Microscopic derivation of the Ginzburg-Landau model[1]

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[1] *Joint work with Rupert Frank, Christian Hainzl, and Robert Seiringer*

Abstract of Talk

I will discuss how the **Ginzburg-Landau** (GL) model of **superconductivity** arises as an **asymptotic limit** of the microscopic **Bardeen-Cooper-Schrieffer** (BCS) model.

The asymptotic limit may be seen as a **semiclassical limit** and one of the main difficulties is to derive a semiclassical expansion with **minimal regularity assumptions**.

It is not rigorously understood how the BCS model approximates the underlying **many-body quantum system**. I will formulate the BCS model as a variational problem, but only heuristically discuss its relation to quantum mechanics.

Outline of Talk

1. Ginzburg-Landau (GL) model
2. The Bardeen-Cooper-Schrieffer (BCS) model
3. BCS Free energy functional
4. The asymptotic regime
5. Main result
6. A few references
7. Sketch of proof
8. Semiclassical estimate

Ginzburg-Landau (GL) model

For superconducting materials on $3D$ box Λ (Could be 1D or 2D):
W potential, $\mathbf{A}$ magnetic vector potential:
GL functional: For constants $B_1, B_3 > 0$ and $B_2 \in \mathbb{R}$:

$$\mathcal{E}^{\mathrm{GL}}(\psi) = \int_\Lambda B_1|(-i\nabla + 2\mathbf{A}(x))\psi(x)|^2 + B_2 W(x)|\psi(x)|^2 + B_3 \left|1 - |\psi(x)|^2\right|^2 dx\,, \quad \psi \in H^1(\Lambda)$$

What is ψ?

What does this have to do with **Bardeen-Cooper-Schrieffer (BCS) theory of superconductivity?**

We will derive GL from BCS in an appropriate limit:
$T \approx T_c$, $\mathbf{A}$, W small and slowly varying on microscopic scale.

The BCS states

Fermionic wave functions $\Psi \in \bigoplus_{N=0}^{\infty} \bigwedge^N L^2(\Xi)$ **(Fock Space)**.
E.g., $\Xi = \Lambda \times \{-1, 1\}$, $\Lambda \subseteq \mathbb{R}^3$, ± 1 =spin-degrees, $\xi = (x, \sigma)$.
Normal state (Slater determinant): For N particles

$$\Psi(\xi_1, \ldots, \xi_N) \approx \phi_1 \wedge \cdots \wedge \phi_N(\xi_1, \ldots, \xi_N) = (N!)^{-1/2} \mathrm{det}(\phi_i(\xi_j))$$

BCS state: Describes an average over $0, 1, \ldots, 2M$ particle states

$$\Psi \approx (\alpha_1 + \beta_1 \phi_1 \wedge \phi_2) \wedge \cdots \wedge (\alpha_M + \beta_M \phi_{2M-1} \wedge \phi_{2M})$$

$\phi_1, \ldots, \phi_{2M}$ orthonormal in $L^2(\Xi)$, $|\alpha_i|^2 + |\beta_i|^2 = 1$.
Describe state in terms of **1-particle density matrices:**

$$\begin{aligned} \boldsymbol{\gamma} &= |\beta_1|^2 (|\phi_1\rangle\langle\phi_1| + |\phi_2\rangle\langle\phi_2|) + \ldots \\ &\quad + |\beta_M|^2 (|\phi_{2M-1}\rangle\langle\phi_{2M-1}| + |\phi_{2M}\rangle\langle\phi_{2M}|) \\ \boldsymbol{\alpha} &= \alpha_1 \overline{\beta_1} \phi_1 \wedge \phi_2 + \ldots + \overline{\alpha_M} \beta_M \phi_{2M-1} \wedge \phi_{2M} \end{aligned}$$

$\boldsymbol{\alpha}$ is the **Cooper pair wave function**. Vanishes in normal state.

BCS States continued

Spin dependence (pairing of spin up and down):

$$\begin{aligned}\boldsymbol{\gamma}(x,\sigma;y,\tau) &= \gamma(x,y)(\delta_{\sigma,1}\delta_{\tau,1}+\delta_{\sigma,-1}\delta_{\tau,-1}),\ \gamma(x,y)=\overline{\gamma(y,x)}\\ \boldsymbol{\alpha}(x,\sigma;y,\tau) &= \alpha(x,y)(\delta_{\sigma,1}\delta_{\tau,-1}-\delta_{\sigma,-1}\delta_{\tau,1}),\ \alpha(x,y)=\alpha(y,x)\end{aligned}$$

2×2-block matrix-operator

$$\Gamma = \begin{pmatrix} \gamma & \alpha \\ \overline{\alpha} & 1-\overline{\gamma} \end{pmatrix}$$

$T=0$ **BCS state**: State is pure (case described above) and Γ is a **projection** with vanishing **entropy**:

$$S(\Gamma) = -\mathrm{Tr}\,[\Gamma\ln\Gamma] = -\frac{1}{2}\mathrm{Tr}\,[\Gamma\ln\Gamma + (1-\Gamma)\ln(1-\Gamma)]$$

$T>0$ **BCS-state**: State is not pure $0<\Gamma<\mathbf{1}$, $S(\Gamma)>0$.

