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Numerical simulation of vortex arrays in thin superconducting films

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Numerical simulations of the evolution of the order parameter and the vector potential in thin type-II superconducting films are reported. The theoretical framework is provided by the well-known time-dependent Ginzburg-Landau (TDGL) equations coupled with the Maxwell equations. The external field is applied parallel to the surfaces. Several maxima appear in the magnetization curve, a phenomenon that has been observed in experiments and up to now only explained using a London approach. It is proved that these maxima are indeed predicted by the full TDGL approach, and are *not* necessarily linked with structural changes in the vortex lattice. A mechanism for the appearance of magnetization maxima in finite samples is identified, based on the behavior of surface supercurrents.

The magnetization of a thin superconducting film as a function of the applied field parallel to its faces is considered. In the last few years this process has attracted attention,[1–3] mainly focused on the oscillations exhibited by the magnetization. Some models, based on a London-type approach, have been able to explain why magnetization peaks appear at certain fields.[1,2] Though the experiments were carried out in layered superconductors and in oriented YBaCuO films, the models make no use of the internal periodic structure of the sample and nevertheless arrive at satisfactory predictions. It is thus interesting to analyze this problem using a fully coupled Ginzburg-Landau approach, by numerically solving the time-dependent Ginzburg-Landau (TDGL) equations coupled with the Maxwell equations in a homogeneous, isotropic, type-II superconducting thin film. Numerical simulations using the same approach have already proved useful in the modeling of other superconductivity phenomena.[4–7]

Our results can be summarized as the following: (i) It is confirmed that the full TDGL approach predicts a series of maxima in the magnetization of a homogeneous type-II film with the applied field parallel to its faces. (ii)It is proved that these maxima are not necessarily linked with structural changes in the vortex lattice. (iii) A mechanism for the appearance of such maxima is identified, strongly linked with the behavior of surface supercurrents. This mechanism is independent of that proposed in Refs. 1 and 2.

Let us briefly describe the mathematical model and the numerical method. We use the time-dependent Ginzburg-Landau (TDGL) equations coupled with Maxwell equations, leading to the following mathematical problem for the order parameter ψ and the vector potential $\mathbf{A}$ (the scalar potential is eliminated through an appropriate choice of gauge):

$$\frac{\partial\psi}{\partial t}=-\frac{1}{\eta}[(-i\nabla-\mathbf{A})^2\psi+(1-T)(|\psi|^2-1)\psi]+\tilde{f}, \quad (1)$$

$$\frac{\partial\mathbf{A}}{\partial t}=(1-T)\mathrm{Re}[\psi^*(-i\nabla-\mathbf{A})\psi]-\kappa^2\nabla\times\nabla\times\mathbf{A}. \quad (2)$$

Lengths have been scaled in units of $\xi(0)$, time in units of $t_0=\pi\hbar/(96k_BT_c)$, $\mathbf{A}$ in units of $H_{c2}(0)\xi(0)$ and temperatures in units of T_c. It has been assumed that $\xi(T)=\xi(0)(1-T/T_c)^{-1/2}$, where T is the temperature and T_c the critical temperature, and that the Ginzburg-Landau parameter κ is independent of temperature. In (1), η is proportional to the ratio of characteristic times for ψ and $\mathbf{A}$. $\tilde{f}$ is a random force simulating thermal fluctuations, selected at each mesh point from a Gaussian distribution with zero mean and standard deviation $\sigma=\sqrt{(\pi E_0\Delta t/6)(T/T_c)}$ where Δt is the time step, as done in Ref. 6. Re stands for "real part of."

Equations (1) and (2) are complemented with initial conditions, together with the condition

$$(-i\nabla-\mathbf{A})\psi\Big|_n=0,$$

where n denotes the normal to the superconductor-vacuum interface; and boundary conditions for $\mathbf{A}$, namely that $B_z=\nabla\times\mathbf{A}|_z$ at the external surfaces must equal H_e, the applied field. The sample is assumed to be infinite in the z direction, and the problem is reduced to two dimensions neglecting all derivatives along z. The magnetization M_z is defined as (see, e.g., Ref. 8)

$$\frac{\int[B_z(x,y)-H_e]dx\,dy}{4\pi\int dx\,dy}.$$

The numerical method is the same as that used in Refs. 4–7. The order parameter is defined at the nodes of a rectangular mesh, while at the links of the mesh the *link variable* $U_\mu=\exp[-i\int A_\mu d\mu]$ is used, with $\mu=x$ or $\mu=y$ depending on the direction of the link.

