# BCS

PRELIMINARY NOTES (IN PROGRESS) BY L. G. MOLINARI

## 1. The BCS Hamiltonian

In electronic systems the low temperature properties are determined by the long-lived quasi-particles in an energy shell $\sim k_B T$ near the Fermi surface. Because of the Debye cutoff, the interaction mediated by phonons

$$U_{\rm ph}(k,\omega) = g\frac{v_s^2 k^2}{\omega^2 - v_s^2 k^2}\theta(\omega_D - v_s\, k)$$

is attractive in the energy shell $|\epsilon - \epsilon_F| < \hbar\omega_D$ and this, at low enough temperatures, leads to the formation of Cooper pairs with binding energy $\Delta \sim \hbar\omega_D \exp(-2/g\rho_F)$ characterising a superconductive phase, with critical temperature $k_B T_C \sim \Delta$. Cooper obtained this important result (1956) by solving a 2-particle problem in presence of a filled Fermi sea [3].
The BCS theory (1957)[1] is a full many-electron model, characterized by the attractive interaction that arises in the static limit, $-g\delta(\mathbf{x}-\mathbf{x}')$, which captures the essence [2]:

$$\hat K = \sum_{\mu\nu}\int d\mathbf{x}\, \delta_{\mu\nu}(\hat\psi^\dagger_\mu k_x \hat\psi_\nu)(\mathbf{x}) - \frac{g}{2}(\hat\psi^\dagger_\mu\hat\psi^\dagger_\nu\hat\psi_\nu\hat\psi_\mu)(\mathbf{x}) \tag{1}$$

where $k_x = \frac{1}{2m}(\mathbf{p}+\frac{e}{c}\mathbf{A})^2 + U(\mathbf{x}) - \mu$ and the Debye cut-off is understood for the interaction. By the exclusion principle, only two spin configurations are allowed, and are equivalent: $\hat\psi^\dagger_\uparrow\hat\psi^\dagger_\downarrow\hat\psi_\downarrow\hat\psi_\uparrow = \hat\psi^\dagger_\downarrow\hat\psi^\dagger_\uparrow\hat\psi_\uparrow\hat\psi_\downarrow$. The quartic interaction gets simplified by replacing pairs of operators with their mean values,

$$\hat\psi^\dagger_\downarrow\hat\psi^\dagger_\uparrow\hat\psi_\uparrow\hat\psi_\downarrow \approx \langle\hat\psi^\dagger_\downarrow\hat\psi^\dagger_\uparrow\rangle\hat\psi_\uparrow\hat\psi_\downarrow + \hat\psi^\dagger_\downarrow\hat\psi^\dagger_\uparrow\langle\hat\psi_\uparrow\hat\psi_\downarrow\rangle$$

This introduces a complex field $\Delta$, which behaves as an order parameter that can be related to the Ginzburg Landau field:

$$\boxed{\Delta(x) = -g\langle\, \hat\psi_\uparrow(x)\hat\psi_\downarrow(x)\rangle} \tag{2}$$

The thermal average is calculated with the effective Hamiltonian, that no longer conserves the number of electrons

$$\hat K_{\rm eff} = \hat K_0 + \int d\mathbf{x}\, \overline{\Delta}(\mathbf{x})\, \hat\psi_\uparrow(\mathbf{x})\hat\psi_\downarrow(\mathbf{x}) + \hat\psi^\dagger_\downarrow(\mathbf{x})\hat\psi^\dagger_\uparrow(\mathbf{x})\,\Delta(\mathbf{x}). \tag{3}$$

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[1] At the time, Leon Cooper and Robert Schrieffer were respectively post-doc and graduate student of John Bardeen. Read the nice hystorical account by Hoddeson [7]

1.1. **The Hartree approximation.** To gain some understanding of the approximation, let $\hat{K} = \hat{K}_0 + \hat{K}_1$, where $\hat{K}_1$ is the quartic term, and consider the (thermal) interaction picture. A thermal average of field operators is

$$\langle \mathcal{T}\hat{\psi}(x_1)\hat{\psi}(x_2)\dots\rangle_K = \frac{\langle \mathcal{T}\mathscr{U}_I(\hbar\beta,0)\hat{\psi}(x_1)\hat{\psi}(x_2)\dots\rangle_{K_0}}{\langle \mathscr{U}_I(\hbar\beta,0)\rangle_{K_0}}.$$

where $x = (\mathbf{x},\tau)$. Consider the discretization of Dyson's T-product expansion:

$$\begin{aligned}\mathscr{U}_I(\hbar\beta,0) &= \mathcal{T}\exp\left(-\frac{1}{\hbar}\right)\sum_x \left[-g\,(\hat{\psi}^\dagger_\downarrow\hat{\psi}^\dagger_\uparrow)(x^+)(\hat{\psi}_\uparrow\hat{\psi}_\downarrow)(x)\right]\\ &= \mathcal{T}\prod_x \exp\left[+\frac{g}{\hbar}\,(\hat{\psi}^\dagger_\downarrow\hat{\psi}^\dagger_\uparrow)(x^+)(\hat{\psi}_\uparrow\hat{\psi}_\downarrow)(x)\right]\end{aligned}$$

where, because with time-ordering, the quadratic operators commute. The four-fermion interaction may be splitted with the introduction of an auxiliary complex field $\Delta'(x)$. At each point $x$ the following complex integral applies

$$\exp\left[\frac{g}{\hbar}AB\right] = \int \frac{d^2z}{\pi g}\exp\left[-\frac{1}{\hbar}\left(\frac{1}{g}|z|^2 + \overline{z}A + Bz\right)\right]$$

With $z = \Delta'(x)$, we obtain a product of integrals which defines a Gaussian functional integral, where all pairs of operators commute because of $\mathcal{T}$-ordering:

$$\begin{aligned}\mathscr{U}_I(\hbar\beta,0) =&\mathcal{T}\prod_x\int\frac{d^2\Delta'(x)}{\pi g}\exp\left[-\frac{1}{\hbar g}|\Delta'(x)|^2 - \frac{1}{\hbar}(\overline{\Delta}'\hat{\psi}_\uparrow\hat{\psi}_\downarrow + \hat{\psi}^\dagger_\downarrow\hat{\psi}^\dagger_\uparrow\Delta')(x)\right]\\ =&\frac{1}{Z_\Delta}\int\mathscr{D}\Delta'\;\mathcal{T}\exp\left[-\frac{1}{\hbar}S[\Delta',\overline{\Delta}']\right]\end{aligned}$$

