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## Gauges for the Ginzburg-Landau Equations of Superconductivity

This note is concerned with gauge choices for the time-dependent GINZBURG-LANDAU equations of superconductivity. The equations model the state of a superconducting sample in a magnetic field near the critical temperature. Any two solutions related through a "gauge transformation" describe the same state and are physically indistinguishable. This "gauge invariance" can be exploited for analytical and numerical purposes. A new gauge is proposed, which reduces the equations to a particularly attractive form.

## 1. The Ginzburg-Landau Model of Superconductivity

In the GINZBURG-LANDAU theory of phase transitions [1], the state of a superconducting material near the critical temperature is described by a complex-valued *order parameter*  $\psi$ , a real-valued *vector potential*  $\mathbf{A}$ , and, when the state changes with time, a real-valued *scalar potential*  $\phi$ . The role of  $\phi$  differs from that of  $\psi$  and  $\mathbf{A}$ : the latter are predictive variables, whose evolution is governed by differential equations; the former is more like a Lagrange multiplier. After suitable nondimensionalization, the equations and boundary conditions satisfied by  $\psi$  and  $\mathbf{A}$  are usually presented in the form

$$\eta \left( \frac{\partial}{\partial t} + i\kappa\phi \right) \psi = - \left( \frac{i}{\kappa} \nabla + \mathbf{A} \right)^2 \psi + (1 - |\psi|^2) \psi \quad \text{in } \Omega \times (0, \infty), \quad (1)$$

$$\frac{\partial \mathbf{A}}{\partial t} + \nabla \phi = -\nabla \times \nabla \times \mathbf{A} - \frac{i}{2\kappa} (\psi^* \nabla \psi - \psi \nabla \psi^*) - |\psi|^2 \mathbf{A} + \nabla \times \mathbf{H} \quad \text{in } \Omega \times (0, \infty), \quad (2)$$

$$\left( \frac{i}{\kappa} \nabla + \mathbf{A} \right) \psi \cdot \mathbf{n} = -\frac{i}{\kappa} \gamma \psi \quad \text{on } \partial\Omega \times (0, \infty), \quad (3)$$

$$(\nabla \times \mathbf{A} - \mathbf{H}) \times \mathbf{n} = \mathbf{0} \quad \text{on } \partial\Omega \times (0, \infty). \quad (4)$$

The domain  $\Omega$  corresponds to the region occupied by the superconducting material. We assume that  $\Omega$  is bounded,  $\Omega \subset \mathbb{R}^D$  with  $D = 2$  or  $D = 3$ , and the boundary  $\partial\Omega$  of  $\Omega$  is sufficiently regular;  $\mathbf{n}$  denotes the outer unit normal to  $\partial\Omega$ . The parameters of the model are  $\eta$ , a (dimensionless) friction coefficient;  $\kappa$ , the (dimensionless) GINZBURG-LANDAU parameter; and  $\gamma$ , a nonnegative parameter, which is zero if the superconducting material is surrounded by vacuum. The vector field  $\mathbf{H}$  is a given *applied magnetic field*; in practice,  $\mathbf{H}$  is either time-independent or time-periodic. As usual,  $\nabla \equiv \text{grad}$ ,  $\nabla \times \equiv \text{curl}$ ,  $\nabla \cdot \equiv \text{div}$ , and  $\nabla^2 = \nabla \cdot \nabla \equiv \Delta$ . Furthermore,  $i$  is the imaginary unit, and a superscript  $*$  denotes complex conjugation.

The system of Eqs. (1)–(4), with appropriate initial conditions, constitutes the *time-dependent GINZBURG-LANDAU (TDGL) model of superconductivity*. It was first proposed by SCHMID [2] and subsequently obtained as an asymptotic limit of the microscopic BARDEEN-COOPER-SCHRIEFFER (BCS) model of superconductivity by GOR'KOV AND ELIASHBERG [3]. Details can be found in the physics literature; standard references are ABRIKOSOV [4], DEGENNES [5], and TINKHAM [6].

