Time-dependent Bogoliubov–de Gennes and Ginzburg–Landau equations

Rupert L. Frank

LMU Munich

Hamiltonian Methods and Asymptotic Dynamics
ICERM Workshop, December 6, 2021

Joint work with C. Hainzl, B. Schlein and R. Seiringer

Effective models

One wants to approximately describe complicated (quantum) many-body systems by simpler, effective models. The effective models involve typically only a single function in $\mathbb{R}^d$ (e.g., $d = 3$), whereas the original models involved functions on $\mathbb{R}^{dN}$.

Such an effective describtion is desirable both in static and dynamic problems.

Examples. (1) Schrödinger equation for bosons: Hartree theory, Gross–Pitaevski theory
(2) Schrödinger equation for fermions: Hartree–Fock theory, Vlasov equations

We approximate Hamiltonian systems by Hamiltonian systems.

Today's topic: Superconductivity
Microscopic description by Bardeen–Cooper–Schrieffer (BCS) (think: Hartree–Fock)
Macroscopic description by Ginzburg–Landau (GL) (think: NLS)

A relation between the micro and the macro description is possible in a static setting. In part., existence of a critical temperature below which one has superconductivity.

Question. Can one derive the time-dependent GL equations from time-dependent BCS equations (aka Bogoliubov-de Gennes (BdG) equations)?

$$id\partial_t\psi = -\Delta\psi + a\psi + b|\psi|^2\psi\,, \qquad a \in \mathbb{R}\,,\ b > 0\,,\ \operatorname{Im} d \geq 0\,.$$

This equation is not Hamiltonian if $\operatorname{Im} d > 0$!

Answer. (=Main result for today) No! (generically)

The BCS minimization problem

Admissible BCS states for us on $\mathbb{R}^d$ (for us, $d = 1, 2, 3$) are $\mathbb{Z}^d$-periodic operators Γ on $L^2(\mathbb{R}^d) \oplus L^2(\mathbb{R}^d)$ that satisfy $0 \leq \Gamma \leq 1$ and are of the form

$$\Gamma = \begin{pmatrix} \gamma & \alpha \\ \overline{\alpha} & 1 - \overline{\gamma} \end{pmatrix} \qquad \text{where } \bar{\cdot} \text{ denotes complex conjugation.}$$

Idea. States with $\alpha = 0$ correspond to usual Hartree–Fock states. Presence of an $\alpha \neq 0$ indicates the presence of superconductivity. (Cooper pair wave function)

Microscopic data. $V : \mathbb{R}^d \to \mathbb{R}$ even (interaction potential), $\mu \in \mathbb{R}$ (chemical potential), $\beta > 0$ (inverse temperature)

Macroscopic data. $W : \mathbb{R}^d \to \mathbb{R}$, $A : \mathbb{R}^d \to \mathbb{R}^d$ $\mathbb{Z}^d$-periodic (external fields),

Ratio between microscopic and macroscopic scale. $h > 0$

Free energy functional.

$$\mathcal{F}_\beta[\Gamma] = \operatorname{Tr}\left(\left(-ih\nabla + hA\right)^2 + h^2 W - \mu\right)\gamma + \frac{1}{2}\iint V\left(\tfrac{x-y}{h}\right)|\alpha(x,y)|^2\, dx\, dy + \beta^{-1}\operatorname{Tr}\Gamma\ln\Gamma$$

Question. Does the minimizer of

$$\inf\left\{\mathcal{F}_\beta[\Gamma] : \ \Gamma \text{ admissible}\right\}$$

have $\alpha \not\equiv 0$? In particular, can one answer this as $h \to 0$ and describe α?

From BCS to GL for the free energy

We denote by $\Gamma^{(\beta)}$ the minimizer of the above problem under the additional restriction that $\alpha \equiv 0$. (normal state)

We will define a critical temperature β_c, a normalized function $a_* \in L^2(\mathbb{R}^d)$, as well as coefficients $\Lambda_0, \ldots, \Lambda_3$ (in terms of V and μ), such that under a simple, explicit generic assumption the following holds.

