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Exercise to the Lecture

Superconductivity and Low Temperature Physics I
WS 2022/2023

4   Microscopic Theory

4.7   The Bogoliubov Quasiparticles – Dispersion Relation

Exercise:

The energy spectrum of the Bogoliubov quasiparticles is given by

$$E_{\mathbf{k}} \;=\; \sqrt{\xi_{\mathbf{k}}^2 + \Delta_{\mathbf{k}}^2}\,,$$

where $\xi_{\mathbf{k}} = \varepsilon_{\mathbf{k}} - \mu = (\hbar^2 k^2/2m) - (\hbar^2 k_{\mathrm{F}}^2/2m)$ is the normal electron energy relative to the chemical potential ($\mu = \hbar^2 k_{\mathrm{F}}^2/2m$ at $T = 0$). We consider the dispersion of the Bogoliubov quasiparticles for an isotropic gap $\Delta_{\mathbf{k}} = \Delta$.

(a) Discuss the energy spectrum of the Bogoliubov quasiparticles close to the Fermi wave number k_{F}.

(b) How does the effective mass m_{qp} of the Bogoliubov quasiparticles compare to that of free electrons?

(c) Discuss the group velocity

$$v_{\mathbf{k}} \;=\; \frac{1}{\hbar}\frac{\partial E_{\mathbf{k}}}{\partial k}$$

close to the Fermi wave number.

Solution:

(a) Close the the Fermi wave number we can use the approximation

$$\xi_{\mathbf{k}} = \frac{\hbar^2 k^2}{2m} - \frac{\hbar^2 k_F^2}{2m} = \frac{\hbar^2 (k_F + \delta k)^2}{2m} - \frac{\hbar^2 k_F^2}{2m}, \tag{1}$$

where $\delta k = k - k_F$ is the deviation from the Fermi wave number. Considering only the regime close to k_F we can neglect quadratic terms in δk and obtain

$$\xi_{\mathbf{k}} = \frac{\hbar^2 k_F \delta k}{m} = v_F \hbar \delta k. \tag{2}$$

Here, $v_F = \hbar k_F / m$ is the Fermi velocity. With (2) the expression for the quasiparticle energy reads as

$$\begin{aligned} E_{\mathbf{k}} &= \sqrt{\xi_{\mathbf{k}}^2 + \Delta^2} = \sqrt{v_F^2 \hbar^2 \delta k^2 + \Delta^2} \\ &= \Delta \sqrt{1 + \frac{v_F^2}{\Delta^2} \hbar^2 \delta k^2}. \end{aligned} \tag{3}$$

For small δk we can use the approximation $\sqrt{1+x} \simeq 1 + \frac{1}{2}x$ and obtain

$$E_{\mathbf{k}} \simeq \Delta \left(1 + \frac{v_F^2}{2\Delta^2} \hbar^2 \delta k^2 \right) = \Delta + \frac{\hbar^2 (k - k_F)^2}{2(\Delta/v_F^2)}. \tag{4}$$

This dispersion relation of the Bogoliubov quasiparticles is shown in Fig. 1 together with that of electrons and holes in a normal metal. It is similar to that of rotons in superfluid ^{4}He. We see that close to the Fermi momentum $\hbar k_F$ the Bogoliubov quasiparticles have a parabolic dispersion. Note that for the energy of normal electrons and holes relative to the chemical potential we have $\xi_{\mathbf{k},h} = -\xi_{\mathbf{k},e}$. The reason is that in order to generate a hole we have to remove an electron. Since removing an electron means to bring it to the chemical potential, we have $\xi_{\mathbf{k},h} = \mu - \varepsilon_{\mathbf{k},e} = -\xi_{\mathbf{k},e}$, since $\varepsilon_{\mathbf{k},e} = \mu + \xi_{\mathbf{k},e}$.

