Lectures on superconductivity

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Lecture 7

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BCS theory at nonzero temperature

BCS theory ($T \neq 0$)

Recap: at $T = 0$ the structure of the MBWF is

$$\Psi = \prod_k \Phi_k \qquad\qquad \left(\boldsymbol{k} \equiv (\boldsymbol{k}\uparrow, -\boldsymbol{k}\downarrow)\right)$$

$$\Phi_k = u_k|00>_k + v_k|11\rangle_k$$

and the specific values of u_k and v_k were found by minimizing $\langle \widehat{\mathrm{H}} - \mu\widehat{\mathrm{N}} \rangle$.

For $T \neq 0$ we expect intuitively that the description of the many-body system can still be factored into a product of descriptions of the occupation of the individual pair states $(\boldsymbol{k}\uparrow, -\boldsymbol{k}\downarrow)$: technically

$$\hat{\rho} = \prod_k \hat{\rho}_k \qquad \longleftarrow \qquad \text{density matrix}$$

but now (a) all 4 occupation states will be realized with some probability

(b) quantities like Δ will be T –dependent

(c) at some $T_c \sim \Delta(T = 0)/k_B$ the collective bound state will cease to exist.

Recall: for given $\boldsymbol{k} \equiv (\boldsymbol{k}\uparrow, -\boldsymbol{k}\downarrow)$ 4 occupation states

$$\begin{matrix} |00\rangle, & |11\rangle, & |01\rangle, & |10\rangle \\ GP & EP & BP_1 & BP_2 \end{matrix}$$

and ground state has

$\psi_k = u_k|00\rangle + v_k|11\rangle$ corresponding to $\boldsymbol{\sigma}_k \parallel \boldsymbol{\mathcal{H}}_k \equiv -\epsilon_k\hat{\boldsymbol{z}} + \Delta\hat{\boldsymbol{x}}$ with an "energy" $-E_k \equiv |\boldsymbol{\mathcal{H}}_k| \equiv \left(\epsilon_k^2 + |\Delta|^2\right)^{1/2}$. The limit $\Delta \to 0$ corresponds to the normal GS, and then $E_k \to |\epsilon_k|$. So the energy of the "ground pair" state relative to the normal ground state is

$$E_{GP} = |\epsilon_k| - E_k.$$

The EP ("excited pair") state is formed by simply reversing the pseudospin k, so that

$$\psi_{k,EP} = v_k^*|00\rangle_k - u_k|11\rangle_k$$

(orthogonal to $\psi_{k,GF}$)

This evidently costs an energy $2E_k$, so

$$E_{EP} = |\epsilon_k| + E_k$$

What about the BP ("broken pair") states $BP_{1,2}$? These each correspond (relative to the N ground state) to kinetic energy (KE) $|\epsilon_k|$ and zero PE (no partner to scatter!), hence

$$E_{BP_{1,2}} = |\epsilon_k|$$

Thus the relative energies of the various states are

$$E_{BP_{1,2}} - E_{GP} = E_k, \quad E_{EP} - E_{GP} = 2E_k$$

and lowest (fermionic) excitation energy is $min_{\in_k}(|\in_k|^2 + |\Delta|^2)^{1/2}$ $= \Delta$ (hence name "energy gap")

Conventional language:

State $BP_1 (BP_2)$ has "Bogoliubov quasiparticle" in state $\boldsymbol{k}\uparrow (-\boldsymbol{k}\downarrow)$; state EP has quasiparticles in both $\boldsymbol{k}\uparrow$ and $\boldsymbol{k}\downarrow$ (hence $E_{EP} = 2\mathrm{E}_{BP_{1,2}}$. ↑ : but EP is really an "excitation of the condensate" whereas $BP_{1,2}$ are not).

