

# MICROSCOPIC DERIVATION OF THE GINZBURG–LANDAU MODEL

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ABSTRACT. We present a summary of our recent rigorous derivation of the celebrated Ginzburg–Landau (GL) theory, starting from the microscopic Bardeen–Cooper–Schrieffer (BCS) model. Close to the critical temperature, GL arises as an effective theory on the macroscopic scale. The relevant scaling limit is semiclassical in nature, and semiclassical analysis, with minimal regularity assumptions, plays an important part in our proof.

## 1. INTRODUCTION

The purpose of this paper is to describe how the celebrated Ginzburg–Landau (GL) model of superconductivity [1] arises as an asymptotic limit of the microscopic Bardeen–Cooper–Schrieffer (BCS) model [2]. The relevant asymptotic limit may be seen as a semiclassical limit, and one of the main difficulties involved in the proof is to derive a semiclassical expansion with minimal regularity assumptions. The present article represents a summary of our recent work in [3] (see also [4] for a simplified model in one dimension) and we shall refer to [3] for all technical details.

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

## 2. THE GINZBURG–LANDAU MODEL

The Ginzburg–Landau model is a phenomenological model for superconducting materials. Imagine a sample of such a material occupying a three-dimensional box  $\Lambda$ .<sup>1</sup> If  $W$  denotes a scalar external potential, and  $\mathbf{A}$  a magnetic vector potential, the Ginzburg–Landau functional is given as

$$(1) \quad \mathcal{E}^{\text{GL}}(\psi) = \int_{\Lambda} \left( |(-i\nabla + 2\mathbf{A}(x))\psi(x)|^2 + \lambda_1 W(x)|\psi(x)|^2 - \lambda_2 |\psi(x)|^2 + \lambda_3 |\psi(x)|^4 \right) dx,$$

where  $\psi \in H^1(\Lambda)$ . Here, the  $\lambda_i$  are real parameters, with  $\lambda_3 > 0$ . Note the factor 2 in front of the  $\mathbf{A}$ -field, which is reminiscent of the fact that  $\psi$  describes pairs of

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<sup>1</sup>For simplicity, we restrict our attention to three dimensions here, but a similar analysis applies in one and two dimensions as well.

particles. The microscopic model discussed in the next section does not have such a factor 2, as it describes single particles.

By simple rescaling, we could take  $\lambda_3 = 2|\lambda_2|$  if  $\lambda_2 \neq 0$ . If  $\lambda_2 > 0$ , one could then complete the square in the second line of (1) and write it as  $\lambda_3(1 - |\psi(x)|^2)^2 - \lambda_3$  instead.<sup>2</sup> Since  $\lambda_2$  can have either sign, however, we prefer to use the more general formulation in (1) here. We shall derive formulas for the coefficients  $\lambda_i$  from the BCS model below.

The function  $\psi$  is interpreted as the order parameter of the system. In the absence of external fields, i.e., for  $W = 0$  and  $\mathbf{A} = \mathbf{0}$ , the minimum of (1) is attained at  $|\psi(x)|^2 = \lambda_2/(2\lambda_3)$  for  $\lambda_2 > 0$ , or at  $\psi = 0$  for  $\lambda_2 \leq 0$ , respectively.

Our main concern here will be the relation of (1) with the Bardeen–Cooper–Schrieffer theory of superconductivity, which we describe in the next section. We will derive GL from BCS in an appropriate limit, where the temperature is close to the critical one, and the external fields  $\mathbf{A}$  and  $W$  are suitably small and slowly varying on a microscopic scale.

We note that there is a considerable literature [5, 6] concerning functionals of the type (1) and their minimizers, usually with an additional term added corresponding to the magnetic field energy. Such a term plays no role here since  $\mathbf{A}$  is considered a fixed, external field.