$S = \int dx(\frac{1}{g}|\Delta'|^2 + \overline{\Delta}'\hat{\psi}_\uparrow\hat{\psi}_\downarrow + \hat{\psi}^\dagger_\downarrow\hat{\psi}^\dagger_\uparrow\Delta')$, $Z_\Delta = \int\mathscr{D}\Delta'\;\exp\left[-\frac{1}{\hbar g}\int dx|\Delta'(x)|^2\right]$.
The partition function is $Z = Z_0\langle\mathscr{U}_I(\hbar\beta,0)\rangle_{K_0}$, with $Z_0 = \mathrm{tr}\,(e^{-\beta K_0})$ and

$$\langle\mathscr{U}_I(\hbar\beta,0)\rangle_{K_0} = \frac{1}{Z_\Delta}\int\mathscr{D}'\Delta\left\langle\mathcal{T}e^{-\frac{1}{\hbar}S[\Delta',\overline{\Delta}']}\right\rangle_{K_0} \tag{4}$$

Now comes the approximation: the main contribution to the functional integral comes from the auxiliary field $\Delta(x)$ that maximises the Boltzmann weight $\langle\mathcal{T}e^{-S/\hbar}\rangle$. The extremum condition for a variation $\delta\bar{\Delta}'$ is an equation for $\Delta(x)$. By retaining only linear terms:

$$\begin{aligned}&\langle\mathcal{T}\exp(-\frac{1}{\hbar}S[\Delta',\bar{\Delta}'+\delta\bar{\Delta}'])\rangle_{K_0}\\ &= \langle\mathcal{T}\exp(-\frac{1}{\hbar}S[\Delta',\bar{\Delta}'])\left[1+\int dx\delta\bar{\Delta}'(x)\left[g^{-1}\Delta'(x)+\hat{\psi}_\uparrow(x)\hat{\psi}_\downarrow(x)\right]+\dots\right]\rangle_{K_0}\end{aligned}$$

The first variation is zero for

$$\Delta(x) = -g\frac{\langle\mathcal{T}e^{-\frac{1}{\hbar}S[\Delta,\overline{\Delta}]}\hat{\psi}_\uparrow(x)\hat{\psi}_\downarrow(x)\rangle_{K_0}}{\langle e^{-\frac{1}{\hbar}S[\Delta,\overline{\Delta}]}\rangle_{K_0}} \tag{5}$$

This is an equation for $\Delta(\mathbf{x})$, which appears on both sides (time-dependence cancels because of equal times). The integral (6) simplifies:

$$\langle\mathscr{U}_I(\hbar\beta,0)\rangle_{K_0} \approx\; N_\Delta\left\langle\mathcal{T}e^{-\frac{1}{\hbar}S[\Delta,\overline{\Delta}]}\right\rangle_{K_0} = e^{\beta\hat{K}_0}e^{-\beta\hat{K}_{\mathrm{eff}}} \tag{6}$$

$N_\Delta$ is a normalization factor. The equation for $\Delta$ corresponds to eq.(2) with the effective Hamiltonian (7) (see Zagoskin, [10]).

**Exercise 1.1.** Prove that, if $A$ and $B$ commute, then

$$\int dx\,dy\ \exp(-\frac{1}{g}|z|^2 + \overline{z}A + Bz) = \pi g \exp(gAB), \qquad z = x + iy$$

1.2. **Matrix formulation.** In the operator $\hat{K}_0$ an integration by parts and an anticommutation bring $\hat{\psi}_\uparrow^\dagger k_x \hat{\psi}_\uparrow$ to $-\hat{\psi}_\uparrow \overline{k}_x \hat{\psi}_\uparrow^\dagger$ up to a constant[2]. Then:

$$\hat{K}_{\text{eff}} = \int d\mathbf{x}\ \left[-\hat{\psi}_\uparrow \overline{k}_x \hat{\psi}_\uparrow^\dagger + \hat{\psi}_\downarrow^\dagger k_x \hat{\psi}_\downarrow + \overline{\Delta}\hat{\psi}_\uparrow\hat{\psi}_\downarrow + \hat{\psi}_\downarrow^\dagger\hat{\psi}_\uparrow^\dagger\Delta\right]$$

The Hamiltonian is now written in a matrix form introduced by Nambu [8]:

$$\boxed{\hat{K}_{\text{eff}} = \int d\mathbf{x}\, \Psi^\dagger(\mathbf{x})(\mathbb{K}_x\Psi)(\mathbf{x})} \tag{7}$$

$$\mathbb{K}_x = \begin{bmatrix} k_x & \Delta(\mathbf{x}) \\ \overline{\Delta}(\mathbf{x}) & -\overline{k}_x \end{bmatrix},\ \Psi(\mathbf{x}) = \begin{bmatrix} \hat{\psi}_\downarrow(\mathbf{x}) \\ \hat{\psi}_\uparrow^\dagger(\mathbf{x}) \end{bmatrix},\ \Psi^\dagger(\mathbf{x}) = \left[\hat{\psi}_\downarrow^\dagger(\mathbf{x}),\ \hat{\psi}_\uparrow(\mathbf{x})\right] \tag{8}$$

The components of $\Psi$ and $\Psi^\dagger$ anticommute (note that $(\Psi_r)^\dagger = (\Psi^\dagger)_r$):

$$\{\Psi_r(\mathbf{x}), \Psi_s^\dagger(\mathbf{y})\} = \delta_{rs}\delta_3(\mathbf{x}-\mathbf{y}), \qquad \{\Psi_r, \Psi_s\} = \{\Psi_r^\dagger, \Psi_s^\dagger\} = 0 \tag{9}$$

As the effective Hamiltonian is quadratic in the fields, the model can be solved like a theory of independent particles or a Hartree theory, with the self-consistency eq.(2), named *gap equation*.
Two equivalent approaches are presented: one, by de Gennes, generalises the canonical transformation introduced by Bogoljubov and Valatin (1958) for homogeneous systems; the other one is based on Green functions, introduced by Gor'kov in 1958 [5] and here expressed with Nambu's matrix formalism.

