Homework #6 — Phys625 — Spring 2002
Deadline: Tuesday, April 2, 2002.
Turn in homework in the class or put it in the box on the door of Phys 2314 by 10 a.m.

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Do not forget to write your name and the homework number!
Equation numbers with the period, like (3.25), refer to the equations of the textbook.
Equation numbers without period, like (5), refer to the equations of this homework.

Peierls Instability as Bose-Condensation of Phonons (start reading Ch. III)

1. *Peierls instability in 1D*

(a) [**6 points**]
For a 1D electron gas with the energy dispersion $\varepsilon(k) = k^2/2m - \mu$ calculate the density-density correlation function $\Pi(\Omega, q)$ given by Eq. (2) of HW 5 *not* assuming that Ω and q are small.
For $\Omega = 0$, sketch $\Pi(0, q)$ as a function of q. What happens when $q \to 2k_F$?

(b) [**2 points**]
Suppose a weak static periodic potential $U(q)$ with the wave vector q is applied to the system. It would create a static periodic perturbation of electron density $\delta n(q)$ with the same wave vector q. Considering $\delta n(q)$ as a linear response to $U(q)$, we can write

$$\delta n(q) = \chi(q)\, U(q). \tag{1}$$

Using Eq. (6) of HW 3, express the static response function $\chi(q)$ in terms of the density-density correlation function $\Pi(0, q)$.
How would you physically interpret the divergence of the response function $\chi(q)$ at $q \to 2k_F$?

(c) [**2 points**]
Using the diagram series shown in Problem 3 of HW 5, describe qualitatively what happens to the phonon frequency $\omega_{ph}(q)$ (renormalized by the electron-hole loops) when $q \to 2k_F$.

2. *Mean-field theory of 1D charge-density wave (CDW)*

Suppose phonons develop a static periodic deformation $u(x) = u_0 \cos(2k_F x + \theta)$ with the wave vector $2k_F$. The electron Hamiltonian becomes

$$\hat{H}_{el} = \int dx\, \left(\hat{\psi}^+(x) \frac{-\partial^2}{2m\, \partial x^2} \hat{\psi}(x) + U(x) \psi^+(x) \hat{\psi}(x) \right), \tag{2}$$

where the deformation potential is $U(x) = g\, \partial u/\partial x$, and g is the electron-phonon interaction constant.

Restricting consideration to the vicinity of the two Fermi points $\pm k_F$, we can represent the electron operator

$$\hat{\psi}(x) = \hat{\psi}_+(x)\, e^{ik_F x} + \hat{\psi}_-(x)\, e^{-ik_F x} \tag{3}$$

in terms of the operators $\psi_\pm$ that describe electron states with momenta close to $\pm k_F$, respectively.

(a) [**4 points**] Show that the electron Hamiltonian (2) can be approximately written as

$$\hat{H}_{el} = \int dx\, [-iv_F \hat{\psi}_+^+(x) \frac{\partial}{\partial x} \hat{\psi}_+(x) + iv_F \hat{\psi}_-^+(x) \frac{\partial}{\partial x} \psi_-(x)$$
$$+ \Delta \hat{\psi}_+^+(x) \psi_-(x) + \Delta^* \hat{\psi}_-^+(x) \psi_+(x)], \tag{4}$$

where $\Delta = gu_0k_Fe^{i\theta}$. Show that in momentum representation, the Hamiltonian (4) can be written in the matrix form

$$\hat{H}_{el} = \begin{pmatrix} v_Fk & \Delta \\ \Delta^* & -v_Fk \end{pmatrix}, \tag{5}$$

which operates of the 2-component vector $[\hat{\psi}_+(k), \hat{\psi}_-(k)]$.

(b) [**4 points**] Diagonalizing Hamiltonian (5) calculate the energy dispersion relation of electrons $E_k(\Delta)$ in the presence of Δ. Discuss which of the states are filled with electrons and which are empty.

(c) [**4 points**] Calculate the change δF_{el} of the total energy of electrons due to opening of the gap Δ:

$$\delta F_{el} = 2\int \frac{dk}{2\pi}\,[E_k(\Delta) - E_k(\Delta = 0)], \tag{6}$$

where the factor 2 comes from spin. If there is a logarithmic divergence, cut it off at the appropriate upper and lower limits.

(d) [**2 points**] Show that, classically, the Hamiltonian of phonons can be written as

$$H_{ph} = \int dx \left[\frac{1}{2M}\left(\frac{\partial u}{\partial t}\right)^2 + \frac{\rho s^2}{2}\left(\frac{\partial u}{\partial x}\right)^2\right], \tag{7}$$

where the first term is kinetic and the second is elastic energy, M is the atomic mass, ρ is the lattice mass density, and s is the sound velocity.

For the static deformation $u(x) = u_0\cos(2k_Fx + i\theta)$, express the phonon energy H_{ph} in terms of $\Delta = gu_0k_Fe^{i\theta}$.

(e) [**2 points**] Find the value Δ_0 that minimizes the total energy of the system $\delta F_{el} + H_{ph}$. Interpret physically why $\Delta_0 \neq 0$ and relate with the instability discussed in Problem 1.

The occurrence of spontaneous lattice deformation with the wave vector $2k_F$ is called the Peierls instability or the charge-density wave. It can be viewed as Bose-condensation of phonons with the wave vector $2k_F$. The mathematical description of this phenomenon is very similar to the BCS theory of superconductivity.

3. [**4 points**] *Bose-condensation of noninteracting bosons*

Consider noninteracting Bose particles in 3D with the parabolic dispersion law $\varepsilon(p) = p^2/2m$ and concentration n. Using the Bose distribution function

$$f(\varepsilon) = \frac{1}{e^{(\varepsilon-\mu)/T} - 1}, \tag{8}$$

determine the temperature of Bose condensation, which is the temperature where the population of the lowest energy state with momentum $p = 0$ becomes macroscopic.

Do you expect Bose-condensation of noninteracting Bose particles with the parabolic dispersion law in 2D and 1D?