Karlsruher Institut für Technologie
Institut für Theorie der Kondensierten Materie

Theorie der Kondensierten Materie II SS 2015

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Blatt 5
Lösungen

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1. Peierls Instability:

(a) *Calculate the polarization operator of free fermions (the so-called Lindhardt function) in three dimensions $d = 3$.*

First, we evaluate the frequency integral, which can be done in arbitrary dimensions. Noticing, that the integral is nonzero only if the two poles lie in different half-planes, we find

$$\Pi(\omega, q) = 2 \int \frac{d^d k}{(2\pi)^d} \frac{n_{\vec{k}} - n_{\vec{k}+\vec{q}}}{\omega + \xi_{\vec{k}} - \xi_{\vec{k}+\vec{q}} + i\delta(\mathrm{sign}\xi_{\vec{k}+\vec{q}} - \mathrm{sign}\xi_{\vec{k}})}$$

Now, there are two possibilities.

1. Often one is interested (as we will be in the next questions) in small momenta $q \ll k_F$. Then the exact form of the spectrum is not important, since one can use the expansion

$$\xi_{\vec{k}+\vec{q}} \approx \xi_{\vec{k}} + v_F q \cos\theta, \qquad \xi_{\vec{k}+\vec{q}} - \xi_{\vec{k}} \approx v_F q \cos\theta.$$

where θ is the angle between $\vec{k}$ and $\vec{q}$.

In this case (hereafter $\xi = \xi_{\vec{k}}$)

$$n_{\vec{k}} - n_{\vec{k}+\vec{q}} = \begin{cases} -1, & \cos\theta < 0;\ 0 < \xi < v_F q |\cos\theta|, \\ 1, & \cos\theta > 0;\ -v_F q \cos\theta < \xi < 0, \\ 0, & \text{otherwise.} \end{cases}$$

The integral over ξ is then trivial.

2. One can choose a spectrum and try to evaluate the momentum integral exactly. A common choice is the quadratic spectrum. For details of this calculation see the book by Giuliani, Vignale, "Quantum theory of the electron liquid", Chapter 4.4.

Here we continue with the first option and evaluate the polarization operator for small q. Integrating over ξ, we find (for the three-dimensional case)

$$\Pi(\omega, q) = \nu_0 \int_0^\pi \sin\theta d\theta \frac{v_F q \cos\theta}{\omega - v_F q \cos\theta + i\delta\ \mathrm{sign}\cos\theta},$$

where $\nu_0 = mk_F/(2\pi^2)$ is the "density of states". Denote $z = \cos\theta$. Then the remaining integral can be evaluated as

$$\Pi(\omega, q) = \nu_0 \int_{-1}^{1} \frac{x dx}{\frac{\omega}{v_F q} - x + i\delta\ \mathrm{sign}x} = -2\nu_0 \left[1 + \frac{\omega}{2v_F q} \ln\left|\frac{\omega - v_F q}{\omega + v_F q}\right| + \frac{i\pi}{2} \frac{|\omega|}{v_F q} \theta(v_F q - |\omega|)\right].$$

(b) *Use the Lindhard function and the phonon Dyson equation to calculate the change (often called the "renormalization") of the speed of sound due to electron-phonon interaction*

$$c^2 = c_0^2(1 - 2\zeta), \qquad \zeta = g^2\nu_0,$$

where g is the electron-phonon coupling constant and ν_0 is the electronic density of states (ζ is the dimensionless coupling constant in the problem).

The phonon spectrum can be found from

$$D^{-1}(\omega, q) = 0,$$

where the phonon Green's function $D(\omega, q)$ is given by the Dyson's equation (g is the electron-phonon coupling constant)

$$D^{-1}(\omega, q) = D_0^{-1}(\omega, q) - g^2\Pi(\omega, q).$$

The polarization operator was found in the previous question.

