Jorge Berger and Jacob Rubinstein

On the zero set of the wave function in superconductivity

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Abstract.
We consider the Ginzburg Landau functional in a multiply connected planar domain with enclosed magnetic flux. Particular attention is given to the zero set of the order parameter. We show that there exist applied fields for which the zero set is of codimension 1.

1 Introduction

The Ginzburg Landau (GL) model of superconductivity concerns an order parameter u which is a complex valued function and the magnetic field vector potential A. The problem is forced by an applied magnetic field H_e. The local minimizers describe the possible equilibrium configurations under the external constraints. The square of the absolute value of u measures the density of the superconducting electrons, while the phase of u is related to the supercurrent.

We shall consider here the GL functional in a two dimensional domain Ω that is homotopic to an annulus. Of particular interest are the zeros of u. It is often argued that the zero set, which we shall denote by S, should consist of isolated points. The heuristic reasoning is that since u is complex, its zeros are the intersection of the zero levels lines of its real and imaginary parts. Morover, Elliott et al. have recently proved [7] that under some smoothness assumptions on the given data, S is indeed a finite collection of points.

We shall show that there exist fields H_e for which S consists of a *curve* connecting the inner boundary of the ring to its outer boundary. When this occurs we say that u is in the *singly connected state* [2]. The solution we discovered exists for some temperature range below the critical temperature T_c in which the transition to superconductivity occurs. A by-product of our result is that the Elliott - Matano - Qi [7] theorem is valid only for simply connected domains.

When the ring is very thin, the GL functional can be approximated by a one dimensional model on a curve [12]. We have studied this model in detail [3] and derived an intricate picture of phase transitions when there exist nonuniformities in the ring's cross section. Our results here give a rigorous justification to the phase transition diagram of [3]. In the thin ring limit the line of zeros collapses to a point. The appearance of a singly connected state has profound effects on the behavior of the supercurrent as a function of H_e. Experimental aspects of the new phase are discussed in [4].

2 Formulation

We write the GL functional in nondimensional form

$$G_\lambda(u, A) = \int_\Omega \left(\lambda[-|u|^2 + |u|^4/2] + |(\nabla - iA)u|^2\right) dx + \frac{\kappa^2}{\lambda}\int_{\mathbb{R}^2} |\nabla \times A - H_e|^2 \, dx. \qquad (2.1)$$

Here λ is a parameter that vanishes at T_c and increases with $T_c - T$, where $T\,(T_c)$ is the temperature (critical temperature), and κ is a material parameter. We chose R, the inner radius of the ring, as a lengthscale (rather than the coherence length or the penetration length). The external field is given in dimensional units by $\Phi_0 H_e/2\pi R^2$, and the dimensional vector potential is $\Phi_0 A/2\pi R$, where Φ_0 is the fundamental flux quantum. We comment that the form (2.1) is slightly different than the form used in other mathematical texts ([6],[11]). In our scaling the temperature appears explicitly in the functional, which is advantageous for the purpose of studying phase transitions.

The Euler Lagrange equations associated with (2.1) are

$$-(\nabla - iA)^2 u + \lambda u(|u|^2 - 1) = 0, \quad x \in \Omega \qquad (2.2)$$

$$\nabla \times (\nabla \times A - H_e) = \lambda\kappa^{-2}\Im(\bar{u}(\nabla - iA)u)1_\Omega, \quad x \in \mathbb{R}^2 \qquad (2.3)$$

$$(\nabla - iA)u \cdot \nu = 0, \quad x \in \partial\Omega, \qquad (2.4)$$

where ν is the unit normal to $\partial\Omega$. We can remove the gauge invariance of (2.1) [6] by imposing the constraint $\nabla \cdot A = 0$.

We assume in sections 3 and 4 that H_e is a smooth vector field in the direction orthogonal to the plane, and that *its support does not intersect* Ω. It is easy to verify that for sufficiently small λ the global minimizer is $(u, A) = (0, A_e)$, where A_e is a solution of $\nabla \times A_e = H_e$. Increasing λ (i.e. decreasing the temperature), we reach a critical (bifurcation) value λ_p where a nonzero solution emerges. The bifurcation equation is

$$-(\nabla - iA_e)^2 u - \lambda_p u = 0, \quad x \in \Omega \qquad (2.5)$$

$$(\nabla - iA_e)u \cdot \nu = 0, \quad x \in \partial\Omega. \qquad (2.6)$$

Since λ_p is the first λ for which there is a nontrivial solution for (2.5), there is a variational characterization for it:

$$\lambda_p = \inf \; GL(u) = \inf \int_\Omega |(\nabla - iA_e)u|^2 \, dx, \qquad (2.7)$$

where the minimization is taken under the constraint $\int_\Omega |u|^2 dx = 1$.