### 3. THE BCS ENERGY FUNCTIONAL

The BCS model is based on the microscopic many-particle Hamiltonian describing the system under consideration. Consider a gas of spin 1/2 fermions confined to the box  $\Lambda$ . With  $\mu$  denoting the chemical potential, the Hamiltonian is given by

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

Here,  $V$  is the two-particle interaction potential, which is taken to be local, i.e., it is a multiplication operator. In the original BCS Hamiltonian [2] it is replaced by an effective, non-local interaction which results from integrating out the phonon variables. For simplicity, we prefer to work with a local interaction of the form (2) here.<sup>3</sup>

The BCS model can be obtained from (2) by an approximation procedure (see Appendix A in [7]). One first restricts the states of the system to quasi-free states on Fock space. These states are completely determined by two quantities, the one-particle reduced density matrix<sup>4</sup>

$$(3) \quad \gamma(x, y) = \langle a^\dagger(x)a(y) \rangle$$

and the Cooper-pair wave function

$$(4) \quad \alpha(x, y) = \langle a(x)a(y) \rangle.$$

One thus obtains an expression for the energy of such states solely in terms of  $\gamma$  and  $\alpha$ . One further ignores the direct and exchange term in this expression, and arrives

<sup>2</sup>This is, in fact, the convention used in [3].

<sup>3</sup>It is not necessary to assume  $V$  to be radial, as done here, but the formulas simplify somewhat in this case.

<sup>4</sup>We suppress the spin dependence in the notation for simplicity.

at the following BCS energy functional. With  $T \geq 0$  denoting the temperature of the system,

$$(5) \quad \begin{aligned} \mathcal{F}(\Gamma) &= \text{Tr} \left[ \left( (-i\nabla + \mathbf{A}(x))^2 - \mu + W(x) \right) \gamma \right] - T S(\Gamma) \\ &+ \int_{\Lambda \times \Lambda} V(|x-y|) |\alpha(x,y)|^2 dx dy. \end{aligned}$$

The BCS states can be expressed as  $2 \times 2$  block matrices

$$(6) \quad \Gamma = \begin{pmatrix} \gamma & \alpha \\ \bar{\alpha} & 1 - \bar{\gamma} \end{pmatrix}$$

satisfying the constraint  $0 \leq \Gamma \leq 1$ . The entropy  $S(\Gamma)$  in (5) takes the usual form  $S(\Gamma) = -\text{Tr} \Gamma \ln \Gamma$ .

One of the main questions concerning the model (5) is whether a minimizing state  $\Gamma$  has  $\alpha$  identically zero or not, i.e., whether or not Cooper pairs exist. The non-vanishing of  $\alpha$  implies a superconducting (or superfluid, depending on the context) behavior of the system.

**3.1. BCS Energy in the Translation-Invariant Case.** It was shown in [7] that in the absence of external fields, i.e., for  $\mathbf{A} = \mathbf{0}$  and  $W = 0$ , there exists a critical temperature  $T_c \geq 0$  such that

- $T \geq T_c$ : Minimizer is *normal*, i.e.,  $\alpha = 0$  and  $\gamma = (1 + \exp((-\nabla^2 - \mu)/T))^{-1}$
- $T < T_c$ : Minimizer has  $\alpha \neq 0$ .

This critical temperature may be characterized by the operator

$$(7) \quad K_{T_c}(-\nabla^2 - \mu) + V(|x|), \quad K_T(\eta) = \frac{\eta}{\tanh(\eta/2T)}$$

having zero as the lowest eigenvalue. Note that the spectrum of  $K_T(-\nabla^2 - \mu)$  equals  $[2T, \infty)$ , hence 0 is necessarily an isolated eigenvalue of (7) if  $T_c > 0$ .

This linear criterion on the critical temperature was used to derive precise asymptotics of  $T_c$  for weak coupling and/or low density, see [8]–[10].

*In the following, we shall assume* that  $V$  is such that  $T_c > 0$ , and that the eigenfunction  $\alpha_0$  corresponding to the zero eigenvalue of (7) is unique. The potential  $V$  also has to be sufficiently regular to be form-bounded with respect to the Laplacian, and should decay at infinity.

**3.2. Microscopic vs. Macroscopic Scales.** Let us introduce a small parameter  $h > 0$ , describing the ratio between the microscopic and macroscopic length scales. The external fields  $\mathbf{A}$  and  $W$  occurring in the GL functional vary on the macroscopic scale, i.e., on the scale of the box  $\Lambda$ . The particle interaction  $V$ , on the other hand, varies on the microscopic scale. To take this into account, we replace the external fields  $\mathbf{A}(x)$  and  $W(x)$  in the BCS functional (5) by

$$(8) \quad \tilde{\mathbf{A}}(x) = h\mathbf{A}(hx), \quad \tilde{W}(x) = h^2W(hx)$$

and define the BCS functional on a rescaled box  $\tilde{\Lambda} = h^{-1}\Lambda$ . Here,  $x$  is the microscopic variable, while  $\tilde{x} = hx$  is the macroscopic variable.

