Algorithm for computer simulations of flux-lattice melting in type-II superconductors

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We derive an algorithm for simulating the dynamical behavior of stochastic diffusive systems. We use this algorithm to simulate flux-lattice melting in thin slabs of type-II superconductor whose thickness is comparable to the penetration depth. The simulations show that the flux lattice can melt at temperatures well below the superconducting transition temperature. In addition we show that the melting behavior of the flux-line lattice is very similar to that seen in both low-density Lennard-Jones and hard-disk systems.

The discovery of high-T_c superconductors has led to renewed interest in the thermal behavior of magnetic flux lattices. Before the discovery of this new class of type-II superconductor, melting of the Abrikosov vortex lattice had only been observed in quasi-two-dimensional samples.[1] However, recent experiments on bulk compounds of high-temperature superconducting material exhibit a melting transition in the vortex lattice.[2] In this note we describe an algorithm which can be used to simulate the dynamical behavior of magnetic vortices at finite temperatures in thin slabs of type-II superconductors. We use this algorithm to examine the phenomenon of flux lattice melting in a superconducting slab of thickness d, d being comparable to the penetration depth, λ. The external magnetic field is normal to the surface of the slab. The restriction to the case $d \approx \lambda$ reduces the computational effort considerably. In the two-dimensional (2D) limit, $d \ll \lambda$, the vortices interact via a logarithmic potential[3] which can only be handled using some form of many-body simulation whereas the 3D potential decays exponentially at large distance. In the 3D limit, $d \gg \lambda$, the flux line bending cannot be neglected and one is faced with the complex task of simulating a large number of interacting vortex lines. In the thin slab case considered here, we use the 3D potential for straight vortex lines.

It is well known that vortices obey a diffusive equation of motion[4]

$$\mathbf{F} - a\mathbf{v} \times \hat{\mathbf{z}} - \eta \mathbf{v} = 0 ,$$

where $\mathbf{F}$ is the total force on a vortex, a is the magnitude of the Magnus force, and η is the viscosity. Solving for the velocities, and adding a stochastic term, χ, to model the interaction of the vortices with a heat bath, we obtain[5]

$$\begin{pmatrix} v_x \\ v_y \end{pmatrix} = \frac{1}{a^2+\eta^2} \begin{pmatrix} \eta F_x - aF_y \\ aF_x + \eta F_y \end{pmatrix} + \begin{pmatrix} \chi_x \\ \chi_y \end{pmatrix} . \tag{1}$$

In the most general case, the force on the vortices can be written as

$$\mathbf{F} = \mathbf{F}_{vv} + \mathbf{F}_{vp} + \mathbf{F}_d , \tag{2}$$

where $\mathbf{F}_{vv}$ is the force on a vortex due to the surrounding vortices, $\mathbf{F}_{vp}$ models the interaction of the vortices with inhomogeneities in the superconductor, and $\mathbf{F}_d$ is the Lorentz force on the vortices due to an applied electric current through the superconductor. The total force on a vortex at $\mathbf{r}_i$ due to the interaction with all the other N_v vortices in the system is[6]

$$\mathbf{F}_{vv}(r_{ij}) = (\Phi_0^2/8\pi^2\lambda^3)(1-b)^{3/2} \sum_{\substack{j=1 \\ j\neq i}}^{N_v} (\mathbf{r}_{ij}/r_{ij})[K_1(r_{ij}\sqrt{(1-b)}/\lambda) - \sqrt{2}\kappa K_1(r_{ij}\kappa\sqrt{2(1-b)}/\lambda)] , \tag{3}$$

where K_1 is a modified Bessel function, Φ_0 is the flux quantum, $b = B/B_{c_2}$ is the reduced magnetic field, $\kappa = \lambda/\xi$, where ξ is the coherence length, and $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$. In this note we will assume that $\mathbf{F}_{vp}$ is negligible and that no external current is transported through the sample.