1.3. **The Bogoljubov - de Gennes equations.** The matrix operator $\mathbb{K}_x$ acts on the Hilbert space $L^2(\mathbb{R}^3)\times\mathbb{C}^2$ and is self-adjoint. It has real eigenvalues, and the eigenvectors form an orthonormal basis. The eigenvalue equation

$$\boxed{\begin{bmatrix} k_x & \Delta(\mathbf{x}) \\ \overline{\Delta}(\mathbf{x}) & -\overline{k}_x \end{bmatrix}\begin{bmatrix} u_a(\mathbf{x}) \\ v_a(\mathbf{x}) \end{bmatrix} = E_a \begin{bmatrix} u_a(\mathbf{x}) \\ v_a(\mathbf{x}) \end{bmatrix}} \tag{10}$$

gives the pair of *Bogoljubov - de Gennes equations*:

$$(ku_a)(\mathbf{x}) + \Delta(\mathbf{x})v_a(\mathbf{x}) = E_a u_a(\mathbf{x})$$
$$(\overline{k}v_a)(\mathbf{x}) - \overline{\Delta}(\mathbf{x})u_a(\mathbf{x}) = -E_a v_a(\mathbf{x})$$

If $(u_a,\, v_a)$ solve them with eigenvalue $E_a > 0$, then $(-\overline{v}_a,\, \overline{u}_a)$ are a solution with eigenvalue $-E_a$. The equations (10) with eigenvalues $\pm E_a$ may be written jointly:

$$\mathbb{K}_x \begin{bmatrix} u_a(\mathbf{x}) & -\overline{v}_a(\mathbf{x}) \\ v_a(\mathbf{x}) & \overline{u}_a(\mathbf{x}) \end{bmatrix} = \begin{bmatrix} u_a(\mathbf{x}) & -\overline{v}_a(\mathbf{x}) \\ v_a(\mathbf{x}) & \overline{u}_a(\mathbf{x}) \end{bmatrix}\begin{bmatrix} E_a & 0 \\ 0 & -E_a \end{bmatrix} \tag{11}$$

[2]The operators $k_x$ and $\overline{k}_x$ differ by the sign of the term linear in $\mathbf{p}$, if any.

The ortho-normalization and completeness of the doublets in Hilbert space may be expressed in matrix form:

$$\int d\mathbf{x} \begin{bmatrix} \overline{u}_b(\mathbf{x}) & \overline{v}_b(\mathbf{x}) \\ -v_b(\mathbf{x}) & u_b(\mathbf{x}) \end{bmatrix} \begin{bmatrix} u_a(\mathbf{x}) & -\overline{v}_a(\mathbf{x}) \\ v_a(\mathbf{x}) & \overline{u}_a(\mathbf{x}) \end{bmatrix} = \delta_{ab}\, \mathbb{I}_2 \tag{12}$$

$$\sum_a \begin{bmatrix} u_a(\mathbf{x}) & -\overline{v}_a(\mathbf{x}) \\ v_a(\mathbf{x}) & \overline{u}_a(\mathbf{x}) \end{bmatrix} \begin{bmatrix} \overline{u}_a(\mathbf{y}) & \overline{v}_a(\mathbf{y}) \\ -v_a(\mathbf{y}) & u_a(\mathbf{y}) \end{bmatrix} = \delta(\mathbf{x}-\mathbf{y})\, \mathbb{I}_2 \tag{13}$$

1.4. **Diagonalization of the many-body Hamiltonian.** The matrix relation (11) suggests that the many body Hamiltonian is diagonalized by the following transformation to new operators:

$$\begin{bmatrix} \hat\psi_\downarrow(\mathbf{x}) \\ \hat\psi_\uparrow^\dagger(\mathbf{x}) \end{bmatrix} = \sum_a \begin{bmatrix} u_a(\mathbf{x}) & -\overline{v}_a(\mathbf{x}) \\ v_a(\mathbf{x}) & \overline{u}_a(\mathbf{x}) \end{bmatrix} \begin{bmatrix} \hat\alpha_a \\ \hat\beta_a^\dagger \end{bmatrix} \tag{14}$$

This and the adjoint are, in detail:

$$\hat\psi_\downarrow(\mathbf{x}) = \sum_a u_a(\mathbf{x})\hat\alpha_a - \overline{v}_a(\mathbf{x})\hat\beta_a^\dagger, \quad \hat\psi_\downarrow^\dagger(\mathbf{x}) = \sum_a \overline{u}_a(\mathbf{x})\hat\alpha_a^\dagger - v_a(\mathbf{x})\hat\beta_a \tag{15}$$

$$\hat\psi_\uparrow(\mathbf{x}) = \sum_a \overline{v}_a(\mathbf{x})\hat\alpha_a^\dagger + u_a(\mathbf{x})\hat\beta_a, \quad \hat\psi_\uparrow^\dagger(\mathbf{x}) = \sum_a v_a(\mathbf{x})\hat\alpha_a + \overline{u}_a(\mathbf{x})\hat\beta_a^\dagger \tag{16}$$

Inversion is done with the aid of (12):

$$\begin{bmatrix} \hat\alpha_a \\ \hat\beta_a^\dagger \end{bmatrix} = \int d\mathbf{x} \begin{bmatrix} \overline{u}_a(\mathbf{x}) & \overline{v}_a(\mathbf{x}) \\ -v_a(\mathbf{x}) & u_a(\mathbf{x}) \end{bmatrix} \begin{bmatrix} \hat\psi_\downarrow(\mathbf{x}) \\ \hat\psi_\uparrow^\dagger(\mathbf{x}) \end{bmatrix} \tag{17}$$

The adjoint operators are also obtained. The transformation is canonical i.e. the new operators have canonical anticommutation relations:

$$\{\hat\alpha_a, \hat\alpha_b^\dagger\} = \delta_{ab}, \qquad \{\hat\beta_a, \hat\beta_b^\dagger\} = \delta_{ab} \tag{18}$$

(all other anticommutators vanish). By eq.(11)

$$(\mathbb{K}_x\Psi)(\mathbf{x}) = \sum_a \begin{bmatrix} u_a(\mathbf{x}) & -\overline{v}_a(\mathbf{x}) \\ v_a(\mathbf{x}) & \overline{u}_a(\mathbf{x}) \end{bmatrix} \begin{bmatrix} E_a & 0 \\ 0 & -E_a \end{bmatrix} \begin{bmatrix} \hat\alpha_a \\ \hat\beta_a^\dagger \end{bmatrix}$$

Evaluation of $\hat K_{\rm eff} = \int d\mathbf{x}\, \Psi^\dagger \mathbb{K}\Psi$ and (12) give a diagonal operator for quasiparticles (*bogolons*):

$$\boxed{\hat K_{\rm eff} = U_0 + \sum_a E_a[\hat\alpha_a^\dagger\hat\alpha_a + \hat\beta_a^\dagger\hat\beta_a]} \tag{19}$$

where $U_0 = -\sum_a E_a$. The ground state is defined by $\hat\alpha_a|BCS\rangle = 0$ and $\hat\beta_a|BCS\rangle = 0$ for all $a$.

