Microscopic Derivation of Ginzburg–Landau Theory

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Abstract of the 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.

Superconductivity and Superfluidity

Superconductivity is the phenomenon that certain materials have zero electrical resistance below a **critical temperature**.
This is a **quantum phenomenon** on a **macroscopic scale**.

A brief history of superconductivity:

1911 **Onnes** discovers superconductivity experimentally

1950 **Ginzburg** and **Landau** provide a phenomenological **macroscopic model** for superconductivity

1957 **Bardeen**, **Cooper** and **Schrieffer** propose a **microscopic theory** and introduce the concept of **Cooper pairs**

1959 **Gor'kov** gives a derivation of GL theory from BCS theory

In addition, important contributions from **Bogoliubov**, **de Gennes**, ...

The related phenomenon of **superfluidity** concerns fluids with **zero viscosity**. While originally discovered in liquid helium, it is currently being explored in experiments on **ultracold atomic gases**.

The Ginzburg–Landau model

Let $\mathcal{C} \subset \mathbb{R}^3$ be a compact set and let A and W be vector and scalar potentials on $\mathcal{C}$. Set

$$\mathcal{E}_D^{\mathrm{GL}}(\psi)=\int_{\mathcal{C}}\Big[B_1|(-i\nabla+2A(x))\,\psi(x)|^2+B_2W(x)|\psi(x)|^2-B_3D|\psi(x)|^2+B_4|\psi(x)|^4\Big]dx$$

Here, $B_1, B_3, B_4 > 0$, $B_2 \in \mathbb{R}$ and $D \in \mathbb{R}$ are coefficients.

Ginzburg–Landau energy $\qquad E_D^{\mathrm{GL}} = \inf_\psi \mathcal{E}_D^{\mathrm{GL}}(\psi)$

A minimizing ψ describes the macroscopic variations in the **superfluid density**. The normal state corresponds to $\psi \equiv 0$, while $|\psi| > 0$ means superfluidity (or supercond.).

Question: Is the optimal $\psi \equiv 0$ or not?

For us, $\mathcal{C} = [0,1]^3$ and ψ satisfies periodic boundary conditions (torus)

One is often interested in minimizing over both ψ and A, adding an additional field energy term. For us, A is **fixed** (but arbitrary).

The BCS model

State of the system described by a 2×2 operator-valued matrix (op. in $L^2(\mathbb{R}^3) \oplus L^2(\mathbb{R}^3)$)

$$\Gamma = \begin{pmatrix} \gamma & \alpha \\ \bar{\alpha} & 1 - \bar{\gamma} \end{pmatrix} \qquad \text{with} \quad 0 \leq \Gamma \leq 1$$

Here, $0 \leq \gamma \leq 1$ is the 1-particle density matrix, and α the **Cooper-pair wavefunction**.

$$\mathcal{F}_T^{\mathrm{BCS}}(\Gamma) := \mathrm{Tr}\left[\left((-ih\nabla + hA(x))^2 - \mu + h^2 W(x)\right)\gamma\right] + T\,\mathrm{Tr}\,\Gamma \ln \Gamma$$
$$+ \iint_{\mathcal{C} \times \mathbb{R}^3} V(h^{-1}(x-y))|\alpha(x,y)|^2\, dx\, dy$$

Again $\mathcal{C} = [0,1]^3$, Γ is periodic and Tr stands for the **trace per unit volume**.

BCS energy $\qquad F_T^{\mathrm{BCS}} = \inf_\Gamma \mathcal{F}_T^{\mathrm{BCS}}(\Gamma)$

The normal state corresponds to $\alpha \equiv 0$, while $|\alpha| > 0$ describes Cooper pairs.

Question: Is the optimal $\alpha \equiv 0$ or not?

Remarks about the BCS model

$$\mathcal{F}_T^{\mathrm{BCS}}(\Gamma) = \mathrm{Tr}\left[\left((-ih\nabla + hA(x))^2 - \mu + h^2 W(x)\right)\gamma\right] + T\,\mathrm{Tr}\,\Gamma\ln\Gamma$$
$$+ \iint_{\mathcal{C}\times\mathbb{R}^3} V(h^{-1}(x-y))|\alpha(x,y)|^2\,dx\,dy$$

- Can be heuristically derived from a many-body Hamiltonian for spin $\frac{1}{2}$ fermions with two-body interaction V via **two simplifications**. First, one restricts to **quasi-free states**, and second one drops the **direct and exchange term** in the interaction energy.