It has been recognized since the classical work of Little and Parks [8] that the flux of H_e through the hole bounded by the ring, i.e. the integral of H_e over this area, is an important physical quantity. The flux times 2π will be denoted by Φ. It will be shown that a necessary condition for the singly connected state to appear is that Φ is as far as possible from an integer.

The following geometrical - spectral characterization will be useful in the sequel:

Definition Q. *Let Ω be a ring-like domain, and let Γ be a curve connecting the inner boundary of the ring to its outer boundary. We denote the class of such curves by $\mathcal{L}$. We introduce the scalar eigenvalue problem*

$$\mu_\Omega(\Gamma) = \inf_{y\in\mathcal{A}} \int_\Omega |\nabla y|^2\, dx, \tag{2.8}$$

where $\mathcal{A} = \{y \in H^1(\Omega),\ \int_\Omega y^2\, dx = 1,\ \ y|_\Gamma = 0\}$. Let

$$\mu_\Omega = \inf \mu_\Omega(\Gamma). \tag{2.9}$$

A domain Ω is said to be of type Q if the infimum in (2.9) is achieved at a finite discrete set of isolated curves $\{\Gamma_1, \Gamma_2, ..., \Gamma_q\}$.

3 The linear problem

We first establish our result for the linear bifurcation problem (2.5)-(2.6).

Theorem 1. *Assume Ω is of type Q. Let*

$$2\Phi = 2l + 1 \tag{3.1}$$

for some integer l. Then every solution of (2.5)-(2.6) vanishes along a curve Γ of class $\mathcal{L}$. Moreover, the polar form of the solution is $u(x) = Y(x)e^{i\phi(x)}$, where $\phi(x)$ satisfies

$$\nabla\phi = A_e. \tag{3.2}$$

The curve Γ, the amplitude Y and the eigenvalue λ_p are the solution to the minimization problem (2.8)-(2.9).

Proof.

Since the solutions of (2.5)-(2.6) are critical points of (2.7), the real and imaginary parts of u are analytic functions [9]. We recall Theorem 2.6 of [7] that states that S consists only of isolated points or curves which end on the boundary of Ω. Thus the phase is well defined almost everywhere. Moreover, using the same arguments as in Corollary 2.7 of [7], S can at most contain curves of type $\mathcal{L}$.

Let ϕ_c be the family of solutions of (3.2) that differ from each other by a constant. Consider first solutions of (2.5) of the form $u_c = Ye^{i\phi_c}$ for some c. Let $\mathcal{C}$ be a curve circulating once around the ring. Integrating (3.2) along $\mathcal{C}$, using (3.1), and applying Stokes theorem, we find that u_c is not single valued unless it has a zero somewhere on $\mathcal{C}$. It follows that Y must vanish along some curve Γ_c of type $\mathcal{L}$. Also, normalizing Y to have a unit L^2 norm, we see by substituting (3.2) into (2.7) that

$$GL(u_c) = \mu_\Omega(\Gamma_c). \tag{3.3}$$

Assume now in contradiction that there exists a solution $u_1 = Y_1e^{i\phi_1}$ of (2.5)-(2.6) whose phase does not satisfy (3.2). Using (3.1), we see that $u_2 = Y_1e^{i(2\phi_c-\phi_1)}$ is also a solution. But since (2.5)-(2.6) is linear, any linear combination of u_1 and u_2 is a solution too. Consider for example

$$u_c^* = Y_c^* e^{i\phi_c^*} = u_1 - u_2 = Y_1 e^{i\phi_1}(1 - e^{2i(\phi_c - \phi_1)}) \tag{3.4}$$

for some c. Clearly we can find a value c such that the equation $\phi_c(x) - \phi_1(x) = 0$ defines a curve γ_c. Since γ_c consists of zeros of u_c^*, it must be of class $\mathcal{L}$.

