Effects of geometrical symmetry on the vortex in mesoscopic superconductors

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Abstract. We first systematically study the multivortex states in mesoscopic superconductors via self-consistent Bogoliubov-de Gennes equations. Our work focuses on how the geometrical symmetry affects the penetration and arrangement of vortices in mesoscopic superconductors and find that the key parameter determining the entrance of the vortex is the current density at the hot spots on the edge of sample. Through determining the spatial distribution of hot spots, the geometrical symmetry of the superconducting sample influences the nucleation and entrance of vortices. Our results propose one possible experimental approach to control and manipulate the quantum states of mesoscopic superconductors with their topological geometries, and they can be easily generalized to the confined superfluids and Bose-Einstein condensates.

The advances in modern nanotechnology and the development of quantum computing have opened many new perspectives for research on mesoscopic superconductors \cite{1}. One fascinating aspect in mesoscopic superconductivity is the novel physics associated with vortices, which has been a subject of great experimental \cite{2-10} and theoretical \cite{11-13} interest in the past decades. In the mesoscopic superconductors, vortices are quantized and confined by the sample geometry, so they can exhibit many unique phenomena compared with conventional bulk superconductors. For example, when the sample is mesoscopic, the giant vortex can form, and there may exhibit the exotic paramagnetic Meissner effect \cite{12}. Further, it is shown that the symmetry of the sample geometry can dramatically affect the properties of the mesoscopic system \cite{9}. Recent experiment has also reported the symmetry-induced antivortices formation \cite{7}, which is a unique character of a mesoscopic superconductor.

Recently, many works \cite{14-21} based on Ginzburg-Landau (GL) theory \cite{22} devote to the study of vortex state and phase transition in superconductor sample. The studies \cite{14,15} point out that the vortex configuration is distinct for different regular geometries of mesoscopic sample. Moreover, the influence of surface defects on these samples are investigated and the results show that the defects can break the original symmetry of system \cite{16-18} and affect dramatically the vortex entry field \cite{19-21}. However, the question how the geometrical symmetry of sample can control the vortex state is hitherto not well solved quantitatively. On the other hand, the GL theory does not work well far below the critical temperature \(T_c\), especially when the quantum limit is realized in the region \(T/T_c \leq 1/(k_F\xi_0)\) with \(\xi_0 = \hbar v_F/\Delta_0\) the coherence length (\(\Delta_0\) the gap at \(T = 0\)) and \(k_F\) the Fermi wave number. Owing to the experimental developments and the study of the high-\(T_c\) superconductors (such as for YBCO, \(k_F\xi_0\) is estimated \cite{23,24} 1 ~ 4 and the quantum temperature \(T < 10\) K), this quantum region of interest is easy to reach, where the multivortex states are not studied systematically.

Prompted by these motivations, in this work, we explore the effect of symmetry on the vortex nucleation and entrance in the mesoscopic superconductor far below the critical temperature. We develop an effective numerical method to generally solve the Bogoliubov-de Gennes (BdG) equations \cite{25}, which is based on the finite element method (FEM) \cite{26,27}. Compared with the conventional GL theory, the BdG equations work well in wider temperature region, and can give the spectrum of excitations for spatially inhomogeneous superconductor self-consistently, supposed the few fundamental material parameters are given. Several groups have successfully used the BdG equations to study the single vortex line \cite{24,28-30}.

Here, we solve the BdG equations self-consistently, and obtain the vortex pattern and the current density
in mesoscopic superconductors with arbitrary and complicated geometries. We first calculate the magnetization and vortex configuration of the system and the results agree very well with the previous work, which confirms the physical scenarios about the vortex state from microscopic theory and meanwhile verifies the our new numerical method. Then we analyze the mechanism of effect of symmetry. Our results show that the current distribution and the penetration of vortices are determined by the symmetry of the sample geometry, and the entrance of the vortex happens only when the current density at the hot spots (i.e. the spots with maximum current density) reaches the depairing current density. These facts reveal unambiguously that the geometrical symmetry of the superconducting sample influences the nucleation and entrance of vortices, through determining the spatial distribution of hot spots. These results provide a practicable route to manipulate the quantum states of a mesoscopic superconductors in future applications.

We start with the BdG equations for the quasiparticle wave functions $u_n(r)$ and $v_n(r)$ in the presence of a magnetic field

$$
\frac{1}{2m} \left( \frac{\hbar}{i} \nabla - \frac{eA}{c} \right)^2 u_n(r) + \Delta(r) v_n(r) = E_n u_n(r),
$$

$$
\frac{1}{2m} \left( \frac{\hbar}{i} \nabla + \frac{eA}{c} \right)^2 v_n(r) + \Delta^*(r) u_n(r) = E_n v_n(r),
$$

where $E_n$ is the $n$th energy eigenvalue, $\Delta(r)$ the pair potential, $A(r)$ the vector potential and $\mu$ the chemical potential.