- **Microscopic data**: chemical potential μ, temperature T, interaction potential V

- **Macroscopic data**: vector magnetic potential A, scalar electric potential W

- **What is h?** It is the **ratio of the microscopic and macroscopic scale**.

- **Technical assumptions**: V real-valued, $V(x) = V(-x)$ and $V \in L^{3/2}(\mathbb{R}^3)$
  W and A periodic and $\widehat{W}(p)$, $|\widehat{A}(p)|(1+|p|) \in \ell^1$

The normal state

Let us first discuss the **non**-superfluid case, i.e.,

$$\inf_{0\le\gamma\le 1} \mathcal{F}_T^{\rm BCS}\left(\begin{pmatrix}\gamma & 0 \\ 0 & 1-\overline{\gamma}\end{pmatrix}\right) = \inf_{0\le\gamma\le 1}\left\{\operatorname{Tr} H\gamma + T\operatorname{Tr}\left(\gamma\ln\gamma + (1-\gamma)\ln(1-\gamma)\right)\right\}$$
$$= -T\operatorname{Tr}\ln\left(1+e^{-H/T}\right)$$

with $H = (-ih\nabla + hA(x))^2 + h^2 W(x) - \mu$.

This infimum is attained iff Γ is the **normal state**

$$\Gamma_T^{\rm normal} = \begin{pmatrix}\gamma_T^{\rm normal} & 0 \\ 0 & 1-\overline{\gamma_T^{\rm normal}}\end{pmatrix}, \qquad \gamma_T^{\rm normal} = \left(1+e^{H/T}\right)^{-1}.$$

Order of magnitude of free energy: By **Weyl's law**,

$$\mathcal{F}_T^{\rm BCS}\left(\Gamma_T^{\rm normal}\right) = -T\operatorname{Tr}\ln\left(1+e^{-H/T}\right) \sim -\frac{T}{(2\pi h)^3}\int_{\mathbb{R}^3}\ln(1+e^{-p^2/T})dp \quad \text{as } h\to 0.$$

The critical temperature

Define

$$\overline{T_c(h)} := \sup \left\{ T \geq 0 : \ F_T^{\rm BCS} < \mathcal{F}_T^{\rm BCS} \left(\Gamma_T^{\rm normal} \right) \right\}$$
$$\underline{T_c(h)} := \inf \left\{ T \geq 0 : \ F_T^{\rm BCS} = \mathcal{F}_T^{\rm BCS} \left(\Gamma_T^{\rm normal} \right) \right\}$$

Lemma 1. $T_c := \lim_{h\to 0} \overline{T_c(h)} = \lim_{h\to 0} \underline{T_c(h)}$ *exists in* $[0,\infty)$ *and is characterized by*

$$\inf \operatorname{spec} \left(K_T + V \right) < 0 \quad \text{if } 0 \leq T < T_c \,,$$
$$\inf \operatorname{spec} \left(K_T + V \right) \geq 0 \quad \text{if } T \geq T_c \,,$$

where $K_T = (-\Delta - \mu) \coth((-\Delta - \mu)/2T)$ *in* $L^2(\mathbb{R}^3)$.

Note that T_c does not depend on the 'macroscopic' A or W.

In the following, we shall **assume** that V and μ are such that $T_c > 0$, and that the eigenvalue 0 of $K_{T_c} + V$ is **simple**. This is satisfied, e.g., if $\widehat{V} \leq 0$ (and $\not\equiv 0$).

Let α_0 denote the normalized eigenfunction of $K_{T_c} + V$ corresponding to its eigenvalue 0.

MAIN RESULTS: ASYMPTOTICS OF ENERGY AND MINIMIZERS

THEOREM 1. *Fix* $D \in \mathbb{R}$ *and let* $T = T_c(1 - h^2 D)$. *For appropriate* $B_1, \ldots, B_4$,

$$\boxed{F_T^{\mathrm{BCS}} = \mathcal{F}_T^{\mathrm{BCS}}(\Gamma_T^{\mathrm{normal}}) + h\left(E_D^{\mathrm{GL}} + o(1)\right)}$$

with $E_D^{\mathrm{GL}} = \inf_\psi \mathcal{E}_D^{\mathrm{GL}}(\psi)$ *and* $\mathrm{const.}\, h^2 \geq o(1) \geq -\mathrm{const.}\, h^{1/5}$ *for small* h.

