A microscopic derivation of Ginzburg–Landau theory

Rupert L. Frank
Department of Mathematics
Princeton University

Joint work with C. Hainzl, R. Seiringer, J. P. Solovej

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The Ginzburg–Landau Model

Introduced in 1950 as a **phenomenological model of a superconductor**. For given vector and scalar potentials A and W on a compact set $\mathcal{C}$,

$$\mathcal{E}^{\mathrm{GL}}(\psi)=\int_{\mathcal{C}}\left[B_1|(-i\nabla+2A(x))\,\psi(x)|^2+B_2W(x)|\psi(x)|^2+B_3\left(|\psi(x)|^4-2D|\psi(x)|^2\right)\right]dx$$

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

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

A minimizing ψ describes the macroscopic variations in the **superfluid density**. The normal state corresponds to $\psi \equiv 0$, while $|\psi| > 0$ describes superconducting particles.

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

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 Functional

Bardeen–Cooper–Schrieffer (1957): a **microscopic theory** of superconductivity
State of the system described by a 2×2 operator-valued matrix

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

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

For chemical potential $\mu \in \mathbb{R}$ and temperature $T > 0$, the **BCS energy functional** is

$$\operatorname{Tr}\left[\left(\left(-i\nabla + \tilde{A}(x)\right)^2 - \mu + \tilde{W}(x)\right)\gamma\right] - T\,S(\Gamma) + \iint \tilde{V}(x-y)|\alpha(x,y)|^2\,dx\,dy\,.$$

The entropy equals $S(\Gamma) = -\operatorname{Tr}\left[\Gamma \ln \Gamma\right]$.

The BCS functional can be heuristically derived from the full many-body Hamiltonian with pair-interaction V via two steps of simplification. First, one considers only **quasi-free states**, and second one neglects the direct and exchange term in the interaction energy.

Microscopic vs. Macroscopic Scale

We are interested in interactions $\tilde{V}(x) = V(h^{-1}x)$ of size one varying on the **microscopic scale** and external fields $\tilde{A}(x) = hA(hx)$ and $\tilde{W}(x) = h^2W(hx)$ which are weak and vary on the **macroscopic scale**. Here h is a small parameter. Thus,

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

To avoid boundary conditions, we assume that the system is periodic (with period 1). $\mathcal{C}$ denotes the unit cube $[0,1]^3$, and Tr stands for the **trace per unit volume**.

We make the following **assumptions** on the functions A, W and V appearing in $\mathcal{F}^{\mathrm{BCS}}$.

- W and A are periodic, and $\widehat{W}(p)$ and $|\widehat{A}(p)|(1+|p|)$ are summable.
- V is real-valued and reflection-symmetric, i.e., $V(x) = V(-x)$, with $V \in L^{3/2}(\mathbb{R}^3)$.

Non-local potentials V (as in the original BCS model) could also be considered.

The Translation-Invariant Case

For $W = 0 = A$, we can restrict to **translation-invariant** states Γ. In this case, there exists a **critical temperature** $T_c \geq 0$ such that

- For $T \geq T_c$, $\alpha = 0$ in any minimizer of $\mathcal{F}^{\mathrm{BCS}}$.
- For $T < T_c$, $\alpha \neq 0$ in any minimizer of $\mathcal{F}^{\mathrm{BCS}}$.

In fact, T_c turns out to be the unique T such that

$$\frac{-\nabla^2 - \mu}{\tanh\left(\frac{-\nabla^2-\mu}{2T}\right)} + V(x) =: K_T(-i\nabla) + V(x)$$

has 0 as its lowest eigenvalue (Hainzl, Hamza, Seiringer, Solovej 2008).

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

Let α_0 denote the eigenfunction of $K_{T_c}(-i\nabla) + V$ corresponding to eigenvalue 0.