We find it more convenient to express the BCS functional in macroscopic variables, and shall henceforth drop the  $\tilde{\cdot}$ 's. The resulting rescaled BCS functional

is

$$(9) \quad \begin{aligned} \mathcal{F}(\Gamma) &= \text{Tr} \left[ \left( (-ih\nabla + h\mathbf{A}(x))^2 - \mu + h^2W(x) \right) \gamma \right] - TS(\Gamma) \\ &+ \int_{\Lambda \times \Lambda} V(h^{-1}|x-y|) |\alpha(x,y)|^2 dx dy, \end{aligned}$$

and it is defined on the  $h$ -independent macroscopic volume  $\Lambda$ . Note the semiclassical nature of the appearance of  $h$  in the various terms in (9). For small  $h$  the energy is of order  $h^{-3}$ .

In order for (9) to be well-defined, suitable boundary conditions have to be imposed on the boundary of  $\Lambda$ . In the limit  $h \rightarrow 0$ , these are not relevant in the bulk of the sample. In order to avoid technical problems related to these boundary condition, we chose in [3] to work with an infinite system instead, which is assumed to be periodic, and all energies are calculated per unit volume. Consequently, also the functions  $\psi$  in the GL functional (1) have to be periodic.

#### 4. MAIN RESULTS

We shall choose the temperature  $T$  in (9) to be close to the critical temperature defined in Subsection 3.1. More precisely, we take

$$(10) \quad T = T_c(1 - Dh^2)$$

for some  $h$ -independent parameter  $D \in \mathbb{R}$ .<sup>5</sup>

Our main result concerns the asymptotic behavior of  $\inf_{\Gamma} \mathcal{F}(\Gamma)$  and the corresponding minimizers as  $h \rightarrow 0$ .

**Theorem 1.** *There exists a  $\lambda_0 > 0$  and parameters  $\lambda_1$ ,  $\lambda_2$  and  $\lambda_3$  in the GL functional such that*

$$(11) \quad \inf_{\Gamma} \mathcal{F}(\Gamma) = \mathcal{F}(\Gamma_0) + \lambda_0 h \inf_{\psi} \mathcal{E}^{\text{GL}}(\psi) + o(h)$$

as  $h \rightarrow 0$ , where  $\Gamma_0$  is the normal state (i.e., the minimizer in the absence of  $V$ ).

Moreover, if  $\Gamma$  is a state such that  $\mathcal{F}(\Gamma) \leq \mathcal{F}(\Gamma_0) + \lambda_0 h \inf_{\psi} \mathcal{E}^{\text{GL}}(\psi) + o(h)$  then the corresponding Cooper pair wave function  $\alpha$  satisfies

$$(12) \quad \|\alpha - \alpha_{\text{GL}}\|_{L^2}^2 \leq o(h) \|\alpha_{\text{GL}}\|_{L^2}^2 = o(h)h^{-1}$$

where

$$(13) \quad \alpha_{\text{GL}}(x,y) = h^{-2} \psi_0 \left( \frac{x+y}{2} \right) \alpha_0 \left( \frac{x-y}{h} \right) = Op(h\psi_0(x)\widehat{\alpha}_0(p))$$

and  $\mathcal{E}^{\text{GL}}(\psi_0) \leq \inf_{\psi} \mathcal{E}(\psi) + o(1)$ .

Theorem 1 represents a rigorous derivation of Ginzburg–Landau theory. Starting from the BCS model, GL arises as an effective theory on the macroscopic scale, in the presence of weak and slowly varying external fields, and for temperatures close to the critical one.

*Remark 1.* As mentioned above,  $\mathcal{F}(\Gamma_0)$  is  $O(h^{-3})$ , hence the GL functional arises as an  $O(h^4)$  correction to the main term.

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<sup>5</sup>The results in [3] were stated for  $D > 0$ , but their proof is equally valid for  $D \leq 0$ .

*Remark 2.* In (13),  $Op$  denotes Weyl quantization. Theorem 1 demonstrates the role of the function  $\psi$  in the GL model: It describes the center-of-mass motion of the Cooper pair wavefunction, which close to the critical temperature equals (13) to leading order in  $\hbar$ .