We assume the following empirical temperature dependence of the thermodynamic critical field and penetration depth;[7] $H_c(t) = H_c(0)(1-t^2)$ and $\lambda(t) = \lambda(0)/\sqrt{(1-t^4)}$, where $t = T/T_c$. We also assume that the upper critical field is given by the usual relation $H_{c_2} = \sqrt{2}\kappa H_c$. The reduced field then satisfies

$$b(t) = B/B_{c_2}(T) = b(0)(1+t^2)/(1-t^2) .$$

The stochastic term in Eq. (1) modeling the interaction with a heat bath needs to be calibrated in such a way that we reach the correct equilibrium distribution at long times. As in the usual case of a Langevin equation for particles with an inertial mass,[8] this is done using the Fokker-Planck equation associated with Eq. (1). Let

$$P(x,t\,|\,x_0,t_0) = P(x,t-t_0\,|\,x_0)$$

denote the probability that a vortex is found at position x at time t if it were at position x_0 at time t_0 [for notational simplicity we discuss the one-dimensional version of Eq. (1) with $a=0$]. P will obey the differential equation

$$\frac{\partial P}{\partial t} = \sum_{n=1}^{\infty} \frac{(-1)^n}{n!} \frac{\partial^n}{\partial x^n}[M_n P(x,t\,|\,x_0)] , \tag{4}$$

where

$$M_n = \frac{1}{\tau}\int \zeta^n P(x+\zeta,\tau\,|\,x)d\zeta .$$

We can make the connection between Eqs. (1) and (4) by replacing the M_n in Eq. (4) by the moments as calculated directly from Eq. (1) to $O(dt^2)$. In order to calculate these moments we assume that χ_i can be expressed as a Gaussian white-noise function

$$\langle \chi_i(t)\rangle = 0 ,$$
$$\langle \chi_i(t_1)\chi_k(t_2)\rangle = A\delta(t_1-t_2)\delta(i-k) , \quad (5)$$

where A is a constant. Calculating the moments from Eq. (1),

$$M_1 \equiv \frac{1}{\tau}\langle \delta x\rangle = \frac{1}{\eta}F, \quad M_2 \equiv \frac{1}{\tau}\langle (\delta x)^2\rangle = A , \quad (6)$$

and substituting them into Eq. (4) we obtain the following Fokker-Planck equation:

$$\frac{\partial P}{\partial t} = -\frac{\partial}{\partial x}\left[\frac{1}{\eta}FP(x,t\,|\,x_0)\right] + \frac{1}{2}\frac{\partial^2}{\partial x^2}[AP(x,t\,|\,x_0)] . \quad (7)$$

The value of A can be obtained by demanding that

$$P(x,\infty\,|\,x_0) \propto \exp[-(1/kT)U(x)] , \quad (8)$$

where $U(x)$ is the total potential energy of the vortices at $t=\infty$. Substituting Eq. (8) into Eq. (7) we finally obtain the result $A=2kT/\eta$.

Special care must be taken in deriving the discrete form of the Gaussian white-noise term in Eq. (1). We assume that the noise term acts with a constant average rate, $1/\tau$, on each particle.[9] The probability that a given vortex will have been acted on by the noise term during a time step of length Δ is $p \approx \Delta/\tau$ for $\Delta \ll \tau$. As we are using a discrete time variable we need to find a representation for the noise term which satisfies Eqs. (8) and (9) (with A replaced by $2kT/\eta$). It is also important that the measured physical quantities are independent of τ. The following prescription[9] for the noise term satisfies all the above requirements

$$\chi(t) = B\sum_j \delta(t-t^j)\gamma(t^j)\Theta(p-q^j) , \quad (9)$$

where j labels the time step, $\gamma(t^j)$ is a random number chosen from a Gaussian distribution of mean 0 and width 1, q^j is a random number uniformly distributed on [0,1], and $\Theta(x)$ is defined by

$$\Theta(x) = \begin{cases} 1, & \text{if } x>0; \\ 0 & \text{if } x<0 . \end{cases}$$

Substituting Eq. (9) into Eq. (5) gives us $B=(2\Delta kT/\eta p)^{1/2}$.

Combining all the results described above, and working in units of

length: $l_0(t)=\lambda(t)=l_0(0)/\sqrt{1-t^4}$,

energy/length: $\varepsilon_0(t)=\Phi_0^2/(8\pi^2\lambda^2)=\varepsilon_0(0)(1-t^4)$,

force/length: $f_0(t)=\Phi_0^2/(8\pi^2\lambda^3)=f_0(0)(1-t^4)^{3/2}$,

time: $\tau_0(t)=8\pi^2\lambda^4\sqrt{a^2+\eta^2}/\Phi_0^2=\tau_0(0)/(1-t^4)^2$, (10)

we get the following discretized equation of motion:

