S7.B. Momentum Condensation in an Interacting Fermi Fluid

This section is an introduction to the BCS theory for superconductivity.

The defining property of super fluids & superconductors, namely, frictionless flows, can be explained by assuming that the "super" states are macroscopic quantum states, i.e., all carriers in the system are in a single coherent quantum state. One way to achieve this is via the Bose-Einstein condensation, which is indeed the case for the super fluids, provided the inter-particle interactions are taken into account. However, the carriers in most superconductors are electrons, which are fermions of spin $1/2$. Bose condensation can occur only if there is a way to convert them into effective bosons of integral spin. In the BCS theory, this is done using the Cooper pairs, which are bound states of two electrons of opposite spins and momenta. To complete the argument, the attractive interaction that causes the binding is assumed to be the side-effects of electron-phonon interactions.

Since the Cooper pairs are composed of electrons with opposite momenta, transition to the super state is actually a condensation in the momentum space, hence the title of this section.

The foregoing argument translates into the model Hamiltonian

$$\begin{aligned}\hat{H} &= \sum_{\boldsymbol{k},\lambda} \varepsilon_{\boldsymbol{k}}\, \hat{a}^{+}_{\boldsymbol{k},\lambda}\, \hat{a}_{\boldsymbol{k},\lambda} + \frac{1}{2} \sum_{\boldsymbol{k},\boldsymbol{l},\lambda} V_{\boldsymbol{k}\boldsymbol{l}}\, \hat{a}^{+}_{\boldsymbol{k},\lambda}\, \hat{a}^{+}_{-\boldsymbol{k},-\lambda}\, \hat{a}_{-\boldsymbol{l},-\lambda}\, \hat{a}_{\boldsymbol{l},\lambda} \\ &= \sum_{\boldsymbol{k},\lambda} \varepsilon_{\boldsymbol{k}}\, \hat{a}^{+}_{\boldsymbol{k},\lambda}\, \hat{a}_{\boldsymbol{k},\lambda} + \sum_{\boldsymbol{k},\boldsymbol{l}} V_{\boldsymbol{k}\boldsymbol{l}}\, \hat{a}^{+}_{\boldsymbol{k},\uparrow}\, \hat{a}^{+}_{-\boldsymbol{k},\downarrow}\, \hat{a}_{-\boldsymbol{l},\downarrow}\, \hat{a}_{\boldsymbol{l},\uparrow}\end{aligned} \tag{7.208}$$

where

$$\lambda = (\uparrow,\downarrow) = \left(\frac{1}{2}\hbar,\ -\frac{1}{2}\hbar\right) = \text{spin component along a quantization axis}$$

$$\varepsilon_{\boldsymbol{k}} = \frac{\hbar^2 \boldsymbol{k}^2}{2\,m^*} \qquad m^* = \text{effective mass of conducting free electrons} \tag{7.208a}$$

$$V_{\boldsymbol{k}\boldsymbol{l}} = \left\langle \boldsymbol{k}, -\boldsymbol{k} \,\middle|\, \hat{V} \,\middle|\, \boldsymbol{l}, -\boldsymbol{l} \right\rangle = \text{matrix elements of the phonon-mediated interaction } V$$

According to the 2nd quantization rules for fermions [see Appendix B], the 1st and 4th operators in the last sum in (7.208) belongs to one electron, the 2nd and 3rd to the other. Note the different ordering for states in $V_{\boldsymbol{k}\boldsymbol{l}}$, where $|\, i, j\,\rangle$ and $\langle\, i, j\,|$ denote particle 1 & 2 are in states i & j, respectively.

Finally, discussions in the last paragraph concerns rules for the translation of the usual quantum Hamiltonian into the 2nd quantization formalism. Thus, each interaction term involves only 2 particles in a Cooper pair. In subsequent applications, $\hat{a}_\alpha$ & $\hat{a}^{+}_\alpha$ are often interpreted as the annihilation & creation of the state α (or more vividly, the particle in state α), respectively. Thus, each interaction term involves 4 particles. The way to reconcile these two seemingly conflicting viewpoints is to treat the interaction as a scattering process in which the pair $(\hat{a}^{+}_\beta, \hat{a}_\alpha)$ represents an incoming particle in state α being scattered into the outgoing state β.

Since superconductivity occurs only at low temperatures, only electrons near the Fermi surface can be affected by the interaction. In the simplest approximation, we set

$$V_{\boldsymbol{k}\boldsymbol{l}} = \begin{cases} -V_0 & \text{for } |\mu' - \varepsilon_{\boldsymbol{k}}| \le \Delta\varepsilon \text{ and } |\mu' - \varepsilon_{\boldsymbol{l}}| \le \Delta\varepsilon \\ 0 & \text{otherwise} \end{cases} \tag{7.209}$$

where μ' is the chemical potential, V_0 & $\Delta\varepsilon$ are both positive constants of order $k_B T_C$, with T_C the transition temperature.

Solutions to (7.208) require mathematical techniques developed especially for the quantum field theory (or the many body problem). In lieu of which, we are confined to the mean field approximation. Thus, we replace $\hat{V}$ with its average using

$$\sum_m V_{\boldsymbol{k}\boldsymbol{m}}\,\hat{a}_{-\boldsymbol{m},\downarrow}\,\hat{a}_{\boldsymbol{m},\uparrow} \to \left\langle \sum_m V_{\boldsymbol{k}\boldsymbol{m}}\,\hat{a}_{-\boldsymbol{m},\downarrow}\,\hat{a}_{\boldsymbol{m},\uparrow} \right\rangle = \Delta_{\boldsymbol{k}} \qquad (7.209a)$$

and its Hermitian conjugate

$$\sum_m V_{\boldsymbol{m}\boldsymbol{k}}\,\hat{a}^+_{\boldsymbol{m},\uparrow}\,\hat{a}^+_{-\boldsymbol{m},\downarrow} \to \left\langle \sum_m V_{\boldsymbol{m}\boldsymbol{k}}\,\hat{a}^+_{\boldsymbol{m},\uparrow}\,\hat{a}^+_{-\boldsymbol{m},\downarrow} \right\rangle = \Delta^*_{\boldsymbol{k}} \qquad (7.209b)$$

where we have used

$$V^*_{\boldsymbol{k}\boldsymbol{m}} = V_{\boldsymbol{m}\boldsymbol{k}} \qquad \& \qquad (a\,b)^+ = b^+\,a^+$$

(7.208) simplifies to

$$\hat{H}_{\text{mf}} = \sum_{\boldsymbol{k},\lambda} \varepsilon_{\boldsymbol{k}}\,\hat{a}^+_{\boldsymbol{k},\lambda}\,\hat{a}_{\boldsymbol{k},\lambda} + \sum_{\boldsymbol{k}} \Delta_{\boldsymbol{k}}\,\hat{a}^+_{\boldsymbol{k},\uparrow}\,\hat{a}^+_{-\boldsymbol{k},\downarrow} + \sum_{\boldsymbol{l}} \Delta^*_{\boldsymbol{l}}\,\hat{a}_{-\boldsymbol{l},\downarrow}\,\hat{a}_{\boldsymbol{l},\uparrow} \qquad (7.210)$$

Since the total number of electrons is fixed, we use the grand canonical ensemble for the averages

$$\langle \hat{A} \rangle = \text{Tr}\left(\hat{\rho}\,\hat{A}\right) \qquad (7.213)$$

$$\hat{\rho} = \frac{1}{\mathcal{Z}_\mu} e^{-\beta\left(\hat{H} - \mu'\hat{N}\right)} \approx \frac{1}{Z_\mu} e^{-\beta\left(\hat{H}_{mf} - \mu'\hat{N}\right)} \qquad (7.214)$$

where

$$\mathcal{Z}_\mu = \text{Tr}\, e^{-\beta\left(\hat{H} - \mu'\hat{N}\right)} \qquad\qquad Z_\mu = \text{Tr}\, e^{-\beta\left(\hat{H}_{mf} - \mu'\hat{N}\right)}$$

Note that the (free) electron number operator

$$\hat{N} = \sum_{\boldsymbol{k},\lambda} \hat{a}^+_{\boldsymbol{k},\lambda}\,\hat{a}_{\boldsymbol{k},\lambda} \qquad (7.215)$$

commutes with $\hat{H}$ but not $\hat{H}_{mf}$. Obviously, by assigning pairs of electrons as Cooper pairs, the number of free electrons given by $\hat{N}$ is no longer conserved.

Putting(7.209) into (7.209a-b) then gives

$$\Delta_{\boldsymbol{k}} = \begin{cases} \Delta & \text{if } \left| \varepsilon_{\boldsymbol{k}} - \mu' \right| \le \Delta\varepsilon \\ 0 & \text{otherwise} \end{cases}$$

$$\Delta^*_{\boldsymbol{k}} = \begin{cases} \Delta^* & \text{if } \left| \varepsilon_{\boldsymbol{k}} - \mu' \right| \le \Delta\varepsilon \\ 0 & \text{otherwise} \end{cases} \qquad (7.211)$$

where

$$\Delta = -V_0 \sum_m{}' \left\langle \hat{a}_{-\boldsymbol{m},\downarrow}\,\hat{a}_{\boldsymbol{m},\uparrow} \right\rangle \qquad\qquad \Delta^* = -V_0 \sum_m{}' \left\langle \hat{a}^+_{\boldsymbol{m},\uparrow}\,\hat{a}^+_{-\boldsymbol{m},\downarrow} \right\rangle \qquad (7.212)$$

The prime on the sum $\sum_m{}'$ means that $\boldsymbol{m}$ is restricted by the condition $\left| \varepsilon_{\boldsymbol{m}} - \mu' \right| \le \Delta\varepsilon$.

Consider now the individual terms in the mean field Hamiltonian (7.210).

$\hat{a}^+_{\boldsymbol{k},\lambda}\,\hat{a}_{\boldsymbol{k},\lambda}$ counts the number of free electrons with energy $\varepsilon_{\boldsymbol{k}}$ and spin λ.

$\hat{a}^+_{\boldsymbol{k},\uparrow}\,\hat{a}^+_{-\boldsymbol{k},\downarrow}$ creates a Cooper pair with coupling constant $\Delta_{\boldsymbol{k}}$.

$\hat{a}_{-\boldsymbol{k},\downarrow}\,\hat{a}_{\boldsymbol{k},\uparrow}$ removes a Cooper pair with coupling constant $\Delta^*_{\boldsymbol{k}}$.

where, for want of a better term, we have called $\Delta_{\boldsymbol{k}}$ & $\Delta^*_{\boldsymbol{k}}$ coupling constants, keeping in mind that

$\hat{a}^+_{\boldsymbol{k},\lambda}\,\hat{a}^+_{-\boldsymbol{k},-\lambda}\,\hat{a}_{-\boldsymbol{k},-\lambda}\,\hat{a}_{\boldsymbol{k},\lambda}$ counts the number of Cooper pairs with binding energy $\Delta^*_{\boldsymbol{k}}\Delta_{\boldsymbol{k}}$ and spin λ.

The quantity Δ is called the gap function [see (7.226c) for reason of name]. Combing (7.211) & (7.212), we see that $|\Delta|^2$ is the average binding energy of a Cooper pair. This means $\Delta = 0$ is the threshold for the formation of a macroscopic number of Cooper pairs. Therefore, $|\Delta|$ is the order parameter of the transition.

