Numerical Method for Zero-Temperature Vortex-Line Phase Diagrams

Welles A. M. Morgado and Gilson Carneiro *

Instituto de Física
Universidade Federal do Rio de Janeiro
C.P. 68528
21945-970, Rio de Janeiro-RJ
Brazil

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A numerical method to calculate equilibrium vortex-line configurations in bulk anisotropic type-II superconductors, at zero temperature, placed in an external magnetic field is introduced and applied to two physical problems. The method is designed to search for the minimum of the Gibbs free-energy in the London approximation and assumes only that the vortex lines are straight and arranged in a periodic lattice. Based on these assumptions a simulated annealing algorithm is developed to find the vortex-line-lattice unit cell shape, and vortex-line positions within it. This algorithm is made fast and accurate by the use of a rapidly converging series to calculate the lattice sums entering the vortex-vortex interaction energy. The method’s accuracy is illustrated by calculating the magnetic induction versus applied field curve for an isotropic superconductor. The method is applied to a superconductor with a square lattice of columnar defects to study selected regions of the zero-temperature-phase diagram where vortex-line-lattices commensurate with the columnar defect lattice exist.

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I. INTRODUCTION

A first step for understanding the behavior of type-II superconducting systems is to determine the equilibrium vortex configurations that occur at temperature zero, or the zero-temperature phase diagram. Although this problem has been under study for many years [1], there are many systems, such as artificial structures, constrained geometries and anisotropic superconductors, for which some questions remain open.

The situation of greater interest is that of a superconductor subjected to an external magnetic field \( H \). The theoretical problem of calculating the zero-temperature phase diagram is then to find the vortex configuration that minimizes the Gibbs free-energy for a given \( H \). The analytical method to solve this problem determines, instead, the vortex configurations that minimize the energy for a given magnetic induction, \( B \), and then calculates \( H \) from the derivatives of the energy with respect to \( B \). Analytical solutions are difficult to obtain and are known only for a few situations. Numerical methods to solve this problem have been proposed. These attempt to find the zero-temperature phase diagram of a large number of vortices by minimizing the energy, if \( B \) is kept constant, or the Gibbs free-energy, if \( H \) is kept constant [2]. These methods are severely limited by finite-size effects.

In this paper we introduce a numerical method to calculate configurations of straight vortex lines that minimize the Gibbs free-energy of bulk superconductors in the London approximation for a given \( H \). The essential ingredients of our methods are two. First, we assume that the vortex lines are straight and restrict the search for the minimum free-energy configurations to periodic vortex-line-lattices (VLL) with a given number of vortex lines per unit cell. This restriction greatly reduces the number of parameters that we have to vary to find the minimum. Second, we use a rapidly converging series to calculate the lattice sums entering the vortex-vortex interaction energy in the London approximation [4]. These ingredients allow us to create a simulated annealing algorithm, using Monte Carlo techniques, that is fast and, as a consequence, highly accurate. A closely related method has been used in Ref. [5] to calculate the zero-temperature phase diagram for films under parallel fields.

To illustrate the accuracy of the method we apply it to the well known problem of a bulk superconductor under a field \( H \) to obtain the \( B \times H \) curve and to compare it with known results at high and low fields [6]. We also apply the method to find some equilibrium vortex-line configurations in bulk superconductors and in films with a square lattice of columnar defects. This system is of experimental interest because there are several studies of vortices in films with a lattice of columnar defects created by lithographic techniques or by bombardment with an electron beam [7-8].

This paper is organized as follows. In Sec. [1] we discuss the details of the theoretical model, numerical method and simulated annealing algorithm. In Sec. [II] we report

*Corresponding author. Fax: 55 21 290 9020. e-mail: gmc@if.ufrj.br
the results of the above mentioned applications. Finally in Sec. IV we state our conclusions.

