The Ginzburg-Landau theory in application

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Abstract

A numerical approach to Ginzburg-Landau (GL) theory is demonstrated and we review its applications to several examples of current interest in the research on superconductivity. This analysis also shows the applicability of the two-dimensional approach to thin superconductors and the re-defined effective GL parameter $\kappa$. For two-gap superconductors, the conveniently written GL equations directly show that the magnetic behavior of the sample depends not just on the GL parameter of two bands, but also on the ratio of respective coherence lengths.

Key words: Ginzburg-Landau; Mass anisotropy; Two-gap superconductors; Josephson coupling.

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Whenever a new scientific discovery is made, researchers must strive to explain it theoretically. In the case of superconductivity, it took more than two decades after its experimental discovery before the London theory was developed [1]. However, the London theory treats vortices as point-like objects and does not take into account the finite size and the inner structure of the vortex. In 1950, Landau and Ginzburg [2] developed a phenomenological theory, which combined Landau’s theory of second-order phase transitions with a Schrödinger-like wave equation. Over the past 50 years, this theory had great success in explaining macroscopic properties of superconductors (such as the division of superconductors into two categories now referred to as type-I and type-II, and the description of the mixed state of type-II superconductors [3]), but it was also immensely useful for description of mesoscopic superconducting samples [4,5]. Even the full, microscopic Bardeen, Cooper, and Schrieffer (BCS) theory of superconductivity reduces to the Ginzburg-Landau (GL) theory close to the critical temperature [6].

The GL theory extends Landau’s theory of second-order phase transitions [7] to a spatially varying complex order parameter $\psi(\vec{r})$ which is nonzero at $T < T_c$ and vanishes at $T \geq T_c$ through a second order phase transition. The resulting gradient term is made gauge-invariant by combining it with the vector potential $\vec{A}(\vec{r})$ where $\nabla \times \vec{A}(\vec{r}) = \vec{h}(\vec{r})$ is the local magnetic field.

The two Ginzburg-Landau equations are obtained by minimization of the GL free energy functional $\mathcal{F}\{\psi, \vec{A}\}$ with respect to $\psi$ and $\vec{A}$

$$
\mathcal{F}\{\psi, \vec{A}\} = \frac{H^2}{4\pi} \int \left[ -|\psi|^2 + \frac{1}{2} |\psi|^4 + \frac{1}{2} |(-i\nabla - \vec{A})\psi|^2 
+ \kappa^2 (\vec{h} - \vec{H}_0)^2 \right] dV, \tag{1}
$$

where $\kappa$ is the GL parameter given as a ratio of magnetic penetration depth $\lambda$ and the coherence length $\xi$, and $\vec{H}_0$ denotes the applied magnetic field. Eq. (1) is given in dimensionless form, where all distances are measured in $\xi(T)$, the vector potential $\vec{A}$ in $ch/2e\xi$, the magnetic field $\vec{H}$ in $H_{c2} = ch/2e\xi^2$, and the order parameter $\psi$ in $\psi_0 = \sqrt{-\alpha/\beta}$, with $\alpha, \beta$ being the material dependent coefficients.
Every part of Eq. (1) describes some physical property. In principle, it is possible to introduce some extra terms in the energy functional in order to describe the superconducting state deeper in the superconducting phase (see, for example, Ref. [8]), but the achieved corrections are very small and are rarely considered. The first part of Eq. (1) is the expansion of the energy difference between the superconducting and normal state for a homogeneous superconductor in the absence of an applied magnetic field $\gamma$ near the zero-field critical temperature $T_c$. The coefficient $\alpha$ is negative and changes sign as temperature is increased over $T_c$ ($\alpha \propto (T - T_c)$), while $\beta$ is a positive constant, independent of temperature. Therefore, the Cooper-pair density corresponding to temperatures below $T_c$ is a positive constant, independent of temperature. Therefore, the Cooper-pair density corresponds to temperatures below $T_c$ and in absence of magnetic field $|\psi_0|^2 = -\alpha/\beta$.

The next term in Eq. (1) is clearly the kinetic energy of the Cooper-pairs $\frac{1}{2m^*} \left( -i \nabla - \frac{2e}{c} \vec{A} \right)^2 \psi$, where $m^*$ is the effective mass of a Cooper-pair. It describes the energy cost when the superconducting density is non-homogeneous.