1.5. **The gap equation.** The change of basis (15) simplifies the gap equation: $\Delta(\mathbf{x}) = -g\sum_{ab} u_a(\mathbf{x})\overline{v}_b(\mathbf{x})\langle\hat\alpha_a^\dagger\hat\alpha_b\rangle - \overline{v}_a(\mathbf{x})u_b(\mathbf{x})\langle\hat\beta_a\hat\beta_b^\dagger\rangle = g\sum_a u_a(\mathbf{x})\overline{v}_a(\mathbf{x})[1 - 2n(E_a)]$ where $n(E_a)$ is the Fermi-Dirac occupation number of the state with energy $E_a$. Then:

$$\boxed{\Delta(\mathbf{x}) = g\sum_a u_a(\mathbf{x})\overline{v}_a(\mathbf{x}) \tanh\left(\frac{\beta}{2}E_a\right)} \tag{20}$$

The equation must be solved self-consistently with the Bogoljubov - de Gennes equations for $u_a$ and $v_a$.

**Remark 1.2.** *As the gap function depends on temperature, the amplitudes $u_a$, $v_a$ as well as the energies $E_a$ and $|BCS\rangle$ depend on $T$.*

**Exercise 1.3.** Show that $\Omega = -\frac{2}{\beta}\sum_a \log\left(2\cosh\frac{1}{2}\beta E_a\right)$.

**Exercise 1.4.** Show that the average density of electrons is:

$$n(\mathbf{x}) = \sum_a |u_a(\mathbf{x})|^2 n_a + |v_a(\mathbf{x})|^2(1-n_a), \qquad n_a = \frac{1}{e^{\beta E_a}+1} \tag{21}$$

1.6. **Nambu - Gorkov theory.** There are advantages in studying the BCS model with the Green function formalism. The imaginary time evolution of operators is $O(\tau) = e^{\tau K/\hbar} O e^{-\tau K/\hbar}$, where $K$ is the effective hamiltonian (7). The equation of motion of $\Psi(\mathbf{x},\tau)$ is:

$$\begin{aligned}
-\hbar\frac{\partial}{\partial\tau}\Psi_r(\mathbf{x},\tau) &= e^{\frac{1}{\hbar}\tau K}[\Psi_r(\mathbf{x}), K]e^{-\frac{1}{\hbar}\tau K} \\
&= e^{\frac{1}{\hbar}\tau K}\int d\mathbf{x}'[\Psi_r(\mathbf{x}), \Psi^\dagger_{s'}(\mathbf{x}')(\mathbb{K}_{s's}\Psi_s)(\mathbf{x}')e^{-\frac{1}{\hbar}\tau K} \\
&= e^{\frac{1}{\hbar}\tau K}\int d\mathbf{x}'\{\Psi_r(\mathbf{x}), \Psi^\dagger_{s'}(\mathbf{x}')\}(\mathbb{K}_{s's}\Psi_s)(\mathbf{x}')e^{-\frac{1}{\hbar}\tau K} \\
&= (\mathbb{K}_{rs}\Psi_s)(\mathbf{x},\tau)
\end{aligned}$$

Let us introduce the thermal Nambu propagator

$$\boxed{-\mathbb{G}(x,x') = \langle \mathcal{T}\Psi(x)\Psi^\dagger(x')\rangle} \tag{22}$$

It is a matrix with components

$$\mathbb{G}(x,x') = -\begin{bmatrix} \langle\mathcal{T}\psi_\downarrow(x)\psi^\dagger_\downarrow(x')\rangle & \langle\mathcal{T}\psi_\downarrow(x)\psi_\uparrow(x')\rangle \\ \langle\mathcal{T}\psi^\dagger_\uparrow(x)\psi^\dagger_\downarrow(x')\rangle & \langle\mathcal{T}\psi^\dagger_\uparrow(x)\psi_\uparrow(x')\rangle \end{bmatrix} = \begin{bmatrix} \mathscr{G}(x,x') & \mathscr{F}(x,x') \\ \mathscr{F}^\dagger(x,x') & -\mathscr{G}(x',x) \end{bmatrix}$$

Note the sign and the exchange of $x$ and $x'$ in one component. The correlators $\mathscr{F}$ and $\mathscr{F}^\dagger$ are named *anomalous* and vanish in the normal phase. In particular:

$$\boxed{\Delta(\mathbf{x}) = -g\mathscr{F}(x,x^+)} \tag{23}$$

The equation of motion of the Nambu propagator,

$$\left[\hbar\frac{\partial}{\partial\tau} + \mathbb{K}_x\right]\mathbb{G}(x,x') = -\hbar\delta_4(x-x')\,\mathbb{I}_2 \tag{24}$$

simplifies in Matsubara (odd) frequency space:

$$\begin{bmatrix} -i\hbar\omega_n + k_x & \Delta(\mathbf{x}) \\ \overline{\Delta}(\mathbf{x}) & -i\hbar\omega_n - \overline{k}_x \end{bmatrix}\mathbb{G}(\mathbf{x},\mathbf{x}';i\omega_n) = -\hbar\delta_3(\mathbf{x}-\mathbf{x}')\,\mathbb{I}_2 \tag{25}$$

$$\mathbb{G}(\mathbf{x},\mathbf{x}',i\omega_n) = \begin{bmatrix} \mathscr{G}(\mathbf{x},\mathbf{x}',i\omega_n) & \mathscr{F}(\mathbf{x},\mathbf{x}',i\omega_n) \\ \mathscr{F}^\dagger(\mathbf{x},\mathbf{x}',i\omega_n) & -\mathscr{G}(\mathbf{x}',\mathbf{x},-i\omega_n) \end{bmatrix} \tag{26}$$