THEOREM 2. *If* Γ *is an* **approximate minimizer** *of* $\mathcal{F}_T^{\mathrm{BCS}}$ *at* $T = T_c(1 - h^2 D)$, *in the sense that*

$$\mathcal{F}_T^{\mathrm{BCS}}(\Gamma) \leq \mathcal{F}_T^{\mathrm{BCS}}(\Gamma_T^{\mathrm{normal}}) + h\left(E_D^{\mathrm{GL}} + \epsilon\right)$$

for some small $\epsilon > 0$, *then the corresponding* α *can be* **decomposed** *as*

$$\boxed{\alpha = \frac{h}{2}\big(\psi(x)\widehat{\alpha}_0(-ih\nabla) + \widehat{\alpha}_0(-ih\nabla)\psi(x)\big) + \sigma}$$

with $\iint_{\mathcal{C}\times\mathbb{R}^3} |\sigma(x,y)|^2\, dx\, dy \leq \mathrm{const.}\, h^{3/5}$ *and*

$$\mathcal{E}_D^{\mathrm{GL}}(\psi) \leq E_D^{\mathrm{GL}} + \epsilon + \mathrm{const.}\, h^{1/5}$$

Remarks on...

... energy asymptotics:

$$\boxed{F_T^{\mathrm{BCS}} = \mathcal{F}_T^{\mathrm{BCS}}(\Gamma_T^{\mathrm{normal}}) + h\left(E_D^{\mathrm{GL}} + o(1)\right)}$$

• $\mathcal{F}_T^{\mathrm{BCS}}(\Gamma_T^{\mathrm{normal}}) \sim Ch^{-3}$, hence GL theory gives an $O(h^4)$ correction to the main term.

• For smooth enough A and W, one could also expand $\mathcal{F}_T^{\mathrm{BCS}}(\Gamma_T^{\mathrm{normal}})$ to order h. We bound directly the energy difference, however!

... asymptotics of almost minimizers:

$$\boxed{\alpha = \frac{h}{2}\big(\psi(x)\widehat{\alpha}_0(-ih\nabla) + \widehat{\alpha}_0(-ih\nabla)\psi(x)\big) + \sigma}$$

• That is,

$$\alpha(x,y) = \frac{1}{2h^2}\left(\psi(x)+\psi(y)\right)\alpha_0\left(\tfrac{x-y}{h}\right) + \sigma(x,y) \approx \frac{1}{h^2}\,\psi\left(\tfrac{x+y}{2}\right)\alpha_0\left(\tfrac{x-y}{h}\right)$$

• To appreciate $\iint |\sigma(x,y)|^2\,dx\,dy \leq \mathrm{const.}\,h^{3/5}$, note that for the main term $\iint |h^{-2}\psi((x+y)/2)\alpha_0((x-y)/h)|^2\,dx\,dy = \mathrm{const.}\,h^{-1}$.

The coefficients in the GL functional

$$\mathcal{E}_D^{\mathrm{GL}}(\psi) = \int_{\mathcal{C}} \left[\left| \mathbb{B}_{\mathbf{1}}^{1/2} (-i\nabla + 2A)\, \psi \right|^2 + \mathbf{B_2} W |\psi|^2 - \mathbf{B_3} D |\psi|^2 + \mathbf{B_4} |\psi|^4 \right] dx$$

Let t be the Fourier transform of $2K_{T_c}\alpha_0 = -2V\alpha_0$, where $\|\alpha_0\|_2 = 1$. Let

$$g_1(z) = \frac{e^{2z} - 2ze^z - 1}{z^2(1+e^z)^2}\,, \qquad g_2(z) = g_1'(z) + 2g_1(z)/z\,.$$

Then the matrix $\mathbb{B}_{\mathbf{1}}$ and the numbers $\mathbf{B_2}$, $\mathbf{B_3}$ and $\mathbf{B_4}$ are given by ($\beta_c = T_c^{-1}$)

$$(\mathbb{B}_1)_{ij} = \frac{\beta_c^2}{16} \int_{\mathbb{R}^3} t(p)^2 \left(\delta_{ij} g_1(\beta_c(p^2-\mu)) + 2\beta_c p_i p_j\, g_2(\beta_c(p^2-\mu)) \right) \frac{dp}{(2\pi)^3}\,, \qquad \mathbb{B}_{\mathbf{1}} > \mathbf{0}$$