(b) The effective mass of the Bogoliubov quasiparticles is given by the curvature of their dispersion relation (4). We find

$$m_{\mathrm{qp}} = \left(\frac{1}{\hbar^2} \frac{\partial^2 E_{\mathbf{k}}}{\partial k^2} \right)^{-1} = \frac{\Delta}{v_F^2}. \tag{5}$$

To compare this effective mass with the free electron mass m we can rewrite (5) and obtain the reduced effective mass

$$\frac{m_{\mathrm{qp}}}{m} = \frac{\Delta}{mv_F^2} = \frac{\Delta}{2E_F}, \tag{6}$$

where $E_F = \frac{1}{2}mv_F^2$ is the Fermi energy. Typically, $\Delta/E_F \sim 10^{-4} - 10^{-3}$ for metallic superconductors. Therefore, the effective mass of the Bogoliubov quasiparticles is orders of magnitude smaller than the free electron mass.
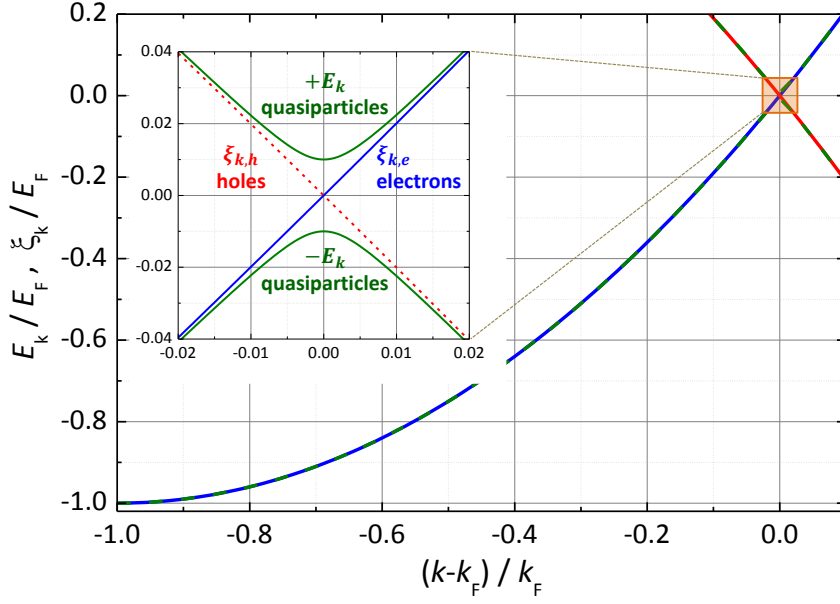
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Figure 1: Energy dispersion of Bogoliubov quasiparticles (olive) close to the Fermi momentum calculated for $\Delta/E_F = 0.01$. For comparison, the energy dispersion $\xi_{\mathbf{k},e}$ of free electrons (blue) and holes $\xi_{\mathbf{k},h} = -\xi_{\mathbf{k},e}$ (red) is also plotted. Due to the small value of Δ/E_F differences are seen only in the regime very close to k_F shown in the inset.

(c) We can use eqs. (2) to (4) to derive the group velocity

$$
\begin{aligned}
v_{\mathbf{k}} &= \frac{1}{\hbar}\frac{\partial E_{\mathbf{k}}}{\partial k} = \frac{1}{2\hbar}\frac{2\xi_{\mathbf{k}}}{E_{\mathbf{k}}}\hbar v_F = v_F \frac{\xi_{\mathbf{k}}}{E_{\mathbf{k}}} \\
&= v_F \frac{v_F \hbar(k-k_F)}{\Delta + \frac{\hbar^2(k-k_F)^2}{2m_{qp}}} = \frac{\hbar(k-k_F)}{\frac{\Delta}{v_F^2} + \frac{\hbar^2(k-k_F)^2}{2m_{qp}v_F^2}} .
\end{aligned}
\tag{7}
$$

Considering only the regime close to the Fermi momentum we can neglect terms of order $\mathcal{O}\left([k-k_F]^2\right)$. In this approximation the group velocity is given by

$$
v_{\mathbf{k}} = \frac{\hbar(k-k_F)}{m_{qp}} + \mathcal{O}\left([k-k_F]^2\right) \simeq \frac{\hbar(k-k_F)}{m_{qp}} .
\tag{8}
$$