In this article, we will work mostly with a rescaled version of the TDGL model, because the equations are somewhat simpler. Let  $\sigma = 1/(\eta\kappa^2)$ . In the *rescaled TDGL model*, time is measured in units of  $1/\sigma$ , the scalar potential in units of  $\sigma/\kappa$ , and the vector potential and applied magnetic field in units of  $1/\kappa$ . The model consists of the equations

$$(\partial_t + i\phi) \psi = -(i\nabla + \mathbf{A})^2 \psi + \kappa^2 (1 - |\psi|^2) \psi \quad \text{in } \Omega \times (0, \infty), \quad (5)$$

$$\sigma (\partial_t \mathbf{A} + \nabla \phi) = -\nabla \times \nabla \times \mathbf{A} + \mathbf{J}_s + \nabla \times \mathbf{H} \quad \text{in } \Omega \times (0, \infty), \quad (6)$$

$$(i\nabla + \mathbf{A}) \psi \cdot \mathbf{n} = -i\gamma \psi \quad \text{on } \partial\Omega \times (0, \infty), \quad (7)$$

$$(\nabla \times \mathbf{A} - \mathbf{H}) \times \mathbf{n} = \mathbf{0} \quad \text{on } \partial\Omega \times (0, \infty), \quad (8)$$

together with the appropriate initial conditions. Here, we have introduced the abbreviation  $\partial_t = \partial/\partial t$ . Furthermore,

$$\mathbf{J}_s = (2i)^{-1} (\psi^* \nabla \psi - \psi \nabla \psi^*) - |\psi|^2 \mathbf{A} = -\text{Re} [\psi^* (i\nabla + \mathbf{A}) \psi]. \quad (9)$$

The quantity  $\mathbf{J}_s$  is the so-called *supercurrent* or, more correctly, *supercurrent density*. The supercurrent is a phenomenological quantity, which is thought of as a flux of moving "superelectrons." The superelectrons (or COOPER

pairs), whose density is  $n_s = |\psi|^2$ , are responsible for the superconducting properties of the material. For example, the supercurrent prevents a magnetic field from penetrating a superconducting region.

Note that  $\mathbf{E} = -\partial\mathbf{A}/\partial t - \nabla\phi$  is the *electric field* and  $\mathbf{B} = \nabla \times \mathbf{A}$  the *magnetic induction*. Therefore, Eq. (6) may be viewed as Faraday's law,  $\nabla \times \mathbf{B} = \mathbf{J}$ , where the total current  $\mathbf{J}$  is the sum of the supercurrent  $\mathbf{J}_s$ , a "normal" current  $\mathbf{J}_n = \sigma\mathbf{E}$ , and the transport current  $\mathbf{J}_t = \nabla \times \mathbf{H}$ . The normal current obeys OHM's law with a "normal conductivity" coefficient  $\sigma$ .

In the steady state, the TDGL model admits the trivial solution  $\psi = 0$ ,  $\nabla \times \mathbf{A} = \mathbf{H}$ . (Recall that the scalar potential vanishes in the steady state.) This solution represents the superconductor in the *normal state*, where the magnetic field penetrates the sample uniformly and the material has lost all superconducting properties.

## 2. Gauge Invariance

Equations (5) and (6) require initial conditions for the order parameter and the vector potential. Here, the concept of *gauge invariance* enters. Because the physical state of the system at  $t = 0$  is completely determined by the magnetic induction  $\mathbf{B}$ , the superelectron density  $n_s$ , and the supercurrent  $\mathbf{J}_s$ , we have a significant degree of freedom in the choice of initial data for  $\psi$  and  $\mathbf{A}$ . In fact, if the pair  $(\psi_0, \mathbf{A}_0)$  properly specifies the physical initial state, then so does any other pair  $(\psi'_0, \mathbf{A}'_0)$  that is related to  $(\psi_0, \mathbf{A}_0)$  by a transformation

$$\mathcal{G}_{\chi_0}: (\psi_0, \mathbf{A}_0) \mapsto (\psi'_0, \mathbf{A}'_0) = (\psi_0 e^{i\chi_0}, \mathbf{A}_0 + \nabla\chi_0). \quad (10)$$

Here,  $\chi_0$  can be any (sufficiently smooth) real-valued function of position. Equation (10) is the *gauge transformation* for the stationary GINZBURG-LANDAU model.

