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Relation of BCS and GL Theories

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

$$\mathcal{F}\{\Psi(r){:}\,T\} = \alpha(T)|\Psi(r)|^2 + \frac{1}{2}\beta(T)|\Psi(r)|^4 + \frac{\hbar^2}{2m}\left|\boldsymbol{\nabla} - 2\frac{ie}{\hbar}A(rt)\Psi(r)\right|^2 + \frac{1}{2}\mu_0^{-1}\big(\boldsymbol{\nabla}\times\boldsymbol{A}(r)\big)^2$$

with $\alpha(T) = \alpha_0(T - T_c), \beta(T) = \beta_0 = const.$

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

What is relation between these two descriptions?

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

$$F(\boldsymbol{r})(\equiv F(\boldsymbol{r}_1 - \boldsymbol{r}_2) \Longrightarrow F(\boldsymbol{r}_1, \boldsymbol{r}_2) \equiv F(\boldsymbol{R}, \boldsymbol{r})$$

← generalized pair wave function

($\boldsymbol{R}$: COM; $\boldsymbol{r}$: relative)

[Technical Definition of $F(\boldsymbol{r}_1, \boldsymbol{r}_2)$:

(a) probability amplitude to add an electron of spin ↑ at $\boldsymbol{r}_1$, and one of spin ↓ at $\boldsymbol{r}_2$ 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 $\hat{\rho}_2(\boldsymbol{r_1}\sigma_1\boldsymbol{r_2}\sigma_2 : \boldsymbol{r'_1}\sigma'_1\boldsymbol{r'_2}\sigma'_2)$ corresponding to single macroscopic eigenvalue].

Crudely:

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

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

Expect theory to be "simple" only if scale of variation with respect to $\boldsymbol{R}$ is large compared to "scale of confinement" in $\boldsymbol{r}$, *i.e.* to pair radius ξ'. This is always true for $T \to T_c$, since scale of variation in $\boldsymbol{R}$ 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 ξ' 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 $\boldsymbol{R}$ can become $\lesssim \xi'$. Theory is then very messy – do not attempt to cover here.

Define quite generally:

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

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 $(V_{kk'} = -V_o)$

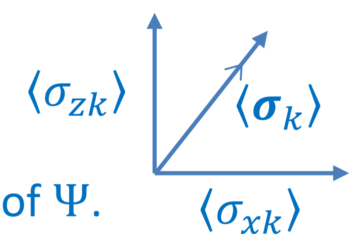
1. Consider spatially uniform case, *i.e.* $F(\boldsymbol{R}, \boldsymbol{r}) \neq f(\boldsymbol{R})$, so that from our definition

$$\Psi(\boldsymbol{R}) = \text{const.} \equiv \Psi \equiv F(\boldsymbol{r} = \boldsymbol{O}) \equiv \sum_k F_k \qquad (F_k \equiv \langle u_k v_k^* \rangle)$$

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

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

$$\langle V \rangle_{pair} = -V_o \sum_{kk\prime} F_k \, F_{k\prime}^* \equiv -V_o |\Psi|^2.$$



so always favors nonzero (and large) value of Ψ.

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

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

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: or rather general grounds expect this to be a decreasing function of $|\Psi|^2$, so if it is analytic expect again terms in $|\Psi|^2$ and $|\Psi|^4$.

Quantitative calculation*: gives precise values for coefficients $\alpha(T)$ and $\beta(T)$ as well as for T_c.

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

and so if we write F in terms of a normalized order parameter $\widetilde{\Delta} \equiv |V_0|\Psi$, then

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

and differentiation with respect to $\widetilde{\Delta}$ gives back the BCS result

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

* See *e.g.* AJL, Quantum Liquids, section 5

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

$$\Psi(\boldsymbol{r}:\boldsymbol{T}) = \left|\Psi_{eq}(T)\right| \exp i\,\varphi(r)$$

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

$$\boldsymbol{v}_s = \frac{\hbar}{2m}\boldsymbol{\nabla}\varphi$$ ← "superfluid velocity"

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

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

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 by applying a vector potential $\boldsymbol{A} = m\mathbf{v}/e$; the required momentum P is by definition $(\rho_n\,(T)/\rho)Nm\mathbf{v}$, and the extra KE is $\frac{1}{2}\rho_n(T)\mathrm{v}_n^2 \equiv \frac{1}{2}\rho_n\mathrm{v}^2$. On the other hand, the extra energy acquired by boosting the condensate to velocity $\mathbf{v}$ is, as above, $\frac{1}{2}\rho_s\mathrm{v}_s^2 \equiv \frac{1}{2}\rho_s\mathrm{v}^2$. Since the total energy due to the boost must by Galilean invariance be $\frac{1}{2}\rho\mathrm{v}^2$, we have

$$\rho_n(T) + \rho_s(T) = \rho$$

and thus by result of Lecture 7

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

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

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

by comparing this with $\frac{1}{2}\rho_s(T)\mathrm{v}_s^2$, 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 $\Psi(T) = \Delta(T)$.

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

Generalizations:

effect of vector potential: $\boldsymbol{\nabla} \to \nabla - 2\frac{ie}{\hbar}\boldsymbol{A}(r)$ (since Cooper pair has charge $2e$)

spatially varying case: provide scale of variation ≫ pair radius able to replace

$$\mathcal{F}(\Psi{:}\,T) \to \mathcal{F}\{\Psi(r){:}\,T\}$$

$\Longrightarrow$ complete GL free energy, QED

↑: have assumed (rather than demonstrated) that correct form of gradient term in const$|\nabla\Psi|^2 \equiv$ const $(|\Psi|^2(\nabla\varphi)^2 + (\nabla|\Psi|)^2)$