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Extended Molecular Dynamics Methods for Vortex Dynamics in Nano-structured Superconductors

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Abstract

Using improved molecular dynamics simulation method, we study vortex dynamics in nano-scaled superconductors. Heat generations during vortex motion, heat transfer in superconductors, and entropy forces to vortices are incorporated. Also quasi-particle relaxations after vortex motion, and their attractive "retarded" forces to other vortices are incorporated using the condensation-energy field. We show the time development of formation of vortex channel flow in a superconducting Corbino-disk.

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Keywords: Vortex dynamics; molecular dynamics; heat transport; quati-particle realxation; Corbino-disk; finite element method

1. Introduction

For applications of superconductors, vortex dynamics is a key feature, because when vortices move, the zero resistivity of a superconductor is broken. In order to investigate the dynamics of vortices theoretically or by computer simulations, we use phenomenological time-dependent Ginzburg-Landau equations [1] or the molecular dynamics method. Especially, the molecular dynamics method is effective when we consider many vortices in superconductors [2], because we only consider classical equations of motion of the vortices. However, in this method, several features are missing, when we consider real superconducting systems. For example, when vortices move, heat generation occurs. If the vortex motion is uniform, this heat generation is also uniform. But when vortex motion is not uniform, such as in a corbino disk [3], non-uniform heat generation occurs and then non-uniform temperature distribution appears. A vortex has a transport-entropy [4,5], and then motion of the vortex is affected by this temperature distribution. In order to incorporate such effect, we must solve the heat transport equation with the molecular dynamics equation for vortices. Another feature is a retardation effect, which comes from quasi-particle recombination after fast movement of vortices [6,7]. After a vortex moves, the order parameter that was inside of the vortex core is restored to the uniform value, but it takes a time for recombining Cooper pairs. Then, if vortices move fast, the vortex motion is affected by a preceding vortex. In order to incorporate such retarded effect, we introduce a condensation energy field, which is proportional to the square of the absolute value of the order parameter. In Sec. 2, we explain our method, and in Sec. 3 we show our numerical results.

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2. Method

In usual molecular dynamics method, we ignore the inertia mass term because of dissipative dynamics of vortices and then we treat the overdamped equations of motions, where a damping term is large. We denote the position of i-th vortex $\boldsymbol{r}_i$. Forces on this vortex are, the vortex-vortex interaction force $\boldsymbol{f}_i^{vv}$, and the force of vortex interaction with the Meissner shielding current $\boldsymbol{f}_i^H$, the pinning force from the impurities $\boldsymbol{f}_{pi}^{imp}$, and a driving force from an external current is $\boldsymbol{f}_{di}$. Also thermal fluctuation force $\boldsymbol{f}_{fi}$ from the environment is incorporated and the equation of motion is based on the Langevin dynamics as follows,

$$\eta \frac{d\boldsymbol{r}_i}{dt} = \boldsymbol{f}_{di} + \boldsymbol{f}_i^{vv} + \boldsymbol{f}_{pi}^{imp} + \boldsymbol{f}_i^H + \boldsymbol{f}_{fi} \ , \tag{1}$$

where η is the viscosity. The driving, pinning and fluctuation forces are defined as,

$$\boldsymbol{f}_{di} = \frac{1}{c}\boldsymbol{j}(\boldsymbol{r}_i) \times \Phi_0 , \tag{2}$$

$$\boldsymbol{f}_i^{imp} = \sum_j^{imp} \frac{f_p}{r_p} \left| \boldsymbol{r}_i - \boldsymbol{r}^p{}_j \right| \Theta\left(\frac{r_p - \left| \boldsymbol{r}_i - \boldsymbol{r}^p{}_j \right|}{\lambda} \right) \hat{\boldsymbol{r}}_{ij} \ , \tag{3}$$

$$\left\langle \boldsymbol{f}_i^f(t_1) \cdot \boldsymbol{f}_j^f(t_2) \right\rangle = 2\eta k_B T \delta_{ij} \delta(t_1 - t_2) , \tag{4}$$

where $\boldsymbol{j}(\boldsymbol{r}_i)$ is an external current at the vortex position $\boldsymbol{r}_i$, $\boldsymbol{r}^p{}_j$ is the position of j-th impurity, r_p is the size of impurities, f_p is the strength of pinning force, λ is the penetration depth, and $\Theta(x)$ is a step function. Thermal fluctuation force depends on the temperature T. In Sec. 3, we show numerical simulation results for a superconducting corbino-disk with radius R, and in such geometry, the vortex-vortex interaction force and the force from shielding current are given as,

$$\boldsymbol{f}_i^{vv} = f_0 \sum_j \left(\frac{\hat{\boldsymbol{r}}_{ij}}{\frac{r_{ij}}{R}} - \frac{r_j^2}{R} \frac{\frac{r_j^2}{R^2}\boldsymbol{r}_i - \boldsymbol{r}_j}{\left| \frac{r_j^2}{R^2}\boldsymbol{r}_i - \boldsymbol{r}_j \right|^2} \right) , \tag{5}$$

$$\boldsymbol{f}_i^H = f_0 \left(\frac{1}{1-(r_i/R)^2} - \frac{\pi R^2 H}{\Phi_0} \right) \frac{\boldsymbol{r}_i}{R} \ , \tag{6}$$

where f_0 is the strength of vortex-vortex interaction. In previous our work [8], we use a vortex-vortex interaction in 3-dimensional superconductors. But in this work, we use a vortex-vortex interaction in 2-dimensional superconductors.

For the heat generation by the vortex motion, we must solve the heat transport equation and we use the finite element method (FEM),

$$\sum_j \left(a_{ij}\dot{T}_j + c_{ij}T_j \right) = Q_j \ , \tag{7}$$

where temperature is expanded as $T(x,y;t) = \sum_{e,k} T_k(t) N_k^e(x,y)$, using area coordinates $N_k^e(x,y)$. And $c_{ij} = \alpha I_{ij}^e + \lambda_h h\left(K_{ij}^{exx} + K_{ij}^{eyy} \right)$, $a_{ij} = chI_{ij}$ and $Q_i = \alpha T_a \sum_j I_{ij}^e + \sum_j h q_j I_{ij}^e$. Here c, λ_h and h are the specific heat, thermal conductivity, and he thickness of the superconductor, respectively. α and T_a are thermal conductance between the superconductor and substrate and temperature of the substrate, respectively. The heat generation by the vortex motion is given by,