*Remark 3.* The method of our analysis can also be used to show that the GL model predicts the correct change in critical temperature in the BCS theory due to the external field [11]. As discussed in the next subsection, the parameter  $\lambda_2$  is proportional to the difference between the critical and the actual temperature (more precisely, to  $D$  in (10)), and the mentioned shift corresponds to the largest  $\lambda_2$  with the property that  $\psi = 0$  is a GL minimizer. This can have either sign, depending on the external fields  $\mathbf{A}$  and  $W$ .

*Remark 4.* A similar analysis can be used at  $T = 0$  to study the low-density limit of the BCS model. In this limit, one obtains a Bose-Einstein condensate of fermion pairs, described by the Gross-Pitaevskii equation [12, 13].

**4.1. The Coefficients  $\lambda_i$ .** The coefficients  $\lambda_0$ ,  $\lambda_1$ ,  $\lambda_2$  and  $\lambda_3$  in Theorem 1 can be explicitly calculated. They are all expressed in terms of the eigenfunction  $\alpha_0$  corresponding to the zero eigenvalue of (7), the critical temperature  $T_c$  and the coefficient  $D$  in (10).

Specifically, if we denote by  $t$  the Fourier transform of  $2K_{T_c}\alpha_0$ , we have<sup>6</sup>

$$(14) \quad \lambda_0 = \frac{1}{16T_c^2} \int_{\mathbb{R}^3} t(q)^2 \left( g_1(\beta_c(q^2 - \mu)) + \frac{2}{3}\beta_c q^2 g_2(\beta_c(q^2 - \mu)) \right) \frac{dq}{(2\pi)^3},$$

$$(15) \quad \lambda_1 = \lambda_0^{-1} \frac{1}{4T_c^2} \int_{\mathbb{R}^3} t(q)^2 g_1(\beta_c(q^2 - \mu)) \frac{dq}{(2\pi)^3},$$

$$(16) \quad \lambda_2 = \lambda_0^{-1} \frac{D}{8T_c} \int_{\mathbb{R}^3} t(q)^2 \cosh^{-2} \left( \frac{\beta_c}{2}(q^2 - \mu) \right) \frac{dq}{(2\pi)^3}$$

and

$$(17) \quad \lambda_3 = \lambda_0^{-1} \frac{1}{16T_c^2} \int_{\mathbb{R}^3} t(q)^4 \frac{g_1(\beta_c(q^2 - \mu))}{q^2 - \mu} \frac{dq}{(2\pi)^3}.$$

Here  $\beta_c = T_c^{-1}$ , and  $g_1$  and  $g_2$  denote the functions

$$(18) \quad g_1(z) = \frac{e^{2z} - 2ze^z - 1}{z^2(1 + e^z)^2} \quad \text{and} \quad g_2(z) = \frac{2e^z(e^z - 1)}{z(e^z + 1)^3},$$

respectively. One can show [3] that  $\lambda_0 > 0$ . Note that  $g_1(z)/z > 0$ , hence also  $\lambda_3 > 0$ . The coefficient  $\lambda_2$  is proportional to  $D$ , defined in (10).

As mentioned in Section 2, the terms in the second line of the GL functional (1) are often written as  $\frac{\kappa^2}{2}(1 - |\psi(x)|^2)^2$  instead, with a suitable coupling constant  $\kappa > 0$ . In our notation,  $\kappa$  corresponds to

$$(19) \quad \kappa = \sqrt{\lambda_2}$$

(in case  $D > 0$ , i.e.,  $T < T_c$ ).

Note that the normalization of  $\alpha_0$  is irrelevant. If we multiply  $\alpha_0$  by a factor  $\lambda > 0$ , then  $\lambda_0$  and  $\lambda_3$  get multiplied by  $\lambda^2$ , while  $\lambda_1$  and  $\lambda_2$  stay the same. Hence

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<sup>6</sup>In the published version, there is a misprint in Eq. (14): the factor  $\frac{2}{3}$  in front of the second term in the integrand is wrongly written as 2.

the GL minimizer  $\psi_0$  gets multiplied by  $\lambda^{-1}$ , leaving both  $\lambda_0 \mathcal{E}^{\text{GL}}(\psi_0)$  and the product  $\psi_0 \alpha_0$  unchanged. In particular, (13) is independent of the normalization of  $\alpha_0$ .