**Exercise 1.5.** The propagators can be represented as expansions in the Bogoljubov - de Gennes eigenstates. Show that:

$$\mathscr{G}(\mathbf{x},\mathbf{x}',i\omega_n) = \sum_a \frac{u_a(\mathbf{x})\overline{u}_a(\mathbf{x}')}{i\omega_n - E_a/\hbar} + \frac{\overline{v}_a(\mathbf{x})v_a(\mathbf{x}')}{i\omega_n + E_a/\hbar} \tag{27}$$

$$\mathscr{F}(\mathbf{x},\mathbf{x}',i\omega_n) = \sum_a -\frac{u_a(\mathbf{x})\overline{v}_a(\mathbf{x}')}{i\omega_n - E_a/\hbar} + \frac{\overline{v}_a(\mathbf{x})u_a(\mathbf{x}')}{i\omega_n + E_a/\hbar} \tag{28}$$

and recover the gap equation (20) by evaluating the Matsubara sum

$$\Delta(\mathbf{x}) = -g\frac{1}{\hbar\beta}\sum_n \mathscr{F}(\mathbf{x},\mathbf{x},i\omega_n)e^{i\omega_n\eta}$$

1.7. **Perturbative expansion.** When $\Delta = 0$, eq.(25) is solved by the normal Nambu propagator $\mathbb{G}_n(x,x')$, which can be used to transform (25) into a Dyson equation (integration and summation of repeated variables is implicit):

$$\mathbb{G}(x,y) = \mathbb{G}_n(x,y) + \frac{1}{\hbar}\mathbb{G}_n(x,x')\mathbb{D}(\mathbf{x}')\mathbb{G}(x',y), \quad \mathbb{D}(\mathbf{x}) = \begin{bmatrix} 0 & \Delta \\ \overline{\Delta} & 0 \end{bmatrix} \tag{29}$$

In BCS model the self-energy $\mathbb{D}$ is local and time-independent. When this description is inadeguate, one has to consider a microscopic model with the actual phonon-electron interaction. The Dyson's equation becomes

$$\mathbb{G}(x,y) = \mathbb{G}_n(x,y) + \mathbb{G}_n(x,x')\mathbb{S}(x',x'')\mathbb{G}(x'',y). \tag{30}$$

where $\mathbb{S}$ is a non-local self-energy matrix. In a 1-phonon exchange approximation, $\mathbb{S}(x,y) = -\frac{1}{\hbar}\mathbb{G}(x,y)U^0_{\rm ph}(x-y)$, the coupled equations for $\mathscr{G}$ and $\mathscr{F}$ are:

$$\mathscr{G}(x,y) = \mathscr{G}_n(x,y) + \mathscr{G}_n(x,x')S_{11}(x',x'')\mathscr{G}(x'',y) + \mathscr{G}_n(x,x')S_{12}(x',x'')\mathscr{F}(x'',y)$$
$$\mathscr{F}(x,y) = -\mathscr{G}_n(x,x')S_{12}(x',x'')\mathscr{G}(y,x'') + \mathscr{G}_n(x,x')S_{11}(x',x'')\mathscr{F}(x'',y).$$

with the addition of the gap equation.

## 2. Homogeneous systems

In homogeneous problems there is no external field and $\Delta$ is constant. An analytic solution is found in momentum space.

2.1. **The Bogoljubov - Valatin canonical transformation.** We seek for a solution of the Bogoljubov - de Gennes equations of the form

$$\begin{bmatrix} u_k(\mathbf{x}) \\ v_k(\mathbf{x}) \end{bmatrix} = \frac{e^{i\mathbf{k}\cdot\mathbf{x}}}{\sqrt{V}}\begin{bmatrix} u_k \\ v_k \end{bmatrix} \tag{31}$$

Then

$$\begin{bmatrix} \xi_k & \Delta \\ \overline{\Delta} & -\xi_k \end{bmatrix}\begin{bmatrix} u_k \\ v_k \end{bmatrix} = E_k\begin{bmatrix} u_k \\ v_k \end{bmatrix}$$

where $\xi_k = \epsilon_k - \mu$ are the single-particle energies (normal phase) measured with respect to the chemical potential. The homogeneous system admits a nontrivial solution if

$$\boxed{E_k = \sqrt{\xi_k^2 + |\Delta|^2}} \tag{32}$$

(the positive root is selected for stability). The **energy gap** $|\Delta|$ separating the Fermi surface $\xi = 0$ from the lowest excitation, profoundly modifies the properties of the electron gas at low temperatures.

The amplitudes solve the normalization condition $|u_k|^2 + |v_k|^2 = 1$ and the condition $\xi_k u_k + \Delta\, v_k = E_k u_k$. The latter gives $|\Delta||v_k| = (E_k - \xi_k)|u_k|$, with solutions

$$|u_k|^2 = \frac{1}{2}\left(1 + \frac{\xi_k}{E_k}\right), \quad |v_k|^2 = \frac{1}{2}\left(1 - \frac{\xi_k}{E_k}\right) \tag{33}$$

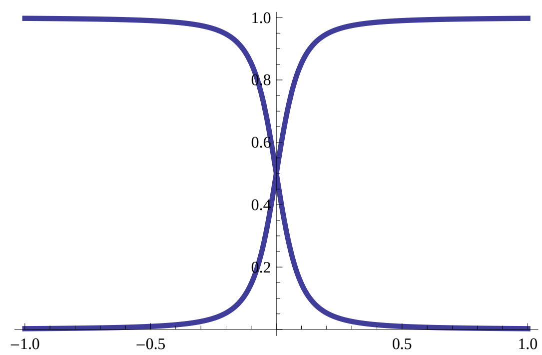


FIGURE 1. The parameters $|u_k|^2$ and $|v_k|^2$ as functions of $\xi_k$ for $|\Delta| = 0.1$.