There is a similar, though more complicated, gauge transformation for the time-dependent GINZBURG-LANDAU model. In terms of the rescaled variables, it is

$$\mathcal{G}_\chi: (\psi, \mathbf{A}, \phi) \mapsto (\psi', \mathbf{A}', \phi') = (\psi e^{i\chi}, \mathbf{A} + \nabla\chi, \phi - \partial_t\chi). \quad (11)$$

Here,  $\chi$  can be any (sufficiently smooth) real-valued function of position and time. Mathematically, gauge invariance reflects a lack of uniqueness. The TDGL model defines only an equivalence class of solutions, and by choosing a particular gauge  $\chi$  we select a representative from this class. The physical relevance of gauge invariance is the following. At each instant, the macroscopic state of the superconductor is entirely specified in terms of the electromagnetic variables  $\mathbf{E}$  and  $\mathbf{B}$ , the superelectron density  $n_s$ , and the supercurrent  $\mathbf{J}_s$ . These quantities are invariant under the gauge transformation (11), so the states  $(\psi, \mathbf{A}, \phi)$  and  $(\psi', \mathbf{A}', \phi')$  are macroscopically indistinguishable. The choice of a particular gauge  $\chi$  does not affect the specification of the physical state of the system.

## 3. Gauge Choices

The most common gauge is the "COULOMB gauge," where the vector potential is divergence-free at all times. If  $(\psi_0, \mathbf{A}_0)$  are the initial data given with Eqs. (5) and (6), one determines the initial gauge  $\chi_0$  by solving the boundary value problem

$$\Delta\chi_0 = -\nabla \cdot \mathbf{A}_0 \text{ in } \Omega, \quad \nabla\chi_0 \cdot \mathbf{n} = -\mathbf{A}_0 \cdot \mathbf{n} \text{ on } \partial\Omega, \quad (12)$$

and changes to the image  $(\psi'_0, \mathbf{A}'_0)$  of  $(\psi_0, \mathbf{A}_0)$  under the gauge transformation  $\mathcal{G}_{\chi_0}$ . At any time  $t > 0$ , one takes the solution  $(\psi, \mathbf{A}, \phi)$  of the rescaled TDGL model, solves the boundary value problem

$$\Delta\chi = -\nabla \cdot \mathbf{A} \text{ in } \Omega, \quad \nabla\chi \cdot \mathbf{n} = -\mathbf{A} \cdot \mathbf{n} \text{ on } \partial\Omega, \quad (13)$$

and changes to the image  $(\psi', \mathbf{A}', \phi')$  of  $(\psi, \mathbf{A}, \phi)$  under the gauge transformation  $\mathcal{G}_\chi$ . As a result,  $\mathbf{A}'_0$  and  $\mathbf{A}'$  are divergence-free. The procedure amounts effectively to integrating Eqs. (5) and (6), together with the equations

$$\sigma\Delta\phi = \nabla \cdot \mathbf{J}_s, \quad \nabla \cdot \mathbf{A} = 0 \text{ in } \Omega \times (0, \infty), \quad (14)$$

$$\nabla\psi \cdot \mathbf{n} = -\gamma\psi, \quad \nabla\phi \cdot \mathbf{n} = 0, \quad \mathbf{A} \cdot \mathbf{n} = 0, \quad (\nabla \times \mathbf{A} - \mathbf{H}) \times \mathbf{n} = 0 \text{ on } \partial\Omega \times (0, \infty), \quad (15)$$

starting from initial data  $(\psi_0, \mathbf{A}_0)$  with  $\nabla \cdot \mathbf{A}_0 = 0$ .

