Condensed Matter Theory problem set 10

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Problem 26: Density of states of a linear chain

Consider the quantum version of the one-dimensional harmonic chain with the Hamiltonian $H = \sum_k \omega_k(a_k^\dagger a_k + 1/2)$ with bosonic operators a_k describing phonons with dispersion relation $\omega_k = \omega_0|\sin(ka/2)|$.

(a) Show that the specific heat C_V is given by

$$C_V = \frac{1}{2\pi}\frac{\partial}{\partial T}\int_{1.\mathrm{BZ}} dk \frac{\omega_k}{e^{\omega_k/(k_B T)} - 1}\,. \tag{1}$$

(b) Calculate the specific heat explicitly, using two simplifications: (a) linearize the dispersion relation, and (b) extend the integral bounds $\frac{1}{2\pi}\int_{1.\mathrm{BZ}} dk \to \frac{1}{2\pi}\int_{-\infty}^{\infty} dk$. Discuss whether the second simplification is valid at low temperatures.

(c) We introduce the density of states of the phonons as

$$g(\omega) = \int_{1.\mathrm{BZ}} \frac{dk}{2\pi}\delta(\omega - \omega_k)\,. \tag{2}$$

Show that the density of states for the linear harmonic chain is given by

$$g(\omega) = \frac{2}{\pi a\sqrt{\omega_-^2 - \omega^2}}. \tag{3}$$

Problem 27: Einstein phonons

If electrons scatter off phonons, their self-energy is given to leading order by

$$\Sigma(\boldsymbol{p}, i\epsilon_n) = -\frac{1}{\beta V}\sum_{\boldsymbol{q}, i\omega_m} \mathcal{G}_0(\boldsymbol{p}+\boldsymbol{q}, i\epsilon_n + i\omega_m)\, V_{\mathrm{ph}}(\boldsymbol{q}, i\omega_m). \tag{4}$$

The free fermionic Green function $\mathcal{G}_0(\boldsymbol{p}, i\epsilon_n) = (i\epsilon_n - \xi_{\boldsymbol{p}})^{-1}$ for electrons with dispersion relation $\xi_{\boldsymbol{p}} = \boldsymbol{p}^2/(2m) - \mu$, while the phonon-induced interaction can be written as

$$V_{\mathrm{ph}}(\boldsymbol{q}, i\omega_m) = M^2\left(\frac{1}{i\omega_m - \omega_{\boldsymbol{q}}} + \frac{1}{-i\omega_m - \omega_{\boldsymbol{q}}}\right) \tag{5}$$

for bosonic Matsubara frequencies ω_m and real electron-phonon coupling M.

(a) Show that the bosonic Matsubara sum over $i\omega_m$ leads to the expression

$$\Sigma(\boldsymbol{p}, i\epsilon_n) = M^2 \int \frac{d^3q}{(2\pi)^3} \left[\frac{b(\omega_{\boldsymbol{q}}) + f(\xi_{\boldsymbol{p}+\boldsymbol{q}})}{i\epsilon_n - \xi_{\boldsymbol{p}+\boldsymbol{q}} + \omega_{\boldsymbol{q}}} + \frac{b(\omega_{\boldsymbol{q}}) + 1 - f(\xi_{\boldsymbol{p}+\boldsymbol{q}})}{i\epsilon_n - \xi_{\boldsymbol{p}+\boldsymbol{q}} - \omega_{\boldsymbol{q}}} \right] \tag{6}$$

where $b(\omega)$ is the Bose and $f(\omega)$ the Fermi distribution.

(b) Consider specifically Einstein phonons with constant energy $\omega_{\boldsymbol{q}} = \omega_0 > 0$. Compute the momentum sum in the electronic self-energy at zero temperature $T = 0$ where the phonon occupation $b(\omega_0) = 0$ vanishes. Assume further a constant density of states at all energies, $g(\xi) = g(0)$ for $-\infty < \xi < \infty$. Derive the self-energy

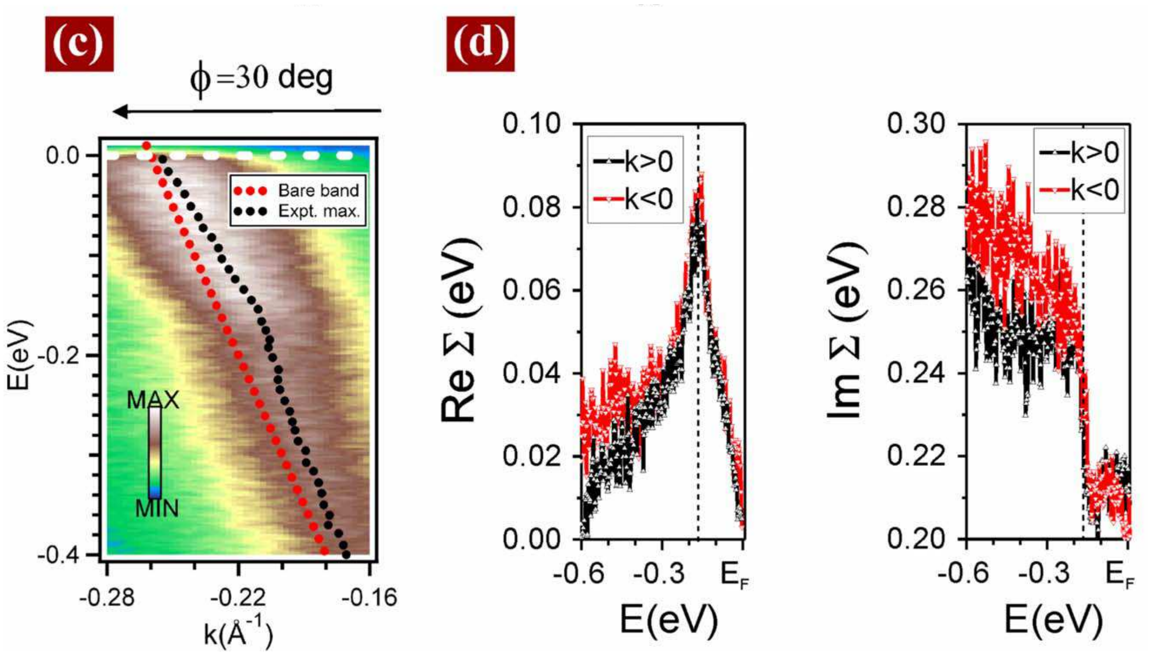
$$\Sigma(\boldsymbol{p}, i\epsilon_n) = \alpha \log \frac{\omega_0 - i\epsilon_n}{\omega_0 + i\epsilon_n} \tag{7}$$