Equation (2.5) implies that the supercurrent $J = Y_c^{*2}(\nabla\phi_c^* - A_e)$ is a divergence free vector field. Therefore the streamlines satisfy the dynamical system

$$\dot{x_1} \doteq J_1 = -\psi_{x_2} \tag{3.5}$$

$$\dot{x_2} \doteq J_2 = \psi_{x_1} \tag{3.6}$$

for some stream function $\psi(x)$. Consider now the domain $\Omega \setminus \gamma_c$. The boundary conditions (2.6) imply that ψ is constant on its boundary. We shall first prove that the dynamical system (3.5)-(3.6) has no periodic solutions. Assume in contradiction that there exists some periodic orbit. Dividing J by Y_c^{*2}, integrating along the periodic orbit and denoting the tangential direction on the orbit by τ, we get

$$\int \frac{J}{Y_c^{*2}} \cdot d\tau = \int (\nabla\phi_c^* - A_e) d\tau = 0, \tag{3.7}$$

where we used in the last equality the single valuedness of u_c^* and the fact that $H_e = 0$ in Ω. But since the integrand in (3.7) is nonnegative, we conclude that $J \equiv 0$, and therefore all the points on the orbits are in fact critical. ¿From the Poincare-Bendixon theorem we now infer that all the orbits are either critical points, or converging to critical points. But since ψ is constant on the orbit, it follows that all the values taken by ψ are critical. If ψ takes more than one value, it must then take values in some interval, which is impossible according to Sard's theorem. Hence ψ is constant in $\Omega \setminus \gamma_c$, which implies $J \equiv 0$ and therefore $\nabla\phi_c^* = A_e$ there.

Returning to (2.7), normalizing Y_c^* to have a unit L^2 norm, and using (3.2), we obtain the following identity for u_c^*:

$$\lambda_p = GL(u_c^*) = \mu_\Omega(\gamma_c). \tag{3.8}$$

But varying c we obtain a smooth family of curves γ_c satisfying (3.8) in contradiction to our assumption that Ω is of type Q. Moreover, property Q implies that the zero set of u consists of any single member Γ_j of the set $\{\Gamma_1, \Gamma_2, ..., \Gamma_q\}$. For each one of them there corresponds a unique amplitude Y_j.

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4 The nonlinear equations

The existence of minimizers of (2.1) in the singly connected state is established in the following theorem

Theorem 2. *Assume Ω is of type Q, and (3.1) holds. Then there exists an interval $I_\delta = (\lambda_p, \lambda_p + \delta)$, $\delta > 0$, such that for every $\lambda \in I_\delta$, the global minimizer of (2.1) vanishes* *along a curve of class $\mathcal{L}$. The phase of the global minimizer satisfies (3.2) and the current vanishes everywhere.*

Proof.

Fix $\lambda > \lambda_p$, and let $(u, A) = (Ye^{i\phi}, A_e + A_i)$ be a global minimizer of G_λ. If ϕ satisfies (3.2), then $A_i = 0$, and the result follows by the same arguments as in Theorem 1.

If, on the other hand, ϕ does not satisfy (3.2), then from equation (2.3) A_i cannot vanish identically. Consider now

$$(v, B) = (Ye^{i(2\phi_c - \phi)}, A_e - A_i), \tag{4.1}$$

where ϕ_c is a solution of (3.2). Condition (3.1) implies that (v, B) is smooth, and it is easy to check that $G_\lambda(v, B) = G_\lambda(u, A)$. We remark that u and v are of different homotopy types: Let the homotopy type of u be d_1. This means $\int_{\mathcal{C}} \nabla\phi = d_1$, where $\mathcal{C}$ is any curve circulating once about the ring. But then the homotopy type of v is $d_2 = 2l + 1 - d_1$, and since d_1 and l are integers, $d_1 \neq d_2$.

We have shown (Theorem 1) that a unique solution u_p bifurcates at $\lambda = \lambda_p$, $2\Phi = 2l + 1$. Applying the Crandall - Rabinowitz abstract bifurcation theory ([5], Theorem 2.4), one can show that there is a unique branch originating at u_p. The details are similar to the examples in [5] and to Theorem 8..6 of [1], so we do not spell them out. It follows that at least at a small λ interval to the right of λ_p, the phase ϕ must satisfy (3.2)

Substituting (3.2) and $A_i = 0$ in (2.2)-(2.4) we find that the amplitude Y solves

$$-\Delta Y + \lambda Y(Y^2 - 1) = 0, \quad x \in \Omega \tag{4.2}$$

$$\nu \cdot \nabla Y = 0, \; x \in \partial\Omega \tag{4.3}$$

Multiplying (4.2) by Y, integrating by parts and using (3.2) again, we get

$$G = -\frac{\lambda}{2} \int_\Omega Y^4 \, dx \; < \; 0. \tag{4.4}$$

Thus the pair (u, A_e), where u is in the singly connected state, is the global minimizer of G.