The last term in Eq. (1) describes the energy of the magnetic field of the supercurrents, which measures the response of the superconductor to an external field and is nothing else than the difference between the local and applied magnetic field. Note that for a superconductor in an external field, the equilibrium state is not defined by the Helmholtz free energy but the Gibbs free energy.

The phenomenological GL theory is one of the most elegant and powerful concepts in physics, which was applied not only to superconductivity (see textbooks [9–12]) but also to other phase transitions, to nonlinear dynamics, to dissipative systems with self-organizing pattern formation, and even to cosmology. In what follows, we describe a numerical approach towards solving the GL equations, with several particular modifications for special problems in superconductivity.

### Numerical approach in general

In what follows, we describe a numerical method used to solve the Ginzburg-Landau equations, whose solution minimizes the free energy. Using the dimensionless variables as explained above and the Lorenz gauge, $\text{div} \vec{A} = 0$, GL equations can be written in the following form:

\[
\left( -i \nabla - \vec{A} \right)^2 \psi = \psi \left( 1 - |\psi|^2 \right),
\]

\[
-\kappa^2 \Delta \vec{A} = \frac{1}{2i} \left( \psi^* \nabla \psi - \psi \nabla \psi^* \right) - |\psi|^2 \vec{A}.
\]

The Neumann boundary condition on the sample surfaces takes the form

\[
\vec{n} \cdot \left( -i \nabla - \vec{A} \right) \psi \bigg|_{\text{boundary}} = 0.
\]

For the fixed applied magnetic field, we solve the two coupled Ginzburg-Landau equations self-consistently. Both equations are solved using the link variable approach [13] for a finite-difference computational lattice, which is achieved by introducing the link variables between $\vec{r}_1$ and $\vec{r}_2$ as

\[
U_{\mu}^{\vec{r}_1,\vec{r}_2} = \exp \left[ -i \int_{\vec{r}_1}^{\vec{r}_2} \vec{A}_\mu (\vec{r}) \cdot d\vec{\mu} \right],
\]

with $\mu = x, y, z$.

In our calculation, the whole system is mapped on a rectangular grid. The first term from Eq. (5) is discretized as (the index $j$ denotes the lattice point of interest)

\[
\left( \nabla_{\mu} - A_{\mu} \right)^2 \psi_j = -\nabla_{\mu}^2 \psi_j + i e \nabla_{\mu} (A_{\mu} \psi_j) +
A_{\mu}^2 \psi_j + i A_{\mu} \nabla_{\mu} \psi_j = \frac{1}{U_{\mu}^2} \left( -2i A_{\mu} U_{\mu} \nabla_{\mu} \psi_j \right.

\left. -i U_{\mu}^2 \psi_j (\nabla_{\mu} A_{\mu} - i A_{\mu}^2) + U_{\mu}^2 \nabla_{\mu}^2 \psi_j \right).
\]

After substituting $\nabla_{\mu} U_{\mu} = -i A_{\mu} U_{\mu}^{\dagger}$ and $\nabla_{\mu}^2 U_{\mu} = -i U_{\mu}^2 (\nabla_{\mu} A_{\mu} - i A_{\mu}^2)$, and some trivial transformations, we obtain

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1 It can be shown from the microscopic theory that only even powers of $|\psi|$ appear in this expansion.
\[
\left( \frac{\nabla \mu}{\mu} - A_\mu \right)^2 \psi_j = \frac{1}{U_\mu^2} \nabla_\mu (\nabla_\mu (U_\mu \psi_j)).
\]  
(8)

Finally, for \( \mu = x \) (analogously for \( \mu = y, z \)) we have

\[
\left( \frac{\nabla x}{x} - A_x \right)^2 \psi_j = \frac{1}{U_x^2} \left( U_x^{j+1} \psi_{j+1} - U_x^j \psi_j - U_x^j \psi_{j-1} - U_x^{j-1} \psi_{j-1} \right)
= \frac{U_x^{j+1} \psi_{j+1} - 2 \psi_j + U_x^{j-1} \psi_{j-1}}{a_x^2}.
\]  
(9)

