Technische Universität Berlin
Institut für Theoretische Physik
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Exercises: Dr. Christian Carbogno, Henrik Kowalski et al.

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Theoretical Material Science: Exercise Sheet 12

Please hand in solutions by: Tuesday, July 18, start of the exercise class

Exercise 26 (8 additional points): *Cooper pairing*

The wavefunction for electron states in the superconducting phase is qualitatively different from that of the ordinary phase and the electrons' behaviour is determined by strong pair correlations. In this exercise, we will try to understand the qualitative nature of the pairing mechanism that was first discussed by Leon Cooper and is essential to the BCS formalism.[1]

We begin with two electrons in planewave states in a box of volume V with periodic boundary conditions as usual. By allowing an attractive interaction between the electrons, a bound state with pair wavefunction $\psi_{\rm pair}$ can form that we expand in the product states of the single electrons with some function χ describing the pairing amplitude, so that

$$\psi_{\rm pair}(\mathbf{r}_1, \mathbf{r}_2) = \sum_{\mathbf{k}_1\mathbf{k}_2} \chi(\mathbf{k}_1, \mathbf{k}_2)\ \mathrm{e}^{\mathrm{i}\mathbf{k}_1\cdot\mathbf{r}_1}\mathrm{e}^{\mathrm{i}\mathbf{k}_2\cdot\mathbf{r}_2}\ . \tag{1}$$

The pairing amplitude χ must not be confused with the spin function that is sometimes denoted by χ as well.

a) Show that after changing to center of mass and relative momentum coordinates

$$\mathbf{K} = \mathbf{k}_1 + \mathbf{k}_2\ , \qquad \mathbf{k} = \frac{\mathbf{k}_1 - \mathbf{k}_2}{2}\ , \tag{2}$$

$$\mathbf{R} = \frac{\mathbf{r}_1 + \mathbf{r}_2}{2}\ , \qquad \mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2, \tag{3}$$

and using translational invariance, it is sufficient to consider the pair wavefunction

$$\psi_{\rm pair}(\mathbf{r}_1 - \mathbf{r}_2) = \sum_{\mathbf{k}} \chi(\mathbf{k})\ \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot(\mathbf{r}_1-\mathbf{r}_2)} \tag{4}$$

in the following. Why is it beneficial to choose $\mathbf{K} = 0$? (*Hint:* We want to minimize energy.)

In momentum representation, the Schrödinger equation for the pairing amplitude χ has the form

$$\left(E - 2\frac{\hbar^2 k^2}{2m}\right)\chi(\mathbf{k}) = \sum_{\mathbf{k}'\neq\mathbf{k}} V(\mathbf{k}, \mathbf{k}')\chi(\mathbf{k}')\ . \tag{5}$$

We assume that the two electrons interact in the presence of a degenerate free electron gas whose existence is felt only via the exclusion principle: electron states with $k < k_{\rm F}$ are forbidden for both of the two electrons. This gives rise to the constraint

$$\chi(\mathbf{k}) = 0 \quad \text{for} \quad k < k_{\rm F}\ . \tag{6}$$

We take the interaction of the pair to have a simple attractive form in a thin shell of thickness $\hbar\omega_{\rm D}$ around the Fermi level, where $\omega_{\rm D}$ is the phononic Debye frequency,

$$V(\mathbf{k}_1, \mathbf{k}_2) = \begin{cases} -g\ , & \epsilon_{\rm F} < \frac{\hbar^2 k_i^2}{2m} \leq \epsilon_{\rm F} + \hbar\omega_{\rm D} \\ 0\ , & \text{otherwise} \end{cases}\ , \tag{7}$$

with $i = 1, 2$. The origin of the attractive interaction lies in the electron-phonon coupling, hence the energy scale $\hbar\omega_{\rm D}$. We search for a bound-state solution to the Schrödinger equation (5) consistent with constraint (6).

b) Show that a solution to Eq. (5) exists, provided that

$$1 = g\int_{\epsilon_{\rm F}}^{\epsilon_{\rm F}+\hbar\omega_{\rm D}} \frac{\rho(\epsilon)}{2\epsilon - E}\ \mathrm{d}\epsilon \tag{8}$$

is satisfiable, where $\rho(\epsilon)$ is the density of one-electron levels per unit volume for a given spin.

