levels. Why is there a total of four bands, and why are some of them dispersionless?