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5 The one dimensional model

When the ring is very thin, the GL model can be approximated by a functional on a curve M forming the ring's skeleton. The one dimensional model was used by several authors (see e.g. [10]). It was rigorously derived in [12]:

$$G^1_\lambda(u) = \int_M \left(\lambda[-|u|^2 + |u|^4/2] + |(\partial_\theta - iA_e)u|^2\right) D(\theta)\, d\theta. \tag{5.1}$$

Here θ is a variable along M and $D(\theta)$ is a strictly positive function that measures the thickness of the ring at θ. The Euler Lagrange equation associated with (5.1) is

$$(\partial_\theta - A_e)D(\partial_\theta - A_e)u + \lambda D u(1 - |u|^2) = 0, \tag{5.2}$$

with periodic boundary conditions.

The Q property is now replaced by

Definition Q1. *Consider the scalar eigenvalue problem*

$$\mu_M(\alpha) = \inf_{y\in\mathcal{B}} \int_M |\partial_\theta y(\theta)|^2 D(\theta+\alpha)\, d\theta \tag{5.3}$$

where $\mathcal{B} = \{y \in H^1(M),\ \int_M y^2 = 1,\ y(0) = 0\}$. *Let*

$$\mu_M = \inf \mu_M(\alpha). \tag{5.4}$$

A pair (M, D) is said to be of type Q1 if the infimum in (5.4) is achieved at a discrete set of points α.

The phase diagram for the model (5.1) was systematically studied in [3]. The following theorem provides theoretical support to the overall structure of the diagram:

Theorem 3. *Assume (M, D) is of type Q1, and Φ satisfies (3.1). Then*

1. *There exists a critical value λ^1_p where the trivial solution to (5.2) bifurcates into a singly connected state, and an interval $I^1_\delta = (\lambda^1_p, \lambda^1_p + \delta)$, $\delta > 0$, where the global minimizer for (5.1) is singly connected.*
2. *There is another value λ^1_q, such that for all $\lambda \in (\lambda^1_q, \infty)$ the global minimizer is not singly connected*

Proof.

The first part of the theorem follows by the same arguments as in Theorem 2. Notice, though, that in the one dimensional setup, the equation $\partial_\theta \phi = A_e$, replacing (3.2), is always solvable.

To prove the second part, we recall [3] that in the one dimensional case the Euler Lagrange equation for the phase of the order parameter can be integrated explictly in terms of the applied magnetic field. The energy functional for doubly connected functions (i.e. functions that do not vanish on M [2]) takes the form

$$G^1_\lambda(Y) = \int_M \left(\lambda[-Y^2 + Y^4/2] + (\partial_\theta Y)^2\right) D(\theta)\, d\theta + \frac{(2\pi k)^2}{\Lambda}. \tag{5.5}$$

Here Y is the amplitude of u, $k = N - \Phi$, where N is the circulation of the phase, and $\Lambda = \int_M \frac{d\theta}{DY^2}$. Clearly, to minimize the energy, N is chosen to minimize k^2. Our assumption on Φ implies $k^2 = 1/4$. The energy functional for singly connected functions is similar except that the last term is ommitted.

The Euler Lagrange equation for the amplitude of the singly connected state is

$$\partial_\theta(D\partial_\theta Y) + \lambda D(Y - Y^3) = 0,\ \ Y(0) = Y(2\pi) = 0, \tag{5.6}$$

where, without loss of generality, we chose the angle at which Y vanishes to be $\theta = 0$. It is easy to verify that the solution to (5.6) satisfies $0 \le Y \le 1$.

Set $e = D(\partial_\theta Y)^2 + \lambda D(Y^2 - Y^4/2)$. Differentiating e with respect to θ and using (5.6) we get

$$\partial_\theta e + D^{-1}\partial_\theta D e = 2\lambda D^{-1}\partial_\theta D(Y^2 - Y^4/2). \tag{5.7}$$

If the singly connected state is a global minimizer, its energy should be negative. Therefore there must be at least one point where $|\partial_\theta Y| \leq C\lambda^{1/2}$ for some constant C. Applying Gronwall's lemma to (5.7), we conclude that $|\partial_\theta Y| \leq C\lambda^{1/2}$ for all θ.

Multiplying (5.6) by Y and integrating by parts, we get for the singly connected state [3]

$$G^1_\lambda(Y) = -\frac{\lambda}{2}\int_M DY^4\, d\theta. \tag{5.8}$$

We also compute

$$G^1_\lambda(Y=1) = -\frac{\lambda}{2}\int_M D + \frac{\pi^2}{\int_M D^{-1}}. \tag{5.9}$$

The singly connected state vanishes at some point, and the derivative estimate we have obtained implies that, for large λ, Y is small at some interval of size λ^{-p} about this point for every $p \in (1/2, 1)$. Thus

$$\frac{\lambda}{2}\int_M D - \frac{\lambda}{2}\int_M DY^4\, d\theta \geq O(\lambda^{1-p}), \;\; p \in (1/2, 1). \tag{5.10}$$

Therefore for λ sufficiently large the constant solution $Y \equiv 1$ has a lower energy than any singly connected state.

