Numerical study of vortex system quantum melting

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We report a numerical study of the vortex system in the two dimensional II-type superconductors. We have proposed a phenomenological model that takes into account quantum fluctuations of Abrikosov’s vortices. The results of the quantum Monte-Carlo simulations by the SSE algorithm show that the thermal fluctuations are dominated by quantum fluctuations at low temperatures. In particular, we demonstrate the possibility of the quantum melting transition for vortex system in the temperature region where thermal melting transition is improbable.

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INTRODUCTION

Physics of the vortex systems is a very attractive field of the modern condensed matter physics due to various phases and phase transitions associated with vortex matter. Nature of the phase transitions in the vortex system is a subject of numerous both theoretical and experimental studies (see, for example, the reviews [1, 2]). It is well known that at low temperatures vortex system is in solid phase. Structure (quenched) disorder or other kinds of fluctuations have an influence on vortex system state. Thus as the thermal fluctuations increase the vortex lattice melts and system undergoes transition from solid to the liquid phase. Some peculiarities of vortex lattice melting at the presence of structure defects have been obtained by numerical simulations and were discussed in Refs. [3, 4, 5, 6, 7, 8, 9, 10, 11].

Recent experimental results demonstrate an alternative mechanism of the order destruction of vortex systems. This mechanism is associated by the some researches with quantum fluctuations in the vortex system [12, 13, 14, 15, 16]. So the authors of the paper [16] investigated magnetic relaxation in MgB2 thin film and made a conclusion on the presence of the quantum creep of the vortices at T → 0. They supposed that the creep is induced by quantum fluctuations. The transport properties investigations of k - (BEDT - TTF)2Cu(NCS)2 organic superconductor [13] as well as the measurements of dc and ac complex resistivities for thick α - MoxSi1−x films [14] indicated, in the author’s opinion, a presence of quantum fluctuations too. Note that the quantum fluctuations are supposed to be essential for thin superconducting films and high-layered superconductors, i.e. for systems with reduced dimensions. The quantum fluctuations became potentially significant at low temperatures T → 0, where the thermal fluctuations are negligibly small. In other words, quantum fluctuations can give rise to melting of the vortex system in the temperature range where the vortex system is expected to be in solid phase from the classical point of view.

Though there are many experimental researches of the quantum fluctuations influence on properties of the vortex system, simulations of vortex system with quantum fluctuations are practically absent in literature. One exception is the paper [17] where study of two dimensional vortex system has been done. However world-line Monte-Carlo algorithm in discrete imaginary time used in [17] did not allow the authors of the paper to simulate the processes of creation-annihilation of vortices in external magnetic field.

In this Letter we propose a phenomenological model for description of quantum fluctuations in the vortex system and report simulation results which were obtained by the loop quantum Monte Carlo algorithm in continuous imaginary time.

MODEL

To describe the quantum fluctuations of vortex system we propose to consider the vortices as hard-core bosons and introduce quantum tunneling term into Hamiltonian. So, Hamiltonian of vortex system takes the form:

\[ \hat{H} = -t \sum_{i,j} a_i^+ a_j + h.c. + \frac{1}{2} \sum_{i \neq j} V(r_{i,j}) n_i n_j - \sum_i h_i n_i, \]  \hspace{1cm} (1)

where the first term describes the quantum tunneling of the vortices between sites ij with hoping amplitude t - the phenomenological parameter for describing of the wave function overlap. In the general case vortex can hope between any different sites, but for the simplicity of the model we take into account the hopping between only nearest neighboring sites. The second term describes a pairwise interaction between vortices. And the third term includes all linear interactions, namely vortex self-energy, interaction between vortices and pinning centers, interaction between vortices and external magnetic field. Quantum behavior of the vortex system is described by the first term. The second and third terms are the same...
as for classical vortex system (see, for example Ref. [1]).

In this paper we choose:

\[ V(r_{i,j}) = U K_0 \left( \frac{r_{i,j}}{\lambda} \right), \quad \text{(2)} \]

\[ h_i = h + \mu_i, \quad \text{(3)} \]

where \( h \) - external field, \( \mu_i \) - pinning potential, \( K_0 \) - Bessel function, \( \lambda \) - penetration depth, \( r_{i,j} \) - a distance between the vortices at sites \( i \) and \( j \).

A study of the system described by equation (1) is a very complicated problem. Analytic solutions of the model [1] are do not available. Therefore it is necessary to use simulation methods. The quantum Monte Carlo algorithms are the most powerful tools for exploring quantum many body systems, such as a system (1). Quantum Monte Carlo methods allow us to calculate thermodynamic characteristics of the model and obtain visual qualitative picture of complex physical processes [18, 19, 20, 21, 22].

Note that by use of equation (1) we can describe both quantum and classical regimes of the vortex system.

To analyze the model (1) we use SSE (stochastic series expansion) algorithm modified for long-range potential. The algorithm is an exact numerical method and allows us to simulate quantum many body system in wide region of external fields and temperatures [22]. The method can be implemented in the both site [21, 22] and interaction representations [23]. In the case of long-range potential an interaction representation is preferable. For the interaction representation Hamiltonian splits into a diagonal part \( \hat{D} \) and a perturbation part \( \hat{V} \) [23, 24]:

\[ \hat{H} = \hat{D} + \hat{V}. \quad \text{(4)} \]

The partition function takes the form:

\[ Z = \sum_{n=0}^{\infty} (-1)^n \int_0^\beta d\tau_1 \int_0^{\tau_1} d\tau_2 ... \int_0^{\tau_{n-1}} d\tau_n \text{Tr} \{ \hat{V}(\tau_1) \hat{V}(\tau_2) ... \hat{V}(\tau_n) \}, \quad \text{(5)} \]

where

\[ \hat{V}(\tau) = e^{\tau \hat{D}} \hat{V} e^{-\tau \hat{D}}. \quad \text{(6)} \]