Population of states: since all 4 states distinguishable, simple Maxwell-Boltzmann-Gibbs statistics applies, *i.e.* $P_n \propto exp - \beta E_n$. Thus (taking E_{GP} as zero of E)

$$P_{GP} = Z^{-1}, P_{BP_1} = P_{BP_2} = Z^{-1} exp - \beta E_k, P_{EP} = Z^{-1} exp - 2\beta E_k$$

$$\left(E_k \equiv E_k(T)\right)$$

$$Z = 1 + 2exp - \beta E_k + exp - 2\beta E_k$$

A quantity of special interest is

$$F_k(T) \equiv \frac{1}{2}\langle\sigma_{xk}\rangle(T) = (\Delta(T)/2E_k)(P_{GP} - P_{EP})$$

$$= \left(\Delta(T)/2E_k(T)\right) tanh \beta E_k(T)/2$$

Putting this into the equation

$$\Delta(T) = -V_0 \sum_k F_k(T)$$

we find

$$\Delta(T) = -V_0 \sum_k (\Delta(T)/2E_k(T)) tanh \beta E_k\,(T)/2)$$

or in the more general case $(V_0 \longrightarrow V_{kk'})$

$$\Delta_k(T) = -_{k'} \sum V_{kk'} (\Delta_{k'}\,(T)/2E_{k'}(T)) tanh \beta E_{k'}\,(T)/2$$

↑

Finite-temperature BCS gap equation

As T increases from 0, $\Delta(T)$ decreases from $\Delta(0)$ to zero at a temperature T_c given by the linearized equation

$$\Delta_k(T_c) = -\sum_{k'} (V_{kk'}\Delta_{k'}(T_c)/2|\epsilon_{k'}|)\, tanh\beta_c\, |\epsilon_{k'}|/2 \quad (\beta_c \equiv 1/k_B T_c)$$

For the BCS contact potential $(V_{kk'} \to V_0)$ this yields

$$[\mathrm{N}(0)V_0]^{-1} = \int_0^{\epsilon_c} \frac{tanh\beta\, \epsilon/2}{\epsilon} d\epsilon = \ell n(1\cdot 14\beta_c\epsilon_c)$$

so comparing this with zero-T gap equation

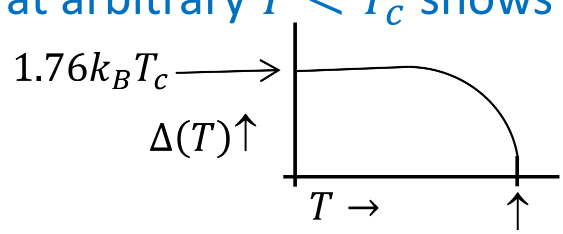
$$[\mathrm{N}(0)V_o]^{-1} = \ell n(2\epsilon_c/\Delta(T=0)) \;\Rightarrow\; 1\cdot 14\beta_c\epsilon_c = 2\epsilon_c/\Delta(T=0))$$

we have

$$\Delta(T=0) = 1.76 k_B T_c$$

reasonably well satisfied for most "classical" superconductors

Examination of the gap equation at arbitrary $T < T_c$ shows that it is a function only of T/T_c



$$\Delta(T) = 1.76 k_B T_c f(T/T_c)$$

with $f(z) \cong (1 - z^4)^{1/2}$

approximate form

(so for $T \to T_c, \Delta(T) \propto (1 - T/T_c)^{1/2}$)

Properties of a BCS superconductor at nonzero T.

A. Condensate:

As we saw, the (F.T. of the) condensate wave function has the form at $T \neq 0$

$$F_k(T) = \big(\Delta(T)\big)/2E_k(T))tanh\beta E_k\,(T)/2$$

so, in the wave function

$$F(\boldsymbol{r}) = \sum_k F_k expi\boldsymbol{k}\cdot\boldsymbol{r}$$

$$\equiv N(0)\int d\epsilon_k \frac{\sin kr}{kr}\frac{\Delta(T)}{\left(\epsilon_k^2+\Delta^2(T)\right)^{1/2}} tanh\,\beta\left(\epsilon_k^2+\Delta^2\right)^{1/2}/2$$

the low energy cutoff (which determines the long-distance behavior) gradually changes from $\sim\Delta(T=0)$ to $\sim k_B T$. Since for $T \lesssim T_c$ these are of same order of magnitude, we have approximately

$$F(r\colon T) \cong \Delta(T)\cdot N(0)\frac{\sin k_F r}{k_F r} exp - r/\xi'(T)$$

where $\xi'(T){\sim}\xi'(0).\, i.e.,$

Cooper-pair radius is not sharply T-dependent

(in particular, does not diverge for $T \to T_c$ from below).