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6 Discussion

We have shown that the zero set of the order parameter can be of codimension 1. Our construction is based on the solvability of the phase equation (3.2), which requires the applied magnetic field to vanish in Ω, while still allowing for nonzero flux. Therefore the topology of the ring is crucial.

Elliot, Matano and Qi proved in [7] that the zero set of the minimizers to the Ginzburg Landau functional in two dimensional domains consists of isolated points. We have given here an example of domains for which the zero set consists of a curve. The reason for the disagreement is that the construction in Lemma 2.7 of [7] is valid only for singly connected domains.

The bifurcation equation (2.5)-(2.6) can also be interpreted as the Schrödinger equation for a charged particle in a ring under an external magnetic field and with zero probability current through the boundary. Thus Theorem 1 implies that whenever the magnetic flux, measured in fundamental flux units, is an integer plus half, then there exists a 'forbidden curve' for the ground state.

In [2] and [3] we have used asymptotic and numerical calculations to study a weighted GL energy on a circle. We predicted the existence of a temperature range in which a new superconducting phase will emerge if the weight is nontrivial. The new phase is characterized by a smooth transition between states with different angular quantum numbers. Theorem 3 provides a theoretical support to the phase transition picture we computed. On the other hand, the standard GL energy in thin annular domains can be shown [12] to converge to the weighted GL energy on a circle, where the weight is determined by the local thickness of the annulus. Thus we have rigourosly established the existence of the new phase for asymmetric thin rings.

The geometrical-spectral characterization of Ω we introduced in Definition Q poses a novel challenging problem in calculus of variations. Essentially condition Q (or Q1) means that the domain is not symmetric. It does not hold for the symmetric annulus confined between two concentric circles. We conjecture that Q is a generic property.

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References

[1] P. Bauman, D. Phillips and T. Qi, "Stable nucleation of the Ginzburg Landau system with an applied magnetic field", *Arch. Rat. Mech. Anal.* to appear.

[2] J. Berger and J. Rubinstein, "Topology of the order parameter in the Little Parks experiment", *Phys. Rev. Lett. 75,* 320-322, 1995.

[3] J. Berger and J. Rubinstein, "Bifurcation analysis for phase transitions in nonuniform superconducting rings", *SIAM J. Appl. Math.,* to appear.

[4] J. Berger and J. Rubinstein, "Signatures for the second critical point in the phase diagram of a superconducting ring", *Phys. Rev. B 56,* 5124-5127, 1997.

[5] M.G. Crandall and P.H. Rabinowitz, "Bifurcation from simple eigenvalues", *J. Func. Anal. 8,* 321-340, 1971.

[6] Q. Du, M.D. Gunzburger and J. Peterson, "Analysis and approximation of the Ginzburg Landau model of superconductivity", *SIAM Review 34,* 529-560, 1992.

[7] C.M. Elliott, H. Matano and T. Qi, "Zeros of complex Ginzburg Landau order parameter with application to superconductivity", *Europ. J. Appl. Math. 5,* 431-448, 1994.

[8] W.A. Little and R.D. Parks, "Observation of quantum periodicity in the transition temperature of a superconducting cylinder", *Phys. Rev. Lett. 9,* 9-12, 1962.

[9] C.B. Morrey, *Multiple Integrals in the Calculus of Variations,* Springer-Verlag, 1966.

[10] B. Pannetier, "Superconducting wire networks", In *Quantum Coherence in Mesoscopic Systems* (ed. B. Kramer) Plenum Press, 457-484, 1991.

[11] J. Rubinstein, "Six lectures on superconductivity", in *Boundaries, Interfaces and Transitions,* M. Delfour Ed. CRM Series, American Mathematical Society, in press.

[12] J. Rubinstein and M. Schatzman, "Asymptotics for thin superconducting rings", *J. Math. Pure Appl.*, to appear.

[13] M. Tinkham, *Introduction to Superconductivity* McGraw-Hill, 1996.

Address: J.B.: Department of Physics, Technion, 32000 Haifa, Israel; `e-mail:phr76jb@vmsa.technion.ac.il`
J.R.: Department of Mathematics, Technion, 32000 Haifa, Israel; `e-mail:koby@leeor.technion.ac.il`