Consider now the effective Hamiltonian

$$\begin{aligned}\hat{K} &= \hat{H}_{mf} - \mu' \hat{N} \\ &= \sum_{\boldsymbol{k},\lambda} (\varepsilon_{\boldsymbol{k}} - \mu') \hat{a}^{+}_{\boldsymbol{k},\lambda} \hat{a}_{\boldsymbol{k},\lambda} + \sum_{\boldsymbol{k}} \Delta_{\boldsymbol{k}} \hat{a}^{+}_{\boldsymbol{k},\uparrow} \hat{a}^{+}_{-\boldsymbol{k},\downarrow} + \sum_{\boldsymbol{k}} \Delta^{*}_{\boldsymbol{k}} \hat{a}_{-\boldsymbol{k},\downarrow} \hat{a}_{\boldsymbol{k},\uparrow} \\ &= \sum_{\boldsymbol{k}} \left[(\varepsilon_{\boldsymbol{k}} - \mu') \hat{a}^{+}_{\boldsymbol{k},\uparrow} \hat{a}_{\boldsymbol{k},\uparrow} + (\varepsilon_{\boldsymbol{k}} - \mu') \hat{a}^{+}_{\boldsymbol{k},\downarrow} \hat{a}_{\boldsymbol{k},\downarrow} \right] + \sum_{\boldsymbol{k}} \Delta_{\boldsymbol{k}} \hat{a}^{+}_{\boldsymbol{k},\uparrow} \hat{a}^{+}_{-\boldsymbol{k},\downarrow} + \sum_{\boldsymbol{k}} \Delta^{*}_{\boldsymbol{k}} \hat{a}_{-\boldsymbol{k},\downarrow} \hat{a}_{\boldsymbol{k},\uparrow}\end{aligned} \tag{7.216a}$$

The spin down term can be written as

$$\sum_{\boldsymbol{k}} (\varepsilon_{\boldsymbol{k}} - \mu') \hat{a}^{+}_{\boldsymbol{k},\downarrow} \hat{a}_{\boldsymbol{k},\downarrow} = \sum_{\boldsymbol{k}} (\varepsilon_{\boldsymbol{k}} - \mu') \hat{a}^{+}_{-\boldsymbol{k},\downarrow} \hat{a}_{-\boldsymbol{k},\downarrow} \qquad [\ \varepsilon_{-\boldsymbol{k}} = \varepsilon_{\boldsymbol{k}} \text{ used.}\ ]$$

Using the anti-commutation relations

$$\begin{aligned}&\left[\hat{a}_{\boldsymbol{k},\lambda}, \hat{a}^{+}_{\boldsymbol{l},\lambda'} \right]_{+} = \delta_{\boldsymbol{k}\boldsymbol{l}}\, \delta_{\lambda\lambda'} \\ &\left[\hat{a}_{\boldsymbol{k},\lambda}, \hat{a}_{\boldsymbol{l},\lambda'} \right]_{+} = \left[\hat{a}^{+}_{\boldsymbol{k},\lambda}, \hat{a}^{+}_{\boldsymbol{l},\lambda'} \right]_{+} = 0\end{aligned} \tag{7.216b}$$

we have

$$\begin{aligned}\sum_{\boldsymbol{k}} (\varepsilon_{\boldsymbol{k}} - \mu') \hat{a}^{+}_{\boldsymbol{k},\downarrow} \hat{a}_{\boldsymbol{k},\downarrow} &= \sum_{\boldsymbol{k}} (\varepsilon_{\boldsymbol{k}} - \mu') \left[1 - \hat{a}_{-\boldsymbol{k},\downarrow} \hat{a}^{+}_{-\boldsymbol{k},\downarrow} \right] \\ &= -\sum_{\boldsymbol{k}} \xi_{\boldsymbol{k}} \hat{a}_{-\boldsymbol{k},\downarrow} \hat{a}^{+}_{-\boldsymbol{k},\downarrow} + E_0\end{aligned} \tag{7.216c}$$

where

$$\xi_{\boldsymbol{k}} = \varepsilon_{\boldsymbol{k}} - \mu' = \frac{\hbar^2 \boldsymbol{k}^2}{2 m^*} - \mu' \qquad E_0 = \sum_{\boldsymbol{k}} (\varepsilon_{\boldsymbol{k}} - \mu') \tag{7.217}$$

Putting (7.216b) into (7.216a) and dropping the infinite constant E_0, we have,

$$\hat{K} = \sum_{\boldsymbol{k}} \xi_{\boldsymbol{k}} \left(\hat{a}^{+}_{\boldsymbol{k},\uparrow} \hat{a}_{\boldsymbol{k},\uparrow} - \hat{a}_{-\boldsymbol{k},\downarrow} \hat{a}^{+}_{-\boldsymbol{k},\downarrow} \right) + \sum_{\boldsymbol{k}} \Delta_{\boldsymbol{k}} \hat{a}^{+}_{\boldsymbol{k},\uparrow} \hat{a}^{+}_{-\boldsymbol{k},\downarrow} + \sum_{\boldsymbol{k}} \Delta^{*}_{\boldsymbol{k}} \hat{a}_{-\boldsymbol{k},\downarrow} \hat{a}_{\boldsymbol{k},\uparrow} \tag{7.216}$$

(7.214) thus becomes

$$\hat{\rho} = \frac{1}{Z} e^{-\beta \hat{K}} \qquad Z = \mathrm{Tr}\, e^{-\beta \hat{K}} \tag{7.218}$$

which takes the form of a canonical ensemble, as befit a system that does not conserve N.

Reminder: The canonical ensemble with $\hat{H}$ written explicitly for N particles does indeed conserve particle numbers. However, for Hamiltonians like $\hat{K}$ that involves sum over states, particle numbers are not necessarily conserved. Another example is the black-body radiation. Remember: all applications need only abide by the constraints imposed in the variational derivation of the statistical operator $\hat{\rho}$, namely

$\mathrm{Tr}\left(\hat{\rho}\hat{H}\right) = U$ for canonical ensemble

$\mathrm{Tr}\left(\hat{\rho}\hat{H}\right) = U$ & $\mathrm{Tr}\left(\hat{\rho}\hat{N}\right) = N$ for grand canonical ensemble

The advantage of (7.126) is that it can be written in matrix form as

$$\hat{K} = \sum_{\boldsymbol{k}} \hat{\boldsymbol{\alpha}}^{+}_{\boldsymbol{k}} \mathbb{K}_{\boldsymbol{k}} \hat{\boldsymbol{\alpha}}_{\boldsymbol{k}} = \sum_{\boldsymbol{k}} \begin{pmatrix} \hat{a}^{+}_{\boldsymbol{k},\uparrow} & \hat{a}_{-\boldsymbol{k},\downarrow} \end{pmatrix} \begin{pmatrix} \xi_{\boldsymbol{k}} & \Delta_{\boldsymbol{k}} \\ \Delta^{*}_{\boldsymbol{k}} & -\xi_{\boldsymbol{k}} \end{pmatrix} \begin{pmatrix} \hat{a}_{\boldsymbol{k},\uparrow} \\ \hat{a}^{+}_{-\boldsymbol{k},\downarrow} \end{pmatrix} \tag{7.219}$$

where

$$\mathbb{K}_{\boldsymbol{k}} = \begin{pmatrix} \xi_{\boldsymbol{k}} & \Delta_{\boldsymbol{k}} \\ \Delta^{*}_{\boldsymbol{k}} & -\xi_{\boldsymbol{k}} \end{pmatrix} \qquad \hat{\boldsymbol{\alpha}}_{\boldsymbol{k}} = \begin{pmatrix} \hat{a}_{\boldsymbol{k},\uparrow} \\ \hat{a}^{+}_{-\boldsymbol{k},\downarrow} \end{pmatrix}$$

$\rightarrow \quad \hat{\boldsymbol{\alpha}}_{\boldsymbol{k}}^{+} = \left(\hat{a}_{\boldsymbol{k},\uparrow}^{+} \quad \hat{a}_{-\boldsymbol{k},\downarrow} \right)$ (7.220)

Note that $\mathbb{K}_{\boldsymbol{k}}$ is a matrix of numbers while $\hat{\boldsymbol{\alpha}}_{\boldsymbol{k}}$($\hat{\boldsymbol{\alpha}}_{\boldsymbol{k}}^{+}$) is a column (row) matrix of operators. Matrix manipulations that follow are therefore merely rearrangement of linear combinations of operators. No new mathematical concepts are involved.

Since $\mathbb{K}_{\boldsymbol{k}}$ is Hermitian, its eigenvalues are real and it can be diagonalized by a unitary transform so that

$$\mathbb{U}_{\boldsymbol{k}}^{+} \mathbb{K}_{\boldsymbol{k}} \mathbb{U}_{\boldsymbol{k}} = \mathbb{E}_{\boldsymbol{k}} = \begin{pmatrix} E_{\boldsymbol{k},0} & 0 \\ 0 & E_{\boldsymbol{k},1} \end{pmatrix} \qquad \mathbb{U}_{\boldsymbol{k}}^{+} \mathbb{U}_{\boldsymbol{k}} = \mathbb{U}_{\boldsymbol{k}} \mathbb{U}_{\boldsymbol{k}}^{+} = \mathbb{I} \qquad (7.225)$$

where $E_{\boldsymbol{k}0}$ & $E_{\boldsymbol{k}1}$ are real eigenvalues of $\mathbb{K}_{\boldsymbol{k}}$. Assuming

$$\mathbb{U}_{\boldsymbol{k}} = \begin{pmatrix} u_{\boldsymbol{k}}^{*} & v_{\boldsymbol{k}} \\ -v_{\boldsymbol{k}}^{*} & u_{\boldsymbol{k}} \end{pmatrix} \qquad \rightarrow \qquad \mathbb{U}_{\boldsymbol{k}}^{+} = \begin{pmatrix} u_{\boldsymbol{k}} & -v_{\boldsymbol{k}} \\ v_{\boldsymbol{k}}^{*} & u_{\boldsymbol{k}}^{*} \end{pmatrix} \qquad (7.221)$$

we have

$$\mathbb{U}_{\boldsymbol{k}}^{+} \mathbb{U}_{\boldsymbol{k}} = \begin{pmatrix} u_{\boldsymbol{k}} & -v_{\boldsymbol{k}} \\ v_{\boldsymbol{k}}^{*} & u_{\boldsymbol{k}}^{*} \end{pmatrix} \begin{pmatrix} u_{\boldsymbol{k}}^{*} & v_{\boldsymbol{k}} \\ -v_{\boldsymbol{k}}^{*} & u_{\boldsymbol{k}} \end{pmatrix} = \begin{pmatrix} |u_{\boldsymbol{k}}|^2 + |v_{\boldsymbol{k}}|^2 & 0 \\ 0 & |u_{\boldsymbol{k}}|^2 + |v_{\boldsymbol{k}}|^2 \end{pmatrix}$$

$$= \begin{pmatrix} u_{\boldsymbol{k}}^{*} & v_{\boldsymbol{k}} \\ -v_{\boldsymbol{k}}^{*} & u_{\boldsymbol{k}} \end{pmatrix} \begin{pmatrix} u_{\boldsymbol{k}} & -v_{\boldsymbol{k}} \\ v_{\boldsymbol{k}}^{*} & u_{\boldsymbol{k}}^{*} \end{pmatrix} = \mathbb{U}_{\boldsymbol{k}} \mathbb{U}_{\boldsymbol{k}}^{+}$$

so that (7.225) is satisfied if

$$|u_{\boldsymbol{k}}|^2 + |v_{\boldsymbol{k}}|^2 = 1 \qquad (7.221a)$$

Putting (7.220-1) into (7.225) gives

$$\begin{pmatrix} u_{\boldsymbol{k}} & -v_{\boldsymbol{k}} \\ v_{\boldsymbol{k}}^{*} & u_{\boldsymbol{k}}^{*} \end{pmatrix} \begin{pmatrix} \xi_{\boldsymbol{k}} & \Delta_{\boldsymbol{k}} \\ \Delta_{\boldsymbol{k}}^{*} & -\xi_{\boldsymbol{k}} \end{pmatrix} \begin{pmatrix} u_{\boldsymbol{k}}^{*} & v_{\boldsymbol{k}} \\ -v_{\boldsymbol{k}}^{*} & u_{\boldsymbol{k}} \end{pmatrix}$$

$$= \begin{pmatrix} u_{\boldsymbol{k}} & -v_{\boldsymbol{k}} \\ v_{\boldsymbol{k}}^{*} & u_{\boldsymbol{k}}^{*} \end{pmatrix} \begin{pmatrix} \xi_{\boldsymbol{k}} u_{\boldsymbol{k}}^{*} - \Delta_{\boldsymbol{k}} v_{\boldsymbol{k}}^{*} & \xi_{\boldsymbol{k}} v_{\boldsymbol{k}} + \Delta_{\boldsymbol{k}} u_{\boldsymbol{k}} \\ \Delta_{\boldsymbol{k}}^{*} u_{\boldsymbol{k}}^{*} + \xi_{\boldsymbol{k}} v_{\boldsymbol{k}}^{*} & \Delta_{\boldsymbol{k}}^{*} v_{\boldsymbol{k}} - \xi_{\boldsymbol{k}} u_{\boldsymbol{k}} \end{pmatrix}$$