The number of Cooper pairs,

$$N_c(T) \equiv \int |F(\boldsymbol{r}\colon T)|^2 d\boldsymbol{r}$$

is proportional to $\Delta^2(T)$, hence for $T \to T_c$

$$N_c(T) \propto (1 - T/T_c)\big(\times\, O(N\Delta(O)/E_F)\big)$$

B. The Normal Component

Condensate is very "inert", e.g. cannot be spin-polarized or (usually) flow in a way determined by walls. This applies both to GP and EP states (both have $S = 0$, COM momentum = 0). Hence such responses determined entirely by BP states. However, response is not simply proportional to the probability of occupation of BP states:

Ex: Pauli spin susceptibility

In field $\boldsymbol{\mathcal{H}}$, $\Delta \mathrm{E} = -\mu_B \mathcal{H} \sum_i S_i^z$. Hence, does not affect $|00\rangle$ or $|11\rangle$, but

↑ real spin not pseudospin!

shifts energies of BP states,

$$\Delta E_{BP_1} = -\mu_B \mathcal{H},\ \ \Delta E_{BP_2} = +\mu_B \mathcal{H}$$

Hence:

$$P_{BP_1} = exp - \beta(\mathrm{E}_k - \mu_B \mathcal{H}), \qquad P_{BP_2} = exp - \beta(\mathrm{E}_k + \mu_B \mathcal{H}))$$

and

$$\langle M_z \rangle \equiv \mu_B \langle S_z \rangle$$

$$= \mu_B^\mu \sum_k (Z_k^{-1}) \big(exp - \beta(\mathrm{E}_k - \mu_B \mathcal{H}) - exp - \beta(\mathrm{E}_k + \mu_B \mathcal{H}) \big).$$

with $Z_k(\mathcal{H}) = Z_k(0) + 0(\mathcal{H}^2)$

For $\mu_8\mathcal{H} \ll k_BT, \Delta(T)$ this gives

$$\langle M_z\rangle = 2\mu_B^2\mathcal{H}\sum_k \frac{d}{dE_k}(exp - \beta E_k)\Big/Z_k = \mu_B^2\mathcal{H}\frac{\beta}{2}\sum_k sech^2\,\beta E_k/2$$

and so

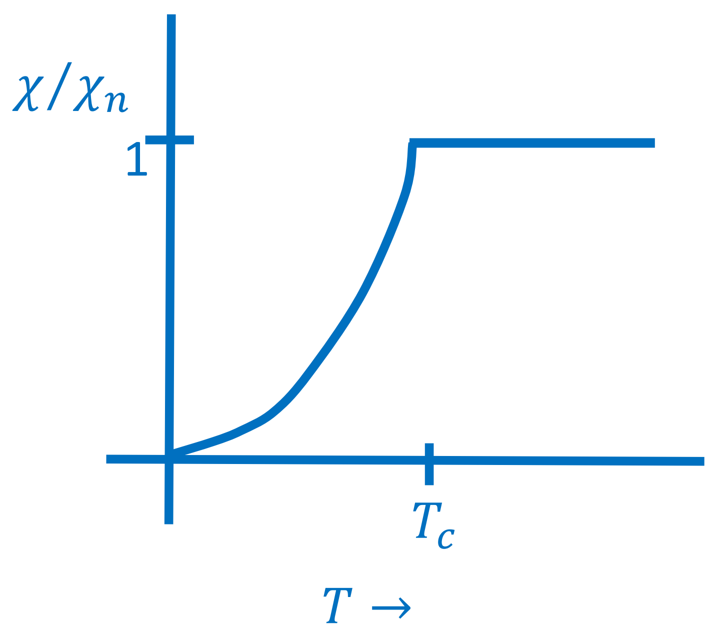
$$\chi \equiv \langle \mathrm{M}_z\rangle/\mathcal{H} = \mu_B^2\left(\frac{dn}{d\epsilon}\right)\frac{\beta}{2}\int_0^\infty sech^2(\beta E/2)d\epsilon$$

In the normal state $(E \to \epsilon)$ this correctly gives $\chi_n = \mu_B^2\, dn/d\epsilon$, so

$$\chi(T)\Big/\chi_n = \frac{\beta}{2}\int_0^\infty sech^2\,(\beta E\,(T)/2)d\epsilon$$

↑ "Yosida function"

Note: Reason argument is relatively simple is that energy eigenstates $(\boldsymbol{k}\uparrow)$ and $(-\boldsymbol{k}\downarrow)$ carry a spin +1/2 (–1/2) respectively



The normal density

The "normal density" is defined as the fraction of the electrons which can respond to a (transverse) static vector potential, in following sense:

In presence of vector potential $\boldsymbol{A}(\boldsymbol{r})$

$$\boldsymbol{p} \rightarrow \boldsymbol{p} - e\boldsymbol{A}(\boldsymbol{r})$$

So KE becomes

$$\sum_i \left(\widehat{\boldsymbol{p}}_i - e\boldsymbol{A}_i(\boldsymbol{r})\right)^2/2m \equiv \sum_i \left(\frac{\hat{p}_i^2}{2m} - \frac{e}{m}\hat{p}_i \cdot A + \frac{e^2 A_i^2(\boldsymbol{r})}{2m}\right)$$

and the current density $\boldsymbol{j}(\boldsymbol{r})$ is

$$\boldsymbol{j}(\boldsymbol{r}) = \frac{e}{2}\sum_i \left(\delta(\boldsymbol{r} - \boldsymbol{r}_i)\right)\left\{\left(\widehat{\boldsymbol{p}}_i - e\boldsymbol{A}(\boldsymbol{r}_i)\right)/m + H.C.\right\}$$

We already saw that the explicit term in $\boldsymbol{A}(\boldsymbol{r}_i)$ gives rise in the S phase, to $\boldsymbol{j}(\boldsymbol{r}) = -\frac{Ne^2}{m}\boldsymbol{A}(\boldsymbol{r})$, *i.e.* the Meissner effect. But in the normal phase it is cancelled by the response of $\hat{p}_i$ to the perturbation $\boldsymbol{p}_i \cdot A(r_i)$.

$$(\delta j/\delta \mathrm{A})_{pert} = +\frac{Ne^2}{m}$$

So: in S phase at $0 < T < T_c$ what is perturbative response of $\boldsymbol{p}$ to $\boldsymbol{A}$?

(almost) exact analogy to calculation of spin susceptibility:

$|00\rangle$ and $|11\rangle$ have total $\boldsymbol{P} = 0$, so cannot respond

$|10\rangle$ has momentum $\boldsymbol{p} = \hbar\boldsymbol{k}$, $|01\rangle$ has $\boldsymbol{p} = -\hbar\boldsymbol{k}$. Hence

$$\Delta E_{BP_1} = -e\hbar\boldsymbol{k}\cdot\boldsymbol{A}/m \qquad\qquad \Delta E_{BP_2} = +e\hbar\boldsymbol{k}\cdot\boldsymbol{A}/m$$

Total induced momentum is

$$\boldsymbol{P} = \sum_k \hbar\boldsymbol{k}\left(Z_k^{-1}\right)\left(exp - \beta\left(E_k - \frac{e\hbar\boldsymbol{k}\cdot\boldsymbol{A}}{m}\right) - exp - \beta\left(E_k + \frac{e\hbar\boldsymbol{k}\cdot\boldsymbol{A}}{m}\right)\right)$$

and for $\hbar k\cdot\boldsymbol{A} \ll k_B T, \Delta(T)$ this reduces to

$$J \equiv e\frac{\boldsymbol{P}}{m} \cong$$

$$2e^2\hbar^2\frac{k_F^2}{3m}\boldsymbol{A}\sum_k\left(Z_k^{-1}\right)\frac{d}{dE_k}exp - \beta E_k \cong e^2\frac{p_F^2}{3m}\frac{\beta}{2}\sum_k sech^2(\beta E_k/2)\cdot\boldsymbol{A}$$

↑ directional averaging

In N state ($E \to \epsilon$) this correctly reduces to Ne^2/m, so ratio ("ρ_n/ρ") of response in S state at temperature T to N −state value is

$$\rho_n/\rho = \frac{\beta}{2}\int_0^\infty \left(sech^2\,\beta E/2\right)d\epsilon$$

↑ Yosida function

↑ χ and ρ_n/ρ are untypically simple, because energy eigenstates are also eigenstates of $\boldsymbol{\sigma}$ and $\boldsymbol{p}$.

Properties of a BCS superconductor at nonzero T (cont.)