II. THEORETICAL MODEL AND NUMERICAL METHOD

We consider a bulk uniaxially anisotropic superconductor with a lattice of columnar defects (CD). We assume that both the vortex lines and the CD are straight and parallel to the c-axis, and that the vortex lines form a periodic VLL. Our problem is then to determine, for a given external field parallel to the c-direction, $H$, the VLL primitive unit cell, the number of vortex lines and their positions within this cell, that give the absolute minimum of the Gibbs free energy per volume

$$G = E_{vv} + E_{v-cd} - \frac{1}{4\pi} B(H - H_{c1}) , \tag{1}$$

where $E_{vv}$ is the vortex line-vortex line interaction energy, $E_{v-cd}$ is the vortex-CD-lattice interaction energy, $B$ is the magnetic induction, $H_{c1} = 4\pi\epsilon/\phi_0$ is the lower critical field, and $\epsilon = (\phi_0/16\pi^2\lambda_{cd}^2)\ln(\lambda_{ab}/\xi)$ is the vortex line self-energy ($\lambda_{ab}$ = penetration depth for currents parallel to the ab-plane, $\xi$ = vortex core radius).

We first solve the simpler problem of finding the VLL with a fixed number of vortex lines per unit cell, $n_v$, that minimizes $G$. To find which one of these gives the absolute minimum of $G$ we have to compare the free energies of the VLL obtained for the same $H$ and different $n_v$, if these are distinct.

Assuming that the VLL unit cell is defined by the vectors $\mathbf{L}_1$ and $\mathbf{L}_2$, as shown in Fig. 1 or by the corresponding reciprocal lattice vectors $\mathbf{G}$, the London approximation expression for $E_{vv}$ is

$$E_{vv} = \frac{\phi_0^2}{8\pi} \left[ \sum_{\alpha, \beta=1}^{n_v} \frac{1}{A_c} \sum_{\mathbf{G}} e^{i\mathbf{G} \cdot (\mathbf{x}_\alpha - \mathbf{x}_\beta)} \frac{1}{1 + \lambda_{cd}^2 G^2} - n_v \int \frac{d^2 k}{(2\pi)^2} \frac{1}{1 + \lambda_{ab}^2 k^2} \right] , \tag{2}$$

where $A_c$ is the unit cell area and $\mathbf{x}_\alpha$ ($\alpha = 1, ..., n_v$) denotes the vortex positions within the unit cell. For the VLL shown in Fig. 1 $B = n_v\phi_0/A_c$ and $A_c = L_1L_2\sin \phi$.

The vortex-line CD-lattice interaction energy is assumed to be the sum of the single vortex-single CD interaction energies, namely

$$E_{v-cd} = \frac{1}{NA_c} \sum_{j=1}^{N} \sum_{\alpha=1}^{n_v} U_{v-cd}(\mathbf{R}_j + \mathbf{x}_\alpha - \mathbf{R}_d) , \tag{3}$$

where $N$ is the number of vortex-lattice unit cells, $\mathbf{R}_j$ denotes the cell positions, $\mathbf{R}_d$ denotes the CD positions.

$U_{v-cd}$ is the single vortex- single CD interaction energy per unit length. The validity of Eq. (3) requires that the CD radius $R$ be such that $R \sim 2\xi$, so that only a single vortex line can be trapped by the CD, and that the vortex lines mean separation is large compared to $\xi$.

We use for $U_{v-cd}$ an approximation based on the London theory results derived in Ref. 4, namely

$$U_{v-cd}(r) = \epsilon \ln \left[ 1 - \frac{R^2}{r^2} \right] \quad (r > 2R) \tag{4}$$

$$U_{v-cd}(r) = \epsilon \left( 2 - \frac{r}{2R} \right) \ln \frac{3}{4} \quad (r \leq 2R) . \tag{5}$$

This expression interpolates smoothly between the large $r$ behavior and the value of the energy per unit length of a vortex line pinned by a CD $\sim \epsilon \ln(\sqrt{2}\xi/R)$, for $R \sim \sqrt{2}\xi$.

In order to study both bulk samples and films of thickness $D < \lambda_{ab}$ in the above described framework, we use in the expression for $E_{vv}$, Eq. (2), instead of $\lambda_{ab}$ an effective penetration depth $\Lambda \sim \lambda_{ab}/D$. This mimics the dominant logarithmic vortex-vortex interactions at distances short compared to the film screening length. The vortex-CD interaction is assumed to be the same for bulk and films.