$$= \begin{pmatrix} u_{\boldsymbol{k}} \xi_{\boldsymbol{k}} u_{\boldsymbol{k}}^{*} - u_{\boldsymbol{k}} \Delta_{\boldsymbol{k}} v_{\boldsymbol{k}}^{*} - v_{\boldsymbol{k}} \Delta_{\boldsymbol{k}}^{*} u_{\boldsymbol{k}}^{*} - v_{\boldsymbol{k}} \xi_{\boldsymbol{k}} v_{\boldsymbol{k}}^{*} & u_{\boldsymbol{k}} \xi_{\boldsymbol{k}} v_{\boldsymbol{k}} + u_{\boldsymbol{k}} \Delta_{\boldsymbol{k}} u_{\boldsymbol{k}} - v_{\boldsymbol{k}} \Delta_{\boldsymbol{k}}^{*} v_{\boldsymbol{k}} + v_{\boldsymbol{k}} \xi_{\boldsymbol{k}} u_{\boldsymbol{k}} \\ v_{\boldsymbol{k}}^{*} \xi_{\boldsymbol{k}} u_{\boldsymbol{k}}^{*} - v_{\boldsymbol{k}}^{*} \Delta_{\boldsymbol{k}} v_{\boldsymbol{k}}^{*} + u_{\boldsymbol{k}}^{*} \Delta_{\boldsymbol{k}}^{*} u_{\boldsymbol{k}}^{*} + u_{\boldsymbol{k}}^{*} \xi_{\boldsymbol{k}} v_{\boldsymbol{k}}^{*} & v_{\boldsymbol{k}}^{*} \xi_{\boldsymbol{k}} v_{\boldsymbol{k}} + v_{\boldsymbol{k}}^{*} \Delta_{\boldsymbol{k}} u_{\boldsymbol{k}} + u_{\boldsymbol{k}}^{*} \Delta_{\boldsymbol{k}}^{*} v_{\boldsymbol{k}} - u_{\boldsymbol{k}}^{*} \xi_{\boldsymbol{k}} u_{\boldsymbol{k}} \end{pmatrix}$$

$$= \begin{pmatrix} (u_{\boldsymbol{k}}^{*} u_{\boldsymbol{k}} - v_{\boldsymbol{k}}^{*} v_{\boldsymbol{k}}) \xi_{\boldsymbol{k}} - u_{\boldsymbol{k}} v_{\boldsymbol{k}}^{*} \Delta_{\boldsymbol{k}} - u_{\boldsymbol{k}}^{*} v_{\boldsymbol{k}} \Delta_{\boldsymbol{k}}^{*} & 2 u_{\boldsymbol{k}} v_{\boldsymbol{k}} \xi_{\boldsymbol{k}} + u_{\boldsymbol{k}}^2 \Delta_{\boldsymbol{k}} - v_k^2 \Delta_{\boldsymbol{k}}^{*} \\ 2 u_{\boldsymbol{k}}^{*} v_{\boldsymbol{k}}^{*} \xi_{\boldsymbol{k}} - v_{\boldsymbol{k}}^{*2} \Delta_{\boldsymbol{k}} + u_{\boldsymbol{k}}^{*2} \Delta_{\boldsymbol{k}}^{*} & -(u_{\boldsymbol{k}}^{*} u_{\boldsymbol{k}} - v_{\boldsymbol{k}}^{*} v_{\boldsymbol{k}}) \xi_{\boldsymbol{k}} + u_{\boldsymbol{k}} v_{\boldsymbol{k}}^{*} \Delta_{\boldsymbol{k}} + u_{\boldsymbol{k}}^{*} v_{\boldsymbol{k}} \Delta_{\boldsymbol{k}}^{*} \end{pmatrix}$$

$$= \begin{pmatrix} E_{\boldsymbol{k},0} & 0 \\ 0 & E_{\boldsymbol{k},1} \end{pmatrix}$$

$$\rightarrow \quad E_{\boldsymbol{k},0} = (u_{\boldsymbol{k}}^{*} u_{\boldsymbol{k}} - v_{\boldsymbol{k}}^{*} v_{\boldsymbol{k}}) \xi_{\boldsymbol{k}} - u_{\boldsymbol{k}} v_{\boldsymbol{k}}^{*} \Delta_{\boldsymbol{k}} - u_{\boldsymbol{k}}^{*} v_{\boldsymbol{k}} \Delta_{\boldsymbol{k}}^{*} = -E_{\boldsymbol{k},1} \qquad (a)$$

$$2 u_{\boldsymbol{k}} v_{\boldsymbol{k}} \xi_{\boldsymbol{k}} + u_{\boldsymbol{k}}^2 \Delta_{\boldsymbol{k}} - v_k^2 \Delta_{\boldsymbol{k}}^{*} = 2 u_{\boldsymbol{k}}^{*} v_{\boldsymbol{k}}^{*} \xi_{\boldsymbol{k}} - v_{\boldsymbol{k}}^{*2} \Delta_{\boldsymbol{k}} + u_{\boldsymbol{k}}^{*2} \Delta_{\boldsymbol{k}}^{*} = 0 \qquad (b)$$

Comparing $(b)^{*}$ with (b) gives

$$\xi_{\boldsymbol{k}}^{*} = \xi_{\boldsymbol{k}}$$

Using (7.221a) to eliminate $u_{\boldsymbol{k}}$ & $v_{\boldsymbol{k}}$ from (a) & (b) gives [see §Code]

$$E_{\boldsymbol{k},0}^2 = \xi_{\boldsymbol{k}}^2 + |\Delta_{\boldsymbol{k}}|^2 = E_{\boldsymbol{k},1}^2$$

To be more definite, we set

$$E_{\boldsymbol{k}} = \xi_{\boldsymbol{k}} \sqrt{1 + \frac{|\Delta_{\boldsymbol{k}}|^2}{\xi_{\boldsymbol{k}}^2}} \qquad (7.226)$$

so that the sign of $E_{\boldsymbol{k}}$ is determined by $\xi_{\boldsymbol{k}}$, and

$$E_{\boldsymbol{k},0} = E_{\boldsymbol{k}} = -E_{\boldsymbol{k},1} \qquad (7.226a)$$

Note that the special form of (7.226) is necessary to ensure a smooth transit to the spectrum of normal electrons when $\Delta_{\boldsymbol{k}} = 0$.

Coupled with (7.211), (7.226) becomes

$$E_{\boldsymbol{k}} = \begin{cases} \xi_{\boldsymbol{k}} \sqrt{1 + \frac{|\Delta|^2}{\xi_{\boldsymbol{k}}^2}} & \text{if } |\varepsilon_{\boldsymbol{k}} - \mu'| \le \Delta\varepsilon \\ \xi_{\boldsymbol{k}} & \text{otherwise} \end{cases} \qquad (7.226b)$$

Since the energy spectrum depends only on $|\Delta|^2$, so does the partition function Z and hence all other thermodynamic functions. Therefore, we can replace $|\Delta|^2$ with Δ^2 , where $\Delta > 0$ is real. This may be taken either as a harmless assumption or simply writing $|\Delta|$ as Δ. (7.226b) thus simplifies to

$$E_{\boldsymbol{k}} = \begin{cases} \xi_{\boldsymbol{k}} \sqrt{1 + \frac{\Delta^2}{\xi_{\boldsymbol{k}}^2}} & \text{if } |\varepsilon_{\boldsymbol{k}} - \mu'| \le \Delta\varepsilon \\ \xi_{\boldsymbol{k}} & \text{otherwise} \end{cases} \qquad (7.226c)$$

with

$$\lim_{\xi_{\boldsymbol{k}} \to 0_\pm} E_{\boldsymbol{k}} = \pm\Delta \qquad (7.226d)$$

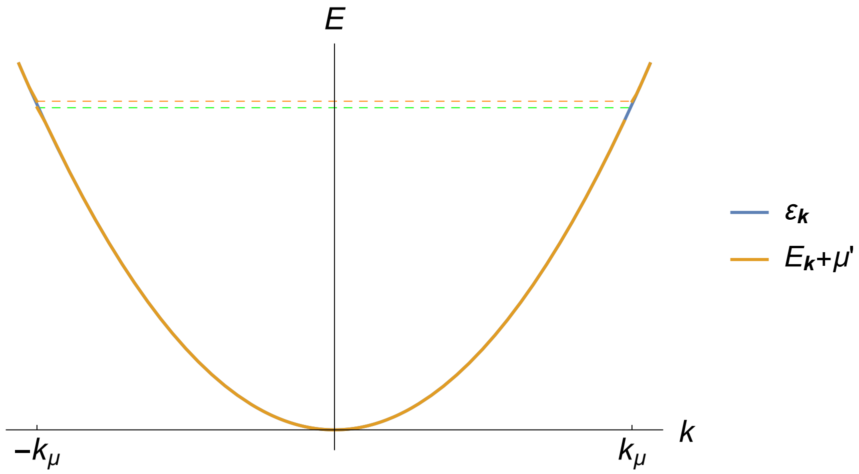

Fig.7.24a. Energy spectra where $k_\mu = \sqrt{\frac{2 m^* \mu'}{\hbar^2}}$ is the k-vector at the chemical potential.

Details near k_μ is shown in Fig.7.24b.

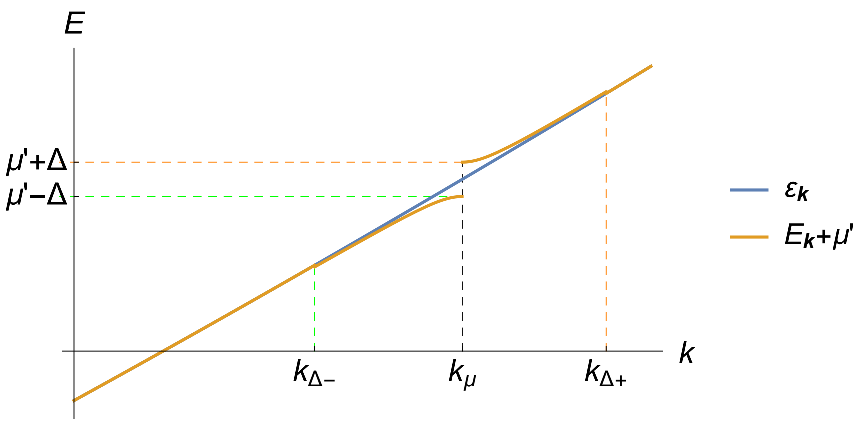

Fig.7.24b. Energy spectra near the chemical potential with

$$k_\mu = \sqrt{\frac{2\, m^*\, \mu'}{\hbar^2}} \qquad \text{and} \qquad k_{\Delta\pm} = \sqrt{\frac{2\, m^* (\mu' \pm \Delta\varepsilon)}{\hbar^2}}\,.$$

A gap of magnitude $2\,\Delta$ appears in the bogolon spectra.

Plots of the energy spectra (7.226c) are given in Fig.7.24a, with the region near k_μ is blown up in Fig.7.24b. For $k \in \{k_{\Delta-}, k_{\Delta+}\}$, the phonon mediated interaction lifts the spin degeneracy of each $\varepsilon_{\boldsymbol{k}}$ and splits it into two levels $\mu' \pm E_{\boldsymbol{k}}$. The splitting is minimum at the chemical potential where

$$\xi_{\boldsymbol{k}} = 0 \qquad \to \qquad E_{\boldsymbol{k}} = \pm\Delta$$

which gives a gap of $2\,\Delta$ in the spectrum. The metal thus becomes a semiconductor of very narrow and temperature sensitive gap, as far as the single particle spectrum is concerned.

Using (7.225), we can write (7.219) as

$$\hat{K} = \sum_{\boldsymbol{k}} \hat{\boldsymbol{\alpha}}_{\boldsymbol{k}}^{+} \mathbb{U}_{\boldsymbol{k}} \mathbb{U}_{\boldsymbol{k}}^{+} \mathbb{K}_{\boldsymbol{k}} \mathbb{U}_{\boldsymbol{k}} \mathbb{U}_{\boldsymbol{k}}^{+} \hat{\boldsymbol{\alpha}}_{\boldsymbol{k}}$$

$$= \sum_{\boldsymbol{k}} \hat{\boldsymbol{\Gamma}}_{\boldsymbol{k}}^{+} \mathbb{E}_{\boldsymbol{k}} \hat{\boldsymbol{\Gamma}}_{\boldsymbol{k}} \qquad (7.227a)$$

where,

$$\hat{\boldsymbol{\Gamma}}_{\boldsymbol{k}} = \mathbb{U}_{\boldsymbol{k}}^{+} \hat{\boldsymbol{\alpha}}_{\boldsymbol{k}} \qquad \to \qquad \hat{\boldsymbol{\alpha}}_{\boldsymbol{k}} = \mathbb{U}_{\boldsymbol{k}} \hat{\boldsymbol{\Gamma}}_{\boldsymbol{k}} \qquad (7.223)$$

$$= \begin{pmatrix} \hat{\gamma}_{\boldsymbol{k},0} \\ \hat{\gamma}_{\boldsymbol{k},1}^{+} \end{pmatrix} \qquad (7.222a)$$

$$\to \quad \hat{\boldsymbol{\Gamma}}_{\boldsymbol{k}}^{+} = \hat{\boldsymbol{\alpha}}_{\boldsymbol{k}}^{+} \mathbb{U}_{\boldsymbol{k}} \qquad \to \qquad \hat{\boldsymbol{\alpha}}_{\boldsymbol{k}}^{+} = \hat{\boldsymbol{\Gamma}}_{\boldsymbol{k}}^{+} \mathbb{U}_{\boldsymbol{k}}^{+} \qquad (7.223a)$$

$$= \begin{pmatrix} \hat{\gamma}_{\boldsymbol{k},0}^{+} & \hat{\gamma}_{\boldsymbol{k},1} \end{pmatrix} \qquad (7.222b)$$

The designation of the components of $\hat{\boldsymbol{\Gamma}}_{\boldsymbol{k}}$ is in accordance with (7.220).

