

# LECTURES ON SUPERCONDUCTIVITY

**Anthony J. Leggett**

Department of Physics

University of Illinois at Urbana-Champaign, USA

Hong Kong University

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**LECTURE 8**

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**RELATION OF BCS AND GL THEORIES**



## Relation of BCS and GL Theories

Recap: GL is phenomenological theory of superconductivity, whose output is a free energy density  $\mathcal{F}$  expressed as a function of a (complex scalar) **order parameter**  $\Psi(\mathbf{R})$ : in its original (and only subsequently rigorously justified) form

$$\mathcal{F}\{\Psi(\mathbf{R}); T\} = \alpha(T)|\Psi(\mathbf{R})|^2 + \frac{1}{2}\beta(T)|\Psi(\mathbf{R})|^4 + \gamma(T) \left| \nabla - 2 \frac{ie}{\hbar} \mathbf{A}(\mathbf{R}, t) \Psi(\mathbf{R}) \right|^2 + \frac{1}{2} \mu_0^{-1} (\nabla \times \mathbf{A}(\mathbf{R}))^2$$

with

(for  $T \rightarrow T_c$ )  $\alpha(T) = \alpha_0(T - T_c)$ ,  $\beta(T) = \beta_0 = \text{const.}$   $\gamma(T) = \gamma_0 = \text{const.}$

On the other hand, BCS theory introduces a **pair wave function**  $F(\mathbf{r}; T)$  which has a spatial extent  $\xi' \sim \hbar v_F / \Delta(0)$ , and an **energy gap**  $\Delta(T)$ .

What is relation between these two descriptions?

Clue: BCS approach as developed so far assumed pairing between  $(\mathbf{k} \uparrow)$  and  $(-\mathbf{k} \downarrow)$ , *i.e.* **COM of pairs at rest**. But must be possible to generalize to COM in motion  $(\mathbf{k} + \mathbf{q}/2 \uparrow)$  paired with  $(-\mathbf{k} + \mathbf{q}/2, \downarrow)$  and even to spatially nonuniform behavior. So consider generalization

$$F(\mathbf{r}) (\equiv F(\mathbf{r}_1 - \mathbf{r}_2)) \Rightarrow F(\mathbf{r}_1, \mathbf{r}_2) \equiv F(\mathbf{R}, \mathbf{r}) \quad \leftarrow \text{generalized pair wave function}$$

COM  $\uparrow$  relative  $\uparrow$



[Technical definition of  $F(\mathbf{r}_1, \mathbf{r}_2)$  (for current or would-be experts only):

- (a) probability amplitude to add an electron of spin  $\uparrow$  at  $\mathbf{r}_1$ , and one of spin  $\downarrow$  at  $\mathbf{r}_2$  to ground state (thermal equilibrium state) of  $N$ -particle system and reach ground state (thermal equilibrium state) of  $N + 2$  – particle system.
- (b) eigenfunction of 2 – particle density matrix  $\hat{\rho}_2(\mathbf{r}_1\sigma_1\mathbf{r}_2\sigma_2; \mathbf{r}'_1\sigma'_1\mathbf{r}'_2\sigma'_2)$  corresponding to single macroscopic eigenvalue].

Others: just think of  $F(\mathbf{r}_1, \mathbf{r}_2) \equiv F(\mathbf{r}, \mathbf{R})$  as 2-particle wave function into which a macroscopic **number** of pairs is condensed.

Crudely:

BCS theory discusses the dependence of  $F(\mathbf{R}, \mathbf{r})$  on **relative coordinate  $\mathbf{r}$**

GL theory discusses the dependence of  $F(\mathbf{R}, \mathbf{r})$  on **COM coordinate  $\mathbf{R}$** .

Expect theory to be “simple” only if scale of variation with respect to  $\mathbf{R}$  is large compared to “scale of confinement” in  $\mathbf{r}$ , *i.e.* to pair radius  $\xi'$ . This is always true for  $T \rightarrow T_c$ , since scale of variation in  $\mathbf{R}$  set by two characteristic lengths of GL theory,  $\xi_{GL}(T)$  and  $\lambda(T)$ , both of which diverge as  $(T_c - T)^{-1/2}$ , while  $\xi'$  remains finite in this limit.

For  $T$  well below  $T_c$ ,  $\xi_{GL}(T)$  and  $\lambda(T)$  can become  $\lesssim \xi'$ , so scale of variation in  $\mathbf{R}$  can become  $\lesssim \xi'$ . Qualitative picture is still valid, but quantitative theory is then very messy – do not attempt to cover here.