Main Results: Energy Asymptotics

Let Γ_0 denote the minimizer of $\mathcal{F}^{\mathrm{BCS}}$ for $V = 0$, i.e.,

$$\Gamma_0 := \begin{pmatrix} \gamma_0 & 0 \\ 0 & 1 - \bar{\gamma}_0 \end{pmatrix} \quad \text{with } \gamma_0 = \left(1 + \exp\left((-ih\nabla + hA(x))^2 + h^2 W(x) - \mu)/T\right)\right)^{-1}$$

Define the **energy difference**

$$F^{\mathrm{BCS}}(T, \mu) = \inf_{0 \leq \Gamma \leq 1} \mathcal{F}^{\mathrm{BCS}}(\Gamma) - \mathcal{F}^{\mathrm{BCS}}(\Gamma_0)\,.$$

Note that $\mathcal{F}^{\mathrm{BCS}}(\Gamma_0) = T\,\mathrm{Tr}\ln(1 - \gamma_0) = O(h^{-3})$ for small h.

THEOREM 1. *Fix $D > 0$. For appropriate coefficients B_1, B_2 and B_3*

$$\boxed{F^{\mathrm{BCS}}(T_c(1 - h^2 D), \mu) = h\left(E^{\mathrm{GL}} + o(1)\right)}$$

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

For smooth enough A and W, one could also expand $\mathcal{F}^{\mathrm{BCS}}(\Gamma_0)$ to order h. We bound directly the energy difference, however!

Macroscopic Variations in the Superfluid Density

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

$$\mathcal{F}^{\rm BCS}(\Gamma) \le \mathcal{F}^{\rm BCS}(\Gamma_0) + h\left(D\,E^{\rm GL} + \epsilon\right)$$

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 $\mathcal{E}^{\rm GL}(\psi) \le E^{\rm GL} + \epsilon + \text{const.}\, h^{1/5}$ *and*

$$\int_{\mathcal{C}\times\mathbb{R}^3} |\sigma(x,y)|^2\,dx\,dy \le \text{const.}\, h^{1-2/5}$$

To appreciate the bound on σ, note that the square of the $L^2(\mathcal{C}\times\mathbb{R}^3)$ norm of the main term in α is of the order $h^{-1} = h^{-3}h^2$. To leading order in h, we thus have

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

The Coefficients in the GL Functional

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

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

and

$$C = \left(\beta_c \int_{\mathbb{R}^3} t(q)^4\, \frac{g_1(\beta_c(q^2-\mu))}{q^2-\mu}\, dq\right)^{-1} \int_{\mathbb{R}^3} \frac{t(q)^2}{\cosh^2\left(\frac{\beta_c}{2}(q^2-\mu)\right)}\, dq\,.$$

Then the matrix B_1 and the numbers B_2 and B_3 are given by

$$(B_1)_{ij} = C\,\frac{\beta_c^2}{16} \int_{\mathbb{R}^3} t(q)^2 \left(\delta_{ij} g_1(\beta_c(q^2-\mu)) + 2\beta_c q_i q_j\, g_2(\beta_c(q^2-\mu))\right) \frac{dq}{(2\pi)^3}\,,$$

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

$$B_3 = C^2\,\frac{\beta_c^2}{16} \int_{\mathbb{R}^3} t(q)^4\, \frac{g_1(\beta_c(q^2-\mu))}{q^2-\mu}\, \frac{dq}{(2\pi)^3}\,.$$

KEY SEMICLASSICAL ESTIMATES

For $\psi \in H^2_{\mathrm{loc}}(\mathbb{R}^d)$ 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 $f(z) = -\ln(1+e^{-z})$ 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

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

Upper Bound to the Energy

One simple takes as **trial state**

$$\Gamma = \Gamma_\Delta := \left[1 + e^{\beta H_\Delta}\right]^{-1}$$

with t the Fourier transform of $2K_{T_c}\alpha_0 = -2V\alpha_0$, and computes

$$\mathcal{F}^{\mathrm{BCS}}(\Gamma_\Delta) - \mathcal{F}^{\mathrm{BCS}}(\Gamma_0) = -\frac{1}{2\beta}\mathrm{Tr}\left[\ln(1+e^{-\beta H_\Delta}) - \ln(1+e^{-\beta H_0})\right]$$

$$- h^{2-2d}\int_{\mathcal{C}\times\mathbb{R}^d} V(\tfrac{x-y}{h})\left|\tfrac{1}{2}(\psi(x)+\psi(y))\alpha_0(\tfrac{x-y}{h})\right|^2 \frac{dx\,dy}{(2\pi)^d}$$

$$+ \int_{\mathcal{C}\times\mathbb{R}^d} V(\tfrac{x-y}{h})\left|\frac{h^{1-d}}{2(2\pi)^{d/2}}\left(\psi(x)+\psi(y)\right)\alpha_0(\tfrac{x-y}{h}) - \alpha_\Delta(x,y)\right|^2 dx\,dy$$