To numerically minimize $G$, Eq. (1), it is necessary to evaluate $E_{vv}$, Eq. (2). Because the lattice sum in this expression converges very slowly, a numerical method based on it requires considerable amount of computer time. Doria showed that the lattice sum in Eq. (2) can be transformed into a series that converges much faster. We use this series in our calculation to generate an efficient numerical algorithm.

Our minimization procedure, based on standard simulated annealing and Monte Carlo techniques, is as follows. For a given $H$ and $n_v$, we start with a chosen unit cell shape and vortex lines located within it. By moving the vortex lines, one at a time, and deforming the unit cell continuously we generate, using a Metropolis algorithm, the equilibrium configurations of the cell shapes and vortex lines positions within it, for a given fictitious temperature $T$. The changes in $G$ caused by vortex line motion or by unit cell deformation are calculated using Doria’s fast convergent series for $E_{vv}$, and a direct summation over a large CD-lattice for $E_{v-cd}$. The VLL that minimizes $G$ is identified with the configuration at very low $T$. In order to reduce trapping in metastable states, $T$ is cycled appropriately.

The VLL found by the above described method can be either commensurate or incommensurate with the CD-lattice. Only the commensurate ones correspond to true minima of the Gibbs free-energy, since we restrict our search for the $G$ minima to periodic vortex-line arrangements. The incommensurate VLL, being periodic, feel only the space average of the vortex-CD-lattice potential, that is, a constant. Consequently, these are triangular VLL that minimize $G$, Eq. (1), in the absence of the vortex-CD- lattice interaction. As discussed in
detail in Sec. III B we expect that in situations where vortex-vortex interactions are strong, such as the ones considered here, our method is capable of predicting not only the commensurate phases, but also of giving reasonable estimates for the range of \( H \) values over which they minimize \( G \).

III. APPLICATIONS

In this section we apply the method described above to two physical problems.

A. Defect-free superconductor

To illustrate the accuracy of our method, we first apply it to the well known problem of vortex lines in a defect-free superconductor subjected to an external magnetic field \( H \) pointing in the c-direction. In this case \( G \) is minimized by a triangular VLL with a single vortex line in the primitive unit cell. We minimize \( G \) for several \( H \) assuming \( n_v = 1 \) and \( n_e = 2 \). We find the triangular lattice in all cases considered. For a given \( H \), we compare the minima obtained for \( n_v = 1 \) and \( n_v = 2 \). We find for \( n_v = 2 \) a unit cell that has twice the area as that for \( n_v = 1 \) and a value of \( G \) that differs from that for \( n_v = 1 \) by less than 3 parts in 10\(^6\). We also find that \( B_c \), calculated by our method, is very accurate when compared with the known analytic expressions for \( H \sim H_{\phi} \) and for \( H_{\phi} \ll H \ll H_{c2} \). This is illustrated in Fig. 3 for the \( M \times H \) curve, instead of the \( B \times H \) because \( B \sim H \). The errors seen in this figure indicate that our \( B \) values differ from the theoretical ones by less than 1%.

B. Regular array of columnar defects

Now we consider a superconductor with a CD-lattice. We assume that the CD radius is \( R = 2\xi = 0.02\lambda_{ab} \) and that the CD-lattice is square and commensurate with the CD-lattice, with one vortex-line pinned at each CD. We find that for both bulk and films with \( n_v = 1 \) the matching phase minimizes \( G \) in the range of \( H \) values \( H_{\phi}^c < H < H_{\phi}^r \). We obtain for bulk \( H_{\phi}^c = 1.01B_\phi \), \( H_{\phi}^r = 1.10B_\phi \), and for films \( H_{\phi}^c = H_{\phi}^r = 1.00B_\phi \). When \( H \) is just outside this range we find that a VLL is commensurate with the CD-lattice minimizes \( G \). The \( H \)-range for films is smaller than that for bulk due to the value of \( \Lambda = 5\lambda_{ab} \).