C. Specific heat

The entropy S, and hence the specific heat c_{v}, has contributions from both the BP states ("normal component") and the EP state ("distortion of condensate"). If we consider a given pair state $(\boldsymbol{k}\uparrow, -\boldsymbol{k}\downarrow)$ and devote the contribution to these quantities by a subscript $(\boldsymbol{k})$, then we have after tedious but straightforward algebra

$$S_{(\boldsymbol{k})}^{(T)} \equiv -k_{\beta} \sum_{n} P_n \, \ell n P_n = -k_{\beta}(P_{GP} \ell n P_{GS} + 2P_{Br} \ell n P_{BP} + P_{EP} \ell n E_P)$$

$$= 2k_B \left\{ \frac{\beta E_k}{e^{\beta Ek} + 1} + \ell n\left(1 + e^{-\beta E_k}\right) \right\} \qquad (E_k) \equiv E_k(T)$$

and so

$$C_{\mathrm{v}(\boldsymbol{k})}(T) \equiv T\,\frac{dS_k}{dT} = \frac{1}{2}\beta^2 E_k \left(E_k + \beta\,\frac{dE_k}{d\beta} \right) sech^2(\beta\, E_k/2)$$

where as usual $\beta \equiv 1/k_B T$. The total (electronic) specific heat $C_{\mathrm{v}}(T)$ of the system is given by summing this over $\boldsymbol{k}$ (no sum over spins).

The qualitative behavior of $C_v(T)$ normalized to its N-state value at T_c is similar to that of the Yosida function (except that it overshoots 1 for $T \to T_c$, see below). Two important limits:

(1) $T \to 0$: since $d\Delta/dT$ and hence dE/dT is negligible in this limit, and $sech^2\beta\, E/2 \to -\frac{d}{d\beta}\left(\frac{1}{e^{\beta E}+1}\right)$, this gives

$$C_v(T)_{T\to 0} = \frac{d}{dT}\sum_k \left\{\frac{2E_k(0)}{e^{\beta E_k(0)}+1}\right\} = const\beta^{3/2}[\Delta(0)]^{5/2} exp - \beta\Delta(0)$$

= specific heat of 2 independent Fermi particles of energy $E_k(0)$

(2) $T \to T_c$: in this limit we can set $E_k \to |E_k|$ except in the $dE_k/d\beta$ term. Then the first term simply gives the N-state specific heat, $\left(\pi^2/3\, k_g^2 T\, dn/d \in\right)$. The difference Δc_{sn} between the superconducting and normal states at T_c (*i.e.* the specific heat "jump") is given by

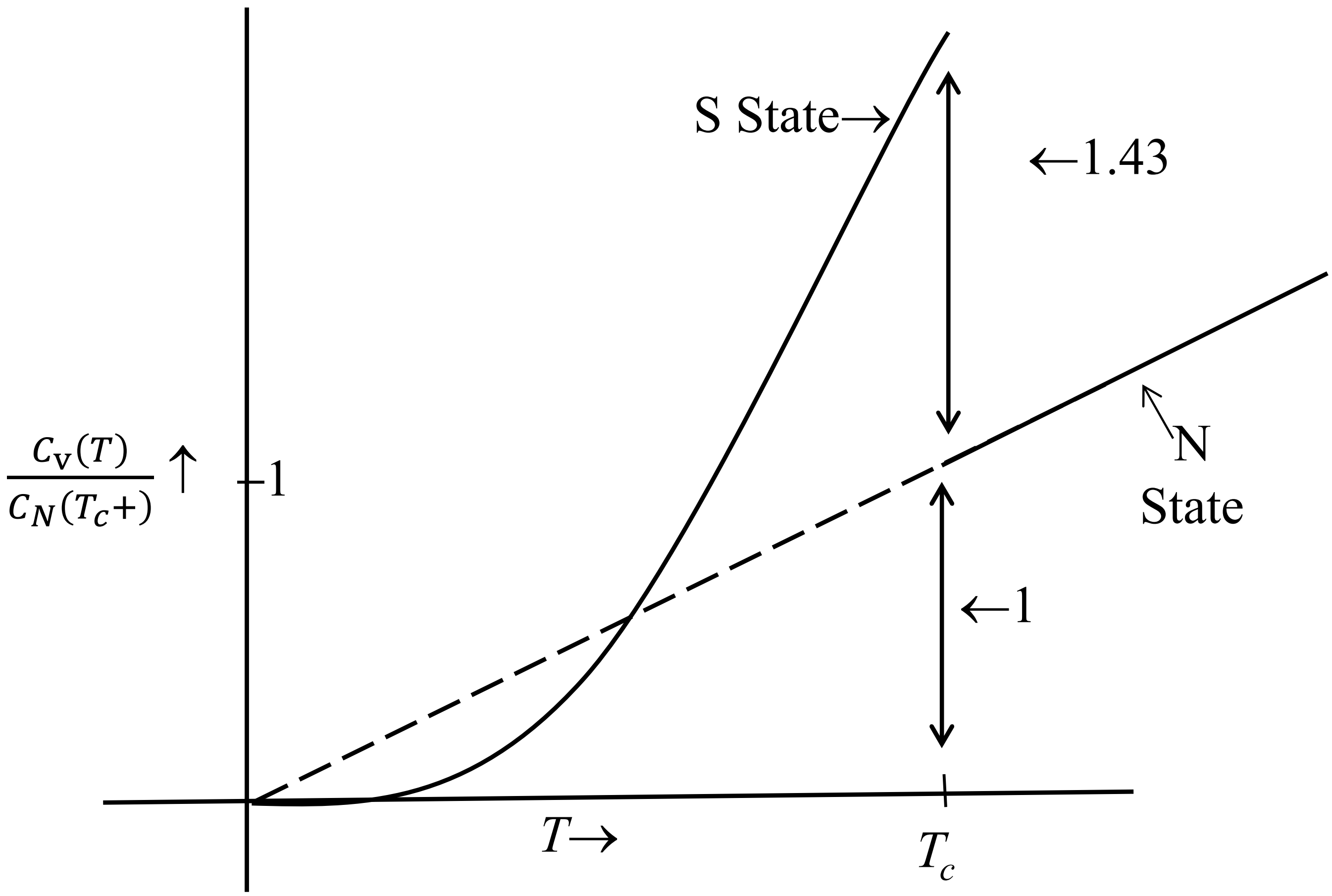
$$\Delta c_{sn} = \frac{1}{2}k_\sigma \beta_c^3 \sum_k E_k (dE_k/d\beta)_{\beta=\beta_c} sech^2(\beta_c/E_k\, 1/2)$$