## 5. SKETCH OF PROOF

In the following, we present a very brief sketch of the main ideas in the proof of Theorem 1. The actual proof is rather lengthy and we have to refer to [3] for details.

The starting point is the identity

$$\begin{aligned} \mathcal{F}(\Gamma) - \mathcal{F}(\Gamma_0) &= -\frac{T}{2} \text{Tr} \left[ \ln \left( 1 + e^{-H_\Delta/T} \right) - \ln \left( 1 + e^{-H_0/T} \right) \right] \\ &\quad - \int V(|x-y|/h) |\alpha_{\text{GL}}(x,y)|^2 dx dy \\ (20) \quad &\quad + \frac{T}{2} \mathcal{H}(\Gamma, \Gamma_\Delta) + \int V(|x-y|/h) |\alpha_{\text{GL}}(x,y) - \alpha(x,y)|^2 dx dy \end{aligned}$$

where  $\Gamma_\Delta = (1 + e^{H_\Delta/T})^{-1}$ ,

$$(21) \quad H_\Delta = \begin{pmatrix} \mathfrak{h} & \Delta \\ \Delta & -\mathfrak{h} \end{pmatrix}, \quad \mathfrak{h} = (-ih\nabla + h\mathbf{A}(x))^2 - \mu + h^2W(x)$$

and  $\Delta$  denotes the operator with integral kernel

$$(22) \quad \Delta(x,y) = 2V(|x-y|/h)\alpha_{\text{GL}}(x,y) = 2h\text{Op}(\psi_0(x)(\widehat{\alpha_0 V})(p)).$$

Moreover,  $\mathcal{H}(\Gamma, \Gamma_\Delta)$  denote the relative entropy

$$(23) \quad \mathcal{H}(\Gamma, \Gamma_\Delta) = \text{Tr} \left[ \Gamma (\ln \Gamma - \ln \Gamma_\Delta) + (1 - \Gamma) (\ln(1 - \Gamma) - \ln(1 - \Gamma_\Delta)) \right].$$

It is non-negative, and vanishes only for  $\Gamma = \Gamma_\Delta$ . The latter property can be quantified in the form

$$(24) \quad T \mathcal{H}(\Gamma, \Gamma_\Delta) \geq \text{Tr} \left[ K_T(H_\Delta) (\Gamma - \Gamma_\Delta)^2 \right].$$

The identity (20) and the inequality (24) hold true for any choice of the function  $\psi_0$  in (13). It is used in two separate steps. One first simply takes  $\psi_0 = 0$ , and uses the gap of the operator  $K_{T_e}(H_0) + V$  to conclude that  $\alpha$  is close to an  $\alpha_{\text{GL}}$  for a suitable  $\psi_0$ , i.e.,  $\alpha$  is of the form (13) to leading order. One then repeats the argument with this choice of  $\psi_0$ , to conclude that the two terms in the last line of (20) are negligible for small  $h$ .

To conclude the proof, it remains to calculate the terms in the first two lines in (20). For this purpose one needs semiclassical estimates with good regularity bounds. The relevant estimates can be summarized as follows:

**Theorem 2.** *With errors controlled by  $H^1$  and  $H^2$  norms of  $\psi_0$*

$$\begin{aligned} &-\frac{h^3}{2} T \text{Tr} \left[ \ln \left( 1 + e^{-H_\Delta/T} \right) - \ln \left( 1 + e^{-H_0/T} \right) \right] \\ (25) \quad &= h^2 \mathcal{D}_2(\psi_0) + h^4 \mathcal{D}_4(\psi_0) + \lambda_0 h^4 \mathcal{E}^{\text{GL}}(\psi_0) + O(h^5) \end{aligned}$$

and

$$(26) \quad h^3 \int V(|x-y|/h) |\alpha_{\text{GL}}(x,y)|^2 dx dy = h^2 \mathcal{D}_2(\psi_0) + h^4 \mathcal{D}_4(\psi_0) + O(h^5)$$

for suitable  $\mathcal{D}_2$  and  $\mathcal{D}_4$ .

In (25) we have already taken into account the choice (10) for the temperature  $T$ . For this choice, all the terms of order  $h^2$  cancel, and one is left with  $\lambda_0 h^4 \mathcal{E}^{\text{GL}}(\psi_0)$  after taking the difference between (25) and (26).

This completes our very brief sketch of the proof of Theorem 1.

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