The computational domain is a two-dimensional layer of thickness $d=12\xi(0)$ and length $L=80\xi(0)$, aligned with the x axis (see insert in Fig. 1). The rectangular domain $(-40\xi(0),40\xi(0))\times(-6\xi(0),6\xi(0))$ is divided into square cells with edge $h=0.5\xi(0)$, resulting in a 160×24 mesh. At the boundaries $y=\pm6\xi(0)$ the y component of the current density is set to zero. Periodic conditions are imposed at $x=\pm40\xi(0)$ to approximate an infinitely long film. The external field H_e is applied along the z direction. H_e is increased linearly with time from 0 to 1, that is $H_e(t)=\dot{H}_et$. $\dot{H}_e$ is given the value 1.333×10^{-5} in the dimensionless units

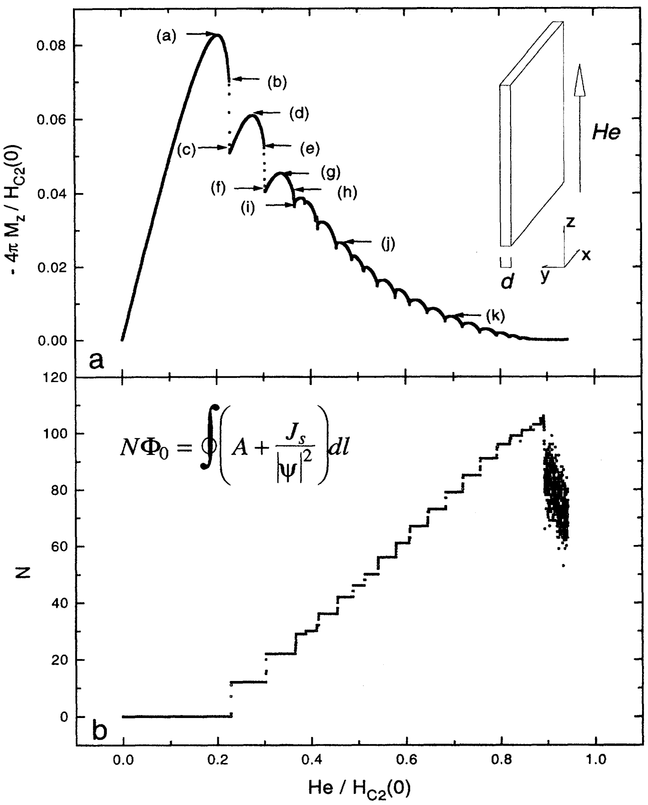

FIG. 1. (a) Magnetization curve obtained for a film of thickness $d=12\xi(0)$. Points (a) to (k) correspond to the contour plots of Fig. 2. (b) Number N of fluxoid quanta in the computational domain. The cloud of points for $H_e \sim 0.9$ and above indicates that the sample has become normal. In the definition of N (inset), J_s is the supercurrent density and the integration path coincides with the border of the computational domain.