$$= \frac{1}{2}\left(\frac{dn}{d\epsilon}\right)\left[-\frac{d}{dT}\Delta^2(T)\right]_{T\to T_c}$$

and since $\Delta^2(T)_{T\to T_c}$ in is $(3\cdot 06)^2(1-T/T_c)$, this gives

$$\Delta c_{sn} = \frac{1}{2}(3\cdot 06 k_B)^2 T_c (dn/d\epsilon) = 1\cdot 43 c_n (T \to T_c +)$$

reasonably well satisfied for most BCS superconductors other than Hg and Pb.



Specific heat normalized to N-state value at T_c

Summary of lecture 7

At $T \neq 0$ the BCS description is still a product over the different pair states $\boldsymbol{k} \equiv |\boldsymbol{k}\uparrow, -\boldsymbol{k}\downarrow\rangle$, but now all four states

$$|GP\rangle \equiv u_k|00\rangle + v_k|11\rangle$$

$$|BP1\rangle \equiv |10\rangle$$

$$|BP2\rangle \equiv |01\rangle$$

$$|EP\rangle \equiv v_k^*|00\rangle - u_k|11\rangle$$

are populated, and u_k and v_k are functions of T. The relative energies of the 4 states are

$$\left.\begin{aligned} E_{BP}(T) - E_{GP}(T) &= E_k(T) \\ E_{EP}(T) - E_{GP}(T) &= 2E_k(T) \end{aligned}\right\} E_k(T) \equiv \left(\epsilon_k^2 + |\Delta_k(T)|^2\right)^{1/2}$$

The self-consistent equation for the gap is

$$\Delta_k(T) = -\sum_{k'} V_{kk'}\big(\Delta_{k'}(T)/2E_{k'}(T)\big)\tanh(\beta E_{k'}(T)/2)$$

and has a nontrivial ($\Delta_k \neq 0$) solution only for $T < T_c$, where

$$k_B T_c = \Delta(T=0)/1.76$$

Condensate wave function $F(r{:}\,T)$ not strongly T-dependent: no. of Cooper pairs $N_c(T) \sim \Delta^2(T)$, near $T_c \sim (1 - T/T_c)$
"Normal component" is essentially BP states: contributes to "simple" quantities $(\chi, \rho_n \ldots)$ an amount $Y(T)$, *e.g.*

$$\chi(T)/\chi_n = Y(T) \equiv \frac{\beta}{2}\int_0^\beta \mathrm{sech}^2(\beta E(T)/2)\,d\epsilon$$