Since the osund velocity is much smaller than v_F, we are interested in the limit $\omega \ll v_F q$. In this limit, the polarization operator is given by

$$\Pi(\omega, q) \to -2\nu_0.$$

Therefore, the phonon Green's function is given by

$$D^{-1}(\omega, q) \approx \frac{\omega^2 - c_0^2 q^2}{c_0^2 q^2} + 2\zeta.$$

As a result, we find the phonon dispersion relation as

$$\omega = cq, \qquad c^2 = c_0^2(1 - 2\zeta).$$

(c) *Consider now the polarization operator in one dimension, $d = 1$. For large momenta $q \approx 2k_F$, the polarization operator exhibits a logarithmic singularity. Show that this leads to the phonon frequency becoming imaginary.*

In one dimension, the polarization operator is given by the same expression

$$\Pi(\omega, q) = 2\int \frac{dk}{2\pi} \frac{n_{\vec{k}} - n_{\vec{k}+\vec{q}}}{\omega + \xi_{\vec{k}} - \xi_{\vec{k}+\vec{q}} + i\delta(\mathrm{sign}\xi_{\vec{k}+\vec{q}} - \mathrm{sign}\xi_{\vec{k}})}$$

Here we're looking to evaluate the integral for arbitrary values of q. Assuming parabolic spectrum,

$$\xi_{\vec{k}} = \frac{k^2 - k_F^2}{2m}, \qquad \xi_{\vec{k}+\vec{q}} = \frac{k^2 - k_F^2}{2m} + \frac{kq}{m} + \frac{q^2}{2m}.$$

The integrand is nonzero when either (i) $\xi_{\vec{k}} > 0$, $\xi_{\vec{k}+\vec{q}} < 0$, or (ii) $\xi_{\vec{k}} < 0$, $\xi_{\vec{k}+\vec{q}} > 0$. Let us consider (for brevity) momenta q belonging to the interval $0 < q < 2k_F$. Then the above two cases can be realized of the momentum k is confined to the following intervals: (i) $-k_F - q < k < -k_F$, (ii) $k_F - q < k < k_F$.

Consequently,

$$\Pi(\omega, q) = -\frac{1}{\pi}\int\limits_{-k_F-q}^{-k_F} \frac{dk}{\omega - kq/m - q^2/(2m) - i\delta} + \frac{1}{\pi}\int\limits_{k_F-q}^{k_F} \frac{dk}{\omega - kq/m - q^2/(2m) + i\delta}.$$

The intergals can now be easily evaluated.

Consider now the static limit $\omega = 0$ with $q = 2k_F(1 - x/2)$, $x \ll 1$. The integral simplifies and we find

$$\Pi(\omega = 0, q = 2k_F - k_F x) \approx \frac{m}{\pi k_F} \ln \frac{x}{4}.$$

The result is diverging!

Consider now the phnon spectrum. Obtaining the phonon Green's function from the Dyson's equation, we find the following equation for the phonon spectrum near $q \approx 2k - F$:

$$\frac{\omega^2 - c_0^2 4k_F^2}{c_0^2 4k_F^2} + \frac{g^2 m}{\pi k_F} \ln \frac{k_F}{|q - 2k_F|} = 0.$$

Thus

$$\omega^2 = \omega_{2k_F}^2 \left(1 - \frac{g^2 m}{\pi k_F} \ln \frac{k_F}{|q - 2k_F|}\right).$$

If q is close enough to $2k_F$ then the second term exceeds the first and the phonon frequency becomes imaginary.

What does it mean? What happens to the system?

The true excitation frequency cannot be imaginary. The above result indicates that the system exhibits an instability and the perturbative approach is no longer valid.

Physically, we can argue, that since the instability develops near the wavevector $2k_F$, the lattice experiences a corresponding deformation, which has a period π/k_F. Sometimes this processis called "dimerization". The density in that state exhibits modulation with the same period. The transition to the dimerized state is called the Peierls transition.

If the lattice exhibits the periodic modulation, then the electrons see this as a periodic potential. In periodic potential electrons form bands and typically open gaps in the spectrum. This is illustrated in the next question.

(d) *In order to clarify the physics of the previous question, consider the one-dimensional model of electrons subjected to a periodic potential*

$$H = H_0 + V, \qquad V(x) = V(x + a),$$

where H_0 describes non-interacting electrons with the usual kinetic energy $p^2/2m$. Overall we assume the system to contain N ions, i.e. to have the length $L = Na$. We also assume periodic boundary conditions. Arrive at the same instability as in the previous question by making the following steps:

1. Consider fermions without the potential: find the normalized wave functions and the energy spectrum.

For free fermions on a chain of length $L = Na$ (where N is the number of lattice sites and a is the lattice spacing), the wavefunctions are given by the plane waves

$$|k\rangle^{(0)} = \frac{1}{\sqrt{L}} e^{ikx},$$

with the usual additional assumption of periodic boundary conditions that yields

$$e^{ikL} = 1 \quad \Rightarrow \quad k = \frac{2\pi n}{L},$$

n being an integer.
The energy spectrum (assuming the usual parabolic dispersion) is

$$H^{(0)}|k\rangle^{(0)} = E_k^{(0)}|k\rangle^{(0)}, \qquad E_k^{(0)} = \frac{k^2}{2m}.$$