Consider now two sets of operators related by a unitary transform:

$$\hat{\boldsymbol{b}} = \mathbb{U}^{+} \hat{\boldsymbol{a}} \qquad \hat{\boldsymbol{b}}^{+} = \hat{\boldsymbol{a}}^{+} \mathbb{U}$$

where the components of $\hat{\boldsymbol{a}}$ & $\hat{\boldsymbol{b}}$ can be a mixture of creator and destruction operators. With implicit summation for repeated indices enforced, we have

$$\left[\hat{b}_i, \hat{b}_j\right]_\pm = \left[U_{i\lambda}^{+} \hat{a}_\lambda, U_{j\lambda'}^{+} \hat{a}_{\lambda'}\right]_\pm = U_{i\lambda}^{+} U_{j\lambda'}^{+} \left[\hat{a}_\lambda, \hat{a}_{\lambda'}\right]_\pm$$

$$\left[\hat{b}_i, \hat{b}_j^{+}\right]_\pm = \left[U_{i\lambda}^{+} \hat{a}_\lambda, \hat{a}_{\lambda'}^{+} U_{\lambda' j}\right]_\pm = U_{i\lambda}^{+} U_{\lambda' j} \left[\hat{a}_\lambda, \hat{a}_{\lambda'}^{+}\right]_\pm$$

If $\hat{\boldsymbol{a}}$ consists of only one kind of operators, then

$$\left[\hat{a}_\lambda, \hat{a}_{\lambda'}\right]_\pm = 0 \qquad \to \qquad \left[\hat{b}_i, \hat{b}_j\right]_\pm = 0$$

$$\left[\hat{a}_\lambda, \hat{a}_{\lambda'}^{+}\right]_\pm = c\, \delta_{\lambda\lambda'} \qquad \to \qquad \left[\hat{b}_i, \hat{b}_j^{+}\right]_\pm = c\, U_{i\lambda}^{+} U_{\lambda j} = c\, \delta_{ij} \qquad (7.222c)$$

where $c = \text{const}$. Thus, $\hat{\boldsymbol{b}}$ obeys the same commutation relations as $\hat{\boldsymbol{a}}$.

Now, if we switch, say, the n^{th} component of $\hat{\boldsymbol{a}}$ to the opposite kind of operator, (7.222c) will still hold with the n^{th} component of $\hat{\boldsymbol{b}}$ similarly switched. Obviously, this pair-wise switching can continue for any number of the rest of the components.

Thus, a unitary transformation preserves the commutation relations as well as the arrangement (or positions) of the different kinds of component operators.

The anti-commutation relations (7.216b) thus transform under (7.223-a) into

$$\left[\hat{\gamma}_{\boldsymbol{k},i}, \hat{\gamma}_{\boldsymbol{l},j}^{+}\right]_+ = \delta_{\boldsymbol{k}\boldsymbol{l}}\, \delta_{ij} \qquad \left[\hat{\gamma}_{\boldsymbol{k},i}, \hat{\gamma}_{\boldsymbol{l},j}\right]_+ = \left[\hat{\gamma}_{\boldsymbol{k},i}^{+}, \hat{\gamma}_{\boldsymbol{l},j}^{+}\right]_+ = 0 \qquad (7.224)$$

Putting (7.222a-b) into (7.227a) gives

$$\hat{K} = \sum_{\boldsymbol{k}} \begin{pmatrix} \hat{\gamma}_{\boldsymbol{k},0}^{+} & \hat{\gamma}_{\boldsymbol{k},1} \end{pmatrix} \begin{pmatrix} E_{\boldsymbol{k},0} & 0 \\ 0 & E_{\boldsymbol{k},1} \end{pmatrix} \begin{pmatrix} \hat{\gamma}_{\boldsymbol{k},0} \\ \hat{\gamma}_{\boldsymbol{k},1}^{+} \end{pmatrix}$$

$$= \sum_{\boldsymbol{k}} \left(E_{\boldsymbol{k},0}\, \hat{\gamma}^{+}_{\boldsymbol{k},0}\, \hat{\gamma}_{\boldsymbol{k},0} + E_{\boldsymbol{k},1}\, \hat{\gamma}_{\boldsymbol{k},1}\, \hat{\gamma}^{+}_{\boldsymbol{k},1} \right)$$

$$= \sum_{\boldsymbol{k}} \left(E_{\boldsymbol{k},0}\, \hat{\gamma}^{+}_{\boldsymbol{k},0}\, \hat{\gamma}_{\boldsymbol{k},0} - E_{\boldsymbol{k},1}\, \hat{\gamma}^{+}_{\boldsymbol{k},1}\, \hat{\gamma}_{\boldsymbol{k},1} + E_{\boldsymbol{k},1} \right) \qquad [\text{ (7.226a) used. }] \qquad (7.227)$$

$$= \sum_{\boldsymbol{k}} \left(E_{\boldsymbol{k},0}\, \hat{n}_{\boldsymbol{k},0} - E_{\boldsymbol{k},1}\, \hat{n}_{\boldsymbol{k},1} \right) + \mathcal{E}_0 \qquad [\ \mathcal{E}_0 = \sum_{\boldsymbol{k}} E_{\boldsymbol{k},1} = -\sum_{\boldsymbol{k}} E_{\boldsymbol{k}}\ ] \qquad (7.227a)$$

$$= \sum_{\boldsymbol{k}} E_{\boldsymbol{k}} \left(\hat{n}_{\boldsymbol{k},0} + \hat{n}_{\boldsymbol{k},1} \right) + \mathcal{E}_0 \qquad [\text{ (7.224) used. }] \qquad (7.227b)$$

which describes a system of two types of free fermions of the same energy spectrum $E_{\boldsymbol{k}}$. Since $\hat{\gamma}^{+}_{\boldsymbol{k},1}$ actually destroys an eigenstate of $\hat{K}$ (or a particle) of energy $-E_{\boldsymbol{k}}$, it is similarly to the hole operator in semiconductors. In honor of Bogoliubov, who pioneered this formalism, the free fermions in (7.227) are called bogolons.

The next order of business is to calculate the gap function Δ as given by (7.212), which needs to be expressed in terms of the bogolons. Using (7.223-a), we have

$$\langle \hat{\boldsymbol{\alpha}}_{\boldsymbol{k}}\, \hat{\boldsymbol{\alpha}}^{+}_{\boldsymbol{k}} \rangle = \mathbb{U}_{\boldsymbol{k}} \left\langle \hat{\boldsymbol{\Gamma}}_{\boldsymbol{k}} \hat{\boldsymbol{\Gamma}}^{+}_{\boldsymbol{k}} \right\rangle \mathbb{U}^{+}_{\boldsymbol{k}}$$

$$= \mathbb{U}_{\boldsymbol{k}} \left\langle \begin{pmatrix} \hat{\gamma}_{\boldsymbol{k},0} \\ \hat{\gamma}^{+}_{\boldsymbol{k},1} \end{pmatrix} \begin{pmatrix} \hat{\gamma}^{+}_{\boldsymbol{k},0} & \hat{\gamma}_{\boldsymbol{k},1} \end{pmatrix} \right\rangle \mathbb{U}^{+}_{\boldsymbol{k}} \qquad [\text{ (7.222a-b) used. }]$$

$$= \mathbb{U}_{\boldsymbol{k}} \left\langle \begin{pmatrix} \hat{\gamma}_{\boldsymbol{k},0}\, \hat{\gamma}^{+}_{\boldsymbol{k},0} & \hat{\gamma}_{\boldsymbol{k},0}\, \hat{\gamma}_{\boldsymbol{k},1} \\ \hat{\gamma}^{+}_{\boldsymbol{k},1}\, \hat{\gamma}^{+}_{\boldsymbol{k},0} & \hat{\gamma}^{+}_{\boldsymbol{k},1}\, \hat{\gamma}_{\boldsymbol{k},1} \end{pmatrix} \right\rangle \mathbb{U}^{+}_{\boldsymbol{k}} \qquad (7.227c)$$

Since there are two kinds of particles, the basis is the orthonormal set $\left\{ \prod_{\boldsymbol{k}} \left| n_{\boldsymbol{k},0}, n_{\boldsymbol{k},1} \right\rangle \right\}$.

$$Z = \left\langle e^{-\beta \hat{K}} \right\rangle = \prod_{\boldsymbol{k}} \sum_{n_{\boldsymbol{k},0},\, n_{\boldsymbol{k},1} = 0}^{1} \left\langle n_{\boldsymbol{k},0}, n_{\boldsymbol{k},1} \right| e^{-\beta \hat{K}_{\boldsymbol{k}}} \left| n_{\boldsymbol{k},0}, n_{\boldsymbol{k},1} \right\rangle \qquad [\text{ c.f. (7.157) of §7.H.2. }]$$

$$= \prod_{\boldsymbol{k}} Z_{\boldsymbol{k}}$$

where, with the constant $\mathcal{E}_0$ dropped,

$$\hat{K}_{\boldsymbol{k}} = E_{\boldsymbol{k}} \left(\hat{n}_{\boldsymbol{k},0} + \hat{n}_{\boldsymbol{k},1} \right)$$

and

$$Z_{\boldsymbol{k}} = \sum_{n_{\boldsymbol{k},0},\, n_{\boldsymbol{k},1} = 0}^{1} \left\langle n_{\boldsymbol{k},0}, n_{\boldsymbol{k},1} \right| e^{-\beta \hat{K}_{\boldsymbol{k}}} \left| n_{\boldsymbol{k},0}, n_{\boldsymbol{k},1} \right\rangle$$

$$= \left\langle 00 \right| e^{-\beta \hat{K}_{\boldsymbol{k}}} \left| 00 \right\rangle + \left\langle 01 \right| e^{-\beta \hat{K}_{\boldsymbol{k}}} \left| 01 \right\rangle + \left\langle 10 \right| e^{-\beta \hat{K}_{\boldsymbol{k}}} \left| 10 \right\rangle + \left\langle 11 \right| e^{-\beta \hat{K}_{\boldsymbol{k}}} \left| 11 \right\rangle$$

$$= 1 + e^{\beta E_{\boldsymbol{k},1}} + e^{-\beta E_{\boldsymbol{k},0}} + e^{-\beta E_{\boldsymbol{k},0} + \beta E_{\boldsymbol{k},1}} \qquad [\text{ (7.227) with } \mathcal{E}_0 \text{ dropped used. }]$$

$$= \left(1 + e^{-\beta E_{\boldsymbol{k},0}}\right)\left(1 + e^{\beta E_{\boldsymbol{k},1}}\right)$$

$$= 1 + e^{-\beta E_{\boldsymbol{k}}} + e^{-\beta E_{\boldsymbol{k}}} + e^{-2\beta E_{\boldsymbol{k}}} \qquad [\text{ (7.227a) used. }]$$

$$= \left(1 + e^{-\beta E_{\boldsymbol{k}}}\right)^2$$

Using (7.224), we have

$$\langle \hat{\gamma}_{\boldsymbol{k},0}\, \hat{\gamma}^{+}_{\boldsymbol{k},0} \rangle = 1 - \langle \hat{n}_{\boldsymbol{k},0} \rangle$$

with

$$\langle \hat{n}_{\boldsymbol{k},0} \rangle = \langle \hat{\gamma}^{+}_{\boldsymbol{k},0}\, \hat{\gamma}_{\boldsymbol{k},0} \rangle = \frac{1}{Z_{\boldsymbol{k}}} \sum_{n_{\boldsymbol{k},0},\, n_{\boldsymbol{k},1} = 0}^{1} \left\langle n_{\boldsymbol{k},0}, n_{\boldsymbol{k},1} \right| e^{-\beta \hat{K}_{\boldsymbol{k}}}\, \hat{n}_{\boldsymbol{k},0} \left| n_{\boldsymbol{k},0}, n_{\boldsymbol{k},1} \right\rangle$$

$$= \frac{1}{Z_{\boldsymbol{k}}} \left(0 + 0 + e^{-\beta E_{\boldsymbol{k},0}} + e^{-\beta E_{\boldsymbol{k},0} + \beta E_{\boldsymbol{k},1}} \right)$$

$$= \frac{1}{Z_{\boldsymbol{k}}} e^{-\beta E_{\boldsymbol{k},0}} \left(1 + e^{\beta E_{\boldsymbol{k},1}} \right)$$
$$= \frac{e^{-\beta E_{\boldsymbol{k},0}}}{1 + e^{-\beta E_{\boldsymbol{k},0}}}$$
$$= \frac{1}{e^{\beta E_{\boldsymbol{k},0}} + 1} = \frac{1}{e^{\beta E_{\boldsymbol{k}}} + 1} \qquad (7.228a)$$

which is the same as the fermion occupation number for state $| \boldsymbol{k}, 0 \rangle$, as expected. An alternative form of (7.228a) that will be useful later is

$$\langle \hat{n}_{\boldsymbol{k},0} \rangle = \frac{e^{-\beta E_{\boldsymbol{k},0}/2}}{e^{\beta E_{\boldsymbol{k},0}/2} + e^{-\beta E_{\boldsymbol{k},0}/2}} = \frac{1}{2}\left(1 - \frac{e^{\beta E_{\boldsymbol{k},0}/2} - e^{-\beta E_{\boldsymbol{k},0}/2}}{e^{\beta E_{\boldsymbol{k},0}/2} + e^{-\beta E_{\boldsymbol{k},0}/2}} \right)$$
$$= \frac{1}{2}\left(1 - \tanh \frac{\beta E_{\boldsymbol{k},0}}{2} \right) \qquad (7.228)$$
$$= \frac{1}{2}\left(1 - \tanh \frac{\beta E_{\boldsymbol{k}}}{2} \right) \qquad [\text{ (7.226a) used. }]$$

