Theorie der Kondensierten Materie II SS 2015

Prof. Dr. A. Shnirman
Dr. B. Narozhny

Blatt 5
Besprechung 29.05.2015

---

1. Peierls Instability:

Consider electron-phonon interaction, described by the Frölich Hamiltonian

$$\hat{H}_{int} = g \int d^d r \hat{\psi}^\dagger(\vec{r})\hat{\psi}(\vec{r})\hat{\phi}(\vec{r}).$$

The free phonon Green's function is given by

$$D_0(\omega, \vec{k}) = \frac{\omega_0^2(\vec{k})}{\omega^2 - \omega_0^2(\vec{k}) + i0}.$$

Here $\omega_0(\vec{k})$ is the phonon spectrum (in the absence of any interactions). Consider the simplest case of a single acoustic branch with $\omega_0(\vec{k}) = ck$, $k < k_D$, where c is the speed of sound and k_D is the Debye wave-vector.

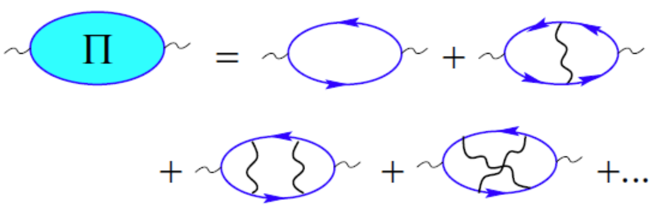
Electron-phonon interaction results in a modification of the phonon spectrum. Similarly to the case of electrons, we describe this effect by means of the Dyson's equation

$$D = D_0 + D_0 \Pi D.$$

The role of the phonon self-energy Π is played by the electronic "density-density" correlator also known as the "polarization operator":

$$\Pi = \langle T\hat{n}(\vec{r}, t)\hat{n}(\vec{r'}, t')\rangle.$$

In the presense of electron-phonon interaction the polarization operator is given by a series of diagrams shown in the Figure, as follows from the Frölich Hamiltonian.



In the simplest case we consider only the first term in the series, corresponding to the polarization operator of free fermions

$$\Pi(\omega, q) = -2i \int \frac{d^d k}{(2\pi)^d} \frac{d\epsilon}{2\pi} G_0(\epsilon, \vec{k}) G_0(\epsilon + \omega, \vec{k} + \vec{q}),$$

where the free-fermion Green's finction is

$$G_0(\epsilon, \vec{k}) = \frac{1}{\epsilon - \xi_{\vec{k}} + i0\mathrm{sign}\xi_{\vec{k}}}.$$

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

(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).

Hint: Recall that the speed of sound is much smaller than the Fermi velocity and focus on the limit $\omega \ll kv_F$.

(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.

What does it mean? What happens to the system?

(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.

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).

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.

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.

5. Show that the result might contain a singularity.

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.

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