$$\frac{\mathbf{r}^{n+1}}{l_0(t)} = \frac{\mathbf{r}^n}{l_0(t)} + \begin{pmatrix} [1+(a/\eta)^2]^{-1/2} & -[1+(\eta/a)^2]^{-1/2} \\ [1+(\eta/a)^2]^{-1/2} & [1+(a/\eta)^2]^{-1/2}\end{pmatrix}\frac{1}{f_0(t)}\begin{pmatrix}F_x^n \\ F_y^n\end{pmatrix}\frac{\Delta}{\tau_0(t)} + \left[\frac{2kT_c}{d\varepsilon_0(t)}\frac{t}{[1+(a/\eta)^2]^{1/2}}\frac{\Delta}{\tau_0(t)}\frac{1}{p}\right]^{1/2}\begin{pmatrix}\gamma_x \\ \gamma_y\end{pmatrix}\Theta(p-q^j) , \quad (11)$$

where F_x and F_y are defined by Eq. (3).

The final stage in the derivation of the numerical integration algorithm is to decide on the sizes of Δ and τ. This can be done by ensuring that the moments calculated using Eq. (11) agree with those given in Eq. (6) [to $O(\Delta^2)$]. Two conditions have to be fulfilled;

$$\frac{\tau}{\tau_0(0)} \gg \frac{2kT_c}{d\varepsilon_0(0)}\left[\frac{f_0(0)}{\bar{f}}\right]^2 t ,$$

$$\frac{\Delta}{\tau_0(0)} \ll \frac{2kT_c}{d\varepsilon_0(0)}\left[\frac{f_0(0)}{\bar{f}}\right]^2 t ,$$

where $\bar{f}$ denotes the average net deterministic force on a vortex. In the program we explicitly calculate the second moment of the Fokker-Planck equation and check that it has the expected equilibrium value.

We have used the algorithm described above to model the melting transition for a system of 340 vortices with periodic boundary conditions in a model superconductor with the following set of parameters: $\kappa(0)=2$, $b(0)=0.1$, $a/\eta=0$, $2kT_c/d\varepsilon_0(0)=0.516$ cm$^{-1}\lambda^2T_c/d$, where $\lambda^2T_c/d=10^{-3}$ cm.

We investigated the melting behavior by measuring the self-diffusion coefficient and the angular susceptibility function, χ_6 for the vortices as a function of temperature. The diffusion coefficient was calculated from the graph of mean-squared displacement versus time. For large values of time this graph has a constant gradient, the gradient being a measure of the self-diffusion coefficient.[10] The function χ_6 is defined by

$$\chi_6 = \langle |\phi_6|^2\rangle - \langle |\phi_6|\rangle^2 ,$$

where

$$\phi_6 = \left\langle \left| \frac{1}{N_v}\sum_l \frac{1}{n_l}\sum_j e^{6i\theta_{lj}}\right|^2 \right\rangle ,$$

and where the sum on l is over all vortices, the sum j is

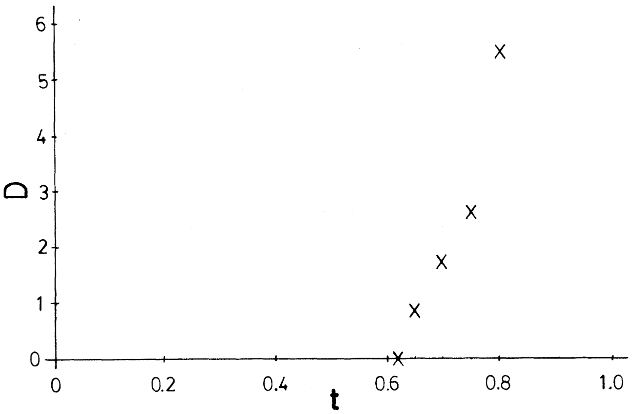

FIG. 1. The self-diffusion coefficient (in arbitrary units) as a function of reduced temperature for the model superconductor.

over nearest neighbors, n_l is the number of nearest neighbors of particle l, N_v is the number of vortices in the system, and θ_{lj} is the angle that the nearest-neighbor bond between vortices l and j makes with an arbitrary axis. Following the example of Strandburg, Zollweg, and Chester,[11] we have used this quantity to examine the system on different length scales. This was done by dividing the system of 340 particles into smaller subsystems and calculating the average value of χ_6 for each subsystem. At each temperature we typically ran 50 000 updating steps of the stochastic dynamics algorithm. We can use this function to determine whether the bond-angle order observed at melting can be explained by coexisting patches of solid and liquid. If this is the case, then the distribution of the χ_6 values for sufficiently small subsystems should be given by a sum of χ_6 in the solid near melting and the liquid near freezing.