Similarly,

$$\langle \hat{n}_{\boldsymbol{k},1} \rangle = \langle \hat{\gamma}^{+}_{\boldsymbol{k},1} \hat{\gamma}_{\boldsymbol{k},1} \rangle = \frac{1}{e^{-\beta E_{\boldsymbol{k},1}} + 1} = \frac{1}{e^{\beta E_{\boldsymbol{k}}} + 1} = \frac{1}{2}\left(1 + \tanh \frac{\beta E_{\boldsymbol{k},1}}{2} \right) \qquad (7.229)$$
$$= \frac{1}{2}\left(1 - \tanh \frac{\beta E_{\boldsymbol{k}}}{2} \right) \qquad [\text{ (7.226a) used. }]$$

Using the general relations

$$\hat{a} \mid n \rangle = n \mid n-1 \rangle \qquad \hat{a}^{+} \mid n \rangle = (1-n) \mid n+1 \rangle \qquad [\, n = 0, 1 \,]$$

for fermions, we have

$$\langle \hat{\gamma}_{\boldsymbol{k},0} \hat{\gamma}_{\boldsymbol{k},1} \rangle = \frac{1}{Z_{\boldsymbol{k}}} \sum_{n_{\boldsymbol{k},0}, n_{\boldsymbol{k},1} = 0}^{1} \left\langle n_{\boldsymbol{k},0}, n_{\boldsymbol{k},1} \,\middle|\, e^{-\beta \hat{K}_{\boldsymbol{k}}} \hat{\gamma}_{\boldsymbol{k},0} \hat{\gamma}_{\boldsymbol{k},1} \,\middle|\, n_{\boldsymbol{k},0}, n_{\boldsymbol{k},1} \right\rangle$$
$$= \frac{1}{Z_{\boldsymbol{k}}} \sum_{n_{\boldsymbol{k},0}, n_{\boldsymbol{k},1} = 0}^{1} \left\langle n_{\boldsymbol{k},0}, n_{\boldsymbol{k},1} \,\middle|\, e^{-\beta \hat{K}_{\boldsymbol{k}}} n_{\boldsymbol{k},0} n_{\boldsymbol{k},1} \,\middle|\, n_{\boldsymbol{k},0} - 1, n_{\boldsymbol{k},1} - 1 \right\rangle$$
$$= 0 \qquad (7.229a)$$
$$\langle \hat{\gamma}^{+}_{\boldsymbol{k},1} \hat{\gamma}^{+}_{\boldsymbol{k},0} \rangle = \frac{1}{Z_{\boldsymbol{k}}} \sum_{n_{\boldsymbol{k},0}, n_{\boldsymbol{k},1} = 0}^{1} \left\langle n_{\boldsymbol{k},0}, n_{\boldsymbol{k},1} \,\middle|\, e^{-\beta \hat{K}_{\boldsymbol{k}}} (1 - n_{\boldsymbol{k},0})(1 - n_{\boldsymbol{k},1}) \,\middle|\, n_{\boldsymbol{k},0} + 1, n_{\boldsymbol{k},1} + 1 \right\rangle$$
$$= 0 \qquad (7.229b)$$

Putting (7.228) & (7.229-b) into (7.227c) gives

$$\langle \hat{\boldsymbol{\alpha}}_{\boldsymbol{k}} \hat{\boldsymbol{\alpha}}^{+}_{\boldsymbol{k}} \rangle = \mathbb{U}_{\boldsymbol{k}} \begin{pmatrix} 1 - \langle \hat{n}_{\boldsymbol{k},0} \rangle & 0 \\ 0 & \langle \hat{n}_{\boldsymbol{k},1} \rangle \end{pmatrix} \mathbb{U}^{+}_{\boldsymbol{k}}$$
$$= \mathbb{U}_{\boldsymbol{k}} \begin{pmatrix} \frac{1}{2}\left(1 + \tanh \frac{\beta E_{\boldsymbol{k}}}{2} \right) & 0 \\ 0 & \frac{1}{2}\left(1 - \tanh \frac{\beta E_{\boldsymbol{k}}}{2} \right) \end{pmatrix} \mathbb{U}^{+}_{\boldsymbol{k}}$$
$$= \frac{1}{2} \mathbb{I} + \frac{1}{2} \tanh \frac{\beta E_{\boldsymbol{k}}}{2} \, \mathbb{U}_{\boldsymbol{k}} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \mathbb{U}^{+}_{\boldsymbol{k}}$$
$$= \frac{1}{2} \mathbb{I} + \frac{1}{2 E_{\boldsymbol{k}}} \tanh \frac{\beta E_{\boldsymbol{k}}}{2} \, \mathbb{U}_{\boldsymbol{k}} \begin{pmatrix} E_{\boldsymbol{k}} & 0 \\ 0 & -E_{\boldsymbol{k}} \end{pmatrix} \mathbb{U}^{+}_{\boldsymbol{k}}$$
$$= \frac{1}{2} \mathbb{I} + \frac{1}{2 E_{\boldsymbol{k}}} \tanh \frac{\beta E_{\boldsymbol{k}}}{2} \, \mathbb{K}_{\boldsymbol{k}} \qquad [\text{ (7.225) used. }] \qquad (7.230)$$
$$= \frac{1}{2} \mathbb{I} + \frac{1}{2 E_{\boldsymbol{k}}} \tanh \frac{\beta E_{\boldsymbol{k}}}{2} \begin{pmatrix} \xi_{\boldsymbol{k}} & \Delta_{\boldsymbol{k}} \\ \Delta^{*}_{\boldsymbol{k}} & -\xi_{\boldsymbol{k}} \end{pmatrix} \qquad [\text{ (7.220) used. }] \qquad (7.230a)$$

Comparing (7.230a) with

$$\langle \hat{\boldsymbol{\alpha}}_k \hat{\boldsymbol{\alpha}}_k^+ \rangle = \left\langle \begin{pmatrix} \hat{a}_{k,\uparrow} \\ \hat{a}^+_{-k,\downarrow} \end{pmatrix} \begin{pmatrix} \hat{a}^+_{k,\uparrow} & \hat{a}_{-k,\downarrow} \end{pmatrix} \right\rangle \qquad \text{[(7.220) used.]}$$

$$= \begin{pmatrix} \langle \hat{a}_{k,\uparrow} \hat{a}^+_{k,\uparrow} \rangle & \langle \hat{a}_{k,\uparrow} \hat{a}_{-k,\downarrow} \rangle \\ \langle \hat{a}^+_{-k,\downarrow} \hat{a}^+_{k,\uparrow} \rangle & \langle \hat{a}^+_{-k,\downarrow} \hat{a}_{-k,\downarrow} \rangle \end{pmatrix}$$

we get

$$\langle \hat{a}_{k,\uparrow} \hat{a}_{-k,\downarrow} \rangle = \frac{\Delta_k}{2 E_k} \tanh \frac{\beta E_k}{2}$$

$$= -\langle \hat{a}_{-k,\downarrow} \hat{a}_{k,\uparrow} \rangle \qquad \text{[(7.216b) used.]} \qquad (7.231)$$

Putting (7.231) into (7.212) then gives

$$\Delta = V_0 \sum_k{}' \frac{\Delta_k}{2 E_k} \tanh \frac{\beta E_k}{2}$$

$$= V_0 \sum_k{}' \frac{\Delta}{2 E_k} \tanh \frac{\beta E_k}{2} \qquad \text{[(7.211) used.]}$$

so that we arrive finally at the so called gap equation:

$$1 = V_0 \sum_k{}' \frac{1}{2 E_k} \tanh \frac{\beta E_k}{2} \qquad (7.232)$$

$$= V_0 \sum_k{}' \frac{1}{2 \xi_k \sqrt{1 + \frac{\Delta^2}{\xi_k^2}}} \tanh \frac{\beta \xi_k \sqrt{1 + \frac{\Delta^2}{\xi_k^2}}}{2} \qquad \text{[(7.226) used with (7.211).]}$$

$$= V_0 \sum_k{}' \frac{1}{2 \sqrt{\xi_k^2 + \Delta^2}} \tanh \frac{\beta \sqrt{\xi_k^2 + \Delta^2}}{2} \qquad (7.232a)$$

where we have taken advantage of the fact that the sign of E_k is cancelled out here.

For large volume V, we have

$$\sum_k \approx \frac{V}{(2\pi)^3} \int d\Omega \int_0^\infty dk\, k^2$$

$$= \frac{V}{(2\pi)^3} \frac{1}{2} \left(\frac{2 m^*}{\hbar^2} \right)^{3/2} \int d\Omega \int_{-\mu'}^\infty d\xi_k \sqrt{\xi_k + \mu'}$$

where [see (7.217)]

$$\xi_k = \frac{\hbar^2 k^2}{2 m^*} - \mu' \qquad \rightarrow \qquad k = \sqrt{\frac{2 m^* (\xi_k + \mu')}{\hbar^2}}$$

Since the integrand is independent of angles,

$$\sum_k \approx \frac{V}{4\pi^2} \left(\frac{2 m^*}{\hbar^2} \right)^{3/2} \int_{-\mu'}^\infty d\xi_k \sqrt{\xi_k + \mu'} \qquad (7.233)$$

$$= \frac{V}{\sqrt{2}\, \pi^2} \frac{m^{*3/2}}{\hbar^3} \int_{-\mu'}^\infty d\xi \sqrt{\xi + \mu'}$$

$$= \int_{-\mu'}^\infty d\xi\, N(\xi) \qquad (7.233a)$$

where

$$N(\xi) = \frac{V}{\sqrt{2}\,\pi^2} \frac{m^{*3/2}}{\hbar^3} \sqrt{\xi + \mu'}$$

= Density of states at $\xi > -\mu'$ for 1 spin degree of freedom. (7.233b)

(7.211) then gives

$$\sum_{k}' = \int_{-\Delta\varepsilon}^{\Delta\varepsilon} d\xi\, N(\xi)$$

$$\approx N(0) \int_{-\Delta\varepsilon}^{\Delta\varepsilon} d\xi \qquad (7.234)$$

where

$$N(0) = \frac{V}{\sqrt{2}\,\pi^2} \frac{m^{*3/2}}{\hbar^3} \sqrt{\mu'} \qquad (7.234a)$$

= Density of states at the chemical potential for 1 spin degree of freedom.

(7.232a) thus becomes [see (7.211)]

$$1 \approx V_0 N(0) \int_{-\Delta\varepsilon}^{\Delta\varepsilon} d\xi \frac{1}{2\sqrt{\xi^2+\Delta^2}} \tanh \frac{\beta\sqrt{\xi^2+\Delta^2}}{2}$$

$$= V_0 N(0) \int_{0}^{\Delta\varepsilon} d\xi \frac{1}{\sqrt{\xi^2+\Delta^2}} \tanh \frac{\beta\sqrt{\xi^2+\Delta^2}}{2} \qquad (7.235)$$

since integrand is even in ξ. Owing to the presence of β, the solution to (7.235) is necessarily a function of T, i.e., $\Delta = \Delta(T)$.

At the transition temperature T_C, $\Delta = 0$ so that (7.235) becomes

$$\frac{1}{V_0 N(0)} = \int_0^{\Delta\varepsilon} d\xi_k \frac{1}{\xi_k} \tanh \frac{\beta_C \xi_k}{2}$$

$$= \int_0^{\beta_C \Delta\varepsilon/2} dx \frac{1}{x} \tanh x \qquad \left[x = \frac{\beta_C \xi_k}{2} \right]$$

$$= (\ln x) \tanh x \Big|_0^{\beta_C \Delta\varepsilon/2} - \int_0^{\beta_C \Delta\varepsilon/2} dx\, (\ln x) \operatorname{sech}^2 x \qquad (7.236a)$$

where the last expression was obtained via integration by part.

