Exercise-sheet 1 (May 9, 2017)

1 In-class exercises. Free phonons: a short tour

In this first session we will revisit the classical vibrations of a systems of ions within the harmonic approximation, and their quantization into phonons. As an example, we will consider the *jellium model* and determine its normal modes.

2 Homework - due date: May 16, 2017 (35 points).

2.1 Revisiting Debye's model of phonons (10 points).

Consider an elastic medium of volume V. The frequency associated to the $3N$ normal modes of a N-atom solid can be approximated by the lowest $3N$ normal frequencies of the elastic medium.

(a) Find the number of normal modes $g(\omega)d\omega$ for an elastic medium whose frequencies lie between ω and $d\omega$, assuming the system has periodic boundary conditions.

(b) In a uniform medium, the normal frequencies have no upper limit. In a real crystal however, the wavenumber propagation cannot exceed the reciprocal of the interparticle spacing. Hence, there exist a natural high frequency cutoff ω_D. Find ω_D from the condition

$$3N = \int_0^{\omega_D} g(\omega)d\omega, \tag{1}$$

and estimate the corresponding wavelength λ_D.

(c) Show the total energy of the system, defined as $E = \sum_i \hbar\omega_i \langle n_i \rangle$, with $\langle n_i \rangle$ the Bose function, can be written as

$$E = \alpha \int_0^{T_D/T} dx \frac{x^3}{e^x - 1}, \tag{2}$$

where $\alpha = \alpha(T)$ is to be determined and $kT_D \equiv \hbar\omega_D$.

(d) Find the leading terms of the total energy and specific heat in both, the high ($T \gg T_D$) and low ($T \ll T_D$) temperature expansion of Eq. (2). You may need to use $\zeta(4) = \frac{\pi^4}{90}$, with $\zeta(n)$ the Riemann zeta function.

2.2 Free electron Green's function (10 points).

Consider the free electron Hamiltonian

$$\hat{H} = \sum_{\boldsymbol{k}\sigma} \epsilon_{\boldsymbol{k}} \hat{c}^{\dagger}_{\boldsymbol{k}\sigma} \hat{c}_{\boldsymbol{k}\sigma}, \quad \epsilon_{\boldsymbol{k}} = \frac{k^2}{2m}, \tag{3}$$

where $\hat{c}_{\boldsymbol{k}\sigma}$ ($\hat{c}^{\dagger}_{\boldsymbol{k}\sigma}$) annihilates (creates) a σ-spin electron in a plane wave state $\boldsymbol{k}$.

The single particle Green's function is defined as the ground state expectation value of the *time-ordered product*

$$G^{(0)}(\boldsymbol{k}t) = -i\langle 0|T\hat{c}_{\boldsymbol{k}}(t)\hat{c}^{\dagger}_{\boldsymbol{k}}(0)|0\rangle, \tag{4}$$

where $|0\rangle$ labels the filled Fermi sea and $\hat{c}_{\mathbf{k}}(t)$ is a Heisenberg operator, with $\hat{c}_{\mathbf{k}}(t) = e^{i\hat{H}t}\hat{c}_{\mathbf{k}}e^{-i\hat{H}t}$. Furthermore, the time ordering operator is defined as

$$T\hat{a}(t)\hat{b}(t') = \theta(t-t')\hat{a}(t)\hat{b}(t') \pm \theta(t'-t)\hat{b}(t')\hat{a}(t), \tag{5}$$

where the upper (lower) sign refers to bosons (fermions) and $\theta(t)$ is the Heaviside step function.

(a) Use Heisenberg's equation of motion to find the explicit time dependence of $\hat{c}_{\boldsymbol{k}}$.

(b) Show

$$G^{(0)}(\boldsymbol{k}t) = -i\theta(t)(1-f_{\boldsymbol{k}})e^{-i\epsilon_{\boldsymbol{k}}t} + i\theta(-t)f_{\boldsymbol{k}}e^{-i\epsilon_{\boldsymbol{k}}t} \tag{6}$$

where $f_{\boldsymbol{k}}$ is the Fermi function.

(c) Show the time Fourier transform of Eq. (6) is given by

$$G^{(0)}(\boldsymbol{k}\omega) = \frac{1}{\omega - \epsilon_{\boldsymbol{k}} + i\eta_{\boldsymbol{k}}}, \tag{7}$$

where $\eta_{\boldsymbol{k}}$ is a positive (negative) infinitesimal for $\boldsymbol{k}$ greater (less) than the Fermi momentum k_F.

2.3 Free phonon Green's function (10 points).

Consider the free phonon Hamiltonian

$$\hat{H} = \sum_{\boldsymbol{q}} \Omega_{\boldsymbol{q}} \hat{a}^{\dagger}_{\boldsymbol{q}} \hat{a}_{\boldsymbol{q}}, \tag{8}$$

where $\hat{a}_{\boldsymbol{q}}$ ($\hat{a}^{\dagger}_{\boldsymbol{q}}$) annihilates (creates) a phonon with wave vector $\boldsymbol{q}$.

The phonon Green's function is defined as the ground state expectation value of the *time-ordered product*

$$D^{(0)}(\boldsymbol{q}t) = -i\langle 0|T\hat{A}_{\boldsymbol{q}}(t)\hat{A}^{\dagger}_{\boldsymbol{q}}(0)|0\rangle, \tag{9}$$

where $\hat{A}_{\boldsymbol{q}} = a_{\boldsymbol{q}} + a^{\dagger}_{-\boldsymbol{q}}$ and T is defined in Eq. (5). Note that the ground state for a system of free phonons is the empty state.

Show

$$D^{(0)}(\boldsymbol{q}\omega) = \frac{2\Omega_{\boldsymbol{q}}}{\omega^2 + \Omega^2_{\boldsymbol{q}} + i\delta}. \tag{10}$$

2.4 Matrix order parameter (5 points).

Consider the matrix order parameter

$$\Delta = (d_0\sigma_0 + \boldsymbol{d}\cdot\boldsymbol{\sigma})\, i\sigma^2, \tag{11}$$

where σ^0 is the 2×2 identity matrix, σ^i ($i = 1, 2, 3$) the Pauli matrices, and d_j ($j = 0, 1, 2, 3$) are complex numbers. Show the gauge-invariant matrix

$$\Delta\Delta^{\dagger} = (|d_0|^2 + |\boldsymbol{d}|^2)\,\sigma^0 + \boldsymbol{q}\cdot\boldsymbol{\sigma}, \tag{12}$$

where $\boldsymbol{q}$ is to be determined.