The discretized Ginzburg-Landau equation can be now written in full as

\[
\frac{\partial \psi}{\partial t} = \frac{U_x^{j+1} \psi_{j+1} - 2 \psi_j + U_x^{j-1} \psi_{j-1}}{a_x^2} + \frac{U_y^{j+1} \psi_{j+1} - 2 \psi_j + U_y^{j-1} \psi_{j-1}}{a_y^2} + \frac{U_z^{j+1} \psi_{j+1} - 2 \psi_j + U_z^{j-1} \psi_{j-1}}{a_z^2} - \left( |\psi_j|^2 - 1 \right) \psi_j + f_j(t),
\]  
(10)

where different indices denote adjacent grid points to point \( j \) along three axis. In general, this approach works for \( a_x \neq a_y \neq a_z \).

Using Eq. (10), with chosen initial vector potential, we solve for the value of the order parameter \( \psi \) in every grid point. These values we can implement to calculate the local current densities \( j_x, y, z \). The right side of Eq. (3) can be written as

\[
j = \frac{1}{2} \left[ \psi^* \left( \frac{1}{i} \nabla - \vec{A} \right) \psi + \psi \left( \frac{1}{i} \nabla - \vec{A} \right)^* \psi^* \right],
\]  
(11)

where again link variable approach comes into play through similar transformations as in Eqs. (7)-(10)

\[
\left( \frac{1}{i} \nabla_x - A_x \right) \psi_j \rightarrow -i \frac{1}{U_x^2} \nabla_x (U_x^j \psi_j) = -i \frac{U_x^{j+1} \psi_{j+1} - \psi_j}{a_x},
\]  
(12)

From the supercurrents a new value for the vector potential can be calculated using the second GL equation. This is a Poisson-type of equation, which we solve using a Fourier transformation. The then obtained vector potential is used (in part, typically 5%) to update the current vector potential gradually. The updated vector potential is substituted back in the first GL equation and the whole procedure is repeated until a convergent solution of both GL equations is found.

Temperature dependence

The temperature dependence of characteristic lengths \( \xi \) and \( \lambda \) and the critical field is incorporated in GL theory as \( \xi(T) = \frac{\xi(0)}{\sqrt{1-T/T_c}} \), \( \lambda(T) = \frac{\lambda(0)}{\sqrt{1-T/T_c}} \), and \( H_{c2}(T) = H_{c2}(0) \left| 1 - \frac{T}{T_c} \right| \). However, if GL equations are scaled to temperature dependent units as given above, that allows us to consider any temperature dependence of the parameters prior to the start of the simulation. A number of works in the past were dedicated to theoretically improved temperature dependence of \( \xi, \lambda, \) and \( \kappa \). Underlying effects for reported differences may be nonlocality, clean/dirty limit effects, strong coupling. GL parameter \( \kappa \) is temperature independent in GL theory, but for e.g. type-I superconductors Ginzburg himself suggested the correction \( \kappa(T) = \kappa(0)/(1+t^2) \) (the two-fluid model), Bardeen gave \( \kappa(T) = \kappa(0)/\sqrt{1+t^2} \), while Gorkov found \( \kappa(T) = \kappa(0)(1-0.24t^2+0.04t^4) \), where \( t = T/T_c \). Although these formulae go beyond GL theory, we emphasize here that they can be implicitly included in the calculation, with aim to improve the overall validity of the theory.

It is also worth mentioning that simulations can account for the exact experimental procedure with respect to cooling. For the zero-field cooled regime the initial value of \( \psi \) should be taken \( \approx 1 \), and in the field-cooled regime opposite, i.e. \( \psi \approx 0 \) since superconductivity nucleates from the normal state.

Fourier transform and 2D approximation

It is well known that in superconductors the magnetic field penetrates only into a relatively small depth \( \lambda \) and that screening currents flow in the surface layer, decaying exponentially in the bulk beyond this length. However, one question arises: what happens when the superconductor is thinner than the London penetration depth? Tinkham argued, as is now generally accepted, that the currents in thin superconductors may be considered constant over the thickness. Consequently, they have no z-component, and the boundary condition (4) is automatically fulfilled at top and bottom surfaces of the sample. Prozorov et al. [14] confirmed Tinkham’s original assumption, considering in detail the current density (in)homogeneity throughout the thickness of superconducting films.
Therefore, for a superconductor with thickness $d < \lambda, \xi$ we assume the uniform distribution of current in the $z$ direction. From the first GL equation (2) then follows the same behavior for the order parameter, and the 3D problem is reduced to a 2-dimensional superconductor. However, an issue of solving the GL equation for the vector potential remains, and here we discuss the details.