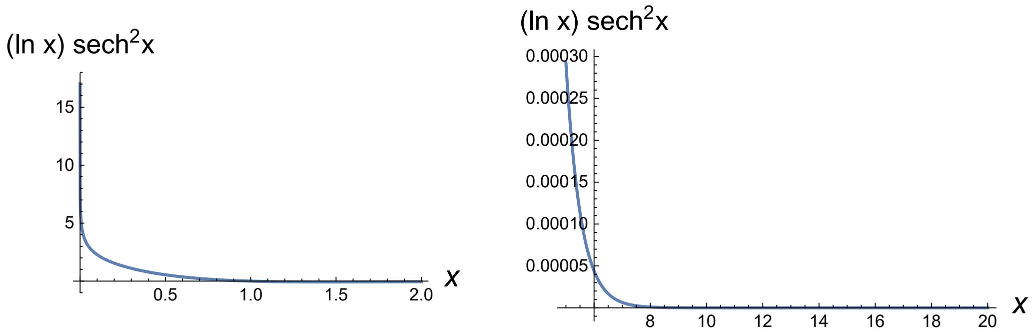

Fig.7.24c. Plots of $(\ln x) \operatorname{sech}^2 x$.

Fig.7.24c shows that for

$\beta_C \Delta\varepsilon / 2 \gtrsim 10$

we can safely replace (7.236a) with

$$\frac{1}{V_0 N(0)} = (\ln x) \tanh x \Big|_0^{\beta_C \Delta\varepsilon/2} - \int_0^{\infty} dx\, (\ln x) \operatorname{sech}^2 x \qquad (7.236b)$$

Using [see §Code]

$\tanh(x > 10) \approx 1$ & $\int_0^{\infty} dx\, (\ln x) \operatorname{sech}^2 x = -\gamma + \ln \frac{\pi}{4}$

where $\gamma \approx 0.577216$ is the Euler-Gamma constant, (7.236a) becomes

$$\begin{aligned}\frac{1}{V_0 N(0)} &= \ln\left(\frac{1}{2}\beta_C \Delta\varepsilon\right) + \gamma - \ln\frac{\pi}{4} \\ &= \ln\left(\frac{2}{\pi}\beta_C \Delta\varepsilon\, e^{\gamma}\right) \\ &= \ln\left(\frac{\alpha}{2}\beta_C \Delta\varepsilon\right)\end{aligned} \qquad (7.236)$$

with

$$\alpha = \frac{4}{\pi} e^{\gamma} \approx 2.26773 \qquad (7.236c)$$

(7.236) can be inverted to give

$$k_B T_C = \frac{\alpha}{2}\Delta\varepsilon \exp\left(-\frac{1}{V_0 N(0)}\right) \qquad (7.238)$$

For $T \to 0$, (7.235) reduces to

$$\frac{1}{V_0 N(0)} \approx \int_0^{\Delta\varepsilon} d\xi\, \frac{1}{\sqrt{\xi^2 + \Delta_0^2}} \qquad \Delta_0 \equiv \Delta(0)$$

$$= \frac{1}{2}\ln \left.\frac{1 + \frac{\xi}{\sqrt{\xi^2+\Delta_0^2}}}{1 - \frac{\xi}{\sqrt{\xi^2+\Delta_0^2}}}\right|_0^{\Delta\varepsilon} \qquad \text{[See §Code.]}$$

$$= \frac{1}{2}\ln\left(\frac{1 + \frac{\Delta\varepsilon}{\sqrt{(\Delta\varepsilon)^2+\Delta_0^2}}}{1 - \frac{\Delta\varepsilon}{\sqrt{(\Delta\varepsilon)^2+\Delta_0^2}}}\right)$$

$$\approx \frac{1}{2}\ln\left(\frac{1 + \left[1 + \left(\frac{\Delta_0}{\Delta\varepsilon}\right)^2\right]^{-1/2}}{1 - \left[1 + \left(\frac{\Delta_0}{\Delta\varepsilon}\right)^2\right]^{-1/2}}\right) \qquad \text{[} \Delta\varepsilon >> \Delta_0 \text{ assumed.]}$$

$$= \frac{1}{2}\ln\left(\frac{2 - \frac{1}{2}\left(\frac{\Delta_0}{\Delta\varepsilon}\right)^2 + \ldots}{\frac{1}{2}\left(\frac{\Delta_0}{\Delta\varepsilon}\right)^2 + \ldots}\right)$$

$$= \frac{1}{2}\ln\left[4\left(\frac{\Delta\varepsilon}{\Delta_0}\right)^2 + \ldots\right]$$

$$\approx \ln\left(2\frac{\Delta\varepsilon}{\Delta_0}\right) \qquad (7.239)$$

$$\rightarrow \quad \Delta_0 \approx 2\,\Delta\varepsilon \exp\left(-\frac{1}{V_0 N(0)}\right) \qquad (7.240)$$

Combining (7.238) & (7.240) gives

$$\frac{\Delta_0}{k_B T_C} \approx \frac{4}{\alpha} \approx 1.764 \qquad (7.241)$$

which was found to be in good argument with experiments on low-temperature superconductors.

For $0 \le T \le T_C$, we can write (7.235) as

$$\frac{1}{V_0 N(0)} = \int_0^{\Delta\varepsilon/\Delta_0} dx\, \frac{1}{\sqrt{x^2 + \overline{\Delta}^2}} \tanh\left(\frac{\beta\Delta_0}{2}\sqrt{x^2+\overline{\Delta}^2}\right) \qquad (7.241a)$$

where

$$x = \frac{\xi}{\Delta_0} \qquad \overline{\Delta} = \frac{\Delta}{\Delta_0}$$

(7.241) gives

$$\beta\Delta_0 = \frac{4}{\alpha}\frac{T_C}{T}$$

$$\frac{\Delta\varepsilon}{\Delta_0} = \frac{\alpha\,\Delta\varepsilon}{4\,k_B\,T_C} = \frac{\alpha}{4}\beta_C\,\Delta\varepsilon = \frac{1}{2}e^{1/V_0 N(0)}$$

so that (7.235) can be thrown into the dimensionless form

$$\ln(2\,\Delta\varepsilon\,/\,\Delta_0) = \int_0^{\Delta\varepsilon/\Delta_0} d\,x\,\frac{1}{\sqrt{x^2+\overline{\Delta}^2}}\tanh\left(\frac{2}{\alpha}\frac{T_C}{T}\sqrt{x^2+\overline{\Delta}^2}\right) \qquad (7.241b)$$

which can be solved numerically for $\Delta(T)$ for a given choice of $\Delta\,\varepsilon\,/\Delta_0 > 10$ [see Fig.7.24].

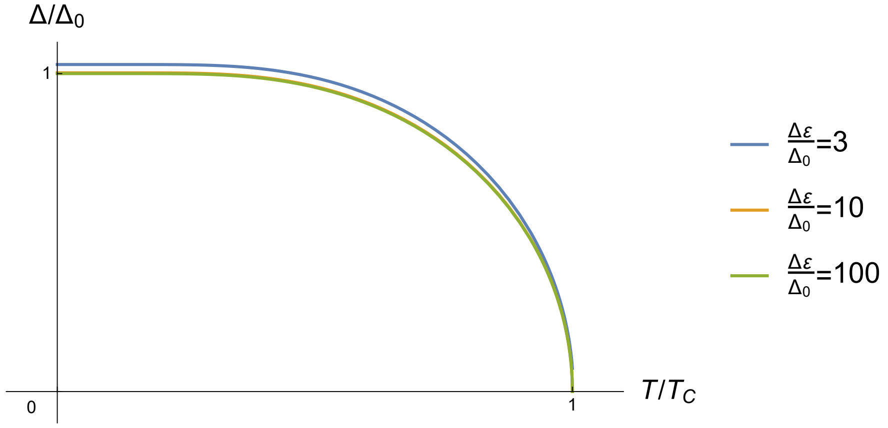

Fig.7.24. Temperature dependence of $\Delta(T)$, which is independent of $\frac{\Delta\varepsilon}{\Delta_0}$ for $\frac{\Delta\varepsilon}{\Delta_0} \gtrsim 10$.

Thus, the curves for $\frac{\Delta\varepsilon}{\Delta_0} = 10$ & $\frac{\Delta\varepsilon}{\Delta_0} = 100$ completely coincide.

Curves for $\frac{\Delta\varepsilon}{\Delta_0} < 10$ are not reliable because (7.236a) assumes $\frac{\Delta\varepsilon}{\Delta_0} \gtrsim 10$.

For example, the curve for $\frac{\Delta\varepsilon}{\Delta_0} = 3$ gives the erroneous $\Delta(0) \neq \Delta_0$.

In Problem 7.23, you are asked to show that the entropy of free fermions is given by

$$S = -k_B\sum_{\boldsymbol{k}}\left[\langle n_{\boldsymbol{k}}\rangle\ln\langle n_{\boldsymbol{k}}\rangle + (1-\langle n_{\boldsymbol{k}}\rangle)\ln(1-\langle n_{\boldsymbol{k}}\rangle)\right] \qquad (7.242a)$$

for each spin degree of freedom. Here, $\langle n_{\boldsymbol{k}}\rangle$ is the fermion occupation number [see (7.161) of §7.H.2].

Since the bogolons are free fermions [see (7.224) & (7.227)], the entropy of $\hat{H}_{\text{mf}}$ is simply

$$S = -k_B\sum_{\boldsymbol{k}}\sum_{j=0}^{1}\left[\langle n_{\boldsymbol{k}}^j\rangle\ln\langle n_{\boldsymbol{k}}^j\rangle + (1-\langle n_{\boldsymbol{k}}^j\rangle)\ln(1-\langle n_{\boldsymbol{k}}^j\rangle)\right] \qquad (7.242b)$$

where

$$\langle n_{\boldsymbol{k}}^0\rangle = \frac{1}{e^{\beta E_{\boldsymbol{k},0}}+1} = \frac{1}{e^{\beta E_{\boldsymbol{k}}}+1} \qquad 1-\langle n_{\boldsymbol{k}}^0\rangle = \frac{e^{\beta E_{\boldsymbol{k}}}}{e^{\beta E_{\boldsymbol{k}}}+1} = \frac{1}{1+e^{-\beta E_{\boldsymbol{k}}}}$$

$$\langle n_{\boldsymbol{k}}^1\rangle = \frac{1}{e^{\beta E_{\boldsymbol{k},1}}+1} = \frac{1}{e^{-\beta E_{\boldsymbol{k}}}+1} = 1-\langle n_{\boldsymbol{k}}^0\rangle \qquad 1-\langle n_{\boldsymbol{k}}^1\rangle = \frac{e^{-\beta E_{\boldsymbol{k}}}}{e^{-\beta E_{\boldsymbol{k}}}+1} = \frac{1}{1+e^{\beta E_{\boldsymbol{k}}}} = \langle n_{\boldsymbol{k}}^0\rangle$$

Hence, (7.242b) can be written as

$$S = -2\,k_B\sum_{\boldsymbol{k}}\left[\langle n_{\boldsymbol{k}}\rangle\ln\langle n_{\boldsymbol{k}}\rangle + (1-\langle n_{\boldsymbol{k}}\rangle)\ln(1-\langle n_{\boldsymbol{k}}\rangle)\right] \qquad (7.242)$$

where

$$\langle n_{\boldsymbol{k}} \rangle = \frac{1}{e^{\beta E_k} + 1} \qquad E_{\boldsymbol{k}} = \xi_{\boldsymbol{k}} \sqrt{1 + \frac{|\Delta_{\boldsymbol{k}}|^2}{\xi_{\boldsymbol{k}}^2}} \tag{7.242c}$$

Note that $E_{\boldsymbol{k}}$ must take the stated form if $\langle n_{\boldsymbol{k}} \rangle$ is to behave properly as $T \to 0$.