[1] L. N. Cooper, "Bound Electron Pairs in a Degenerate Fermi Gas", *Phys. Rev.* **104** (1956), 1189

c) We define the binding energy Δ as the energy gain due to pair formation,

$$\Delta = 2\epsilon_{\mathrm{F}} - E \ . \tag{9}$$

Assuming that $\rho(\epsilon)$ differs only marginally from $\rho(\epsilon_{\mathrm{F}}) \equiv \rho_{\mathrm{F}}$ in the range $\epsilon_{\mathrm{F}} < \epsilon < \epsilon_{\mathrm{F}} + \hbar\omega_{\mathrm{D}}$, show that the binding energy is given by

$$\Delta = 2\hbar\omega_{\mathrm{D}} \frac{\mathrm{e}^{-\frac{2}{g\rho_{\mathrm{F}}}}}{1 - \mathrm{e}^{-\frac{2}{g\rho_{\mathrm{F}}}}} \ , \tag{10}$$

and derive the *weak coupling limit* for $g\rho_{\mathrm{F}} \ll 1$.

d) What are the conditions for Eq. (8) or (10) respectively to yield solutions with a positive definite energy gain Δ? What is the smallest possible coupling strength g in this case? Why is the exclusion principle crucial for this result? (*Hint:* the exclusion principle is responsible for the existence of a low energy cutoff ϵ_{F}.)

Exercise 27 (8 additional points): *BCS Theory*
To further approach the problem of superconductivity, we will discuss the famous BCS Hamiltonian that was introduced by Bardeen, Cooper and Schrieffer in 1957,[2]

$$H^{\mathrm{BCS}} = \sum_{\mathbf{k}} \xi_{\mathbf{k}}\, c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \sum_{\mathbf{k}\mathbf{k}'} V(\mathbf{k},\mathbf{k}')\, c^{\dagger}_{\mathbf{k}\uparrow} c^{\dagger}_{-\mathbf{k}\downarrow} c_{-\mathbf{k}'\downarrow} c_{\mathbf{k}'\uparrow} \ , \tag{11}$$

with electron creation and annihilation operators $c, c^{\dagger}$ that obey the usual fermionic anti-commutation relations $\{c_i, c^{\dagger}_j\} = \delta_{i,j}$, and the same type of interaction $V(\mathbf{k},\mathbf{k}')$ as given in Eq. (7).

We have seen in the previous exercise that an attractive interaction between electrons of this form can lead to the formation of bound states, so called Cooper pairs. These Cooper pairs become manifest in the non-vanishing expectation values

$$\langle c^{\dagger}_{\mathbf{k}\uparrow} c^{\dagger}_{-\mathbf{k}\downarrow}\rangle,\ \langle c_{-\mathbf{k}'\downarrow} c_{\mathbf{k}'\uparrow}\rangle \neq 0 \ ,$$

which are zero in the normal state (why?).

a) *Mean field decoupling*
Perform a mean field decoupling of the Hamiltonian (11) by expanding the operator products in the vicinity of their mean values,

$$cc = \langle cc\rangle + (cc - \langle cc\rangle) \,,$$

and neglecting terms to second order in the fluctuations $\delta = (cc - \langle cc\rangle)$. Use the shorthand

$$\Delta_{\mathbf{k}} \equiv - \sum_{\mathbf{k}_2} V(\mathbf{k},\mathbf{k}') \langle c_{-\mathbf{k}'\downarrow} c_{\mathbf{k}'\uparrow}\rangle \ .$$

b) *Dispersion of the superconducting state*
Show that the mean field Hamiltonian of task a) can be diagonalized by a transformation

$$\begin{aligned} c_{\mathbf{k}\uparrow} &= u_k b_{\mathbf{k}\uparrow} \ \ + v_k b^{\dagger}_{-\mathbf{k}\downarrow} \ , \\ c_{-\mathbf{k}\downarrow} &= u_k b_{-\mathbf{k}\downarrow} - v_k b^{\dagger}_{\mathbf{k}\uparrow} \ \ , \end{aligned} \tag{12}$$

with real u_k, v_k that fulfill $u_k^2 + v_k^2 = 1$. Alternatively, represent the Hamiltonian as a matrix product in the fermionic operators $(c^{\dagger}_{\mathbf{k}\uparrow}, c_{-\mathbf{k}\downarrow})$ and diagonalize the corresponding matrix. Either way, show that the mean field Hamiltonian can be written in the form

$$H^{\mathrm{MF}} = \sum_{\mathbf{k}\sigma} \tilde{\epsilon}_{\mathbf{k}}\, b^{\dagger}_{\mathbf{k}\sigma} b_{\mathbf{k}\sigma} + \mathrm{const.}, \tag{13}$$

and express the dispersion $\tilde{\epsilon}_{\mathbf{k}}$ of the SC state in terms of the electronic dispersion $\xi_{\mathbf{k}}$ and gap function $\Delta_{\mathbf{k}}$. Make a qualitative sketch of $\tilde{\epsilon}_{\mathbf{k}}$ and its associated density of states, assuming that $\Delta_{\mathbf{k}} = \Delta = \mathrm{const}$, $\xi_{\mathbf{k}} = \frac{\hbar^2 k^2}{2m} - \epsilon_{\mathrm{F}}$, and $\Delta \ll \epsilon_{\mathrm{F}}$.

[2] J. Bardeen, L. N. Cooper, and J. R. Schrieffer, "Theory of Superconductivity", *Phys. Rev.* **108** (1957), 1175.