In the normal phase $E_k = |\xi_k|$; then: $|u_k| = \theta(\epsilon_k - \mu)$ and $|v_k| = \theta(\mu - \epsilon_k)$.
The equation $\xi_k u_k + \Delta\, v_k = E_k u_k$ gives $\Delta |v_k|^2 = (E_k - \xi_k) u_k \overline{v}_k$ i.e. the useful relation:

$$u_k \overline{v}_k = \frac{\Delta}{2E_k} \tag{34}$$

The expansion of the field operators in the two canonical basis,

$$\begin{bmatrix} \hat\psi_\downarrow(\mathbf{x}) \\ \hat\psi^\dagger_\uparrow(\mathbf{x}) \end{bmatrix} = \sum_{\mathbf{k}} \frac{e^{i\mathbf{k}\cdot\mathbf{x}}}{\sqrt{V}} \begin{bmatrix} \hat a_{\mathbf{k},\downarrow} \\ \hat a^\dagger_{-\mathbf{k},\uparrow} \end{bmatrix} = \sum_{\mathbf{k}} \frac{e^{i\mathbf{k}\cdot\mathbf{x}}}{\sqrt{V}} \begin{bmatrix} u_k & -\overline{v}_k \\ v_k & \overline{u}_k \end{bmatrix} \begin{bmatrix} \hat\alpha_{\mathbf{k}} \\ \hat\beta^\dagger_{-\mathbf{k}} \end{bmatrix}$$

implies the Bogoljubov - Valatin transformation:

$$\begin{bmatrix} \hat a_{\mathbf{k},\downarrow} \\ \hat a^\dagger_{-\mathbf{k},\uparrow} \end{bmatrix} = \begin{bmatrix} u_k & -\overline{v}_k \\ v_k & \overline{u}_k \end{bmatrix} \begin{bmatrix} \hat\alpha_{\mathbf{k}} \\ \hat\beta^\dagger_{-\mathbf{k}} \end{bmatrix} \tag{35}$$

and the Hermitian conjugate. Inversion gives:

$$\hat\alpha_{\mathbf{k}} = \bar u_k \hat a_{\mathbf{k},\downarrow} + \bar v_k \hat a^\dagger_{-\mathbf{k},\uparrow}, \qquad \hat\alpha^\dagger_{\mathbf{k}} = u_k \hat a^\dagger_{\mathbf{k},\downarrow} + v_k \hat a_{-\mathbf{k},\uparrow} \tag{36}$$

$$\hat\beta_{\mathbf{k}} = -\bar v_k \hat a^\dagger_{-\mathbf{k},\downarrow} + \bar u_k \hat a_{\mathbf{k},\uparrow}, \qquad \hat\beta^\dagger_{\mathbf{k}} = -v_k \hat a_{-\mathbf{k},\downarrow} + u_k \hat a^\dagger_{\mathbf{k},\uparrow} \tag{37}$$

The operators $\hat\alpha_{\mathbf{k}}$ and $\hat\beta_{\mathbf{k}}$ annihilate, for all vectors $\mathbf{k}$, the state

$$|BCS\rangle = \prod_{\mathbf{k}} (\bar u_k + \bar v_k a^\dagger_{\mathbf{k}\uparrow} a^\dagger_{-\mathbf{k}\downarrow})|0\rangle \tag{38}$$

which reads as a sea of Cooper pairs[3]. In the normal phase ($\Delta = 0$) it coincides with the filled Fermi sphere.

$$\begin{aligned} \hat\alpha_{\mathbf{k}}|BCS\rangle &= \prod_{\mathbf{q}\neq\mathbf{k}} (\bar u_q + \bar v_q \hat a^\dagger_{-\mathbf{q}\uparrow} \hat a^\dagger_{\mathbf{q}\downarrow}) \hat\alpha_{\mathbf{k}} (\bar u_k + \bar v_k \hat a^\dagger_{-\mathbf{k}\uparrow} \hat a^\dagger_{\mathbf{k}\downarrow})|0\rangle \\ &= \prod_{\mathbf{q}\neq\mathbf{k}} (\bar u_q + \bar v_q \hat a^\dagger_{-\mathbf{q}\uparrow} \hat a^\dagger_{\mathbf{q}\downarrow})(\bar u_k \bar v_k \hat a_{\mathbf{k},\downarrow} \hat a^\dagger_{-\mathbf{k}\uparrow} \hat a^\dagger_{\mathbf{k}\downarrow} + \bar v_k \bar u_k \hat a^\dagger_{-\mathbf{k},\uparrow})|0\rangle = 0 \end{aligned}$$

[3]In [2] Bardeen, Cooper and Schrieffer (1957) introduced the state with variational parameters $u_k$ and $v_k$ with $|u_k|^2 + |v_k|^2 = 1$ for normalization. Minimization of $\langle BCS|\hat K_{\rm eff}|BCS\rangle$ with respect to the parameters yields the same results presented here. Bogoljubov and Valatin independently simplified the theory by their canonical transformation [1, 9].

$$\begin{aligned}\hat\beta_{-\mathbf{k}}|BCS\rangle &= \prod_{\mathbf{q}\neq\mathbf{k}}(\bar u_q+\bar v_q\hat a^\dagger_{-\mathbf{q}\uparrow}\hat a^\dagger_{\mathbf{q}\downarrow})\hat\beta_{-\mathbf{k}}(\bar u_k+\bar v_k\hat a^\dagger_{-\mathbf{k}\uparrow}\hat a^\dagger_{\mathbf{k}\downarrow})|0\rangle\\ &= \prod_{\mathbf{q}\neq\mathbf{k}}(\bar u_q+\bar v_q\hat a^\dagger_{-\mathbf{q}\uparrow}\hat a^\dagger_{\mathbf{q}\downarrow})(-\bar v_k\bar u_k\hat a^\dagger_{\mathbf{k},\downarrow}+\bar u_k\bar v_k\hat a_{-\mathbf{k}\uparrow}\hat a^\dagger_{-\mathbf{k}\uparrow}\hat a^\dagger_{\mathbf{k},\downarrow})|0\rangle=0\end{aligned}$$

Creation operators create excited states (bogolons) consisting of Cooper pairs and unpaired electrons. For example:

$$\begin{aligned}\hat\alpha^\dagger_{\mathbf{k}}|BCS\rangle &= \prod_{\mathbf{q}\neq\mathbf{k}}(\bar u_q+\bar v_q\hat a^\dagger_{-\mathbf{q}\uparrow}\hat a^\dagger_{\mathbf{q}\downarrow})\hat a^\dagger_{\mathbf{k}\downarrow}|0\rangle\\ \hat\beta^\dagger_{-\mathbf{k}}|BCS\rangle &= \prod_{\mathbf{q}\neq\mathbf{k}}(\bar u_q+\bar v_q\hat a^\dagger_{-\mathbf{q}\uparrow}\hat a^\dagger_{\mathbf{q}\downarrow})\hat a^\dagger_{\mathbf{k}\uparrow}|0\rangle\\ \hat\alpha^\dagger_{\mathbf{k}}\beta^\dagger_{-\mathbf{k}}|BCS\rangle &= \bar u_k\prod_{\mathbf{q}\neq\mathbf{k}}(\bar u_q+\bar v_q\hat a^\dagger_{-\mathbf{q}\uparrow}\hat a^\dagger_{\mathbf{q}\downarrow})\hat a^\dagger_{\mathbf{k}\downarrow}\hat a^\dagger_{\mathbf{k}\uparrow}|0\rangle\end{aligned}$$