2. Consider the situation where there are exactly $2N$ particles in the system. Find the allowed values of electronic momenta and the values of the Fermi momentum (do not forget the electronic spin).
For $2N$ particles with spin, precisely N orbital (or k) states must be occupied. At $T = 0$ this amounts to filling states with n up to $N/2$ (the slight subtleties here have to do with the exact boundary conditions and the exact number of sites, which in turn determine the allowed values of n. Here we disregard these details) or with momenta up to

$$k_F = \frac{\pi}{a}.$$

3. Find the Fourier components of the periodic potential. Determine the allowed values of the wave vector (i.e. those values of q for which $V_q \neq 0$). Justify, why one can disregard the $q = 0$ term.
The potential matrix elements are just the Fourier components

$${}^{(0)}\langle k'|V|k\rangle^{(0)} = \frac{1}{L}\int dx V(x) e^{i(k-k')x}.$$

Since $V(x + a) = V(x)$, the nonzero matrix elements correspond to

$$V_q \neq 0 \Rightarrow q = mK, \quad K = \frac{2\pi}{a},$$

where m is an integer.
The matrix element with $m = 0$ describes the uniform potential which can be disregarded.

4. Consider only the matrix elements V_q with the smallest values of $|q|$. Find the second-order perturbation theory correction to the fermionic spectrum.
Consider the two matrix elements V_q with the lowest values of q, corresponding to $m = \pm 1$:

$$V_q \to V_{-1} + V_1.$$

This way we replace a generic periodic potential with some particular function, which is however sufficient for our exercise.
The second-order perturbation theory then reads

$$E_k^{(2)} = \sum_{k' \neq k} \frac{\left| {}^{(0)}\langle k'|V|k\rangle^{(0)} \right|^2}{E_k^{(0)} - E_{k'}^{(0)}} = \frac{|V_K|^2}{E_k^{(0)} - E_{k+K}^{(0)}} + \frac{|V_{-K}|^2}{E_k^{(0)} - E_{k-K}^{(0)}}.$$

5. Show that the result might contain a singularity.

The free spectrum has a feature for $k = \pi/a$:

$$E^{(0)}_{\pi/a} = E^{(0)}_{\pi/a-K} = E^{(0)}_{-\pi/a}.$$

Then the standard perturbation theory is inapplicable and we have to use the "degenerate perturbation theory".

Again, depending on the precise boundary conditions these states might be not exactly degenerate, but any possible difference is small in the thermodynamic limit, which is why we disregard such details here.

6. Attempt to rectify the problem by focusing on the subspace of the electronic states that involves the two states giving the singularity. These two states have almost identical energy. Use the degenerate perturbation theory to find the spectrum in this subspace.

Consider now the subspace formed by the two states $|k\rangle^{(0)}$ and $|k-K\rangle^{(0)}$, for $k \approx \pi/a$. In this subspace, the Hamiltonian is given by the 2×2 matrix

$$H \to \begin{pmatrix} E^{(0)}_k & V^*_K \\ V_K & E^{(0)}_{k-K} \end{pmatrix}.$$

Diagonalizing this matrix yields the following eigenvalues

$$E_\pm = \frac{E^{(0)}_k + E^{(0)}_{k-K}}{2} \pm \sqrt{\left(\frac{E^{(0)}_k + E^{(0)}_{k-K}}{2}\right)^2 + |V_K|^2}.$$

Exactly for $k = \pi/a$ this lifts the above degeneracy and opens a gap in the spectrum

$$E_\pm = E^{(0)}_{\pi/a} \pm |V_K|.$$

What is the relation between the two calculations? What is the resulting ground state of the system?

Both calculation demonstrate that the system of electrons and phonons is unstable: taking into account electron-phonon interaction leads to a gap opening in the electronic spectrum and to appearance of imaginary phonon frequencies pointing towards deformation (or dimerization) of the original lattice. This is known as the Peierls instability. As a result of the gap opening, the system may undergo a phase transition - at low temperatures the gap prevents thermal excitations and thus the system shows no linear response to weak probes, i.e. behaves as an insulator. The exact nature of the ground state and the transition will be considered later in this course.