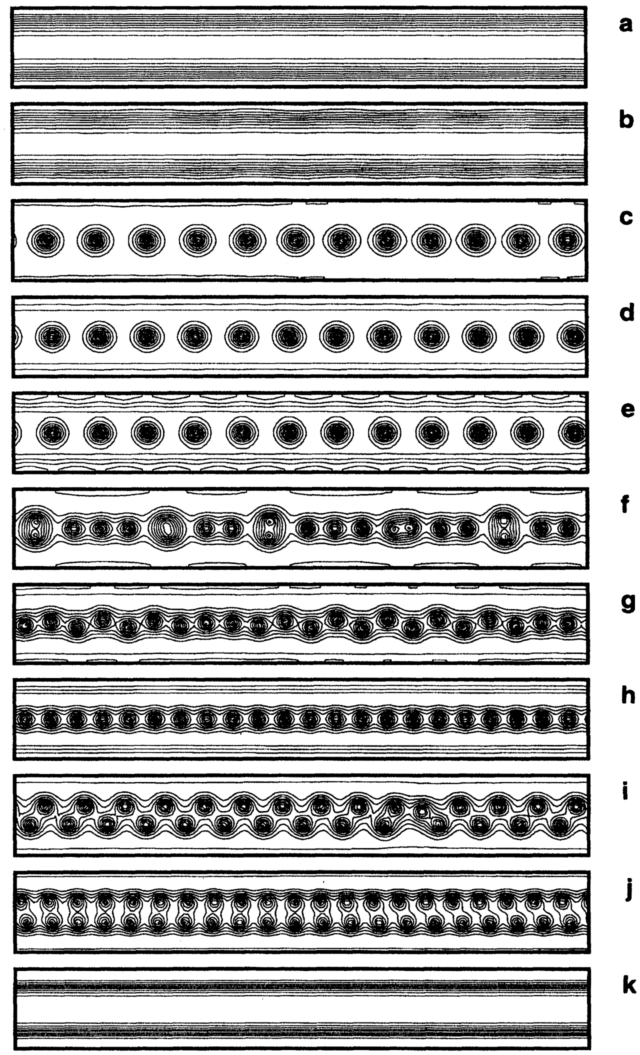

FIG. 2. Contour plots of the magnitude of the order parameter at several stages of the simulation. The corresponding applied fields are $H_e=0.2$ (a), 0.228 (b), 0.232 (c), 0.278 (d), 0.301 (e), 0.305 (f), 0.335 (g), 0.364 (h), 0.37 (i), 0.463 (j) and 0.703 (k). The contour interval is 0.1. The presence of vortices is evidenced by local minima of $|\psi|$. In (a) and (b) a Meissner state holds, so that $|\psi|$ is maximum along the central line. (k) corresponds to surface superconductivity, with $|\psi|$ taking its maximum value at the surfaces.

introduced above. This value corresponds to a slow variation of the applied field, compared to the characteristic times of the system. The time step is $\Delta t=0.015$, $T=0.5$, $\kappa=2$, and $\eta=1$. With these definitions $H_{c1}(T)=0.04$ and $H_{c2}(T)=0.5$ for the bulk material, while $H_{c3}(T)=0.85$ for a semi-infinite domain. Five million time steps are required to simulate the process. Variables are homogeneously initialized to a perfect Meissner state, $\psi(t=0)=1$, $\mathbf{A}(t=0)=0$ (for every point in the domain), implying $U_x(t=0)=U_y(t=0)=1$ and $B_z(t=0)=0$. E_0 is given the value 10^{-5}, as in Ref. 6.

The resulting magnetization curve exhibits a series of maxima, as shown in Fig. 1(a) [notice that the vertical axis in Fig. 1(a) represents $-4\pi M_z$, so the maxima correspond to points of maximal *expulsion* of the external field]. The first three maxima are at $H_e=0.205$, 0.278, 0.335. After each maximum, the curve turns downwards and remains smooth. After a significant decrease in $-4\pi M_z$ from the maximum value a sudden entrance of magnetic flux into the sample takes place, at $H_e=0.229$, 0.303, 0.365. These discontinuities in the magnetization correspond to vortices penetrating into the sample. The number N of vortices as a function of H_e is shown in Fig. 1(b).[9]