Theorem (F.–Hainzl–Seiringer–Solovej (2012))

Assume that $\beta - \beta_c = Dh^2$ for some $D \in \mathbb{R}$. Then, as $h \to 0$,

$$\inf \{\mathcal{F}_\beta[\Gamma] : \ \Gamma \ \textit{admissible}\} - \mathcal{F}_\beta[\Gamma^{(\beta)}] = h^{-d+4} \inf \left\{ \mathcal{E}[\psi] : \ \psi \in H^1(\mathbb{R}^d/\mathbb{Z}^d) \right\} + o(h^{-d+4}) \, ,$$

where

$$\mathcal{E}[\psi] = \int_{\mathbb{R}^d/\mathbb{Z}^d} \left(((-i\nabla + 2A)\psi)^* \Lambda_0 ((-i\nabla + 2A)\psi) + \Lambda_1 W |\psi|^2 - \Lambda_2 D |\psi|^2 + \Lambda_3 |\psi|^4 \right) dx$$

Moreover, if Γ satisfies $\mathcal{F}_\beta[\Gamma] - \mathcal{F}_\beta[\Gamma^{(\beta)}] \leq h^{-d+4}(\inf_\phi \mathcal{E}[\phi] + \epsilon)$ with $\epsilon \lesssim 1$, then

$$\alpha(x,y) \approx h^{-d+1} a_*\left(\tfrac{x-y}{h}\right) \psi\left(\tfrac{x+y}{2}\right) \qquad \textit{with} \qquad \mathcal{E}[\psi] - \inf_\phi \mathcal{E}[\phi] \lesssim \epsilon + o(1) \, .$$

The time-dependent problem

The natural time-dependent equation is the following BdG equation

$$i\partial_t \Gamma = [H_\Delta, \Gamma] \,, \qquad \Delta(x,y) = V(\tfrac{x-y}{h})\alpha(x-y) \,,$$

where

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

This is a Hamiltonian equation that preserves the energy

$$\operatorname{Tr}\left((-ih\nabla + hA)^2 + h^2 W - \mu \right) \gamma + \frac{1}{2} \iint V(\tfrac{x-y}{h}) |\alpha(x,y)|^2 \, dx \, dy \, .$$

Note that there is no temperature in the equation.

Question. Is there a $d \in \mathbb{C}$ (depending on V and μ) with $\operatorname{Im} d \geq 0$ such that, if $|\beta - \beta_c| \lesssim h^2$ and if $\mathcal{F}_\beta[\Gamma_0] - \mathcal{F}_\beta[\Gamma^{(\beta)}] \lesssim h^{-d+4}$, then the solution Γ_t of the BdG equation with initial condition Γ_0 satisfies, for any $t \in \mathbb{R}$,

$$\alpha_t(x,y) \approx h^{-d+1} a_*(\tfrac{x-y}{h}) \, \psi_t(\tfrac{x+y}{2})$$

with ψ_t satisfying

$$id\partial_t \psi_t = (-i\nabla + 2A)^* \Lambda_0 (-i\nabla + 2A)\psi_t + \Lambda_1 W \psi_t - \Lambda_2 D \psi_t + 2\Lambda_3 |\psi_t|^2 \psi_t \, .$$

This equation has been suggested in the physics literature (Stephen–Suhl (1964), Abrahams–Tsuneto (1966), Schmidt (1968)). This derivation was criticized by Eliashberg–Gorkov (1968), but it is still used successfully in theory and applications.

The translation-invariant case

We look at a simple toy problem where $A = 0$, $W = 0$ and where we restrict ourselves to translation-invariant states. (All the noncommutativity disappears!)

$$\mathcal{F}_\beta[\Gamma] = \int_{\mathbb{R}^d} (|\xi|^2 - \mu)\widehat{\gamma}(\xi)\, d\xi + \frac{1}{2}\int_{\mathbb{R}^d} V(x)|\alpha(x)|^2\, dx + \beta^{-1}\int_{\mathbb{R}^d} \operatorname{Tr}\widehat{\Gamma}(\xi)\ln\widehat{\Gamma}(\xi)\, d\xi\,.$$

where

$$\widehat{\Gamma}(\xi) = \begin{pmatrix} \widehat{\gamma}(\xi) & \widehat{\alpha}(\xi) \\ \overline{\widehat{\alpha}(-\xi)} & 1 - \widehat{\gamma}(-\xi) \end{pmatrix}$$

and

$$0 \le \widehat{\gamma}(\xi) \le 1, \qquad \widehat{\alpha}(\xi) = \widehat{\alpha}(-\xi), \qquad |\widehat{\alpha}(\xi)|^2 \le \widehat{\gamma}(\xi)(1 - \widehat{\gamma}(-\xi))\,.$$

Definition of the critical temperature. The operator

$$K_\beta + V := \frac{-\Delta - \mu}{\frac{1}{2}\tanh\frac{\beta}{2}(-\Delta - \mu)} + V \qquad \text{in } L^2_{\rm symm}(\mathbb{R}^d)\,,$$

depends monotonically on β, and so do its eigenvalues. Therefore, there is a unique $\beta_c \in (0, \infty]$ such that

$$\inf \mathrm{spec}\,(K_\beta + V) < 0 \quad \text{for all } \beta > \beta_c\,, \qquad \inf \mathrm{spec}\,(K_\beta + V) \ge 0 \quad \text{for all } \beta \le \beta_c$$