The equations of the TDGL(C) model ("C" for COULOMB gauge) are formally similar to the NAVIER-STOKES equations for an incompressible fluid. This similarity was exploited in recent work by TANG and WANG [7], who proved the existence of strong ( $D = 2, 3$ ) and weak ( $D = 2$ ) solutions and of a global attractor.

Because the COULOMB gauge requires the solution of an elliptic boundary value problem for the scalar potential at each time step, it is less suitable for numerical purposes. Here, one would like to eliminate the scalar potential altogether. This is, in fact, possible. By choosing an arbitrary gauge  $\chi_0$  for the initial data and determining  $\chi$  as the solution of the initial-value problem

$$\partial_t \chi = \phi \text{ in } \Omega \times (0, \infty), \quad \chi|_{t=0} = \chi_0 \text{ in } \Omega, \quad (16)$$

one obtains the "zero-electric potential gauge." (The scalar  $\phi$  is also known as the *electric potential*.) In this gauge, the rescaled TDGL model reduces to

$$\partial_t \psi = -(i\nabla + \mathbf{A})^2 \psi + \kappa^2 (1 - |\psi|^2) \psi \text{ in } \Omega \times (0, \infty), \quad (17)$$

$$\sigma \partial_t \mathbf{A} = -\nabla \times \nabla \times \mathbf{A} + \mathbf{J}_s + \nabla \times \mathbf{H} \text{ in } \Omega \times (0, \infty), \quad (18)$$

$$(i\nabla + \mathbf{A}) \psi \cdot \mathbf{n} = -i\gamma \psi \text{ on } \partial\Omega \times (0, \infty), \quad (19)$$

$$(\nabla \times \mathbf{A} - \mathbf{H}) \times \mathbf{n} = \mathbf{0} \text{ on } \partial\Omega \times (0, \infty). \quad (20)$$

The TDGL(Z) model ("Z" for "zero-electric potential gauge") was used by DU [8] to prove the existence and uniqueness of strong solutions. It is the kernel of the TDGL code used at ARGONNE [9, 10] for the numerical simulation of vortex dynamics in type-II superconductors.

It is not possible to combine the COULOMB gauge and the zero-electric potential gauge. Even when the initial data are divergence-free, the solution obtained in the zero-electric potential gauge does not remain on the divergence-free manifold. To see this, take the divergence of Eq. (18): if  $\text{div } \mathbf{A}$  is zero, it must be the case that  $\text{div } \mathbf{J}_s = 0$ . But from Eq. (17) we obtain the expression  $\text{div } \mathbf{J}_s = (2i)^{-1}(\psi^* \partial_t \psi - \psi \partial_t \psi^*)$ , which is zero if and only if  $\psi = 0$  or the phase of  $\psi$  is constant in time.

It is, however, possible to couple  $\text{div } \mathbf{A}$  to  $\phi$ . The standard gauge is the " $\phi = -\text{div } \mathbf{A}$  gauge," which maintains the identity  $\phi = -\text{div } \mathbf{A}$  between the (unscaled) potentials or, equivalently,  $\sigma\phi = -\text{div } \mathbf{A}$  between the rescaled potentials at all times. The gauge  $\chi$  is the solution of the boundary value problem

$$\sigma \partial_t \chi - \Delta \chi = \text{div } \mathbf{A} + \sigma \phi \text{ in } \Omega \times (0, \infty), \quad \nabla \chi \cdot \mathbf{n} = -\mathbf{A} \cdot \mathbf{n} \text{ on } \partial\Omega \times (0, \infty). \quad (21)$$