Define quite generally:

$$\Psi(\mathbf{R}) \equiv F(\mathbf{R}, \mathbf{r})_{\mathbf{r}=0}$$

**I** *i.e.* GL order parameter is simply **COM wave function of Cooper pairs**. (but with normalization which may be different from that in lecture 4)

Q: Can we derive GL from (generalized) BCS?

A: Yes! (Gor'kov, 1959 – but needs Green's function techniques)

A simplified approach: start from BCS model Hamiltonian  
 $(V_{kk'} = -V_0)$

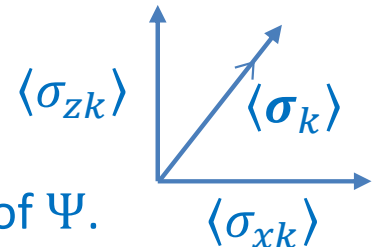
1. Consider spatially uniform case, *i.e.*  $F(\mathbf{R}, \mathbf{r}) \neq f(\mathbf{R})$ , so that from our definition

$$\Psi(\mathbf{R}) = \text{const.} \equiv \Psi \equiv F(\mathbf{r} = \mathbf{0}) \equiv \sum_k F_k \quad (F_k \equiv \langle u_k v_k^* \rangle)$$

where however  $F_k$  and hence  $\Psi$  need not necessarily take its thermal equilibrium value. What is the (free) energy associated with a given value of  $\Psi$ ?

(a) Potential energy: this is just the pairing energy

$$\langle V \rangle_{\text{pair}} = -V_0 \sum_{kk'} F_k F_{k'}^* \equiv -V_0 |\Psi|^2.$$



so always favors nonzero (and large) value of  $\Psi$ .

(b) Kinetic energy: a bit more tricky. Up to a constant,  $KE = \sum_k 2\epsilon_k \langle \sigma_{zk} \rangle$ . Evidently, since  $|\langle \sigma_k \rangle| \leq 1$ , increasing  $F_k \left( \equiv \frac{1}{2} \langle \sigma_{xk} \rangle \right)$  will decrease  $|\langle \sigma_{zk} \rangle|$  from its  $N$ -state value ( $\text{sgn } \epsilon_k$ ) and thus increase  $KE$ . In fact for a single spin  $\mathbf{k}$ ,

$$\Delta T_k = 2|\epsilon_k| \left( 1 - (1 - 4|F_k|^2)^{1/2} \right) = |\epsilon_k| (4|F_k|^2 + 2|F_k|^4 + \dots)$$

so it is plausible that the quantity  $\Delta T \equiv \sum_k \Delta T_k$  will have a similar expansion in terms of  $|\Psi|^2$ : (with the  $|\Psi|^2$  term +ve).



- c) Entropy: on rather general grounds expect this to be a decreasing function of  $|\Psi|^2$ , so if it is analytic expect again terms in the free energy prop. to  $|\Psi|^2$  and  $|\Psi|^4$ , with coefficient of  $|\Psi|^2$  term positive.

Quantitative calculation\*: gives precise values for coefficients  $\alpha(T)$  and  $\beta(T)$  as well as for  $T_c$  (the temperature for which the negative ( $T$ -independent) term in the coefficient of  $|\Psi|^2$  is balanced by the positive term  $-TS(|\Psi|^2)$ ):

$$\alpha(T) = N(0) \frac{(T/T_c - 1)}{|V_0|^2}, \quad \beta(T) = \frac{1}{2} \frac{7\zeta(3)}{8\pi^2} \frac{N(0)}{(k_B T_c)^2 |V_0|^4}$$

and so if we write  $F$  in terms of a normalized order parameter  $\tilde{\Delta} \equiv |V_0|\Psi$  ( $\equiv \mathcal{H}_x$  in Anderson pseudospin picture), then

$$F(\tilde{\Delta}, T) = F_0(T) + N(0) \left\{ - \left( 1 - \frac{T}{T_c} \right) |\tilde{\Delta}|^2 + \frac{1}{2} \frac{7\zeta(3)}{8\pi^2} \frac{1}{(k_B T_c)^2} |\tilde{\Delta}|^4 + \dots \right\}$$

and minimization of  $F(\tilde{\Delta}, T)$  with respect to  $\tilde{\Delta}$  gives back the BCS result that in thermal equilibrium ( $\tilde{\Delta} = \Delta$ )

$$\Delta(T)_{T \rightarrow T_c} = 3.08 k_B T_c (1 - T/T_c)^{1/2}$$



\* See *e.g.* appendix A, and for more details AJL, Quantum Liquids, appendix 5.E