For $\beta^{-1} = T = T_c(1-h^2D)$, the terms in the first two lines yield $h^{4-d}\mathcal{E}^{\mathrm{GL}}(\psi) + O(h^{6-d})$ for $\psi \in H^2(\mathcal{C})$. The last line can be controlled by the $H^1(\mathcal{C})$ norm of the operator, yielding also an error term $O(h^{6-d})$.

Ideas in the Lower Bound

The key is to show that if Γ is an **approximate minimizer**, then $\Gamma \approx [1+e^{\beta H_\Delta}]^{-1}$ for suitable ψ (approximately) minimizing $\mathcal{E}^{\mathrm{GL}}$.

Step 1. For any Γ with $\mathcal{F}^{\mathrm{BCS}}(\Gamma) \leq \mathcal{F}^{\mathrm{BCS}}(\Gamma_0)$, the corresponding α satisfies

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

for some ψ with $H^1(\mathcal{C})$ norm bounded independently of h, and with $\|\sigma\|_{H^1} \leq O(h^{2-d/2})$.

Step 2. With ψ as above, we compute

$$\begin{aligned}\mathcal{F}^{\mathrm{BCS}}(\Gamma) - \mathcal{F}^{\mathrm{BCS}}(\Gamma_0) &= -\frac{T}{2}\mathrm{Tr}\left[\ln(1+e^{-\beta H_\Delta}) - \ln(1+e^{-\beta H_0})\right] \\ &\quad - h^{2-2d}\int_{\mathcal{C}\times\mathbb{R}^d} V(h^{-1}(x-y))\tfrac{1}{4}\left|\psi(x)+\psi(y)\right|^2 \left|\alpha_0(h^{-1}(x-y))\right|^2 \frac{dx\,dy}{(2\pi)^d} \\ &\quad + T\,\mathcal{H}(\Gamma,\Gamma_\Delta) + \int_{\mathcal{C}\times\mathbb{R}^d} V(h^{-1}(x-y))|\sigma(x,y)|^2\,dx\,dy\,,\end{aligned}$$

where $\mathcal{H}$ denotes the **relative entropy**.

Relative Entropy

For general Γ and $\Gamma_\Delta = [1+e^{\beta H_\Delta}]^{-1}$, it is true that

$$\mathcal{H}(\Gamma,\Gamma_\Delta) = \operatorname{Tr}\Gamma\left(\ln\Gamma - \ln\Gamma_\Delta\right) \geq \operatorname{Tr}\left[\frac{\beta H_\Delta}{\tanh\frac{1}{2}\beta H_\Delta}\left(\Gamma-\Gamma_\Delta\right)^2\right]$$

Since $x\mapsto\sqrt{x}/\tanh\sqrt{x}$ is an **operator monotone** function, we can further bound

$$\frac{H_\Delta}{\tanh\frac{1}{2}\beta H_\Delta} \geq (1-O(h))\,\frac{H_0}{\tanh\frac{1}{2}\beta H_0} \geq (1-O(h))\,K_T(-ih\nabla)\otimes\mathbb{I}_{\mathbb{C}^2}$$

Recall that, by definition, $K_{T_c}(-i\nabla)+V(x)\geq 0$, and hence $K_T(-i\nabla)+V(x)\geq -O(h^2)$. Moreover, $\alpha-\alpha_\Delta\approx\sigma$. This allows to get a lower bound on

$$T\,\mathcal{H}(\Gamma,\Gamma_\Delta) + \int_{\mathcal{C}\times\mathbb{R}^d} V(h^{-1}(x-y))|\sigma(x,y)|^2\,dx\,dy$$

that is $o(h^{4-d})$.

Conclusion

- **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 **semiclassical** in nature.

Some open problems:

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

THANK YOU FOR YOUR ATTENTION!