We are actually solving three equations of shape $-\kappa^2 \Delta A = j$. From Fourier theory we know that

$$F(k) = \int_{-\infty}^{\infty} f(x) \exp(-2\pi i x k) dx,$$

(13)

$$f(x) = \int_{-\infty}^{\infty} F(k) \exp(2\pi i x k) dx.$$

(14)

We use this to solve the equation analytically in the $z$-direction. In the $x$- and $y$-direction, we solve numerically using FFT which is based on the following Fourier relationship

$$b_n = \frac{2}{N} \sum_{j=1}^{N-1} f_j \sin(j \pi \frac{n}{N}),$$

(15)

$$f_j = \sum_{n=1}^{N-1} b_n \sin(j \pi \frac{n}{N}),$$

(16)

where we have chosen the sine transform, to respect the boundary condition $A(r \to \infty) \to 0^2$.

Every component of the vector potential can therefore be represented as

$$A(x, y, z) = \sum_{i=1}^{N-1} \sum_{j=1}^{N-1} \int_{-\infty}^{\infty} dk a_{ij}(k) \exp(2\pi i z k) \sin(i \pi x \frac{N}{N}) \sin(j \pi y \frac{N}{N}),$$

(17)

where $x$ and $y$ are integer numbers between 1 and $N$ and $z$ can be any real number. We assume the sample with thickness $d$ to be centered at $z = 0$. The Laplacian of $A$ can be obtained analytically as:

$$\Delta A(x, y, z) = \sum_{i=1}^{N-1} \sum_{j=1}^{N-1} \int_{-\infty}^{\infty} dk (- (2\pi k)^2 - q^2) a_{ij}(k) \exp(2\pi i z k) \sin(i \pi x \frac{N}{N}) \sin(j \pi y \frac{N}{N}),$$

(18)

where we introduced $q^2 \equiv (i \pi/L_x)^2 + (j \pi/L_y)^2$. $L_{x,y}$ is the size of the simulation region in the $x$- and $y$-direction respectively.

Now we introduce $j(x, y)$ as the current uniform over the sample thickness

$$j(x, y, z) = j(x, y) \Pi(z, -d/2, d/2),$$

where $\Pi$ represents the step-like function which is 1 inside the interval $[-d/2, d/2]$ and 0 outside. The Fourier transform of $\Pi$ yields:

$$\Pi(k) = d \sin(\pi kd) / \pi kd.$$

Using sine transform, we can express the current as:

$$j(x, y) = \sum_{i=1}^{N-1} \sum_{j=1}^{N-1} b_{ij} \sin(i \pi x / N) \sin(j \pi y / N),$$

with coefficients:

$$b_{ij} = \frac{4}{N^2} \sum_{x=1}^{N-1} \sum_{y=1}^{N-1} j(x, y) \sin(i \pi x / N) \sin(j \pi y / N).$$

Substituting this into initial GL equation we get:

$$\sum_{i=1}^{N-1} \sum_{j=1}^{N-1} \sin(i \pi x / N) \sin(j \pi y / N) \int_{-\infty}^{\infty} dk \exp(2\pi i z k) \left( \kappa^2 [(2\pi k)^2 + q^2] a_{ij}(k) - b_{ij} d \sin(\pi kd) \right) = 0,$$

(19)

which can only be true if the terms in the brackets equal zero, i.e. when

$$\kappa^2 / d \frac{a_{ij}(k)}{(2\pi k)^2 + q^2} = \frac{b_{ij} \sin(\pi kd) / \pi kd}{(2\pi k)^2 + q^2}.$$

We now revert to the definition of $A$ in terms of its Fourier transform, and obtain:

$$\frac{\kappa^2}{d} A(x, y, z) = \sum_{i=1}^{N-1} \sin(i \pi x / N) \sum_{j=1}^{N-1} \sin(j \pi y / N) b_{ij} \int_{-\infty}^{\infty} dk \exp(2\pi i z k) \frac{1}{(2\pi k)^2 + q^2} \sin(\pi kd) / \pi kd.$$

(20)