## 2. The gradient term in the GL free energy:

To derive this, let's consider the case of uniform flow of the condensate, so that

$$\Psi(\mathbf{r}; T) = |\Psi_{eq}(T)| \exp i \varphi(\mathbf{r})$$

It's useful to define a quantity with the units of velocity:

$$\mathbf{v}_s = \frac{\hbar}{2m} \nabla \varphi \quad \longleftarrow \text{“superfluid velocity”}$$

(note that  $\nabla \times \mathbf{v}_s \equiv 0$ ,  $\oint \mathbf{v}_s \cdot d\ell = nh/2m$ ). From symmetry assume that for small  $v_s$  extra energy due to the flow is proportional to  $v_s^2$ , so define **superfluid density**  $\rho_s$  by

$$\Delta F_{flow}(T) = \frac{1}{2} \rho_s(T) v_s^2$$

Imagine now a thought-experiment in which we start with everything at rest, and “boost” both condensate and normal component to a frame moving with velocity  $\mathbf{v}$ . For the normal component this is achieved (see lecture 7) by applying a vector potential  $\mathbf{A} = m\mathbf{v}/e$ ; the required momentum density is by definition  $(\rho_n(T)/\rho)m\mathbf{v}$ , and the extra *KE* density is  $\frac{1}{2} \rho_n(T) v_n^2 \equiv \frac{1}{2} \rho_n v^2$ . On the other hand, the extra energy density acquired by boosting the condensate to velocity  $\mathbf{v}$  is, as above,  $\frac{1}{2} \rho_s v_s^2 \equiv \frac{1}{2} \rho_s v^2$ . Since the total energy density due to the boost must by Galilean invariance be  $\frac{1}{2} \rho v^2$ , we have

$$\rho_n(T) + \rho_s(T) = \rho \quad (\Rightarrow \text{“2-fluid” picture})$$

and thus by result of Lecture 7

$$\rho_s(T) = \rho(1 - Y(T)) \quad \underset{T \rightarrow T_c}{\cong} \rho(7\zeta(3)/4\pi(k_B T_c)^2) \Delta^2(T)$$

**I** (Note that at nonzero  $T$ , it is  $\rho_s(T)$  rather than  $\rho$  which enters the expression for  $\lambda_L(T)$ )

If now we write the gradient term in the GL free energy in the form (for  $\mathbf{A} = 0$ )

$$\Delta F_{flow}(T) = \gamma(T) |\nabla \Psi|^2 = \gamma(T) |\Psi_{eq}(T)|^2 (\nabla \varphi)^2$$

by comparing this with  $\frac{1}{2} \rho_s(T) v_s^2$ , we have the normalization-independent relation

$$\gamma(T) = \frac{\hbar^2}{8m^2} \frac{\rho_s(T)}{|\Psi|^2(T)}$$

and in particular if we choose the normalization  $\Psi(T) = \Delta(T)$ .

$$\gamma(T) \equiv \rho \frac{\hbar^2}{4m} \frac{7\zeta(3)}{8\pi^2 (k_B T_c)^2} \left( \equiv \frac{\hbar^2}{4m} \beta \right) = \text{const. as } T \rightarrow T_c$$

Generalizations:

effect of vector potential:  $\nabla \rightarrow \nabla - 2 \frac{ie}{\hbar} \mathbf{A}(\mathbf{r})$

(since Cooper pair has charge  $2e$ )

spatially varying case: provide scale of variation  $\gg$  pair radius  
able to regard the local free energy as a function of the local  $\Psi(\mathbf{R})$

$$\mathcal{F}(\Psi; T) \rightarrow \mathcal{F}\{\Psi(\mathbf{R}); T\}, \quad F(T) \equiv \int \mathcal{F}\{\Psi(\mathbf{R}; T)\} d\mathbf{R}$$

$\Rightarrow$  complete GL free energy, QED



$\triangleleft$ : have assumed (rather than demonstrated) that correct form of gradient term is  $\text{const} |\nabla \Psi|^2 \equiv \text{const} (|\Psi|^2 (\nabla \varphi)^2 + (\nabla |\Psi|)^2)$