The initial condition  $\chi|_{t=0} = \chi_0$  can be chosen arbitrarily. Usually, one takes  $\chi_0$  so the initial data are divergence-free, cf. DU [8], but this choice is in no way necessary; in fact, there is a distinct advantage in leaving  $\chi_0$  undetermined. The rescaled TDGL model reduces to the following TDGL(S) model ("S" for "standard  $\phi = -\text{div } \mathbf{A}$  gauge"):

$$\partial_t \psi = -(i\nabla + \mathbf{A})^2 \psi + \kappa^2 (1 - |\psi|^2) \psi + i\sigma^{-1}(\text{div } \mathbf{A})\psi \text{ in } \Omega \times (0, \infty), \quad (22)$$

$$\sigma \partial_t \mathbf{A} = \Delta \mathbf{A} + \mathbf{J}_s + \nabla \times \mathbf{H} \text{ in } \Omega \times (0, \infty), \quad (23)$$

$$\nabla \psi \cdot \mathbf{n} = -\gamma \psi, \quad \mathbf{A} \cdot \mathbf{n} = 0, \quad (\nabla \times \mathbf{A} - \mathbf{H}) \times \mathbf{n} = \mathbf{0} \text{ on } \partial\Omega \times (0, \infty). \quad (24)$$

Here, the initial data  $(\psi_0, \mathbf{A}_0)$  must be consistent with the boundary conditions (24). The TDGL(S) model was analyzed by TAKÁČ [11], who showed that it generates a dynamical process in a Cartesian product of fractional Sobolev spaces.

There are, of course, many other ways to couple  $\text{div } \mathbf{A}$  to  $\phi$ . In fact, we claim that the TDGL model reduces to a more tractable form if the constraint  $\phi = -\text{div } \mathbf{A}$  is applied to the rescaled, rather than the original, potentials. The gauge  $\chi$  which accomplishes this reduction is the solution of the boundary value problem

$$\partial_t \chi - \Delta \chi = \text{div } \mathbf{A} + \phi \text{ in } \Omega \times (0, \infty), \quad \nabla \chi \cdot \mathbf{n} = -\mathbf{A} \cdot \mathbf{n} \text{ on } \partial\Omega \times (0, \infty), \quad (25)$$

with  $\chi|_{t=0} = \chi_0$  arbitrary. In this gauge, the rescaled TDGL model reduces to

$$\partial_t \psi = -(i\nabla + \mathbf{A})^2 \psi + \kappa^2 (1 - |\psi|^2) \psi \text{ in } \Omega \times (0, \infty), \quad (26)$$

$$\sigma \partial_t \mathbf{A} = -\nabla \times \nabla \times \mathbf{A} + \sigma \nabla(\text{div } \mathbf{A}) + \mathbf{J}_s + \nabla \times \mathbf{H} \text{ in } \Omega \times (0, \infty), \quad (27)$$

$$\nabla \psi \cdot \mathbf{n} = -\gamma \psi, \quad \mathbf{A} \cdot \mathbf{n} = 0, \quad (\nabla \times \mathbf{A} - \mathbf{H}) \times \mathbf{n} = \mathbf{0} \text{ on } \partial\Omega \times (0, \infty). \quad (28)$$

We refer to this model as the TDGL(R) model ("R" for "rescaled  $\phi = -\text{div } \mathbf{A}$  gauge").

The TDGL(S) and TDGL(R) models are similar, but not identical. Because  $-\nabla \times \nabla \times \mathbf{A} = \Delta \mathbf{A} - \nabla(\text{div } \mathbf{A})$ , they differ in the way the divergence of  $\mathbf{A}$  is accounted for. In the TDGL(S) model,  $\text{div } \mathbf{A}$  appears in the equation for  $\psi$ , in the TDGL(R) model in the equation for  $\mathbf{A}$ . The difference has an important consequence: the TDGL(R) model describes the gradient flow of an energy functional, the TDGL(S) model does not. In fact, the GINZBURG-LANDAU energy for the TDGL(R) model is

$$E[\psi, \mathbf{A}] = \int_{\Omega} \left( |(i\nabla + \mathbf{A})\psi|^2 + \frac{1}{2}\kappa^2(1 - |\psi|^2)^2 + |\nabla \times \mathbf{A} - \mathbf{H}|^2 + \sigma(\text{div } \mathbf{A})^2 \right) dx + \int_{\partial\Omega} \gamma |\psi|^2 d\tau(x). \quad (29)$$