2.2. **The gap equation.** By means of (34) the gap equation (20) becomes:

$$\Delta = g\frac{1}{V}\sum_{\mathbf{k}}\frac{\Delta}{2E_k}\tanh\left(\frac{\beta}{2}\mathrm{E_k}\right)\theta(\hbar\omega_\mathrm{D}-|\xi_\mathrm{k}|)$$

By introducing the density of states per unit volume and single spin component of the normal phase,

$$\rho_n(\xi)=\frac{1}{V}\sum_{\mathbf{k}}\delta(\xi-\xi_k)$$

the sum in **k**-space is changed into an integral in energy,

$$1=\frac{g}{2}\int d\xi\,\rho_n(\xi)\frac{\tanh\left(\frac12\beta\sqrt{\xi^2+|\Delta|^2}\right)}{\sqrt{\xi^2+|\Delta|^2}}\theta(\hbar\omega_D-|\xi|)$$

With the assumption that the density is almost constant in the energy shell $|\xi|<\hbar\omega_D$ it simplifies to:

$$\boxed{\frac{1}{g\rho_n(0)}=\int_0^{\hbar\omega_D}d\xi\frac{\tanh\left(\frac12\beta\sqrt{\xi^2+\Delta^2}\right)}{\sqrt{\xi^2+\Delta^2}}}\qquad(39)$$

gap equation

where $\rho(0)$ is the density of states at the Fermi energy, $g$ is the squared coupling constant of the phonon to the electron. According to the microscopic theory:

$$\sqrt{g}=\frac{z_c}{v_s}\sqrt{\frac{n_i}{M_i}}\pi^2e^2\frac{a_0}{k_F}$$

$z_c$ is the number of conducting electrons per ion, $n_i$ is the number of ions per unit volume, $M_i$ is the ionic mass, $v_s$ is the speed of sound.

**Exercise 2.1.** Show that the density of states per unit volume and spin component of the free electron gas at the Fermi energy is $\rho_n(0)=\frac34 n/E_F$, where $n$ is the density of electrons and $E_F$ is the Fermi energy. Then show that

$$g\rho_n(0)=\frac{z_c}{6}\frac{m}{M_i}\left(\frac{v_F}{v_s}\right)^2$$

where $m$ is the electron's mass and $v_F$ is the Fermi velocity.

2.3. **The Green functions.** In **k**-space the equation of motion (25) for the Nambu propagator is algebraic

$$\begin{bmatrix} i\hbar\omega_n - \xi_k & -\Delta \\ -\overline{\Delta} & i\hbar\omega_n + \xi_k \end{bmatrix} \mathbb{G}(k; i\omega_n) = \hbar\, \mathbb{I}_2$$

$$\mathbb{G}(k; i\omega_n) = \frac{-\hbar}{\hbar^2\omega_n^2 + \xi_k^2 + |\Delta|^2} \begin{bmatrix} i\hbar\omega_n + \xi_k & \Delta \\ \overline{\Delta} & i\hbar\omega_n - \xi_k \end{bmatrix}$$

The normal and anomalous propagators are obtained, with $E_k = \sqrt{\xi_k^2 + |\Delta|^2}$:

$$\mathscr{G}(k, i\omega_n) = -\hbar \frac{i\hbar\omega_n + \xi_k}{\hbar^2\omega_n^2 + E_k^2} = \frac{|u_k|^2}{i\omega_n - (E_k/\hbar)} + \frac{|v_k|^2}{i\omega_n + (E_k/\hbar)}$$

$$\mathscr{F}(k, i\omega_n) = -\hbar \frac{\Delta}{\hbar^2\omega_n^2 + E_k^2} = \frac{u_k\overline{v}_k}{i\omega_n - (E_k/\hbar)} - \frac{u_k\overline{v}_k}{i\omega_n + (E_k/\hbar)}$$

The Matsubara sum in the gap equation

$$\Delta = -\frac{g}{\hbar\beta} \sum_n \int \frac{d^3k}{(2\pi)^3} \mathscr{F}(k, i\omega_n) e^{i\omega_n \eta}$$

yields the expression (39).

**Example 2.2.** Show that the average number of electrons in a state $(\mathbf{k}, \sigma)$ is

$$n_k = \frac{1}{\hbar\beta} \sum_n \mathscr{G}(k, i\omega_n) = \frac{1}{2} - \frac{1}{2}\frac{\xi_k}{E_k} \tanh \frac{\beta \mathrm{E_k}}{2} \tag{40}$$

**Exercise 2.3** (spectral density)**.** Evaluate the spectral density of the superconducting phase

$$\rho_s(E) = \sum_{\mathbf{k}} |u_k|^2 \delta(E - E_k) + |v_k|^2 \delta(E + E_k)$$

(use the approximation $|\Delta| \ll \mu$). Note the presence of an energy gap of width $2\Delta$ centred at $E = 0$ (chemical potential).

$$\frac{\rho_s(E)}{\rho_n(0)} = \begin{cases} \frac{-E+\sqrt{E^2-\Delta^2}}{\sqrt{E^2-\Delta^2}} \sqrt{1 + \frac{E}{\mu}} + \frac{|E|-\sqrt{E^2-\Delta^2}}{\sqrt{E^2-\Delta^2}} \sqrt{1 - \frac{E}{\mu}} & -\mu < E < -\Delta \\ 0 & |E| < \Delta \\ \frac{E-\sqrt{E^2-\Delta^2}}{\sqrt{E^2-\Delta^2}} \sqrt{1 - \frac{E}{\mu}} + \frac{E+\sqrt{E^2-\Delta^2}}{\sqrt{E^2-\Delta^2}} \sqrt{1 + \frac{E}{\mu}} & \Delta < E < \mu \\ 2\sqrt{1 + \frac{E}{\mu}} & \mu < E \end{cases} \tag{41}$$

$$\rho_n(E) = \frac{1}{4\pi^2} \left(\frac{2m}{\hbar^2}\right)^{\frac{3}{2}} \sqrt{E + \mu} \tag{42}$$

Near the gap $\rho_s(E) \approx 2\rho_n(0)|E|/\sqrt{E^2 - \Delta^2}$.