## A “hand-waving” justification for the form of the gradient energy in GL theory

In their original paper, GL assume without detailed argument that in the limit  $T \rightarrow T_c$ , where their complex order parameter (OP)  $\Psi(\mathbf{R})$  is small, the gradient terms in the free energy density should have the simple form

$$F_{grad}\{\Psi(\mathbf{R})T\} = \gamma(T)|\nabla\Psi(\mathbf{R})|^2$$

However, if we split  $\Psi$  explicitly into its amplitude and phase

$$\Psi(\mathbf{R}) \equiv A(\mathbf{R}) \exp i\varphi(\mathbf{R})$$

then we can form two different real expressions which are bilinear in the gradients and invariant under time reversal, namely

$$F_\varphi(\mathbf{R}) \equiv \gamma_\varphi(T)[A(\mathbf{R})]^2(\nabla\varphi(\mathbf{R}))^2$$

$$F_A(\mathbf{R}) \equiv \gamma_A(T)[\nabla A(\mathbf{R})]^2$$

and it is not immediately obvious that the coefficients are identical, that is that we have

$$\gamma_\varphi(T) = \gamma_A(T) \equiv \gamma(T) \quad (*)$$





The following argument is intended to make it plausible that eqn. (\*) is indeed correct; it is **not** intended (at least in its present form) to give the correct magnitude of  $\gamma(T)$ . The argument is based on an analogy with a particle of spin  $\frac{1}{2}$  whose spin vector  $\boldsymbol{\sigma}(\mathbf{R})$  orients itself parallel to an  $\mathbf{R}$ -dependent magnetic field  $\mathcal{H}(\mathbf{R})$  whose direction makes angles  $\theta(\mathbf{R})$ ,  $\varphi(\mathbf{R})$  with the z-axis. What is the kinetic energy  $|\nabla\psi_{\uparrow}|^2 + |\nabla\psi_{\downarrow}|^2$  associated with this situation? Actually, the question as so stated is not uniquely defined: we need to supplement it with some further piece of information, e.g. that the phase of  $\psi_{\downarrow}(\mathbf{R})$  is constant. Then if we define the complex quantity  $\boldsymbol{\sigma}_{\perp}(\mathbf{R}) \equiv \sigma_x(\mathbf{R}) + i\sigma_y(\mathbf{R})$  and write it in terms of amplitude and phase, we find that in the limit  $\theta(\mathbf{R})$  close to  $\pi$  for all  $\mathbf{R}$  (only) the kinetic energy is a constant times  $|\nabla\boldsymbol{\sigma}_{\perp}(\mathbf{R})|^2$  i.e. the phase and amplitude terms have the same coefficient.



Returning now to our original problem, we note that provided all spatial variations are on a scale  $\gg$  the pair radius  $\xi_0$  (which we recall does **not** diverge in the limit  $T \rightarrow T_c$ ), we can use a semiclassical description in which the quantities  $F_k$  ( $\equiv \frac{1}{2}S_{xk}$  in the Anderson pseudospin representation) are functions of  $\mathbf{R}$ . Moreover, we can generalize the description so as to allow the  $F_k$  to be complex:  $F_k = \frac{1}{2}(S_{xk} + iS_{yk}) \equiv \frac{1}{2}S_{\perp k}$ . Then if we consider  $\epsilon_k = |\epsilon_k| \gg \Delta$  (i.e. a pair state  $\mathbf{k}$  well above the Fermi energy) and postulate that the phase of the vacuum state  $|00\rangle_k$  is independent of  $\mathbf{R}$ , the situation is exactly analogous to that analysed in the preceding paragraph, and we find

$$KE_k \propto |\nabla F_k|^2$$

Of course, this expression is not, when summed over  $k$ , equal to  $|\nabla\Psi|^2 = |\nabla \sum_k F_k|^2$ , so further argument is necessary to obtain the quantitative expression for  $\gamma(T)$ .



At first sight, the above arguments may seem unnecessarily complicated, since we have seen that a possible definition of the order parameter is the “effective” two-particle state  $\psi(r, R)$  into which  $N_c$  Cooper pairs are condensed, why can we not normalize  $\psi$  to 1 and argue that the kinetic energy is apart from constants, simply  $N_c(T)$  times  $|\nabla\varphi|^2$ ?

Equivalently, it would seem that we could write the  $KE$  as

$$\frac{1}{2} \left( \frac{\hbar}{2m} \right)^2 \int d\mathbf{r} \int d\mathbf{R} |\nabla F(r, \mathbf{R})|^2 = (\text{for phase variations})$$

$$\left( \frac{\hbar}{2m} \right)^2 \int \int |F(r, R)|^2 (\nabla\varphi)^2 dr dR \text{ and use the fact that (see lecture 6)}$$

that  $\int \int |F(r, R)|^2 dr dR = N_c(T)$  to find that the coefficient of

$$\left( (\hbar/2m)/\nabla\varphi \right)^2 \equiv v_s^2 \text{ is just } \frac{1}{2} N_c(T), \text{ i.e. that } \rho_s(T)/\rho = N_c(T)/N.$$

