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Effects of Thermal Fluctuations on Vortices in a Layered Superconductor

층 구조를 갖는 초전도체내의 자기 다발선계에서의 열적 요동의 효과

Joonhyun Yeo

여 준 현

Department of Physics, Konkuk University, Seoul, 143-701 Korea

서울특별시 광진구 모진동 93-1 건국대학교 물리학과

We apply the nonperturbative parquet approximation method, which was previously used to study the effect of thermal fluctuations in two-dimensional vortex systems, to vortices in a layered superconductor. We set up the parquet equations for the Lawrence-Doniach model and present two different numerical methods to solve them. The results for a superconductor consisting of two and four layers are also discussed in connection with an observed first order transition line in the vortex liquid regime.

1. Introduction

The phase diagram of a high temperature superconductor in a magnetic field has been the focus of recent theoretical and experimental interest [1]. The mean field theory [2] predicts that the lines of magnetic flux form a triangular array known as the Abrikosov lattice. Because of strong anisotropy, high temperature and short coherence length, thermal fluctuations in the high Tc materials are much more effective than in the conventional low Tc superconductors. Therefore, in a large portion of the phase diagram, flux lines in a high temperature superconducor are believed to be in the vortex liquid phase resulting from the melting of the Abrikosov lattice. Recent experiments [3] detected sharp drops in the resistivity and steps in the magnetization and the specific heat, which were interpreted as resulting from the vortex liquid undergoing a first order phase transition into presumably the Abrikosov lattice as the temperature is lowered.

Theoretical analyses on the vortex system near the first order transition line have mainly been based on the Lindemann criterion or numerical simulations. We note, however, that the Lindemann criterion is not a rigorous thermodynamic treatment and numerical simulations are known to be affected by the boundary conditions in the direction perpendicular to the magnetic field [4,5].

It is noteworthy that a recent numerical simulation [5] on the vortex system in a layered superconductor produced the observed first order transition line which disapeared at an end point at low magnetic field. This kind of behavior has been widely observed in experiments and usually been attributed to the effect of disorder. But the result of this numerical simulation on a system without disorder suggests that there is only one phase below and above the transition, namely the vortex liquid. (The situation is much like a gas-liquid transition.) The only difference between the two phases is the correlation length in the vortex liquid. This is in contrast to other numerical simulation results which use a different boundary condition [4]. In those cases a genuine first order transition between the vortex liquid and the vortex crystal was obtained.

Therefore, an analytical approach is essential to elucidate the nature of flux lines in a layered superconductor. The parquet approximation [6], which was successfully applied to a two-dimensional vortex system, is a nonperturbative analytic method which is free from any finite size effect perpendicular to the field direction. In two dimensions this method was able to capture the growing crystalline order developing in a vortex liquid as the temperature is lowered [6]. In this approximation no finite temperature phase transition was observed in two dimensions. So it would be interesting to see if this conclusion changes when a layered system is considered. In this contribution, we present the first attempt to apply the parquet approximation method to a vortex system in a layered superconductor. The parquet approximation deals with the renormalized four-point function of the vortex system which is obtained by summing an infinte subset of Feynman diagrams, the so-called parquet diagrams. As will be explained below the extra dimension in the parquet approximation method compared to the two dimensional case poses considerable difficulty in practical calculations. In this contribution, we discuss possible numerical methods which can be used to extract useful physical quantities from the parquet approximation. Finally in order to show the applicability of our methods we present the result of these approaches for a superconductor consisting of two and four layers, and discuss its implication on the phase diagram of vortices.

