Fluctuation diamagnetism from a Ginzburg-Landau-like free energy functional for high-$T_c$ superconductors

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Using a recently proposed Ginzburg-Landau-like energy functional due to Banerjee et al. Phys. Rev. B 83, 024510 (2011), we calculate the fluctuation diamagnetism of high-$T_c$ superconductors as a function of doping concentration $x$ in addition to the magnetic field $H$ and temperature $T$ by employing classical Monte Carlo simulations. We show that our results are in good qualitative agreement and reasonable quantitative agreement with recent experimental data. Our calculations show that a model of classical superconducting fluctuations can produce features of the observed magnetization in the pseudogap region. In particular we show that the magnetization tracks the superconducting dome and also comment on the determination and doping dependence of $H_{cd}(T=0)$.

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In recent years fluctuation diamagnetism and the Nernst effect in the vortex-liquid regime of cuprate superconductors have generated great interest both theoretically \cite{1} and experimentally \cite{2,3}. Experiments have found a very large diamagnetic and Nernst response in the enigmatic pseudogap phase of the cuprates, about whose origin there is still no consensus. A close connection between the measured diamagnetism and the Nernst effect was shown by Ong and collaborators \cite{4,5} who have attributed the large observed signals to strong fluctuations of the superconducting order parameter. On the other hand Taillefer and collaborators \cite{6} claim on the basis of their experimental data on the Nernst effect that there could be a dominant contribution from quasiparticles and a negative Nernst signal. Most theoretical studies of the Nernst effect based on superconducting fluctuations yield a positive Nernst coefficient \cite{7,8,9} although a recent study claims to produce a negative Nernst coefficient. The contribution of superconducting fluctuations to the observed Nernst effect thus requires further investigation. On the other hand, the diamagnetism arising from superconducting fluctuations has been calculated numerically in a phase only model \cite{10} as also using renormalization group methods for a 2D system in the vicinity of the Kosterlitz-Thouless transition \cite{11}. While these contributions have been able to reproduce some qualitative and some quantitative features of the experimentally observed diamagnetism in the cuprates, they have been constrained by their nature to specific regions of the phase diagram. In particular, the doping dependence of the observed diamagnetic signal, which has been studied fairly extensively experimentally, has not been included in these calculations.

In this work, we study fluctuation diamagnetism in a recently proposed phenomenological model of high-$T_c$ superconductors by Banerjee et al. \cite{12}. This model is of the Ginzburg-Landau (GL) type with coefficients that depend on temperature and doping. The results quantitatively reproduce several features of the cuprate phase diagram such as the superconducting dome, doping dependence of the phase stiffness etc.. Since the coefficients of this model include a doping dependence, we can use it to calculate the dependence of diamagnetism on doping. Specifically, we obtain the diamagnetism as a function of temperature, doping and magnetic field by performing classical Monte-Carlo simulations on the GL type model. We find that our data matches well with the experimental data of Ong and collaborators and in particular, we comment on their determination of the low-temperature upper critical field $H_{cd}(T=0)$. We will report calculations of the Nernst effect of the same model in a different paper \cite{13}.

The GL free energy functional \cite{12} $\mathcal{F}$ we study is defined on the CuO$_2$ planes of the superconductor. The model describes the free energy as a functional in which the effects of the fluctuations of the order parameter phase and magnitude are coupled, and the relative importance of the latter increase with hole doping $x$. The pairing field $\psi_m = \Delta_m \exp(i \phi_m)$, with amplitude $\Delta_m$ and phase $\phi_m$, is defined on the sites $m$ of a square lattice. Microscopically, the field $\psi_m$ is expected to be related to the complex spin-singlet pairing amplitude defined on the Cu-O-Cu bonds \cite{12,13}. The functional $\mathcal{F}$ is defined as

$$
\mathcal{F}(\{\Delta_m, \phi_m\}) = \mathcal{F}_0(\{\Delta_m\}) + \mathcal{F}_1(\{\Delta_m, \phi_m\}),
$$

$$
\mathcal{F}_0(\{\Delta_m\}) = \sum_m \left( A \Delta_m^2 + B \frac{1}{2} \Delta_m^4 \right),
$$

$$
\mathcal{F}_1(\{\Delta_m, \phi_m\}) = C \sum_{<mn>} \Delta_m \Delta_n \cos(\phi_m - \phi_n),
$$

where $<mn>$ represent pairs of nearest neighbour sites. The coefficients $A$, $B$ and $C$ depend on doping concentration $x$ and temperature $T$ and are parametrized as
The magnetic field is then included via the condition