The heat capacity at constant volume is therefore

$$C_V = T\left(\frac{\partial S}{\partial T}\right)_{V,N} = -2\,k_B\,T \sum_{\boldsymbol{k}} \frac{\partial \beta}{\partial T} \frac{\partial \langle n_{\boldsymbol{k}} \rangle}{\partial \beta} \left[\ln\langle n_{\boldsymbol{k}} \rangle + 1 - \ln\left(1 - \langle n_{\boldsymbol{k}} \rangle\right) - 1 \right]$$

$$= 2\,k_B\,\beta \sum_{\boldsymbol{k}} \frac{\partial \langle n_{\boldsymbol{k}} \rangle}{\partial \beta} \ln \frac{\langle n_{\boldsymbol{k}} \rangle}{1 - \langle n_{\boldsymbol{k}} \rangle} \qquad \left[\frac{\partial \beta}{\partial T} = -\frac{1}{k_B\,T^2} = -k_B\,\beta^2 \right] \tag{7.243a}$$

Using

$$\frac{\partial \langle n_{\boldsymbol{k}} \rangle}{\partial E_{\boldsymbol{k}}} = -\frac{\beta\,e^{\beta E_k}}{\left(e^{\beta E_k} + 1\right)^2} \tag{7.243b}$$

$$\frac{\partial E_{\boldsymbol{k}}}{\partial \beta} = \frac{1}{2\,\xi_{\boldsymbol{k}} \sqrt{1 + |\Delta_{\boldsymbol{k}}|^2 / \xi_{\boldsymbol{k}}^2}} \frac{\partial\,|\Delta_{\boldsymbol{k}}|^2}{\partial \beta} = \frac{1}{2\,E_{\boldsymbol{k}}} \frac{\partial\,|\Delta_{\boldsymbol{k}}|^2}{\partial \beta} \qquad [\,(7.242c)\text{ used.}\,]$$

$$\to \quad \frac{\partial \langle n_{\boldsymbol{k}} \rangle}{\partial \beta} = -\frac{e^{\beta E_k}}{\left(e^{\beta E_k} + 1\right)^2} \left(E_{\boldsymbol{k}} + \beta \frac{\partial E_{\boldsymbol{k}}}{\partial \beta} \right) = \frac{1}{\beta} \frac{\partial \langle n_{\boldsymbol{k}} \rangle}{\partial E_{\boldsymbol{k}}} \left(E_{\boldsymbol{k}} + \beta \frac{1}{2\,E_{\boldsymbol{k}}} \frac{\partial\,|\Delta_{\boldsymbol{k}}|^2}{\partial \beta} \right)$$

and

$$\ln \frac{\langle n_{\boldsymbol{k}} \rangle}{1 - \langle n_{\boldsymbol{k}} \rangle} = \ln \frac{1 + e^{-\beta E_k}}{e^{\beta E_k} + 1} = \ln e^{-\beta E_k} = -\beta\,E_{\boldsymbol{k}}$$

(7.243a) becomes

$$C_V = -2\,k_B\,\beta \sum_{\boldsymbol{k}} \frac{\partial \langle n_{\boldsymbol{k}} \rangle}{\partial E_{\boldsymbol{k}}} \left(E_{\boldsymbol{k}}^2 + \frac{1}{2} \beta \frac{\partial\,|\Delta_{\boldsymbol{k}}|^2}{\partial \beta} \right) \tag{7.243}$$

At $T = 0$, $\langle n_{\boldsymbol{k}} \rangle$ is a step function so that $\frac{\partial \langle n_{\boldsymbol{k}} \rangle}{\partial E_{\boldsymbol{k}}}$ is a delta function at $E_{\boldsymbol{k}} = 0$. Let

$$\frac{\partial \langle n_{\boldsymbol{k}} \rangle}{\partial E_{\boldsymbol{k}}} = c\,\delta(E_{\boldsymbol{k}}) \qquad c = \text{const}$$

$$\to \quad \int_{-\infty}^{\infty} d\,E_{\boldsymbol{k}} \frac{\partial \langle n_{\boldsymbol{k}} \rangle}{\partial E_{\boldsymbol{k}}} = c = \langle n_{\boldsymbol{k}} \rangle \Big|_{-\infty}^{\infty} = -1$$

$$\therefore \quad \frac{\partial \langle n_{\boldsymbol{k}} \rangle}{\partial E_{\boldsymbol{k}}} \approx -\delta(E_{\boldsymbol{k}}) \qquad \text{for } T = 0 \tag{7.243c}$$

For finite T, $-\frac{\partial \langle n_{\boldsymbol{k}} \rangle}{\partial E_{\boldsymbol{k}}}$ is sharply peaked with width of $O(k_B\,T)$, as shown in Fig.7.24d.

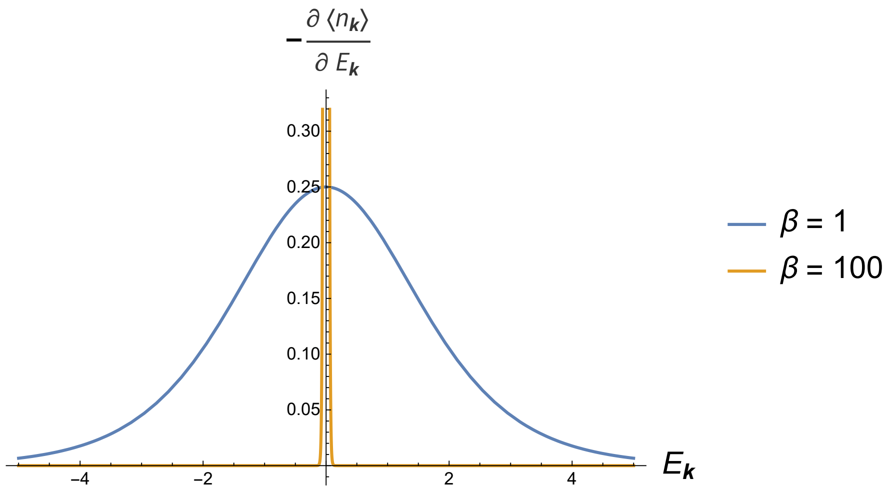

Fig.7.24d. Plots of $-\frac{\partial \langle n_{\mathbf{k}} \rangle}{\partial E_{\mathbf{k}}}$ vs $E_{\mathbf{k}}$ for two different temperatures.

Both β & $E_{\mathbf{k}}$ are normalized to the same unit of energy, say, Δ_0 , to make them dimensionless.

Now for $T \lesssim T_C$,

$$k_B T_C = \frac{\alpha}{4} \Delta_0 \ll \Delta \varepsilon \qquad [\,(7.240\text{-}1)\text{ used.}\,]$$

so that the range of $\mathbf{k}$ included in (7.243) amply satisfies (7.211). Therefore (7.243) can be safely replaced by

$$C_V = -2\, k_B\, \beta \sum_{\mathbf{k} \in \mathcal{I}_T} \frac{\partial \langle n_{\mathbf{k}} \rangle}{\partial E_{\mathbf{k}}} \left(E_{\mathbf{k}}^2 + \frac{1}{2} \beta \frac{\partial \Delta^2}{\partial \beta} \right) \qquad (7.243\text{d})$$

where $\mathcal{I}_T$ is the region of $\mathbf{k}$ for which $E_{\mathbf{k}}$ is of $O(k_B T)$.

For $T > T_C$, we have

$$\Delta \equiv 0 \qquad \to \qquad E_{\mathbf{k}} = \xi_{\mathbf{k}} \qquad \langle n_{\mathbf{k}} \rangle = \frac{1}{e^{\beta \xi_{\mathbf{k}}} + 1} \qquad (7.243\text{e})$$

so that (7.243a) becomes

$$C_V = -2\, k_B\, \beta \sum_{\mathbf{k} \in \mathcal{I}_T} \frac{\partial \langle n_{\mathbf{k}} \rangle}{\partial \xi_{\mathbf{k}}} \xi_{\mathbf{k}}^2 \qquad (\,T > T_C\,) \qquad (7.245\text{a})$$

$$= 2\, k_B\, \beta^2 \sum_{\mathbf{k} \in \mathcal{I}_T} \frac{e^{\beta \xi_{\mathbf{k}}}}{\left(e^{\beta \xi_{\mathbf{k}}} + 1\right)^2} \xi_{\mathbf{k}}^2 \qquad (7.245\text{b})$$

Just above T_C, we have

$$C_V^{>} = -2\, k_B\, \beta_C \sum_{\mathbf{k} \in \mathcal{I}_T} \frac{\partial \langle n_{\mathbf{k}} \rangle}{\partial \xi_{\mathbf{k}}} \xi_{\mathbf{k}}^2 \qquad (7.245)$$

Just below T_C,

$$\Delta = 0 \qquad \text{but} \qquad \frac{\partial \Delta^2}{\partial \beta} \neq 0$$

so that (7.243) becomes

$$C_V^{<} = -2\, k_B\, \beta_C \sum_{\mathbf{k} \in \mathcal{I}_T} \frac{\partial \langle n_{\mathbf{k}} \rangle}{\partial \xi_{\mathbf{k}}} \left(\xi_{\mathbf{k}}^2 + \frac{1}{2} \beta_C \frac{\partial \Delta^2}{\partial \beta} \bigg|_{T = T_C} \right) \qquad (7.244)$$

There is therefore a discontinuity at $T = T_C$ of magnitude

$$\Delta C_V = C_V^{<} - C_V^{>}$$

$$= -k_B \beta_C^2 \sum_{\boldsymbol{k}\in\mathcal{I}_T} \frac{\partial \langle n_{\boldsymbol{k}}\rangle}{\partial \xi_{\boldsymbol{k}}} \frac{\partial \Delta^2}{\partial \beta}\Bigg|_{T=T_C}$$

$$= -k_B \beta_C^2 \int_{-\Delta\varepsilon}^{\Delta\varepsilon} d\xi_{\boldsymbol{k}}\, N(\xi_{\boldsymbol{k}}) \frac{\partial \langle n_{\boldsymbol{k}}\rangle}{\partial \xi_{\boldsymbol{k}}} \frac{\partial \Delta^2}{\partial \beta}\Bigg|_{T=T_C} \quad \text{[(7.233a) used.]} \qquad (7.246a)$$

Putting (7.246b) into (7.246a) gives the lowest order of approximation

$$\Delta C_V \approx k_B \beta_C^2 N(0) \frac{\partial \Delta^2}{\partial \beta}\Bigg|_{T=T_C}$$

$$= -N(0) \frac{\partial \Delta^2}{\partial T}\Bigg|_{T=T_C} \qquad (7.246)$$

which has the opposite sign against Reichl’s (7.246).

From Fig.7.24, we see that

$$\frac{\partial \Delta}{\partial T} < 0 \qquad \to \qquad \Delta C_V > 0 \qquad (7.246c)$$

as shown in Reichl’s Fig.7.25.

Next, we consider the other end of the superconducting phase near $T = 0$. As shown in Fig.7.24,

$$\Delta(0) = \Delta_0 \qquad \& \qquad \frac{\partial \Delta}{\partial T}\Bigg|_{T=0} = 0$$

Therefore, (7.243a) simplifies to

$$C_V = -2 k_B \beta \sum_{\boldsymbol{k}\in\mathcal{I}_T} \frac{\partial \langle n_{\boldsymbol{k}}\rangle}{\partial E_{\boldsymbol{k}}} E_{\boldsymbol{k}}^2$$

$$= 2 k_B \beta \sum_{\boldsymbol{k}\in\mathcal{I}_T} \frac{\beta e^{\beta E_k}}{\left(e^{\beta E_k}+1\right)^2} E_{\boldsymbol{k}}^2 \qquad \text{[(7.243b) used.]} \qquad (7.247)$$

From

$$E_{\boldsymbol{k}}^2 = \xi_{\boldsymbol{k}}^2 + |\Delta_{\boldsymbol{k}}|^2$$

we get, for fixed $\Delta_{\boldsymbol{k}}$,

$$2 E_{\boldsymbol{k}}\, dE_{\boldsymbol{k}} = 2 \xi_{\boldsymbol{k}}\, d\xi_{\boldsymbol{k}}$$

$$\to \quad d\xi_{\boldsymbol{k}} = \frac{E_{\boldsymbol{k}}}{\xi_{\boldsymbol{k}}} dE_{\boldsymbol{k}} = \sqrt{1 + \frac{|\Delta_{\boldsymbol{k}}|^2}{\xi_{\boldsymbol{k}}^2}}\, dE_{\boldsymbol{k}} \qquad \text{[(7.242c) used.]}$$

$$= \sqrt{1 + \frac{|\Delta_{\boldsymbol{k}}|^2}{E_{\boldsymbol{k}}^2 - |\Delta_{\boldsymbol{k}}|^2}}\, dE_{\boldsymbol{k}} = \sqrt{\frac{E_{\boldsymbol{k}}^2}{E_{\boldsymbol{k}}^2 - |\Delta_{\boldsymbol{k}}|^2}}\, dE_{\boldsymbol{k}}$$

$$= \frac{1}{\sqrt{1 - \frac{|\Delta_{\boldsymbol{k}}|^2}{E_{\boldsymbol{k}}^2}}}\, dE_{\boldsymbol{k}} \qquad \text{with} \quad E_{\boldsymbol{k}}^2 \geq |\Delta_{\boldsymbol{k}}|^2$$