Contour lines of the magnitude of the order parameter $|\psi|$ are shown in Fig. 2, for $H_e=0.205$ (a), 0.228 (b), 0.232 (c), 0.278 (d), 0.301 (e), 0.305 (f), 0.335 (g), 0.364 (h), 0.370 (i), 0.463 (j), and 0.703 (k). The corresponding points in the magnetization curve are indicated in Fig. 1(a). For $H_e \leqslant 0.228$ no vortices have entered the sample. The order parameter is depressed at the boundary allowing the magnetic flux to penetrate a depth of order $\lambda(T)$. Twelve vortices enter at $H_e=0.229$, and arrange themselves in an equispaced linear chain. This regular structure can be observed in Figs. 2(d) and 2(e). In Fig. 2(c) ($H_e=0.232$), the vortices have not yet reached the steady configuration. The number N remains equal to 12 until a new vortex penetration event at $H_e=0.303$. The structure in Fig. 2(f) ($H_e=0.305$) is an unsteady configuration of the vortex lattice, a snapshot of the system in its way to equilibrium. This intermediate configuration exhibits the quasicoalescence of vortex pairs. A steady configuration of the 22 vortices at $H_e = 0.335$ is shown in Fig. 2(g). At this field, it is energetically convenient for the vortex lattice to "corrugate." This should not be interpreted as a transition to a two-dimensional structure . When the external field is further increased, it compresses the vortex lattice and, at $H_e = 0.364$ [Fig. 2(h)] a linear chain is again found. The possibility of two maxima in the magnetization curve sharing the same vortex structure is thus proved. After the third vortex-entrance event at $H_e = 0.365$, $N = 29$ is too large for a single chain, and two chains appear [Fig. 2(i)].[10] Though several small maxima can be observed in Fig. 1(a) for fields higher than 0.37, the number of vortex chains remains equal to two up to $H_{c2}(T) = 0.5$. These chains become more and more dense as new vortices enter the sample [see Fig. 2(j)], until the order parameter in the central region becomes essentially zero at $H_e \simeq H_{c2}(T)$ and superconductivity persists only at the surfaces [Fig. 2(k)].

We now propose an alternate mechanism for the phenomenon we have just described. Let us recall the magnetization curve of a superconducting ring, for the case when the thickness of the wire satisfies $a \ll \xi(T)$. If an external field H_e is applied perpendicular to the plane of the ring, a current of density J develops so as to keep fixed the number N of fluxoid quanta trapped. The magnetization of this system has been analyzed in Ref. 11. Denoting by P the perimeter, by A the planar area enclosed, by S the cross-sectional area of the ring, by ϕ_0 the fluxoid quantum, and by Λ the self-inductance, measuring J in units of $c\phi_0/[8\pi^2\kappa^2\xi(T)^3]$ and the magnetization $-4\pi M$ in units of $\phi_0 P/[2\pi A\xi(T)]$, we arrive at[11]

$$-4\pi M = \beta J(\beta, \phi_e), \tag{3}$$

where ϕ_e is a nondimensional measure of the applied flux, namely, $\phi_e = (AH_e/\phi_0 - N)/[P/(2\pi\xi(T)]$ and $\beta = S\Lambda/[2P\kappa^2\xi(T)^2]$. The magnetization is proportional to J, which takes the maximum value $J_c = 2/\sqrt{27}$, independent of β. In Fig. 3 we plot J vs ϕ_e for $\beta = 0$, 0.2, and 0.4. Though only qualitative, the similarity of these curves with each piece of the magnetization of Fig. 1(a) between two vortex penetration events is suggestive. It should be added that all expressions above are valid for a planar superconducting loop of *any* shape, provided the correct value of the self-inductance Λ is used.

As in the case of the loop just discussed, in a finite sample there is a portion of the applied flux that penetrates (in the form of vortices), and a surface current that balances the difference between the average internal field and the applied field. The number of vortices inside a finite sample plays the role of a mesoscopic quantum number (similar to N in the previous paragraph). If the sample contains N vortices, their contribution to the total flux is $N\phi_0$, a constant. The shape of the magnetization curve *between two vortex-penetration events* is thus governed by the surface current, which forms a loop around the vortex array. It is thus natural that, for a finite sample, the magnetization curve is divided into several smooth pieces, each piece corresponding to some number N of vortices inside the sample, and that each smooth piece resembles the magnetization curve of a loop (Fig. 3). The