$$\sum A_{mn} = \Phi,$$

where $\sum_{\square}$ is a sum over a plaquette of the lattice and $\Phi$ is the flux per plaquette in units of the universal flux quantum. Introducing the magnetic field in this manner allows us to determine $H_{c2}(T = 0)$ as follows. It is obtained by locating the value of $\Phi$ at which the magnitude of $\Delta$ at every site goes to zero. This would correspond to the flux per plaquette $\Phi_A$ at the Abrikosov melting field for the square lattice we use in our simulations. For a lattice spacing equal to the zero temperature coherence length $\xi_0$, the melting flux is $\Phi_A = \frac{\Phi_0}{\pi}$ of a flux quantum $\Phi_0$. Numerically we find that the melting flux is roughly 1.18 times this value for all values of the various parameters in Eqn. 4 indicating that spacing in our discrete model is approximately equal to $\xi_0$ for all values of doping. Knowing the exact $x$ dependence of $\xi_0$, one can then obtain the $x$ dependence of $H_{c2}(T = 0)$. One might expect $\xi_0$ to go as $\sqrt{x}$ at least at low doping in our model from the fact that $C \sim x$ suggesting that $H_{c2}(T = 0)$ goes as $1/x$ for low doping. We note that this is indeed the rough $x$ dependence of this quantity obtained by Ong [14] and collaborators.

Magnetization: Introducing a magnetic field gives rise to a diamagnetic moment $M$ in the system. The principal goal our calculation is to find $M$ as a function of $T$, $H$ and $x$. To achieve this we first define the diamagnetic current along a bond between sites $m$ and $n$ as

$$j_{mn} = -\frac{\partial F}{\partial A_{mn}}.$$

$M$ is related to the diamagnetic current density $j$ as $j = \nabla \times M$. $M$ can thus be obtained by an appropriate integration of $j$. To this end we perform our calculations in a cylindrical geometry with periodic boundary conditions along the $\hat{x}$ and zero current conditions along the $\hat{y}$ direction. The magnetic field is radially outwards which yields a magnetization $M$ along the same direction. We
work in the Landau gauge where the $A_{mn}$ are non-zero only for $<mn>$ along the $y$ direction and $\mathbf{j}$ is only along the $x$ direction. We integrate the current along the $y$ direction from the edge of the sample into the middle of the sample to obtain $M$. The precise numerical method we employ is that of classical Monte-Carlo simulations with the Metropolis algorithm. We have verified that our results are independent of gauge choice and also boundary conditions so long as they yield a non-zero magnetization.

Our simulations are on lattice sizes of up to $100 \times 100$. At each value of $T$, $H$ and $x$, we perform $10^6$ Monte-Carlo steps per site for equilibration and a further $4 \times 10^6$ steps for thermal averaging for our largest system size. Even though we perform the simulation for a single 2D layer we assume that the actual 3D system is a collection of 2D layers with a negligible Josephson coupling between them. Thus, the only possible interaction between the pancake vortices is electromagnetic in nature. This type of interaction has been shown to not change the BKT universality class of the superfluid transition and give a very small non-universal correction to the superfluid density jump. We thus ignore the electromagnetic interaction among the vortices in different layers as well.

The conversion from 2D magnetization to 3D magnetization involves division by an appropriate length along the $c$ axis. For Bi2212, the lattice spacing along the $c$ axis is $3.07 \text{nm}$ and the appropriate length is half this value $\sim 1.5 \text{nm}$. The dimensionless temperature is converted into Kelvin by multiplying $T_0$ at each doping. The magnetic field is converted to Tesla by identifying the zero temperature melting flux with the experimental value $\phi_0$. We assume that the actual 3D system is a collection of 2D layers with a negligible Josephson coupling between them.

**Results:** We have obtained the value of magnetization as a function of temperature, doping and field in our model. Fig. 2 is a plot of the magnetization of BSSCO as a function of magnetic field for $x = 0.05$ and $x = 0.15$ at different temperatures. The main qualitative observation that one can immediately make is that as the field decreases the magnetization appears to go to zero for temperatures $T > T_K$ and diverge for $T < T_K$. This is consistent with the predictions of a renormalization group calculation in the vicinity of the Kosterlitz-Thouless transition.

A plot of the magnetization as a function of temperature for different samples (Fig. 3) clearly shows that there is a significant diamagnetic signal above $T_c$ as seen in experiments. Further color plots of the magnetization in the $H - T$ plane (Fig. 4) shows that the variation of magnetization with temperature at fixed field is most gradual for the sample with the largest value of $T_c$ (the OPT sample). This can be seen also in Fig. 5 with color plots of the magnetization at two different fields in the $x - T$ plane. It can be seen that the magnetization curves track the superconducting dome. Experimentally, the Nernst effect has been seen to track the superconducting dome and has been argued to be very closely related to the magnetization. The persistence of the experimental Nernst and diamagnetism signal over a dome-shaped region above $T_c$, instead of the entire pseudogap state all the way up to $T^*$, has been argued as an evidence against the pairing origin of the pseudogap line. This is due to the expectation that the pseudogap line is related to pairing then superconducting fluctuations should continue till $T^*$ on the under-doped side. However, on the basis of our results we can...
argue that this expectation is not justified since pairing fluctuations identifiable as superconducting fluctuations, e.g., those detected through Nernst or diamagnetism, are mainly controlled by superfluid density or the $T_c$ scale. The GL-like model we study has the pseudogap temperature set as the local pairing scale by construction, but the diamagnetic signal tracks the superconducting $T_c$ which is governed by the superfluid density on the underdoped side. The suppression of $T_{KT}(x)$ relative to $T^*(x)$ is an indicator of the strength of superconducting fluctuations.