But this conclusion is wrong. This is related to the fact that at all temperatures, while the “number of pairs” has in it a factor of order  $\Delta/\epsilon_f$ , the superfluid density  $\rho_s$  does not (cf. the fact that the normal-state conductivity does not contain a factor  $k_B T/E_F$ ; in both cases the small shell of states close to the Fermi energy “drags” the whole of the Fermi sea). At nonzero temperature both  $N_c(T)$  and  $\rho_s(T)$  contain an extra  $T$ -dependent factor, which for  $T \rightarrow T_c$  is

**I** proportional to  $(T_c - T)$ .

## Summary of lecture 8

1. The original BCS theory, which assumes the COM of the Cooper pairs to be at rest, may be generalized by assuming their wave function to be a function of COM variable  $\mathbf{R}$  as well as relative variable  $\mathbf{r}$  :

$$F(\mathbf{r}) \rightarrow F(\mathbf{r}, \mathbf{R})$$

2. The GL OP  $\Psi(\mathbf{R})$  may then be identified with  $F(\mathbf{r}, \mathbf{R})_{\mathbf{r}=0}$ , i.e. with the COM wave function of the Cooper pairs. It is “macroscopic” in the sense that a macroscopic number of pairs is condensed into it.
3. In the limit  $T \rightarrow T_c$ , BCS theory allows us to calculate the GL parameters  $\alpha(T), \beta(T), \gamma(T)$  on the basis of microscopic principles.



## Appendix:

A bare-bones sketch of how to get the results (\*) on S8.4 from BCS theory.

As in the main text, we consider a spatially uniform state and define the GL OP  $\Psi$  (which we can take without loss of generality to be real) in terms of the Anderson pseudospins  $\sigma_k$  by

$$\Psi \equiv \sum_k \sigma_{xk} \equiv S_x$$

We do **not** assume that the  $\sigma_k$  's satisfy the self-consistency equation (BCS gap equation); we wish to find an expression for the free energy  $F(\Psi; T)$  for arbitrary (small)  $\Psi$ . As noted in the text, the contribution of the pairing terms is  $-V_0|\Psi|^2$ , independently of  $T$ . It remains to find the minimum value of the remaining terms in the free energy

$$(H_k - \mu N) - TS \equiv F_1 \quad (H_k \equiv \text{kinetic energy})$$

for given  $\Psi$ .



To find  $F_1$  ( $KE$  + entropy terms) as a function of  $\Psi$  :

1. Use Lagrange multiplier technique, i.e. minimize not  $F_1$ , but rather  $F_1 - 2\lambda\Psi$  for fixed  $\lambda$ , and obtain as a result  $\Psi(\lambda)$ .
2. This is nothing but the BCS problem with  $\Delta \rightarrow \lambda$ , so we obtain

$$\begin{aligned}\Psi(\lambda) &= \frac{\lambda}{2} \sum_k E_k^{-1}(\lambda) \tanh[\beta E_k(\lambda)/2] \\ &= \lambda A(T) + \lambda^3 B(T) + O(\lambda^5) \quad E_k(\lambda) \equiv (\epsilon_k^2 + \lambda^2)^{1/2}\end{aligned}$$

3. The rest is algebra: invert to get  $\lambda(\Psi)$  and use  $F_1 = F_0 + 2 \int_0^\Psi \lambda(\Psi') d\Psi'$  to get

$$F_1(\Psi, T) = (\text{const.} +) A^{-1}(T) |\Psi|^2 + \frac{1}{2} B A^{-4}(T) |\Psi|^4$$

where

$$A(T) \equiv \sum_k |\epsilon_k|^{-1} \tanh \beta |\epsilon_k|/2 \equiv \frac{1}{2} \left( \frac{dn}{d\epsilon} \right) \ln(1.14 \epsilon_c / kT)$$

$$B(T) \equiv - \sum_k \frac{d}{d(\epsilon_k^2)} \frac{\tanh \beta \epsilon_k/2}{2\epsilon_k} \equiv \frac{1}{2} \left( \frac{dn}{d\epsilon} \right) \frac{1}{(\pi k_B T)^2} \cdot \frac{7}{8} \zeta(3)$$

The condition that the total coefficient of  $|\Psi|^2$  (including the potential term), namely  $-V_0 + A^{-1}(T)$ , should vanish then gives the BCS equation for  $T_c$ , and an expansion to lowest order in  $T - T_c$  then gives the equations (\*) on S8.4