2.4. **Discussion of the gap equation.**

$\mathbf{T = T_c}$. At the critical temperature the order parameter $\Delta$ is zero, and the gap equation is an equation for $T_c$:

$$\frac{1}{g\rho(0)} = \int_0^{\hbar\omega_D} \frac{d\xi}{\xi} \tanh\left(\frac{1}{2}\beta_c \xi\right) = \int_0^{\mathrm{x_c}} \frac{\mathrm{dx}}{\mathrm{x}} \tanh \mathrm{x} = \tanh(\mathrm{x_c}) \log(\mathrm{x_c}) - \int_0^{\mathrm{x_c}} \mathrm{dx}\, \frac{\log \mathrm{x}}{\cosh^2 \mathrm{x}}$$

$$\approx \log x_c - \int_0^\infty dx \frac{\log x}{\cosh^2 x} = \log x_c + \log(4e^C/\pi), \qquad x_c = \frac{\hbar\omega_D}{2k_B T_c} = \frac{T_D}{2T_c}$$

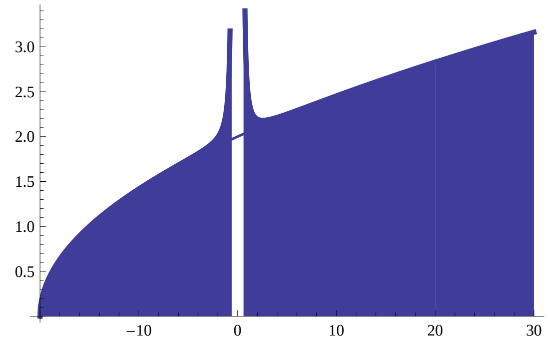


FIGURE 2. The spectral density ($\mu = 20$, $\Delta = 0.6$). The thin line is the square root $\sqrt{E}$ of the normal phase. The gap is centred on the chemical potential.

The approximations are justified by $T_D/T_c \gg 1$. With $C \approx 0.5772..$, the result is

$$\boxed{k_B T_c \; = \; 1.134 \; \hbar\omega_D \; \exp\left(-\frac{1}{g\rho(0)}\right)} \tag{43}$$

**T = 0**. The gap equation becomes:

$$\frac{1}{g\rho(0)} = \int_0^{\hbar\omega_D} d\xi \, \frac{1}{\sqrt{\xi^2 + \Delta_0^2}}$$

with solution

$$\Delta_0 = \frac{\hbar\omega_D}{\sinh \frac{1}{g\rho(0)}} \approx 2\hbar\omega_D \exp\left(-\frac{1}{g\rho(0)}\right) \tag{44}$$

The following universal ratio is then obtained:

$$\boxed{\frac{\Delta_0}{k_B T_c} = \pi e^{-C} \approx 1.76} \tag{45}$$

## 3. THE GINZBURG - LANDAU LIMIT OF BCS

The Ginzburg-Landau theory can be derived from the microscopic BCS model. Near the transition line $H = H_c(T)$, the function $\Delta$ is small, and the Dyson equation (29) for $\mathbb{G}(\mathbf{x}, \mathbf{y}; i\omega_n)$ can be solved by iteration:

$$\mathbb{G} = \mathbb{G}_n + \frac{1}{\hbar}\mathbb{G}_n\mathbb{D}\mathbb{G}_n + \frac{1}{\hbar^2}\mathbb{G}_n\mathbb{D}\mathbb{G}_n\mathbb{D}\mathbb{G}_n + \frac{1}{\hbar^3}\mathbb{G}_n\mathbb{D}\mathbb{G}_n\mathbb{D}\mathbb{G}_n\mathbb{D}\mathbb{G}_n$$

The truncation to third order in $\Delta$ evaluates the anomalous correlator $\mathscr{F}(\mathbf{x}, \mathbf{y}, i\omega_n)$ and the Green function $\mathscr{G}(\mathbf{x}, \mathbf{y}, i\omega_n)$ in terms of the normal Green function and the gap function:

$$\mathscr{F}(1,2,i\omega_n) = -\frac{1}{\hbar}\mathscr{G}_n(1,3,i\omega_n)\Delta(3)\mathscr{G}_n(2,3,-i\omega_n) + \frac{1}{\hbar^3}\mathscr{G}_n(1,3,i\omega_n)\Delta(3)\mathscr{G}_n(4,3,-i\omega_n)\overline{\Delta}(4)\mathscr{G}_n(4,5,i\omega_n)\Delta(5)\mathscr{G}_n(2,5,-i\omega_n); \tag{46}$$

$$\mathscr{G}(1,2,i\omega_n) = \mathscr{G}_n(1,2,i\omega_n) - \frac{1}{\hbar^2}\mathscr{G}_n(1,3,i\omega_n)\Delta(3)\mathscr{G}_n(4,3,-i\omega_n)\overline{\Delta}(4)\mathscr{G}_n(4,2,i\omega_n) \tag{47}$$

The space variables $3, 4, 5$ are integrated. $\mathscr{G}_n$ are the normal Green functions for independent particles in a static magnetic field.
The equations are the starting point for Gor'kov's derivation [6] of the two Ginzburg-Landau equations (1959).
Eq.(46) with $2 = 1^+$ and summation of Matsubara frequencies, is a cubic expansion of the gap equation for $\Delta$, and provides the first G.L. equation with order parameter $\psi \propto \Delta$:

$$\frac{1}{g}\Delta(1) = Q(1,2)\Delta(2) + R(1,2,3,4)\Delta(2)\overline{\Delta}(3)\Delta(4) \tag{48}$$

with weight functions

$$Q(1,2) = \frac{1}{\hbar^2\beta}\sum_n \mathscr{G}_n(1,2,i\omega_n)\mathscr{G}_n(1,2,-i\omega_n)$$
$$R(1,2,3,4) = -\frac{1}{\hbar^4\beta}\sum_n \mathscr{G}_n(1,2,i\omega_n)\mathscr{G}_n(3,2,-i\omega_n)\mathscr{G}_n(3,4,i\omega_n)\mathscr{G}_n(1,4,-i\omega_n)$$

Eq.(47) is an expansion for the Green function, that is used to to evaluate the super-current, and yields the second G.L. equation.
The derivation of G.L. equations relies crucially on the large difference among the length scales involved. We need some preliminaries. ...

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