BCS Free energy functional

Hamiltonian: For gases of fermionic atoms on $3d$-torus Λ:

$$H = \sum_j \left((-i\nabla_j + \mathbf{A}(x_j))^2 - \mu + W(x_j)\right) + \sum_{i\neq j} V(|x_i - x_j|)$$

Remark: The original BCS Hamiltonian obtained after integrating out phonons is similar, but non-local.

BCS free energy functional: Temperature $T \geq 0$

$$\begin{aligned}\mathcal{F}(\Gamma) &= \operatorname{Tr}\left[\left((-i\nabla + \mathbf{A}(x))^2 - \mu + W(x)\right)\gamma\right] - T\,S(\Gamma) \\ &\quad + \int_{\Lambda\times\Lambda} V(|x-y|)|\alpha(x,y)|^2\,dx\,dy\,.\end{aligned}$$

Remark: Would be upper bound except we ignore (absorb in μ)

- **direct term:** $\iint \gamma(x,x)\gamma(y,y)V(|x-y|)dxdy$
- **exhange term:** $-\iint |\gamma(x,y)|^2 V(|x-y|)dxdy$.

BCS free energy in special cases

• **Non-interacting case** $V = 0$: BCS minimizer is **normal** state Γ_0: $\alpha = 0$,

$$\gamma_0 = (1 + \exp(\mathfrak{h}/T))^{-1}, \quad \mathfrak{h} = (-i\nabla + \mathbf{A}(x))^2 + W(x) - \mu$$

• **Translation invariant case** $\mathbf{A} = \mathbf{0}$, $W = 0$: There exists **critical temperature** $T_c \geq 0$ such that.

- $T \geq T_c$: Minimizer is normal (as above with $\mathbf{A} = \mathbf{0}$, $W = 0$)
- $T < T_c$: Minimizer has $\alpha \neq 0$.

The critical temperature may be characterized by the operator

$$K_{\mathrm{T_c}}(-\nabla^2 - \mu) + V(|x|), \qquad K_T(\eta) = \frac{\eta}{\tanh(\eta/2T)}$$

having 0 as the lowest eigenvalue (on symmetric functions).
Note $\sigma(K_T(-\nabla^2 - \mu) = [2T, \infty)$.
We assume $T_c > 0$ and **eigenfunction** α_0 unique (e.g. $\widehat{V} < 0$ OK).

Making the asymptotics precise

Introduce **small parameter** $h > 0$. $\mathbf{A}$, W occuring in GL functional are **rescaled** versions of the potentials in BCS functional. Denote quantities in BCS functional by $\widetilde{\mathbf{A}}, \widetilde{W}, \widetilde{\Lambda}$. In terms of quantities in GL functional:

$$\widetilde{\mathbf{A}}(x) = h\mathbf{A}(hx), \quad \widetilde{W}(x) = h^2 W(hx), \quad \widetilde{\Lambda} = h^{-1}\Lambda$$

In BCS functional $\widetilde{\mathcal{F}}$ insert $\widetilde{\alpha} = h^3\alpha(hx, hy)$, $\widetilde{\gamma} = h^3\gamma(hx, hy)$:

$$\begin{aligned} \widetilde{\mathcal{F}}(\widetilde{\Gamma}) &= \operatorname{Tr}\left[\left((-ih\nabla + h\mathbf{A}(x))^2 - \mu + h^2 W(x)\right)\gamma\right] \\ &\quad -T\,S(\Gamma) + \int_{\Lambda\times\Lambda} V(h^{-1}|x-y|)|\alpha(x,y)|^2\,dx\,dy\,. \end{aligned}$$

Here we assume

$$T = T_c(1 - Dh^2), \quad D > 0.$$

Note the **semiclassical nature** of the asymptotics.
The **order of the free energy** is h^{-3}.