2. Model

Our starting point is the Lawrence-Doniach model for a layered superconductor in a magnetic field perpendicular to the layers. We denote the order parameter in the n-th layer by ψ_n. The free energy is given by

$$F[\psi, \psi^*] = \sum_n d_0 \int d^2r [\, a|\psi_n(r)|^2 + \frac{\beta}{2}|\psi_n(r)|^4 + \frac{1}{2m_{ab}}|(-i\hbar\nabla - \frac{e^*}{c}\vec{A})\psi_n|^2 + \frac{\hbar^2}{2m_c d^2}|\psi_n(r) - \psi_{n+1}(r)|^2]$$

where d_0 is the layer thickness, d the layer spacing and α, β, m_{ab} and m_c phenomenological parameters. We denote by $\tau \equiv \hbar^2/2m_c d^2 = (\xi_c/d)^2$ the dimensionless ratio between the coherence length ξ_c perpendicular to the layers and the layer spacing. We take $\vec{B} = \nabla \times \vec{A}$ as constant and uniform.

We use the lowest Landau level (LLL) approximation which is believed to be valid over a large portion of the vortex liquid regime. We expand the order parameter in terms of the eigenstates of the covariant derivative term and keep only the lowest eigenvalue state. In the symmetric gauge, the LLL wavefunction is given by $\psi_n(r) = \exp(-\mu^2|z|^2/4)\phi_n(z)$ where $\mu^2 = e^*B/\hbar c$ and $\phi_n(z)$ is an arbitrary analytic function of z=x+iy.

We calculate the various correlation functions with respect to a partition function obtained from the LLL free energy by using the parquet approximation. It is a nonperturbative analytic approximation and thus no boundary conditions are used in the direction perpendicular to the magnetic field. Along the field, however, we consider a system consisting of a stack of N layers, for which we impose the periodic boundary condition $\phi_{n+N}(z) = \phi_n(z)$. We introduce, in a usual way, the Fourier transform $\tilde{\phi}_q(z)$ of $\phi_n(z)$.

The main quantity one calculates in the parquet approximation is the renormalized connected four-point function,

$$\langle \widetilde{\phi}^*_{q_1}(z_1^*)\widetilde{\phi}^*_{q_2}(z_2^*)\widetilde{\phi}_{q_3}(z_3)\widetilde{\phi}_{q_4}(z_4)\rangle_c$$

which can be written in terms of the renormalized vertex function [6]

$$\Gamma(q_1, q_2, q_3 ; \vec{k}) = \Gamma(q_1, q_2, q_3, q_1 + q_2 - q_3 ; \vec{k}).$$

Here the momentum $\vec{k}$ corresponds to the two-dimensional space perpendicular to the magnetic field and q_i to the layer index. Note that to the lowest order $\Gamma(q_1, q_2, q_3; \vec{k}) = \Gamma_B(\vec{k})$, the bare vertex which is independent of the momenta across the layers.

In order to make a resummation over all parquet diagrams, we note that the contributions to Γ can be decomposed into a totally irreducible part and a reducible part which in turn can be written as the sum of three parts Π_i $(i=1,2,3)$ representing the contributions from three different channels which can be written in terms of irreducible vertices Λ_i and Γ. (A detailed discussion on the diagrammatic decomposition and a construction of the parquet equations can be found in [6]) The parquet approximation we employ here corresponds to neglecting in the totally irreducible vertex all the higher order ($O(\beta^4)$) diagrams except the bare vertex function $\Gamma_B(\vec{k})$.

Using the solutions to the above equations one can calculate several interesting physical quantities. Among them we focus on the structure factor, which is the measure of correlation between vortices in a vortex liquid. It is calculated from

$$\chi_{n-n'}(r-r') = \langle |\phi_n(r)|^2 |\phi_{n'}(r')|^2\rangle - \langle |\phi_n(r)|^2\rangle\langle |\phi_{n'}(r')|^2\rangle .$$

The structure factor $\Delta_m(\vec{k})$ used in this work is then defined by

$$\Delta_m(\vec{k}) \equiv \left(\frac{d_0\beta}{k_B T}\right) e^{k^2/2\mu^2} \int d^2R\, e^{i\vec{k}\cdot\vec{R}} \chi_m(\vec{R})$$