One readily verifies that the first variations of  $E$  with respect to  $\psi^*$  and  $\mathbf{A}$  are

$$\delta_{\psi^*} E = (i\nabla + \mathbf{A})^2 \psi - \kappa^2 (1 - |\psi|^2) \psi, \quad (30)$$

$$\delta_{\mathbf{A}} E = 2(\nabla \times \nabla \times \mathbf{A} - \sigma \nabla(\operatorname{div} \mathbf{A}) - \mathbf{J}, -\nabla \times \mathbf{H}). \quad (31)$$

The natural boundary conditions associated with  $E$  are

$$\nabla \psi \cdot \mathbf{n} = -\gamma \psi, \quad (\nabla \times \mathbf{A} - \mathbf{H}) \times \mathbf{n} = \mathbf{0}, \quad (32)$$

provided  $\mathbf{n} \cdot \mathbf{A} = 0$  on  $\partial\Omega$ . Hence, the TDGL(R) model corresponds to the dynamical system

$$\partial_t \psi = -\delta_{\psi^*} E, \quad \sigma \partial_t \mathbf{A} = -\frac{1}{2} \delta_{\mathbf{A}} E. \quad (33)$$

A detailed study of this dynamical system will appear in our forthcoming article [12].

In conclusion, we note that the  $\phi = -\operatorname{div} \mathbf{A}$  gauge, in either of the forms discussed here, appears to be the most natural gauge for the TDGL model, as every stationary solution  $(\psi, \mathbf{A})$  of TDGL(S) or TDGL(R) automatically satisfies the COULOMB gauge  $\operatorname{div} \mathbf{A} = 0$ .

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#### 4. References

- 1 GINZBURG, V.L., LANDAU, L.D.: On the theory of superconductivity; Zh. Eksperim. i Teor. Fiz. (USSR) 20 (1950), 1064-1082; Engl. transl. in TER HAAR, D.: L.D. Landau; Men of Physics, Vol. I, Pergamon Press (1965), 138-167.
- 2 SCHMID, A.: Phys. Kondens. Mater. 5 (1966), 302.
- 3 GOR'KOV, L.P., ELIASHBERG, G.M.: Generalizations of the Ginzburg-Landau equations for non-stationary problems in the case of alloys with paramagnetic impurities; Zh. Eksp. Teor. Fiz. 54 (1968), 612-626; Soviet Phys.- JETP 27 (1968), 328-334.
- 4 ABRIKOSOV, A.A.: Fundamentals of the Theory of Metals; North-Holland Publ. Co., Amsterdam 1988.
- 5 DEGENNES, P.: Superconductivity in Metals and Alloys; Benjamin, New York 1966.
- 6 TINKHAM, M.: Introduction to Superconductivity; McGraw-Hill, Inc., New York 1975.
- 7 TANG, Q., WANG, S.: Time dependent Ginzburg-Landau equations of superconductivity; preprint (1995).
- 8 DU, Q.: Global existence and uniqueness of solutions of the time-dependent Ginzburg-Landau model for superconductivity; Applicable Analysis (to appear).
- 9 GALBREATH, N., ET AL.: Parallel solution of the three-dimensional time-dependent Ginzburg-Landau equation; in: Proc. SIAM Conf. on Parallel Processing for Scientific Computing (1993); SIAM, Philadelphia.
- 10 GROPP, W.D., ET AL.: Numerical simulation of vortex dynamics in type-II superconductors; J. Comp. Phys. (1995) (to appear)
- 11 TAKÁČ, P.: On the dynamical process generated by a superconductivity model; Proc. ICIAM 95.
- 12 FLECKINGER-PELLÉ, J., KAPER, H.G., TAKÁČ, P.: Unpublished information, Argonne National Laboratory, 1995.

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