We recall that by our method \( H_{\phi}^c \) and \( H_{\phi}^r \) are the boundaries in the \( B \times H \) phase diagram where the matching state becomes unstable with respect to an incommensurate triangular VLL. We may ask what is the relationship between these boundaries and true ones obtained if \( G \) were minimized without the restrictions imposed by our method. To answer this question it is necessary to guess the state to which the matching phase would become unstable to at these boundaries. One possibility is that the matching state becomes unstable with respect to the state obtained from it by the addition of vacancies or interstitials. Another possibility is that at these boundaries a commensurate-incommensurate (CI) transition takes place. We believe that the former is possible only if the vortex-CD interaction is stronger than vortex-vortex interactions, which is not the case here. In our calculation the parameters are such that these two interactions are of comparable strength so, we believe, that the true boundaries here correspond to a CI transition. It is known that for strong vortex-vortex interactions, and not too close to the CI transition point, the incommensurate state differs from the triangular lattice by small incommensurate elastic distortions. Thus, we believe that our method makes a reasonable approximation for the incommensurate state (except close to the CI transition), and that the estimates obtained from it for the matching state phase boundaries are close to the true ones.

We also apply our method with \( n_v = 2 \) a value of \( H \) in the range \( H_{\phi}^c < H < H_{\phi}^r \). We find that the matching state with a rectangular unit cell twice as large as that for \( n_v = 1 \) minimizes \( G \) and that the \( G \)-value differs from that for \( n_v = 1 \) by less than 1 part in 10\(^4\).

Next we study VLL commensurate with the CD-lattice for \( B < B_\phi \). These can be characterized as follows. We assume that the CD-lattice primitive unit cell is a square of side \( a_{cd} \) with unit vectors \( e_x \) and \( e_y \) oriented along the sides. We expect that for these VLL all vortex lines are pinned by the CD. Thus, the VLL primitive unit cell vectors, \( a_1 \) and \( a_2 \) can be written as

\[
a_i = a_{cd}(n_{1x}e_x + n_{1y}e_y) \quad (i = i, 2).
\]

If there are \( n_v \) vortices in the unit cell, the magnetic induction in this state is

\[
B_c = B_\phi \left| \frac{n_v}{n_{1x}n_{2y} - n_{1y}n_{2x}} \right|,
\]

where \( n_v \) is restricted by \( n_v < \left| n_{1x}n_{2y} - n_{1y}n_{2x} \right| \). Thus, when \( B/B_\phi \) is rational, there are many non-equivalent VLL satisfying the above stated conditions. We apply our numerical method to determine which one of these minimize \( G \), and to estimate the range of \( H \) values over which this minimum is stable.

We study \( B = B_\phi/5, B_\phi/4, B_\phi/3, B_\phi/2, 2B_\phi/3 \) with \( n_v = 1 \) and \( B = 2B_\phi/5 \) with \( n_v = 2 \). We find that for films the commensurate VLL shown in Fig. 3 minimize \( G \) with \( H = B \). The \( H \) range where these minima are stable is around \( H = B \) for which these VLL minimize \( G \) is less than \( 10^{-3}B_\phi \). For bulk we find that for \( B_\phi/4 \) and \( B_\phi/2 \) the same VLL minimize \( G \) for \( H = 0.330B_\phi \).
and \( H = 0.528B_{\phi} \), respectively. The \( H \)-range was not investigated in detail in this case.

Our results for \( B = B_{\phi}/4 \) and \( B = B_{\phi}/2 \) agree with recent Lorentz microscopy experiments reported in Ref[7].

IV. CONCLUSIONS

In conclusion then we develop a numerical method to calculate the zero-temperature phase diagram of a bulk superconductor in the presence of an external field \( H \) and show that it gives accurate results for the \( B \times H \) curve of an ideal superconductor and that it can make predictions about the zero-temperature phase diagram of the non-trivial problem of vortex lines in the presence of a CD-lattice. The method can be extended to study the zero-temperature phase diagram for anisotropic superconductors in tilted fields and to long cylinders of rectangular cross sections in axial fields. Work along these lines is under way and will be reported elsewhere.

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FIG. 1. Vortex-line-lattice unit cell with \( n_v = 3 \).
FIG. 2. Magnetization for a defect free superconductor versus $H$ compared to theoretical results for low $H$ (full curve) and intermediate $H$ (dashed curve).

FIG. 3. Commensurate vortex-line-lattices that minimize the Gibbs free-energy.