where $\alpha = g(0)M^2$. Sketch the real and imaginary parts of the retarded self-energy $\Sigma^R(\boldsymbol{p}, \varepsilon) = \Sigma(\boldsymbol{p}, \varepsilon + i0)$.

(c) The full electronic Green function is given by the Dyson equation

$$G^R(\boldsymbol{p}, \varepsilon) = \frac{1}{\varepsilon + i0 - \xi_{\boldsymbol{p}} - \Sigma^R(\boldsymbol{p}, \varepsilon)} . \tag{8}$$

Plot the spectral function of the electrons as a function of p/k_F and ε/E_F with $\mu = E_F$, phonon frequency $\omega_0 = 0.1\,E_F$ and take for $i0$, e.g., $0.05i$. For $\alpha = 0$ this is the unperturbed parabolic dispersion relation of free fermions; which features appear in the presence of an electron-phonon interaction $\alpha = 0.1\,E_F$? Interpret the experimental spectral function of KC_8 shown below [ARPES data from A. Grünein et al., Physical Review B **79**, 205106 (2009)]; which kind of interaction could the electrons have in this material?



Problem 28: Cooper pairs

On top of a Fermi sea at $T = 0$, two electrons are added which attract each other but interact with the remaining electrons in the Fermi sea only via the Pauli principle, *i.e.*, they can only occupy states with $k > k_F$. The ground state of only these two electrons is a spatially symmetric spin singlet with zero total momentum and can be written as

$$|\psi_0\rangle = \sum_{k>k_F} g_{\boldsymbol{k}} c^\dagger_{\boldsymbol{k}\uparrow} c^\dagger_{-\boldsymbol{k}\downarrow} |0\rangle \,. \tag{9}$$

(a) Consider the Schrödinger equation $\mathcal{H}_{\text{BCS}}|\psi_0\rangle = E|\psi_0\rangle$ with the BCS Hamiltonian

$$\mathcal{H}_{\text{BCS}} = \sum_{\boldsymbol{k}\sigma} \epsilon_{\boldsymbol{k}} c^\dagger_{\boldsymbol{k}\sigma} c_{\boldsymbol{k}\sigma} + \frac{1}{V} \sum_{\boldsymbol{k},\boldsymbol{k}'>k_F} U_{\boldsymbol{k}\boldsymbol{k}'} c^\dagger_{\boldsymbol{k}\uparrow} c^\dagger_{-\boldsymbol{k}\downarrow} c_{-\boldsymbol{k}'\downarrow} c_{\boldsymbol{k}'\uparrow} \tag{10}$$

and the potential $U_{\boldsymbol{k}\boldsymbol{k}'}$ for scattering an electron pair with momenta $(\boldsymbol{k}', -\boldsymbol{k}')$ into a pair $(\boldsymbol{k}, -\boldsymbol{k})$. Show that this leads to the following equation for the energy eigenvalue E and the amplitudes $g_{\boldsymbol{k}}$:

$$(E - 2\epsilon_{\boldsymbol{k}}) g_{\boldsymbol{k}} = \frac{1}{V} \sum_{k'>k_F} U_{\boldsymbol{k}\boldsymbol{k}'} g_{\boldsymbol{k}'} \,. \tag{11}$$

If this equation has a solution for $E < 2E_F$ then there exists a bound state.

(b) Assume the attractive interaction to be constant in a shell around the Fermi surface,

$$U_{\boldsymbol{k}\boldsymbol{k}'} = \begin{cases} -g < 0, & E_F < \epsilon_{\boldsymbol{k}}, \epsilon_{\boldsymbol{k}'} < E_F + \omega_D \\ 0 & \text{otherwise.} \end{cases} \tag{12}$$

Derive the equation

$$\frac{1}{g} = \frac{1}{V} \sum_{k_c>k>k_F} \frac{1}{2\epsilon_{\boldsymbol{k}} - E} \tag{13}$$

where $\epsilon_{k_c} = E_F + \omega_D$. Then integrate the right-hand side in the approximation of a constant density of states $g_\sigma(\xi) \approx \nu_0$ near the Fermi surface. Solve this equation for $E \lesssim 2E_F$ in the limit of weak coupling $\nu_0 g \ll 1$.