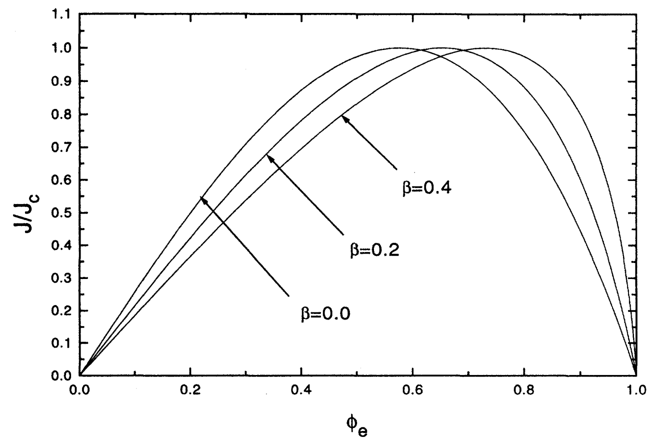

FIG. 3. Current density in a superconducting ring, as a function of the dimensionless measure of the applied flux ϕ_e (see text). Shown are typical plots of J/J_c (specifically, the curves correspond to $\beta = 0$,0.2, and 0.4). The magnetization of the ring is proportional to the current density.

previous argument applies as well to an *infinite* thin film, provided that its behavior can be shown to be equivalent to that of a *finite* film (of length L large enough) with periodic boundary conditions. The approximation of infinite domains by finite ones with periodicity assumptions is usual. Moreover, we have checked that our results are independent of the particular choice of L [whenever $L > 40\xi(0)$]. This implies that an infinite film can be approximated by a finite (periodic) one, which in turn is in the sense described above analogous to a superconducting loop.

In Fig. 1(a), the first maximum corresponds to the Meissner state ($N = 0$), the second to $N = 12$, the third to $N = 22$, and so on. The analogy with the loop also explains the magnetization maxima at fields $H_e > H_{c2}(T)$, for which no vortices exist and thus no explanation based on the vortex-lattice structure (such as that of Refs. 1and 2) applies. The argument suggests that oscillations in the magnetization can occur for *any* finite sample. The effects are of course only measurable when the surface-to-volume ratio is large enough.[12]

The analogy to the superconducting loop can be carried further to explain the *sudden* entrance of vortices at some specific values of H_e. As recently proved by Horane *et al.*,[13] the analytical solutions obtained in Ref. 11 become *unstable* at some value of the difference $AH_e - N\phi_0$. This instability takes the loop to a state in which $|\psi(x)|$ is *not* uniform around the loop. Moreover, as a result of this instability phenomenon there appear points where $|\psi(x)| = 0$. Consequently, the loop "opens" and additional flux quanta are allowed in, just as is observed in Fig. 1(b). By analogy, we propose that the distribution of currents surrounding the vortices becomes *unstable* at some value of $AH_e - N\phi_0$, and that this instability induces the observed spontaneous appearance of points at the sample surface with $|\psi(x)| = 0$ where new vortices nucleate. The number of vortices entering the sample at each instability event can in principle only be predicted by time-dependent simulations as the ones reported here.

The computations presented here are part of a series of computations which will be reported in a future paper. It has been checked that all results from which we draw conclusions are *generic*, and do not depend on purely numerical parameters such as h, Δt, L, E_0, or $\dot{H}$, within reasonable ranges of variation. Also, changes in κ, T, or η modify the results only quantitatively, but not in their essential features.

We believe the mechanism proposed to explain magnetization maxima, is an *alternate* mechanism to that proposed earlier by Guimpel *et al.*[1] The difference is that theirs neglects the fact that the vortices must overcome the surface barrier to enter the sample,[14] while ours is *based* on the *destabilization* of this barrier when the difference between the applied flux and the number of trapped flux quanta is large enough. This is the important part of our argument and leads to the prediction of oscillations in the magnetization curve. The approximation of the surface supercurrents by a *one-dimensional* loop is introduced for clarity but is not essential and only qualitatively valid. Which mechanism applies to a specific situation will depend on the role played by defects in the sample surface. Simulations accounting for defects will be carried out in the near future. We should remark that the relation (if any) between the internal vortex structures and the magnetization maxima can be experimentally determined by carrying out magnetization measurements together with neutron-scattering experiments.

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[9] The magnetization curve of Fig. 1(a) is *not* reversible. If the applied field is decreased from $H_{c2}(0)$ to 0 the magnetization is much weaker ($|M_z|<0.02$) and *positive*. Fig. 1(a) is thus the upper part of a hysteresis loop.

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