The pair potential $\Delta(r)$ is determined self-consistently by

$$
\Delta(r) = g \sum_{|E_n| \leq E_c} u_n(r) v_n^* (r) \left[ 1 - 2 f(E_n) \right],
$$

where $g$ is the interaction constant, $f(E)$ the Fermi distribution function and $E_c$ the cutoff energy which is related by the BCS relation via the transition temperature $T_c$ and the superconducting energy gap $\Delta_0$.

The vector potential $\mathbf{A}(r)$ is related to the current distribution $\mathbf{j}(r)$ by Maxwell’s equation

$$
\nabla \times \nabla \times \mathbf{A}(r) = \frac{4\pi}{c} \mathbf{j}(r),
$$

where the current distribution [25,29] is given by

$$
\mathbf{j}(r) = \frac{e\hbar}{2mi} \sum_n \left[ f(E_n) u_n^*(r) \left( \nabla - \frac{ie}{\hbar c} \mathbf{A}(r) \right) u_n(r) \right. $$

$$
\left. + (1 - f(E_n)) v_n^*(r) \left( \nabla - \frac{ie}{\hbar c} \mathbf{A}(r) \right) v_n(r) - h.c. \right].
$$

The chemical potential $\mu$ is determined by the particle number conservation imposed on this system [28]

$$
N = 2 \int \sum_n \left\{ f(E_n) |u_n(r)|^2 + (1 - 2f(E_n)) |v_n(r)|^2 \right\},
$$

where $N$ is the total number of particles.

The boundary conditions for the above equations are given by

$$
n \cdot \left( \frac{\hbar}{i} \nabla - \frac{eA}{c} \right) u_n = 0, \quad n \cdot \left( \frac{\hbar}{i} \nabla + \frac{eA}{c} \right) v_n = 0,
$$

where we consider two dimensional superconducting samples placed in the $(x,y)$ plane, which are immersed in an insulating medium in the presence of a perpendicular uniform magnetic field along $z$ direction. $\mathbf{n}$ is the normal vector of the boundary.

We numerically solve equations (1)—(6) self-consistently, based on finite elements method [26,27]. All input parameters used in the calculation are microscopic parameters which can in principle be obtained from band structure calculations [29]. These parameters consist of the cutoff energy $E_c$, the coupling constant $g$ and $k_F\xi_0$ [24], where $k_F(v_F)$ is the Fermi wave number (velocity) and $\xi_0 = hv_F/\Delta_0$ the coherence length.

In this paper, we consider the system at the temperature $T = 0.1T_c$, and choose $E_c = 5\xi_0$ and $k_F\xi_0 = 2$. To conveniently compare our results with the experiment, other parameters are chosen so as to make the Ginzburg-Landau parameter $\kappa$ to be a specified value, where $\kappa = 0.96\lambda_L(0)/\xi_0$ [25] and $\lambda_L(0)$ is the London penetration depth. Here without loss of generality, we choose a square superconductor with the length of a side $a = 5\xi_0$ and $\kappa = 20$. The sample is first cooled down into the superconducting state, and then we slowly increase the magnetic field and solve the BdG equations at each field, mimicking the zero field cooling measurements [23]. The global magnetization $M$ can be calculated as $M = 1/(2S) \int \mathbf{r} \times \mathbf{j} \, dxdy$, where $S$ is the sample area. In the frame of BdG theory, the free energy $\mathcal{F}$ of the system is given [31] by

$$
\mathcal{F} = 2 \sum_n E_n f(E_n) - 2 \sum_n E_n \int d^3r |v_n(r)|^2
$$

$$
- 2k_BT \sum_n \{ f(E_n) \ln f(E_n) + [1 - f(E_n)] \ln [1 - f(E_n)] \}
$$

$$
+ \int d^3r \frac{\Delta(r)^2}{g} + \int d^3r \frac{|\mathbf{H}(r) - \mathbf{H}_0|^2}{8\pi},
$$

where $k_B$ is the Boltzmann constant, $\mathbf{H}_0$ the external magnetic field and $\mathbf{H}(r)$ the spatial dependent magnetic field inside the sample.

In order to study the effect of symmetry, we change the symmetry of system through situating one or more defects on the boundary, which mimics the tiny cuts at the edge of sample in practical experiment [6]. The $\mathbf{H}_0$ dependent magnetization and free energy of the square sample with