ETH
Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

Solid State Theory
Exercise 7

SS 08
Prof. M. Sigrist

Exercise 7.1 Van Leeuwen's Theorem

Proof the Van Leeuwen's theorem: There is no diamagnetism in classical physics.
Hint: For $H(p_1, \dots, p_N; q_1, \dots, q_N)$ the Hamiltonian of the N-particle system without a magnetic field, the Hamiltonian with applied magnetic field B is given by $H(p_1 - e/cA_1, \dots, p_N - e/cA_N; q_1, \dots, q_N)$, where $B = \nabla \times A$ and $A_i = A(q_i)$.
Hint: The magnetization can be calculated using

$$M = \left\langle -\frac{\partial H}{\partial B} \right\rangle = \frac{1}{\beta} \frac{\partial \log Z}{\partial B}, \tag{1}$$

with Z the partition function of the system in the magnetic field.

Exercise 7.2 Landau's Diamagnetism

Calculate the orbital part of the magnetization of the free electron gas in 3D in the limit $T \to 0$, $H \to 0$. In addition, show that the magnetic susceptibility at $T = 0$ and $H = 0$ is given by

$$\chi = 2/3 \chi_P, \tag{2}$$

where χ_P is the Pauli (spin-) susceptibility.
Hint: Calculate the free energy (eq. (3.104) in the script) at $T = 0$ in second order in H using the Euler-Mclaurin formula,

$$\sum_0^{n_0} f(n) = \int_{-1/2}^{n_0+1/2} f(n) dn - \frac{1}{24} \left[f'(n_0 + 1/2) - f'(-1/2) \right]. \tag{3}$$

Exercise 7.3 Peierls Instability in 1D

We consider a one-dimensional chain with nearest-neighbor hopping where the position of the electrons is not fixed. The Hamiltonian is thus given by a (renormalized) hopping and an elastic part:

$$\mathcal{H} = \sum_{i,s} (c^\dagger_{i+1,s} c_{i,s} + h.c.)(-t + \alpha \delta u_i) + \lambda \sum_i \frac{\delta u_i^2}{2} \tag{4}$$

where $\delta u_i = u_{i+1} - u_i$ and u_i is the displacement of the atom at site i from its equilibrium position. $\lambda > 0$ is a measure of the stiffness of the system and $\alpha > 0$ is the coupling constant.
In the following, we consider the half filled case (one electron per site) and make for δu_i the ansatz

$$\delta u_i = u_0 \cos(q r_i) \tag{5}$$

a) Calculate for $q = \pi$ the eigenenergies and the eigenstates of the system and the density of states.
Hint: Write the electronic part of the Hamiltonian in the Form

$$\mathcal{H} = \sum_{|k|<\pi/2,s} \vec{c}^{\dagger}_{ks} \mathcal{H}_k \vec{c}_{ks} \tag{6}$$

where $\vec{c}^{\dagger}_{ks} = (c^{\dagger}_{ks}, c^{\dagger}_{k+\pi s})$ and $\mathcal{H}_k$ is a 2×2 matrix which can be written in terms of Pauli matrices. The diagonalization is then just a rotation in the space of these matrices. Note that the sum now only runs over a reduced Brillouin zone, $k \in [-\frac{\pi}{2}, \frac{\pi}{2}]$.

b) Show that in this one-dimensional system, there is always a finite u_0 that minimizes the total energy.
Hint: Show it for large λ and small u_0 by using the elliptic integral of the second kind,

$$E(\varphi, k) = \int_0^{\varphi} \sqrt{1 - k^2 \sin^2 \alpha d\alpha} \tag{7}$$

and its series expansion

$$E(\frac{\pi}{2}, k') = 1 + \frac{1}{2}(\log \frac{4}{k'} - \frac{1}{2})k'^2 + O(k'^4) \tag{8}$$

where $k' = \sqrt{1 - k^2}$.

c) Show that the density of electrons per site, $\rho_i = \sum_s \langle c^{\dagger}_{is} c_{is} \rangle = 1$ for all i but the density per bond, $\tilde{\rho}_i = \sum_s \langle c^{\dagger}_{is} c_{i+1s} \rangle$ oscillates with position i. Discuss also the limits $\lambda \to 0$ and $\lambda \to \infty$ for $\alpha = t$.