Assumptions: $\beta_c < \infty$, $\dim\ker(K_{\beta_c} + V) = \mathrm{span}\{a_*\}$, $\mu > 0$ and

$$\sup_{|\xi|^2 = \mu} |\widehat{a_*}(\xi)| > 0\,.$$

Main result

Time-dependent BdG equation

$$i\partial_t \widehat{\Gamma}(\xi) = \left[H_\Delta(\xi), \widehat{\Gamma}(\xi)\right] , \qquad \widehat{\Delta}(\xi) = (2\pi)^{-d/2} \int_{\mathbb{R}^d} \widehat{V}(\xi - \xi')\widehat{\alpha}(\xi')\, d\xi' ,$$

where

$$\widehat{\Gamma}(\xi) = \begin{pmatrix} \widehat{\gamma}(\xi) & \widehat{\alpha}(\xi) \\ \overline{\widehat{\alpha}(\xi)} & 1 - \widehat{\gamma}(-\xi) \end{pmatrix}, \qquad H_\Delta(\xi) = \begin{pmatrix} |\xi|^2 - \mu & \widehat{\Delta}(\xi) \\ \overline{\widehat{\Delta}(\xi)} & \mu - |\xi|^2 \end{pmatrix},$$

Theorem (F.–Hainzl–Schlein–Seiringer (2016))

Let $\widehat{\Gamma}_t$ be a solution of the time-dependent BdG equation with initial data $\widehat{\Gamma}_0$. Then, if β is sufficiently close to β_c, we have, for all $t \in \mathbb{R}$,

$$\left| |\langle \widehat{a}_*, \widehat{\alpha}_t \rangle|^2 - |\langle \widehat{a}_*, \widehat{\alpha}_0 \rangle|^2 \right| \lesssim \max\left\{ |\beta - \beta_c|^{5/4}, \left(\mathcal{F}_\beta(\Gamma_0) - \mathcal{F}_\beta(\Gamma^{(\beta)}) \right)_+^{5/8} \right\} .$$

- We will see in the proof that, for all $t \in \mathbb{R}$,

$$|\langle \widehat{a}_*, \widehat{\alpha}_t \rangle|^2 \lesssim \max\left\{ |\beta - \beta_c|, \left(\mathcal{F}_\beta(\Gamma_0) - \mathcal{F}_\beta(\Gamma^{(\beta)}) \right)_+^{1/2} \right\}$$

  which is order-sharp, so the theorem shows a cancellation in the difference.
- Thus, $t \mapsto |\langle \widehat{a}_*, \widehat{\alpha}_t \rangle|^2$ is constant to leading order in $\beta - \beta_c$, contradicting that a time-dependent GL equation (with $\operatorname{Im} d > 0$) is satisfied.

Proof of the main result

Step 1. Structure of states with low free energy

Lemma

If $|\beta - \beta_c|$ is sufficiently small, then for any admissible $\widehat{\Gamma}$

$$\widehat{\gamma}(\xi) = \frac{1}{1 + e^{\beta(|\xi|^2 - \mu)}} + \eta(\xi)\,, \qquad \widehat{\alpha}(\xi) = \langle \widehat{a}_*, \widehat{\alpha} \rangle\, \widehat{a}_*(\xi) + \zeta(\xi)$$

with

$$|\langle \widehat{a}_*, \widehat{\alpha} \rangle| \lesssim h\,, \quad \|\eta\|_{L^2(\mathbb{R}^d)} + \|\zeta\|_{L^2(\mathbb{R}^d)} \lesssim h^2\,, \quad h = \max\left\{ |\beta - \beta_c|^{\frac{1}{2}}, \left(\mathcal{F}_\beta(\Gamma) - \mathcal{F}_\beta(\Gamma^{(\beta)})\right)_+^{\frac{1}{4}} \right\}.$$

This follows by variational arguments.

Step 2. Pointwise conservation of the spectrum

Recall that the equation reads $i\partial_t \widehat{\Gamma}(\xi) = [H(\xi), \widehat{\Gamma}(\xi)]$ with $H(\xi)$ Hermitian.
Thus, for each $\xi \in \mathbb{R}^d$, the matrices $\widehat{\Gamma}_t(\xi)$, $t \in \mathbb{R}$, are unitarily equivalent to $\widehat{\Gamma}_0(\xi)$.
Diagonalizing the matrices, we see that

Lemma

For any $\xi \in \mathbb{R}^d$, $t \mapsto (\widehat{\gamma}_t(\xi) - \frac{1}{2})^2 + |\widehat{\alpha}_t(\xi)|^2$ is constant.