As already expected from Fig. 1 we obtain a vanishing group velocity at $k = k_F$ due to the vanishing slope of the dispersion curve $E_{\mathbf{k}}(k-k_F)$. This can be understood by recalling that for $k = k_F$ the Bogoliubov quasiparticles consist of an equal superposition $(|u_{\mathbf{k}}^2| = |v_{\mathbf{k}}^2| = 1/2)$ of an electron and a hole with opposite momentum. For $k < k_F$, they are more hole-like with negative group velocity. For $k > k_F$, they are more electron-like with positive group velocity.

The quasiparticle dispersion curve approaches that of the free electrons and holes moving away from k_F and its maximum slope is given by the Fermi velocity. Then, we can use eq. (8) to estimate the maximum range $(k-k_F)$ in which the Bogoliubov quasiparticles live. We obtain

$$
\delta k = k - k_F \simeq \frac{m_{qp}v_F}{\hbar} = \frac{\Delta}{\hbar v_F} .
\tag{9}
$$

Using the uncertainty relation $\delta k \cdot \delta x \geq 1$, we can estimate the spatial range of the Bogoliubov quasiparticles to

$$
\delta x \simeq \frac{1}{\delta k} = \frac{\hbar v_F}{\Delta} .
\tag{10}
$$

This estimate is close to the BCS coherence length $\xi_0 = \hbar v_F/\pi\Delta$. Obviously, the Bogoliubov quasiparticles are superpositions of electrons and holes living in a volume $\sim \xi_0^3$.

4.8 Spin Susceptibility of BCS Superconductors

Exercise:

The spin polarization of the electrons in a normal metal is defined as $\delta n = \delta N / V = n_\uparrow - n_\downarrow$, i.e., by the difference in the density of spin-up and spin-down electrons. In a spin singlet superconductor, the condensate has vanishing total spin. Therefore, in order to evaluate δn we only have to consider the difference δn for the thermal excitations out of the superconducting ground state, the so-called Bogoliubov quasiparticles. This difference can be expressed in terms of a shifted Fermi-Dirac distribution as

$$\delta N = \sum_{\mathbf{k}\sigma} \sigma\, \delta f_{\mathbf{k}\sigma}^{\text{loc}}, \qquad \delta f_{\mathbf{k}\sigma}^{\text{loc}} = f(E_\mathbf{k} + \delta E_{\mathbf{k}\sigma}) - f_\mathbf{k}^0$$

$$f(E_\mathbf{k}) = \frac{1}{e^{E_\mathbf{k}/k_\text{B}T} + 1}, \qquad E_\mathbf{k} = \sqrt{\xi_\mathbf{k}^2 + \Delta^2} \ .$$

Here, Δ is the energy gap (for simplicity we assume an isotropic energy gap $\Delta_\mathbf{k} = \Delta$), $\sigma = \pm 1$ and $\delta E_{\mathbf{k}\sigma} = -\sigma \mu_\text{B} \mu_0 H_{\text{ext}}$ the Zeeman energy due to an external magnetic field. Show that the modification of the Pauli spin susceptibility χ_P of a normal metal has the following form in the superconducting state:

$$\chi(T) = \chi_\text{P} Y(T) \quad \text{with} \quad Y(T) = \int_0^\infty \frac{dx}{\cosh^2 \sqrt{x^2 + \left(\frac{\Delta(T)}{2k_\text{B}T}\right)^2}} \ .$$

Here, $Y(T)$ is the so-called Yosida function.