The fact that $T_{KT}(x)$ displays a dome shape as a function of $x$ while $T^*(x)$ decreases monotonically with increasing $x$ shows that fluctuations get weaker with increasing doping. The two extremes of the strength of fluctuations are represented by the phase only $XY$ model (strong fluctuations) and the Gaussian model (weak fluctuations). The magnetization in the former model has been calculated and found to be in reasonable agreement with experimental data. Our data for extreme underdoped samples are in agreement with the results of this calculations. The strong fluctuation limit corresponds to fluctuations essentially in the phase $\phi$ of the superconducting order parameter with the amplitude $\Delta$ being frozen. As the doping increases, amplitude fluctuations start becoming more significant even as the overall strength of fluctuations decreases till one arrives at regime where the fluctuations are Gaussian and cannot be divided into contributions from amplitude and phase in any meaningful sense. As can be seen from Fig. 2, our calculations show that the qualitative behaviour obtained from the $XY$ model persists even when amplitude fluctuations develop changing only the overall magnitude of the magnetization.

Essential to a point by point comparison of our simulation results to experimental data is the value of the zero temperature upper critical field $H_{c2}(T = 0)$, which sets the field scale in terms of which all other values of magnetic field are expressed. We use the experimentally determined value of $H_{c2}(T = 0)$ for this purpose. One method to determine the experimentally quoted value involves an extrapolation of the Nernst signal of UD, OPT, OD bilayer Bi2212 cuprates at temperature $T_c$ and obtaining the $H_{c2}(T = 0)$ from a scaled plot of single layer Bi2201 cuprate. This approach was taken by Ong and coworkers where they reported the increase of upper critical field with underdoping. Other approaches utilizing either a Gaussian analysis of fluctuations in the magnetoconductivity of YBCO or obtaining a characteristic field $H^*$ from the peaks of the Nernst signal versus magnetic field isotherms of Eu-LSCO cuprate and fitting $H^*$ to a scaled form give a completely different dependence where $H_{c2}$ decreases with underdoping. The values of $H_{c2}(T = 0)$ obtained from the two methods can differ by as much as a factor of 2 in the UD region. Our simulations can in principle provide a way to test both methods: We can use the experimentally quoted value of $H_{c2}(T = 0)$ for a particular sample from both methods to determine which of the two yields a better comparison to experiment over a large range of temperature and field. While we are constrained in this regard by the fact that both methods have not been applied to data on the same sample, it appears as alluded to earlier that the method of Ong et. al. provides a doping dependence of $H_{c2}(T = 0)$ that is consistent with what we find from our model. We emphasize that our model contains only classical superconducting fluctuations whereas quantum fluctuations could also contribute to physics determin-

![FIG. 4: Color map plots of a) UD($x = 0.05$), b) OPT($x = 0.15$), c) OD($x = 0.25$) BSSCO samples obtained from our calculations. The color bar shows the values of magnetization in $\Lambda/m$ in field temperature ($H - T$) plane.](image1)

![FIG. 5: The diamagnetic signal in the $T - x$ plane obtained form our calculations for two different fields. It can be clearly seen that diamagnetic signal follows the superconducting dome. While converting our field axis we have taken $H_{c2}$ values as 160, 150, 100, 66, 60, 50, 42 Tesla for $x$=0.03, 0.05, 0.10, 0.15, 0.20, 0.25, 0.30 respectively by extrapolating experimental data. The magnetization at all fields is obtained by interpolating between our numerical data points for fixed values of fields.](image2)
ing $H_{c2}(T = 0)$, especially in the underdoped regime. Nevertheless, it appears that the various methods of extrapolation used in the determination of $H_{c2}(T = 0)$ experimentally also essentially take into account only the effect of classical fluctuations like we do here. The effect of quantum fluctuations needs to be considered seriously for a complete picture of the low temperature and high field physics, which task we defer to a later work.

**Conclusion:** This work calculates the diamagnetism in the cuprates described by a Ginzburg-Landau-like energy functional of the superconducting order parameter. Our model allows us to study the doping dependence of the magnetization in addition to its dependence on temperature and magnetic field. We find that our results are in good qualitative agreement and quantitative agreement within a factor of 2 of experimental data obtained on BSSCO [8, 9]. The diamagnetic response as a function of temperature tracks the superconducting dome showing that it is controlled by the superfluid density at low doping and hence supporting the existence of preformed pairs above $T_c$. Finally, our model also seems to suggest that $H_{c2}(T = 0)$ increases with decreasing doping at low values of doping.

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