Proof of the main result, cont'd

Step 3. We abbreviate

$$h := \max\left\{|\beta-\beta_c|^{1/2}, \left(\mathcal{F}_\beta(\Gamma_0)-\mathcal{F}_\beta(\Gamma^{(\beta)})\right)_+^{1/4}\right\}.$$

By conservation of energy and of entropy, we can apply Step 1 at each time and obtain

$$\widehat{\gamma}_t(\xi) = \frac{1}{1+e^{\beta(|\xi|^2-\mu)}} + \eta_t(\xi)\,, \qquad \widehat{\alpha}_t(\xi) = h\ \psi_t\, \widehat{a}_*(\xi) + \zeta_t(\xi)\,, \qquad \psi_t := h^{-1}\langle \widehat{a}_*, \widehat{\alpha}_t\rangle$$

with

$$|\psi_t| \lesssim 1\,, \qquad \|\widehat{\eta}_t\|_{L^2(\mathbb{R}^d)} + \|\widehat{\zeta}_t\|_{L^2(\mathbb{R}^d)} \lesssim h^2\,.$$

By Step 2,

$$\widehat{\eta}_t(\xi)^2 - \widehat{\eta}_0(\xi)^2 - (\widehat{\eta}_t(\xi)-\widehat{\eta}_0(\xi))\tanh\tfrac{\beta}{2}(|\xi|^2-\mu) = |\widehat{\alpha}_t(\xi)|^2 - |\widehat{\alpha}_0(\xi)|^2\,.$$

The left side, integrated over $\{\xi\in\mathbb{R}^d : \left||\xi|-\sqrt{\mu}\right|<\delta\}$, is $\lesssim h^4 + h^2\delta^{3/2}$.
The right side, integrated over the same set, is

$$\geq h^2\left||\psi_t|^2-|\psi_0|^2\right|\int_{||\xi|-\sqrt{\mu}|<\delta} |\widehat{a}_*(\xi)|^2\,d\xi - \mathrm{const.}\left(h^3\delta^{1/2}+h^4\right).$$

Recalling the assumption $\sup_{|\xi|^2=\mu}|\widehat{a}_*(\xi)|$ and picking $\delta = h$, we obtain the assertion. □

What went wrong in the physics literature arguments?

In the physics literature, the BdG equation is first linearized and the linear part of the time-dependent GL equation is derived. Then the nonlinearity is taken into account to lowest order.

When looking at the linearized problem there is a Fermi–Golden Rule mechanism: The zero eigenvalue of $K_{\beta_c} + V$ turns into a resonace. The imaginary part of this resonance gives rise to the imaginary part of d. (We can reproduce the computations in the physics literature.)

An aside: FGR mechanism also appears in the problem of asymptotic stability of ground states of the NLS and in a series of works on 'a tracer particle in a Bose gas'.

The separate treatment of the linear and the nonlinear parts, however, is not rigorous. The equation is

$$i\partial_t \alpha = L\alpha - (\eta + \overline{\eta})V\alpha$$

Away from $|\xi|^2 = \mu$ one has

$$\widehat{\eta}_t(\xi) - \widehat{\eta}_0(\xi) \approx \frac{|\widehat{\alpha}_t(\xi)|^2 - |\widehat{\alpha}_0(\xi)|^2}{\tanh \frac{\beta}{2}(|\xi|^2 - \mu)} ,$$

which looks quadratic in h, but for $|\xi|^2 \sim \mu$ one has

$$\widehat{\eta}_t(\xi) - \widehat{\eta}_0(\xi) \approx \left| |\widehat{\alpha}_t(\xi)|^2 - |\widehat{\alpha}_0(\xi)|^2 \right|^{1/2} \sim h \, |\widehat{a_*}(\xi)| \left| |\psi_t|^2 - |\psi_0|^2 \right|^{1/2},$$

which is linear in h.

Summary

- We have seen that under a generic assumption the time-dependent Ginzburg–Landau equation does not describe solutions of the Bogoliubov–de Gennes equation close to the critical temperature, even though this is natural in view of the results in the static case and this equation is frequently used in theory and applications.
- It remains a challenging open problem to unveil the relevant additional physical effects that are responsible for the possible emergence of a time-dependent GL equation.
- From a mathematical perspective, it would be interesting to study the simple translation invariant BdG equation in more detail and, in particular, understand the behavior close to the Fermi surface $\{|\xi|^2 = \mu\}$.

THANK YOU FOR YOUR ATTENTION!