Solution:

Since the energy shift $\delta E_{\mathbf{k}\sigma} = -\sigma \mu_\text{B} \mu_0 H_{\text{ext}}$ due to the applied magnetic field is small, we can do a Taylor expansion of the Fermi-Dirac distribution for the Bogoliubov quasiparticles $f(E_\mathbf{k} + \delta E_{\mathbf{k}\sigma})$ and keep only the leading term in $\delta E_{\mathbf{k}\sigma}$:

$$f(E_\mathbf{k} + \delta E_{\mathbf{k}\sigma}) = f_\mathbf{k}^0 + \frac{\partial f_\mathbf{k}^0}{\partial E_\mathbf{k}} \delta E_{\mathbf{k}\sigma} = f_\mathbf{k}^0 + \left(-\frac{\partial f_\mathbf{k}^0}{\partial E_\mathbf{k}}\right) \sigma \mu_\text{B} \mu_0 H_{\text{ext}} \ . \tag{1}$$

The deviation from local equilibrium, $f(E_\mathbf{k} + \delta E_{\mathbf{k}\sigma}) - f_\mathbf{k}^0$, then reads as

$$\delta f_{\mathbf{k}\sigma}^{\text{loc}} = \left(-\frac{\partial f_\mathbf{k}^0}{\partial E_\mathbf{k}}\right) \sigma \mu_\text{B} \mu_0 H_{\text{ext}} \tag{2}$$

and we obtain the spin polarization $\delta n = \delta N / V$ to

$$\delta n = \frac{1}{V}\sum_{\mathbf{k}\sigma} \sigma \delta f_{\mathbf{k}\sigma}^{\text{loc}} = \frac{1}{V}\sum_{\mathbf{k}\sigma} \sigma \left(-\frac{\partial f_\mathbf{k}^0}{\partial E_\mathbf{k}}\right) \sigma \mu_\text{B} \mu_0 H_{\text{ext}}$$

$$= \frac{\mu_\text{B}\mu_0 H_{\text{ext}}}{V} \sum_{\mathbf{k}\sigma} \left(-\frac{\partial f_\mathbf{k}^0}{\partial E_\mathbf{k}}\right) \ . \tag{3}$$

With this result the magnetization can be expressed as

$$
M = \mu_B \delta n = \frac{\mu_B^2 \mu_0 H_{\text{ext}}}{V} \sum_{\mathbf{k}\sigma} \left(-\frac{\partial f_{\mathbf{k}}^0}{\partial E_{\mathbf{k}}} \right) \ . \tag{4}
$$

With $M = \chi(T) H_{\text{ext}}$ we obtain

$$
\chi(T) = \frac{\mu_0 \mu_B^2}{V} \sum_{\mathbf{k}\sigma} \left(-\frac{\partial f_{\mathbf{k}}^0}{\partial E_{\mathbf{k}}} \right) \ . \tag{5}
$$

To derive an analytical expression for $\chi(T)$ we have to convert the summation into an integration in k- and finally in energy space. With $Z(k)d^3k = D(E_{\mathbf{k}})dE_{\mathbf{k}} = D(\xi_{\mathbf{k}})d\xi_{\mathbf{k}}$ (conservation of states) we obtain

$$
\frac{\chi(T)}{\mu_0 \mu_B^2} = \frac{1}{V} \int_0^{\infty} d^3k \, Z(k) \left(-\frac{\partial f_{\mathbf{k}}^0}{\partial E_{\mathbf{k}}} \right) = \frac{1}{V} \int_0^{\infty} dE_{\mathbf{k}} \, D(E_{\mathbf{k}}) \left(-\frac{\partial f_{\mathbf{k}}^0}{\partial E_{\mathbf{k}}} \right)
$$

$$
= \frac{1}{V} \int_{\mu}^{\infty} d\xi_{\mathbf{k}} \, D(\mu + \xi_{\mathbf{k}}) \left(-\frac{\partial f_{\mathbf{k}}^0}{\partial E_{\mathbf{k}}} \right) \ . \tag{6}
$$