After that we choose basis \( \{ \alpha \} \) where \( \hat{D} \) is diagonal and decompose the perturbation part into bond operators:

\[ \hat{V} = \sum_b \hat{H}_b, \quad \text{(7)} \]

where \( b \) - bond index. So we can rewrite the partition function in the following way [23]:

\[ Z = \sum_{\alpha} \sum_{n=0}^{\infty} \sum_{T_n} \int_0^\beta d\tau_1 \int_0^{\tau_1} d\tau_2 ... \int_0^{\tau_{n-1}} d\tau_n W(\alpha, T_n, \tau), \]

\[ W = (-1)^n (e^{-\beta E_0} \prod_{p=1}^n e^{-\tau_p (E_p - E_{p-1})}) \langle \alpha | \prod_{p=1}^n \hat{H}_b | \alpha \rangle. \quad \text{(8)} \]
where $E_p = \langle \alpha(p)| \hat{D} | \alpha(p) \rangle$, $T_n$ a sequence of non-diagonal operators. To simplify simulations we add unit operators into the operator sequence $T_n$ and obtain the operator sequence $T_m$. The Monte Carlo simulation is carried out by diagonal and loop updates. The simulation starts with an arbitrary state $| \alpha \rangle$ and the operator sequence $T_m$ containing only unit operators. The diagonal update contains one attempt to interchange diagonal and unit operators. Note that the diagonal update changes the expansion power $n$ by ±1. In a stage of the loop update the interchange of diagonal and non-diagonal operators is carried out with the fixed expansion power $n$. So the loop update provides the creation-annihilation of kinks. At the same time the state of the system $| \alpha \rangle$ can be changed. The method allow us to operate directly with continuous imaginary time $\tau$ and grand canonical ensemble.

RESULTS

We consider a two-dimensional vortex system on triangular grid with periodic boundary conditions. To analyze behavior of the system we calculate a structure factor

$$S_6 = \langle \sum_{i=1}^{N} \frac{1}{Z'_t} \sum_{j=1}^{Z'_t} e^{i\theta_{ij}} \rangle,$$

and so-called superfluid density

$$\rho_s = \frac{1}{2W^2} \langle W^2 \rangle.$$  (10)

Superfluid density is introduced in according to the conventional determination [25]. Superfluid density depends on the mean square of winding number that characterizes a topological configuration of the world lines. Note that the nonzero value of $\rho_s$ means the presence of the energy dissipation as a result of the vortex quantum tunneling, i.e. there is a rise of resistivity. And on the contrary as $\rho_s \rightarrow 0$ quantum creep tends to zero and the only thermal dynamics of vortices is present (in case of current absent).

Calculations have been done for the vortex system on 10 x 10 triangular grid with the periodic boundary conditions. The grid spacing was chosen to be 0.25$\lambda$. One pinning center with the potential $\mu = 0.1U$ was introduced into the system to fix a vortex lattice. Two sets of calculations have been done. The temperature is changed at the fixed hopping amplitude $t$ and vice versa hopping amplitude is changed $t$ at the fixed temperature.

Fig. 1 shows the superfluid density versus temperature at different hopping amplitudes $t$. As seen from the dependencies at small hopping amplitude $t = 0.1$ superfluid density is almost absent in whole range of temperatures. While at $t = 0.5$ well-defined plateau arises on graph. The plateau corresponds to the quantum regime of vortex system. At the same time superfluid density drops rapidly as the temperature increase. This corresponds to transitions of the system to classical regime. As mentioned above, the superfluid density has another meaning for vortex system then usual one for hard-core boson system. Generally if the physical system is in superfluid state the dissipation is absent. However, as well known, high vortex mobility is accompanied by energy dissipation and therefore high value of superfluid density corresponds to high energy dissipation. So quantum fluctuations can give rise to dissipation in the temperature range where there is no dissipation in the classical approach.

The structure characteristics of vortex system along with the superfluid density are of interest. Figure 2 shows the dependencies of the structure factor $S_6$ on temperature at different hopping amplitudes $t$. As seen from the curves the structure factor tend to zero at high temperatures for all considered values of hopping amplitude $t$. As the temperature decreases the structure factor increases. Moreover, in the almost classical case $t = 0.1$ the system is more ordered at low temperatures then in the case of strong quantum fluctuations $t = 0.5$.

To examine a dynamics of the system with the increase of the amplitude of quantum fluctuation, we have done calculations at fixed temperature $T = 0.1U$ and different values of hopping amplitude $t$. As seen from Fig. 3 an enhancement of the hopping amplitude $t$ leads to the increase of the superfluid density. The last one corresponds to the transitions of the system into the quantum regime. Simultaneously the structure factor $S_6$ decreases, i.e. the vortex system disordering takes place. In other words the vortex system melts under quantum fluctuations.

FIG. 3: Superfluid density and structure factor $S_6$ versus hopping amplitude $t$ at temperature $T = 0.1U$, $U = 1.0$, $h = 0.5$. 

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SUMMARY

We have numerically examined the behavior of the Abrikosov’s vortices system in a two dimensional superconductor taking into consideration quantum fluctuations. Simulations have been done in wide range of temperatures at different intensity of quantum fluctuations. We have demonstrated that the enhancement of quantum fluctuations results in the quantum melting of the vortex system. Note that the quantum fluctuations must be essential in thin superconducting films, organic superconductors, high-layered superconductors and can be observed in magnetic and transport experiments at low temperatures.

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