(7.233) then gives

$$\sum_{\boldsymbol{k}} \approx \frac{V}{4\pi^2}\left(\frac{2m^*}{\hbar^2}\right)^{3/2} \int_{-\mu'}^{\infty} d\xi_{\boldsymbol{k}} \sqrt{\xi_{\boldsymbol{k}} + \mu'}$$

$$= \frac{V}{4\pi^2}\left(\frac{2m^*}{\hbar^2}\right)^{3/2} \left[\int_{-\sqrt{(\mu')^2+|\Delta_k|^2}}^{-|\Delta_k|} + \int_{|\Delta_k|}^{\infty} \right] dE_{\boldsymbol{k}} \frac{1}{\sqrt{1 - |\Delta_{\boldsymbol{k}}|^2 / E_{\boldsymbol{k}}^2}} \left(\sqrt{E_{\boldsymbol{k}}^2 - |\Delta_{\boldsymbol{k}}|^2} + \mu'\right)^{1/2}$$

$$(7.248)$$

$$= \frac{N(0)}{\sqrt{\mu'}}\left[\int_{-\sqrt{(\mu')^2+|\Delta_k|^2}}^{-|\Delta_k|} + \int_{|\Delta_k|}^{\infty}\right] d E_k \frac{1}{\sqrt{1-|\Delta_k|^2/E_k^2}}\left(\sqrt{E_k^2-|\Delta_k|^2} + \mu'\right)^{1/2}$$

(7.248a)

so that (7.247) becomes, for $T \to 0$,

$$C_V \approx -2 k_B \beta \frac{N(0)}{\sqrt{\mu'}}\left(\int_{-\sqrt{(\mu')^2+\Delta_0^2}}^{-\Delta_0} + \int_{\Delta_0}^{\infty}\right) d E_k \frac{E_k^2}{\sqrt{1-|\Delta_k|^2/E_k^2}}\left(\sqrt{E_k^2-\Delta_0^2} + \mu'\right)^{1/2} \frac{\partial \langle n_k \rangle}{\partial E_k}$$

(7.248b)

Since $\frac{\partial \langle n_k \rangle}{\partial E_k}$ is sharply peaked symmetrically around $E_k = 0$ with half-width of $O(k_B T)$, the two integrals are essentially the same so that (7.248b) simplifies to

$$C_V \approx -4 k_B \beta \frac{N(0)}{\sqrt{\mu'}} \int_{\Delta_0}^{\infty} d E_k \frac{E_k^2}{\sqrt{1-\Delta_0^2/E_k^2}}\left(\sqrt{E_k^2-\Delta_0^2} + \mu'\right)^{1/2} \frac{\partial \langle n_k \rangle}{\partial E_k} \qquad (7.248c)$$

$$\approx -4 k_B \beta N(0) \int_{\Delta_0}^{\infty} d E_k \frac{E_k^2}{\sqrt{1-\Delta_0^2/E_k^2}} \frac{\partial \langle n_k \rangle}{\partial E_k} \qquad \left[\mu' \gg \sqrt{E_k^2-\Delta_0^2}\right]$$

$$\approx 4 k_B \beta^2 N(0) \int_{\Delta_0}^{\infty} d E_k \frac{E_k^2}{\sqrt{1-\Delta_0^2/E_k^2}} e^{-\beta E_k}$$

$$\approx 4 k_B \beta^2 N(0) \int_{\Delta_0}^{\infty} d E_k \frac{E_k^3}{\sqrt{E_k^2-\Delta_0^2}} e^{-\beta E_k} \qquad (7.250)$$

where we have used, for $E_k > 0$,

$$-\frac{\partial \langle n_k \rangle}{\partial E_k} = \frac{\beta e^{\beta E_k}}{(e^{\beta E_k}+1)^2} = \frac{\beta e^{-\beta E_k}}{(1+e^{-\beta E_k})^2} \xrightarrow[T \to 0]{} \beta e^{-\beta E_k}$$

In[∘]:=
```
Assuming[Δ > 0 && β > 0, ∫_Δ^∞ e/√(e^2 - Δ^2) e^(-β e) ⅆe]
```

Out[∘]=
```
Δ BesselK[1, β Δ]
```

From the code above, we have

$$I = \int_{\Delta_0}^{\infty} d E_k \frac{E_k}{\sqrt{E_k^2-\Delta_0^2}} e^{-\beta E_k} = \Delta_0 K_1(\beta \Delta_0) \qquad (7.251)$$

where K_1 is the modified Bessel function of the 2nd kind. Hence,

$$\frac{\partial^2 I}{\partial \beta^2} = \int_{\Delta_0}^{\infty} d E_k \frac{E_k^3}{\sqrt{E_k^2-\Delta_0^2}} e^{-\beta E_k}$$

$$= \Delta_0^3 \left.\frac{d^2 K_1(x)}{d x^2}\right|_{x=\beta\Delta_0}$$

$$= \frac{1}{4}\Delta_0^3\left[3 K_1(\beta\Delta_0) + K_3(\beta\Delta_0)\right] \qquad [\text{ See code below. }] \qquad (7.252)$$

$$\approx \sqrt{\frac{\pi}{2\beta}}\, \Delta_0^{5/2} e^{-\beta\Delta_0} + \ldots \qquad [\text{ See code below. }] \qquad (7.252a)$$

```
(* (7.252) *)
∂x,x BesselK[1, x] // Simplify
```

Out[∘]=
```
1/4 (3 BesselK[1, x] + BesselK[3, x])
```

```
(* (7.252a) *)
1/4 Δ^3 Series[3 BesselK[1, β Δ] + BesselK[3, β Δ], {β, ∞, 2}] // Normal // Expand
```

Out[∘]= $\frac{11\, e^{-\beta\Delta}\sqrt{\frac{\pi}{2}}\,\Delta^{3/2}}{8\,\beta^{3/2}} + \frac{e^{-\beta\Delta}\sqrt{\frac{\pi}{2}}\,\Delta^{5/2}}{\sqrt{\beta}}$

Keeping only the lowest order term in (7.252a) turns (7.250) into

$$C_V \approx 2\sqrt{2\pi}\; k_B\, \beta^{3/2}\, N(0)\, \Delta_0^{5/2}\, e^{-\beta\Delta_0} \qquad (7.254)$$

C_V as given by (7.254) is twice that given by Reichl's (7.254). However, it agrees with that given by (51.61) of the text "Quantum Theory of Many-Particle Systems" by A.L.Fetter & J.D.Walecka, McGraw Hill (1971).

See Fetter & Walecka for a more comprehensive discussion of the BCS theory.

Code

```
(* (a) & (b)  *)
eq = { e == (u* u - v* v) ξ - u v* Δ - u* v Δ*,
        2 u v ξ + u^2 Δ - v^2 Δ* == 0,
        2 u* v* ξ - (v*)^2 Δ + (u*)^2 Δ* == 0,
        u* u + v* v == 1};
```

In[∘]:= `Eliminate[eq, {u, v}]`

Out[∘]= $\xi^2 + \Delta\, \text{Conjugate}[\Delta] == e^2$

In[∘]:= `Tanh[∞]`

Out[∘]= 1

In[∘]:= $\int \frac{1}{\sqrt{\xi^2+\Delta^2}}\, d\xi$ `// FullSimplify`

Out[∘]= $\text{ArcTanh}\left[\frac{\xi}{\sqrt{\Delta^2+\xi^2}}\right]$

In[∘]:= `ArcTanh[x] + O[x]^3`

Out[∘]= $x + O[x]^3$

In[∘]:= `Ek[k_, μ_, Δ_, Δε_] :=` $\begin{cases} \mu + \left(\frac{1}{2}k^2-\mu\right)\sqrt{1+\Delta^2\Big/\left(\frac{1}{2}k^2-\mu\right)^2} & \left(\frac{1}{2}k^2-\mu\right)^2 \le \Delta\varepsilon^2 \\ \frac{1}{2}k^2 & \text{True} \end{cases}$

In[∘]:=
```
(* Fig.7.24a *)
{μ, Δ, Δε} = {1, .01, .05};
```

```
In[•]:= Plot[{1/2 k^2, Ek[k, μ, Δ, Δε]}, {k, -1.5, 1.5},
      AxesLabel → {"k", "E"},
      Ticks → {{{-√(2 μ), "-kμ"}, {√(2 μ), "kμ"}}, None},
      PlotLegends → {"εk", "Ek+μ'"},
      Prolog → {Orange, {Dashed, Line[{{-√(2 μ), μ + Δ}, {√(2 μ), μ + Δ}}]},
            Line[{{√(2 (μ - Δε)), μ - Δε}, {√(2 (μ - Δε)), Ek[√(2 (μ - Δε)), μ, Δ, Δε]}}],

    Line[{{-√(2 (μ - Δε)), μ - Δε}, {-√(2 (μ - Δε)), Ek[√(2 (μ - Δε)), μ, Δ, Δε]}}],
            Green, {Dashed, Line[{{-√(2 μ), μ - Δ}, {√(2 μ), μ - Δ}}]},

    Line[{{√(2 (μ + Δε)), μ + Δε}, {√(2 (μ + Δε)), Ek[√(2 (μ + Δε)), μ, Δ, Δε]}}],
            Line[{{-√(2 (μ + Δε)), μ + Δε},
      {-√(2 (μ + Δε)), Ek[√(2 (μ + Δε)), μ, Δ, Δε]}}]
  }

]
(* Fig.7.24b *)
y0 = μ - .1;
Plot[{1/2 k^2, Ek[k, μ, Δ, Δε]}, {k, 1.32, 1.46},
      PlotRange → All,
      AxesLabel → {"k", "E"},
      Ticks →
  {{{-√(2 μ), "-kμ"}, {√(2 μ), "kμ"}, {√(2 (μ - Δε)), "kΔ-"}, {√(2 (μ + Δε)), "kΔ+"}},
     {{μ - Δ, "μ'-Δ"}, {μ + Δ, "μ'+Δ"}}},
      PlotLegends → {"εk", "Ek+μ'"},
      Prolog → { Dashed, Line[{{√(2 μ), y0}, {√(2 μ), μ + Δ}}],
            Orange, {Dashed, Line[{{0, μ + Δ}, {√(2 μ), μ + Δ}}]},
            Line[{{√(2 (μ + Δε)), y0}, {√(2 (μ + Δε)), Ek[√(2 (μ + Δε)), μ, Δ, Δε]}}],
            Green, {Dashed, Line[{{0, μ - Δ}, {√(2 μ), μ - Δ}}]},
            Line[{{√(2 (μ - Δε)), y0}, {√(2 (μ - Δε)), Ek[√(2 (μ - Δε)), μ, Δ, Δε]}}]

  }

]
```

$$-\frac{\partial \langle n_k \rangle}{\partial E_k}$$

```
f[e_, β_] := β e^(β e) / (e^(β e) + 1)^2
```

```
(* Fig.7.24d *)
Plot[{f[e, 1], f[e, 100]}, {e, -5, 5},
     AxesLabel → {"Ek", " -∂⟨nk⟩/∂Ek"},
     PlotLegends → { "β = 1", "β = 100"}
]
```

In[∘]:=
```
(* Fig.7.24c *)
Plot[Log[x] Sech[x]^2, {x, 5, 20},
     AxesLabel → {"x", "(ln x) sech^2x"},
     PlotRange → All
]
```

```
(* (7.236) *)
∫_0^∞ Log[x] Sech[x]^2 dx
```

Out[∘]=
```
-EulerGamma + Log[π/4]
```

In[∘]:=
```
{Tanh[10.], EulerGamma, 4/π Exp[EulerGamma]} // N
```

Out[∘]=
```
{1., 0.577216, 2.26773}
```

In[∘]:=
```
α = 4/π ⅇ^EulerGamma // N;

eq[T_, Δ_, Δε_] := 1/Log[2 Δε] NIntegrate[1/Sqrt[x^2 + Δ^2] Tanh[2/(α T) Sqrt[x^2 + Δ^2]], {x, 0, Δε}]
```

In[∘]:=
```
Δs[T_, Δε_: 10^5] := Δ /. FindRoot[eq[T, Δ, Δε] == 1, {Δ, 0.4}]
```

Plot of Fig.7.24 is time consuming. Also, ignore the warning messages.

In[∘]:=
```
(* Fig.7.24) *)
Plot[{Δs[T, 3], Δs[T, 10], Δs[T, 100]}, {T, 0, 1},
     PlotRange → {{-.1, 1.1}, {-.1, 1.1}},
     AxesLabel → {"T/TC", "Δ/Δ0"},
     Ticks → {{0, 1}, {0, 1}},
     PlotLegends → {"Δε/Δ0=3", "Δε/Δ0=10", "Δε/Δ0=100"},
     Epilog → Text["0", -.05 {1, 1}]
]
```