Here, $Z(k)$ and $D(\xi_{\mathbf{k}})$ are the density of states in k- and energy space for both spin directions and $\xi_{\mathbf{k}} = \varepsilon_{\mathbf{k}} - \mu = (\hbar^2 k^2 / 2m) - \mu$ is the energy relative to the chemical potential. Since the function $\partial f_{\mathbf{k}}^0 / \partial E_{\mathbf{k}}$ is finite only in a narrow energy interval $\sim k_B T$ around the chemical potential μ, we can use $D(\mu + \xi_{\mathbf{k}}) \simeq D(E_F) = const$ and obtain

$$
\frac{\chi(T)}{\mu_0 \mu_B^2} = \frac{D(E_F)}{V} \int_{-\mu}^{\infty} d\xi_{\mathbf{k}} \left(-\frac{\partial f_{\mathbf{k}}^0}{\partial E_{\mathbf{k}}} \right) = \frac{D(E_F)}{V} \frac{1}{4k_B T} \int_{-\mu}^{\infty} \frac{d\xi_{\mathbf{k}}}{\cosh^2 \frac{E_{\mathbf{k}}}{2k_B T}} \tag{7}
$$

With the substitution $x = \xi_{\mathbf{k}} / 2k_B T$ and $N_F = D(E_F)/V$ we finally obtain

$$
\chi(T) = \underbrace{\mu_0 \mu_B^2 N_F}_{=\chi_P} \frac{1}{2} \underbrace{\int_{-\infty}^{\infty} \frac{dx}{\cosh^2 \sqrt{x^2 + \left(\frac{\Delta(T)}{2k_B T} \right)^2}}}_{=2Y(T)} \ . \tag{8}
$$

Here we have set the lower integration limit to $-\infty$ since typically $\mu / 2k_B T \gg 1$ for metals.

We see that the spin susceptibility $\chi(T)$ of a BCS superconductor is given by the product of the temperature independent normal state Paul spin susceptibility χ_P and the Yosida function $Y(T)$:

$$
\chi_{\text{BCS}}(T) = \mu_0 \mu_B^2 N_F \cdot Y(T) = \chi_P \cdot Y(T) \tag{9}
$$

$$
\text{with } Y(T) = \int_0^{\infty} \frac{dx}{\cosh^2 \sqrt{x^2 + \left(\frac{\Delta(T)}{2k_B T} \right)^2}} \ . \tag{10}
$$

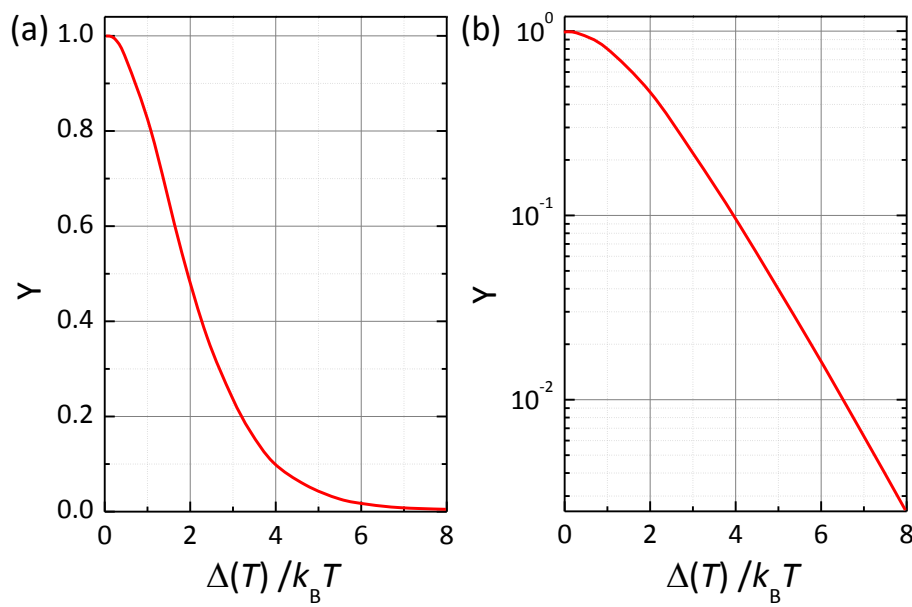The Yosida function is plotted in Fig. 2 as a function of $\Delta(T)/k_B T$.

Figure 2: Yosida function plotted versus $\Delta(T)/k_{\mathrm{B}}T$ using (a) a linear and (b) logarithmic scale.