$$B_2 = \frac{\beta_c^2}{4} \int_{\mathbb{R}^3} t(p)^2\, g_1(\beta_c(p^2-\mu)) \frac{dp}{(2\pi)^3}\,,$$

$$B_3 = \frac{\beta_c}{8} \int_{\mathbb{R}^3} t(p)^2 \cosh^{-2}\left(\tfrac{\beta_c}{2}(p^2-\mu) \right) \frac{dp}{(2\pi)^3}\,, \qquad \mathbf{B_3} > \mathbf{0}\,,$$

$$B_4 = \frac{\beta_c^2}{16} \int_{\mathbb{R}^3} t(p)^4 \frac{g_1(\beta_c(p^2-\mu))}{p^2-\mu} \frac{dp}{(2\pi)^3}\,, \qquad \mathbf{B_4} > \mathbf{0}\,.$$

Main results: Asymptotics of the critical temperature

For every $\psi \in H^1_{\mathrm{per}}(\mathcal{C})$,

$$\mathcal{E}^{\mathrm{GL}}_D(\psi) = \int_{\mathcal{C}} \left[\left| \mathbb{B}_1^{1/2}(-i\nabla + 2A)\,\psi \right|^2 + B_2 W|\psi|^2 - B_3 \mathbf{D}|\psi|^2 + B_4|\psi|^4 \right] dx$$

is an affine-linear, non-increasing function of D with $\mathcal{E}^{\mathrm{GL}}_D(0) = 0$.

Thus, E^{GL}_D is a non-positive, **non-increasing and concave** function of D. Let

$$\begin{aligned} D_c &= \sup\{D \in \mathbb{R} : \ E^{\mathrm{GL}}_D = 0\} \\ &= \inf\{D \in \mathbb{R} : \ E^{\mathrm{GL}}_D < 0\} \\ &= B_3^{-1} \inf \mathrm{spec}\ \left((-i\nabla + 2A)\mathbb{B}_1(-i\nabla + 2A) + B_2 W\right) \end{aligned}$$

Corollary 1.

$$\lim_{h\to 0} \frac{\overline{T_c(h)} - T_c}{T_c h^2} = \lim_{h\to 0} \frac{\underline{T_c(h)} - T_c}{T_c h^2} = -D_c$$

Key Semiclassical Estimates

For $\psi \in H^2_{\rm loc}(\mathbb{R}^d)$ and t "sufficiently nice", let Δ denote the operator

$$\Delta = -\frac{h}{2}\left(\psi(x)t(-ih\nabla) + t(-ih\nabla)\psi(x)\right)$$

The **effective Hamiltonian** on $L^2(\mathbb{R}^d) \otimes \mathbb{C}^2$ is

$$H_\Delta = \begin{pmatrix} (-ih\nabla + hA(x))^2 - \mu + h^2 W(x) & \Delta \\ \bar\Delta & -(ih\nabla + hA(x))^2 + \mu - h^2 W(x) \end{pmatrix}$$

THEOREM 3. *Let $f(z) = -\ln\left(1+e^{-z}\right)$ and $\varphi(p) = \frac{1}{2}\frac{t(p)}{p^2-\mu}\tanh(\frac{\beta}{2}(p^2-\mu))$. Then*

$$\frac{h^d}{\beta}\operatorname{Tr}\left[f(\beta H_\Delta) - f(\beta H_0)\right] = h^2 E_1 + h^4 E_2 + O(h^6)\left(\|\psi\|^6_{H^1(\mathcal{C})} + \|\psi\|^2_{H^2(\mathcal{C})}\right),$$

for explicit E_1 and E_2. Moreover, the off-diagonal entry α_Δ of $[1+e^{\beta H_\Delta}]^{-1}$ satisfies

$$\left\|\alpha_\Delta - \tfrac{h}{2}\left(\psi(x)\varphi(-ih\nabla) + \varphi(-ih\nabla)\psi(x)\right)\right\|_{H^1} \leq \text{const.}\, h^{3-d/2}\left(\|\psi\|_{H^2(\mathcal{C})} + \|\psi\|^3_{H^1(\mathcal{C})}\right)$$

Conclusions

- **Rigorous derivation** of Ginzburg-Landau theory, starting from the BCS model.
- For weak external fields and close to the critical temperature, GL arises as an **effective theory** on the macroscopic scale.
- The relevant scaling limit is **semi-classical** in nature.

Some open problems:

- Treat physical boundary conditions
- Treat self-consistent magnetic fields
- Derive BCS theory from many-body quantum mechanics