Main result

Theorem (GL limit of BCS)

If $T = T_c(1 - Dh^2)$ there exist B_1, B_2, B_3 in GL functional giving

$$\inf_{\Gamma} \mathcal{F}(\Gamma) = \mathcal{F}(\Gamma_0) + h^{-3+4}(\inf_{\psi} \mathcal{E}^{\mathrm{GL}}(\psi) - B_3|\Lambda| + o(1)),$$

as $h \to 0$, where Γ_0 is the **normal state***. Moreover, if $\mathcal{F}(\Gamma) \leq \mathcal{F}(\Gamma_0) + h\left(\inf_{\psi} \mathcal{E}^{\mathrm{GL}}(\psi) - B_3|\Lambda| + o(1)\right)$ then the corresponding* **Cooper pair wave function** *α satisfies:*

$$\|\alpha - \alpha_{\mathrm{GL}}\|_{L^2}^2 \leq o(h)\|\alpha_{\mathrm{GL}}\|_{L^2}^2 = o(h)h^{2-3}$$

$$\alpha_{\mathrm{GL}}(x,y) = h^{-3+1}\psi_0\left(\frac{x+y}{2}\right)\alpha_0\left(\frac{x-y}{h}\right) = \mathit{Op}(h\psi_0(x)\widehat{\alpha}_0(ih\nabla))$$

(α_0 appropriately normalized) and $\mathcal{E}^{\mathrm{GL}}(\psi_0) \leq \inf_{\psi} \mathcal{E}(\psi) + o(1)$.

Short history

- V.L. Ginzburg, L.D. Landau, *On the theory of superconductivity*, Zh. Eksp. Teor. Fiz. **20**, 1064–1082 **(1950)**.
- J. Bardeen, L. Cooper, J. Schrieffer, *Theory of Superconductivity*, Phys. Rev. **108**, 1175–1204 **(1957)**.
- L.P. Gor'kov, *Microscopic derivation of the Ginzburg-Landau equations in the theory of superconductivity*, Zh. Eksp. Teor. Fiz. **36**, 1918–1923 (1959); *English translation* Soviet Phys. JETP **9**, 1364–1367 **(1959)**.
- P.G. de Gennes, *Superconductivity of Metals and Alloys*, Westview Press **(1966)**.
- C. Hainzl, E. Hamza, R. Seiringer, J.P. Solovej, *The BCS functional for general pair interactions*, Commun. Math. Phys. **281**, 349–367 **(2008)**.

Sketch of proof

Rewrite:

$$\mathcal{F}(\Gamma) = \frac{1}{2}\mathrm{Tr}\left[H_\Delta \Gamma\right] - TS(\Gamma) - \int V(|x-y|/h)|\alpha_{\rm GL}(x,y)|^2 dxdy$$
$$+ \int V(|x-y|/h)|\alpha_{\rm GL}(x,y) - \alpha(x,y)|^2 dxdy$$

$$\Delta(x,y) = 2V(|x-y|/h)\alpha_{\rm GL}(x,y) = 2h\mathsf{Op}(\psi_0(x)(\widehat{\alpha_0 V})(-ih\nabla))$$

$$H_\Delta = \begin{pmatrix} \mathfrak{h} & \Delta \\ \overline{\Delta} & -\overline{\mathfrak{h}} \end{pmatrix}, \quad \mathfrak{h} = (-ih\nabla + h\mathbf{A}(x))^2 - \mu + h^2 W(x).$$

$$2T\left[\mathrm{Tr}\left[H\Gamma\right] - TS(\Gamma)\right] \geq \overbrace{-\mathrm{Tr}\,\ln(1+\exp(-H/T))}^{\text{the inf}}$$
$$+ \mathrm{Tr}\,\left[K_T(H)\left(\Gamma - (1+\exp(H/T))^{-1}\right)^2\right],$$

First use this with $\alpha_{\rm GL}$ replaced by 0 and gap in $K_{T_c}(H_0) + V$ to conclude α close to $\alpha_{\rm GL}$ (almost ground state of $K_{T_c} + V$).

Semiclassical estimate

Finally, use semiclassical estimates with good regularity bounds:

Theorem (Semiclassical estimate)

With errors controlled by H^1 and H^2 norms of ψ_0

$$-\frac{h^3}{2}T\Big(\mathrm{Tr}\ \ln(1+\exp(-H_\Delta/T)) - \mathrm{Tr}\ \ln(1+\exp(-H_0/T)\Big)$$
$$= h^2\mathcal{D}_2(\psi_0) + h^4\mathcal{D}_4(\psi_0) + h^4(\mathcal{E}(\psi_0) - B_3|\Lambda|) + O(h^5)$$

$$h^3\int V(|x-y|/h)|\alpha_{\mathrm{GL}}(x,y)|^2 dxdy = h^2\mathcal{D}_2(\psi_0) + h^4\mathcal{D}_4(\psi_0) + O(h^5)$$