We also calculate the Abrikosov ratio β_A defined as

$$\beta_A \equiv \frac{\langle |\phi_n(r)|^4\rangle}{\langle |\phi_n(r)|^2\rangle^2}$$

We solve the parquet equations numerically. The main numerical difficulty arising from the addition of an extra dimension is that Γ and Λ_i now involve the three extra momentum indices, which will require a large amounts of computer memory when the number of layers becomes large. One approach we take is to start from some initial functions, Λ_i, Γ and update these functions iteratively using the parquet equations. At high temperatures, we find that the iteration converges very quickly, but as the temperature is lowered the convergence of this iteration gets slower, and furthermore the results obtained at a closeby temperature have to used as the initial values to get good convergence. For the two dimensional problem it was noticed that the direct iteration approach always produces a slower convergence compared to the matrix inversion method, for which the parquet equations, viewed as Fredholm integral equations of the second kind, are solved numerically by inverting the kernel and by iteratively updating the kernel by using the remaining parquet equations. In the present case the matrix inversion cannot be applied in a straightforward way since they are not in the form of a product of two matrices.

We note, however, that this can in fact be achieved so that the matrix inversion method can be applied in the layered case too. We first cast the parquet equations into the form involving the layer indices instead of the momenta. We find that the parquet equations become much simpler than those written with respect to the layer momenta. (Detailed expressions of the parquet equations in terms of the layer indices can be found in [7].) More importantly, they are in the form of a product of two (big) matrices.

Now we solve the parquet equations using the matrix inversion method. As expected we find that the convergence of the iteration is quicker than the direct iteration method. One shortcoming of this approach, however, is that it involves the inversion of matrices of very big size. In our model we are in general dealing with $(MN^2 \times MN^2)$ matrices where M is the number of grid points in $\vec{k}$ space. Usually one has to use sufficiently large M in order to capture the growing peaks in the structure factor as the temperature is lowered. Therefore when the number of layers N becomes large the numerical inversion method requires a large amount of computer memory and CPU time.

For two-layer and four-layer systems, we find that both methods yield satisfactory results within reasonable amount of computing time. For example for M=300, one iteration for both cases takes around 5 minutes on a DEC workstation. For the calculation of the system with large N, a combination of both methods must be used. We calculate the structure factor for the two-layer and four-layer systems for various values of the temperature and the applied field. We observe that sharp peaks develop, as the we move down below the H_{c2} line, near the value of the first reciprocal lattice vector of a triangular lattice, which indicates the growing crystalline order in the vortex liquid. We can also see the inter-layer correlation is getting larger as the temperature is lowered. In the two-layer system, within the temperature and field range we have studied, we do not see any finite temperature phase transition. In the four-layer system, however, we observe first order transitions in the form of small steps in physical quantities such as the magnetization and the Abrikosov ratio β_A. We detect instabilities in the solution of the parquet equations when these transitions occur. The size of steps gets smaller as we increase the inter-layer coupling, which corresponds to decreasing the applied field in terms of LLL scaling variables. The first order transition line eventually ends at low fields at an critical end point. This behavior is analogous to the result obtained in the simulation in [5], and is consistent with the picture suggested in [5] where the first order transtion line only separates two vortex liquid phases with different correlation lengths and does not correspond to the melting of a vortex lattice.

3. Conclusion

To summarize we presented the parquet equations for the Lawrence-Doniach model and discussed two possible numerical methods for solving them. While, in the two-layer system, we do not see any kind of transition, we see first order transitions and a critical end point in the four-layer system. This is in agreement with the simulation result [5] which indicates that only the vortex liquid phase exists above and below the first order transtion line. As emphasized above the parquet approximation is a very powerful tool to study the phase diagram of vortices in a layered superconductor. In order to elucidate the nature of the vortex liquid phase we need to consider a system with more layers, which is left to the future work [8]. We can then extract useful information on the nature of phase transitions in the vortex liquid using a kind of finite size scaling. For this we have to make an appropriate use of the two methods presented here.

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