The value of the self-diffusion coefficient (in arbitrary units) versus the temperature of the system is shown in Fig. 1. It can be seen from this figure that the vortex lattice melts at a temperature $t_m = T_m/T_c \approx 0.65$. Figure 2 shows the distribution of χ_6 for a variety of subsystem sizes for $t = 0.65$. The χ_6 distributions for the vortices are very similar to those observed in low-density Lennard-Jones and hard-disk systems. Figure 3 shows the trajectories of the vortices for the run at $t = 0.65$ for a run of 50 000 time steps. It can be seen from this figure that although large areas of the sample have melted there are still regions in which the vortices remain localized. This figure is consistent with the idea of the existence of an inhomogeneous two-phase coexistence region just above the melting temperature. As in Ref. 11, we are able to accurately model the χ_6 distributions functions in the intermediate regime as combinations of the distribution functions in the liquid and the solid. From these results we conclude that the topological melting behavior of the vortex lattice is analogous to that observed in low-density 2D Lennard-Jones and hard-disk systems. However, from these results it is impossible to say whether the melting transition is first order or Kosterlitz-Thouless-like.[12]

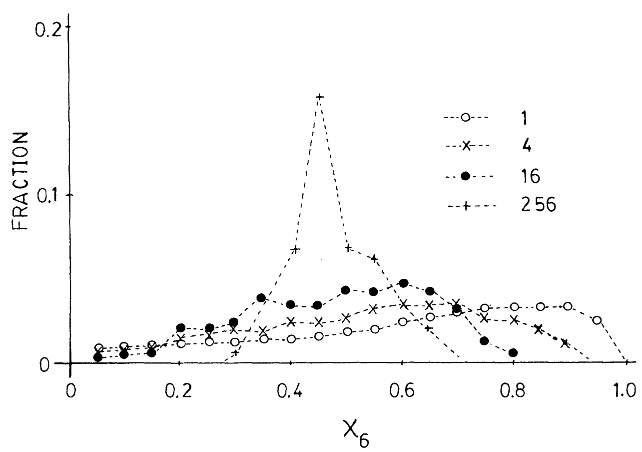

FIG. 2. Distribution of the bond-angle susceptibility, χ_6, for the vortex system at a temperature $t = 0.60$. Data are shown for subsystems containing 256, 16, 4, and 1 vortices.

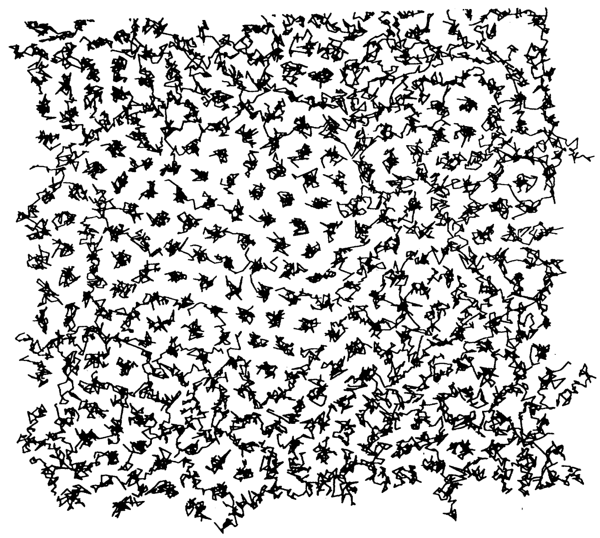

FIG. 3. A plot showing the trajectories of the vortices for a run of 50 000 updating steps at a temperature of $t = 0.65$.

In summary, we have developed an algorithm which can be used to study the dynamical behavior of diffusive stochastic systems. We have used this algorithm to examine flux lattice melting in a thin slab ($d \approx \lambda$) of model type-II superconductor in which the vortex-vortex interaction is described by the 3D vortex potential for straight flux lines. We see a melting transition in this system at a temperature well below the superconducting transition temperature. As long as the flux lines can be considered as rigid rods the melting temperature will scale approximately linearly with the thickness of the sample. By examining the bond-angle correlation functions we have shown that the topological melting behavior is very similar to that seen in Lennard-Jones or hard-disk systems.

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