The last term can be integrated analytically to get:

$$\frac{1}{dq^2} (1 - \cosh(qz) \exp(-dq/2)) \text{, if } z < d/2,$$

$$\frac{1}{dq^2} (\sinh(dq/2) \exp(-qz)) \text{, if } z > d/2.$$

We insert $z = 0$ directly in above equation, and obtain $\frac{1}{dq^2} (1 - \exp(-dq/2))$. 

\[ \]
Recapitulating, we can express $A(x, y, z = 0)$ in its Fourier components:

$$A(x, y, 0) = \sum_{i=1}^{N-1} \sin(i\pi x/N) \sum_{j=1}^{N-1} \sin(j\pi y/N)a_{ij},$$

with as coefficients:

$$a_{ij} = \frac{b_{ij} 1 - \exp(-dq/2)}{\kappa^2 q^2}.$$

Note that the common definition for effective GL parameter for thin superconductors $\kappa_{eff} = \kappa^2/d$ is therefore just a limiting case obtained for extremely thin samples ($j(x, y, z) = \delta(z) j(x, y)$).

Alternatively, one can calculate the mean vector potential (averaged in $z$-direction) inside the sample, instead of the values in $z = 0$ plane only. In that case, the Fourier coefficients become:

$$<a_{ij}>_z = \frac{1}{d} \frac{b_{ij}}{\kappa^2 q^2} \left( d - 2 \frac{\sinh(dq/2)}{q} \right) \exp(-dij/2).$$

The anisotropy

Modern fabrication methods enable experiments on various hybrid structures. Among others, one can think of complex 3D superconductor-metal hybrids, as well as samples made of different superconducting materials. In addition, materials such as high-$T_c$ superconductors are mostly layered, and exhibit clear anisotropy in different directions. In what follows, we show how those are incorporated in our GL formalism.

To begin with, we consider a superconductor-metal hybrid. As already pointed out by deGennes, the leakage of Cooper-pairs from the superconductor into the metal can be modeled through the additional equation describing the Josephson current as

$$\vec{n} \cdot (-i\hbar \nabla - \frac{2e^*}{c} \vec{A}) \psi |_{interface} = \frac{i}{b} \psi,$$

where quantity $b$ is positive and measures the distance outside the boundary (in the normal metal) where the order parameter becomes zero if the slope at the interface is maintained. As a consequence, the discretized first GL equation (10) must be modified at the boundary of the superconductor, and the terms $\psi_j/\alpha^2_n$ perpendicular to the interface get a prefactor $(1 - b)$.

In the case of a superconductor-superconductor hybrid, the situation is far more complex. The simplest scenario is that only $T_c$ is different between two materials, in which case the only parameter $\alpha$ varies in the sample. This is put in GL equations directly, and generates no extra terms in the discretization. Note that the crossing currents are also calculated directly, and no special boundary condition (such as Eq. (23)) is needed. In the case of varied mean free path, both $\alpha$ and $\beta$ change (proportional to $l$ and $l^2$ respectively), but this still does not generate additional terms in GL equations and can be put in the calculations directly. However, to consider mass anisotropy in the sample, one must go back to the very derivation of GL equations to establish that an additional term $\nabla_{int}^{-1} (\vec{A} - \vec{A}^*) \psi$ appears on the right side of Eq. (2). This term is then discretized using Eq. (12) and added to Eq. (10) in the numerical procedure.

Note that for real layered samples (such as high-$T_c$ ones) the coupling between the layers must also be introduced into GL equations. This is the known Lawrence-Doniach extension to the GL model, where Josephson coupling is active between the superconducting layers separated by an insulator of thickness $d_i$. As a result, at planes $z = \pm d_i/2$ a term $[\psi_{\pm d_i/2}^* \psi_{\pm d_i/2} \exp(\pm iA^z_{int})]/d_i$ is added to the first GL equation (here $A^z_{int} = \int_{-d_i/2}^{d_i/2} A_z dz$). The second GL equation remains the same, but an additional equation describing the Josephson current enters the calculation at all S-I boundaries as

$$j_z = \frac{i}{2d_i} \left[ \psi_{d_i/2}^* e^{-iA^z_{int}} \psi_{-d_i/2} - \psi_{d_i/2}^* e^{iA^z_{int}} \psi_{-d_i/2} \right].$$

Two-band superconductivity

Multi-band superconductivity has stirred great interest in the scientific community following the discovery and further studies of MgB$_2$ [15], having the highest critical temperature for a non-copper-oxide and non-fullerene superconductor. This material and some others such as boro-carbides can be described by two superconducting order parameters (hence the name ‘two-band’ or ‘two-gap’ superconductor). However the real boom in two- and multi-band superconductivity followed the last year’s discovery of iron pnictides [16]. The concentration of different dopants and applying of external pressure can tune the electronic, magnetic and structural properties of these materials. Provided that their
critical temperature is increased above liquid air, the impact of these materials on technology is already seen as a ‘new iron age’.

In cases when microscopic structure of the material is not relevant, the Ginzburg-Landau theory can describe two-gap superconductors. The first GL equation, for each of the two order parameters now reads:

\[
(-i\nabla - \vec{A})^2\psi_1 - (\chi_1 - |\psi_1|^2)\psi_1 - \frac{\gamma}{\delta}\psi_2 \\
- \frac{n}{\delta} \left(-i\nabla - \vec{A} \right)^2 \psi_2 = 0 \quad (25)
\]

\[
\frac{1}{\alpha}(-i\nabla - \vec{A})^2\psi_2 - (\chi_2 - |\psi_2|^2)\psi_2 - \frac{\gamma\delta}{m\alpha}\psi_1 \\
- \frac{n\delta}{m\alpha} \left(-i\nabla - \vec{A} \right)^2 \psi_1 = 0, \quad (26)
\]

where \(\chi_i = 1 - T/T_{ci} \) (\(T_{ci}\) being the critical temperature of gap \(i\)). \(\alpha = (\xi_{10}/\xi_{20})^2\) and \(\delta = \psi_{10}/\psi_{20} = \sqrt{\frac{\xi_{10}\xi_{20}}{\xi_{100}\xi_{200}}}\), all measured at \(T = 0\) and in absence of magnetic field and coupling. \(\gamma\) and \(\eta\) are the coupling constants representing Josephson and drag effect respectively. \(m = m_1/m_2\) is the ratio of the effective masses in two gaps. Lengths are expressed in \(\xi_{10}\), and the order parameters in \(\psi_{10}\).

The second GL equation is a single equation, with contribution from both condensates. We write it in the following form using the relation \(\frac{\kappa_1^2}{\kappa_2} = \frac{m}{\sigma_{10}}\):

\[
\begin{align*}
-\Delta \vec{A} &= 1 \kappa_1 R \left[ \psi_1^* \left(-i\nabla - \vec{A} \right) \psi_1 \right] \\
&+ \frac{\alpha}{\kappa_2^2} R \left[ \psi_2^* \left(-i\nabla - \vec{A} \right) \psi_2 \right] \\
&+ \eta \sqrt{\frac{\alpha}{m}} \kappa_1 \kappa_2 R \left[ \psi_1^* \left(-i\nabla - \vec{A} \right) \psi_2 \right] \\
&+ \eta \sqrt{\frac{\alpha}{m}} \kappa_1 \kappa_2 R \left[ \psi_2^* \left(-i\nabla - \vec{A} \right) \psi_1 \right], \quad (27)
\end{align*}
\]

where we singled out the GL parameters for both condensates, although this is not realistic. However, the latter equation makes directly visible that the magnetic behavior of the sample will depend not only on \(\kappa_1\) and \(\kappa_2\), but also on the ratio of coherence lengths in two condensates (parameter \(\alpha\), and this is of direct relevance to the recently observed type-1.5 superconductivity [17]. Note also that all terms in Eqs. (25-27) were already present in the same shape in the single-gap GL equations. Therefore, Eqs. (25-27) can be discretized and solved using the same numerical scheme as given in preceding sections.

In summary, we have explained in more detail the numerical approach that discretizes Ginzburg-Landau equations on a three-dimensional Cartesian grid. We further reviewed its applications on superconducting samples of different topologies, the hybrid systems, anisotropic samples, layered superconductors, and two-gap superconductors. For thin samples, we show the modification of the approach that allows fast solving for order parameter in the 2D plane, while the vector potential is generally solved in all three dimensions. We therefore hope to have presented a brief manual which will be of use for young researchers in the years to come.

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