Anisotropy in the helicity modulus of a 3D XY-model: application to YBCO

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Abstract. We present a Monte Carlo study of the helicity moduli of an anisotropic classical three-dimensional (3D) XY-model of YBCO in superconducting state. It is found that both the $ab$-plane and the $c$-axis helicity moduli, which are proportional to the inverse square of the corresponding magnetic field penetration depth, vary linearly with temperature at low temperatures. The result for the $c$-axis helicity modulus is in disagreement with the experiments on high quality samples of YBCO. Thus we conclude that purely classical phase fluctuations of the superconducting order parameter cannot account for the observed $c$-axis electrodynamics of YBCO.

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1. Introduction

Emery and Kivelson presented [1,2] very strong physical arguments that in systems with low superfluid density \( n_s \) (e.g., high-\( T_c \) copper oxide superconductors and the organic superconductors) the fluctuations in phase of the superconducting order parameter play a significant role. In essence, the superfluid density is proportional to the helicity modulus of a superconductor [3], which measures the stiffness of the superconductor with respect to twists in phase of the order parameter; hence a low value of \( n_s \) implies a low value of the maximum possible phase ordering temperature \( T_\phi \). If \( T_\phi \) is comparable to the measured physical superconducting temperature \( T_c \), the observed superconducting properties may be very different from what is predicted by the mean-field BCS/Eliashberg theory. They further argued that in the case of poor screening, as indicated by a low conductivity, the Coulomb interaction suppresses the local Cooper pair density fluctuations \( \Delta n_s \), which in turn enhances the phase fluctuations \( \Delta \phi \) (\( \Delta n_s \Delta \phi \geq 1/2 \)). Thus, the phase fluctuations might influence the superconducting properties over a wide range of temperatures below and above \( T_c \). Indeed, measurements of the \( ab \)-plane magnetic field penetration depth \( \lambda(T) \) (\( \lambda^{-2} \propto n_s \)) on \( \text{YBa}_2\text{Cu}_3\text{O}_{6.95} \) [4] gave unambiguous evidence for three-dimensional (3D) XY critical scaling behavior in a temperature interval of about 10 K below \( T_c = 92.74 \text{ K} \). Roddick and Stroud [5] were the first to point out that classical phase fluctuations in a nodeless order parameter could produce a low-temperature \( \lambda(T) \) which varies linearly with \( T \) in an isotropic three-dimensional superconductor. They also showed that this dependence persists when combined effects associated with Coulomb energy of local charge density fluctuations and Ohmic dissipation are included in the model. This important result showed that the observed linear temperature dependence of the \( ab \)-plane \( \lambda^{-2} \) in YBCO at low \( T \) [6] does not necessarily originate from quasiparticle excitations near the lines of the gap nodes at the Fermi surface. The same idea was advanced independently by Emery and Kivelson [1], who also argued that a large \( ab \)-plane conductivity in YBCO implies that the phase fluctuations are predominantly classical down to low temperature. More recently, Emery and Kivelson [7] argued that very extensive angle-resolved photoemission spectroscopy experiments found no evidence of quasiparticle excitations near the nodes of the gap even just below \( T_c \), and therefore the existence of nodes is not responsible for the observed linear \( T \)-dependence of the \( ab \)-plane \( \lambda^{-2} \) in YBCO at low temperatures.

If, indeed, the phase fluctuations in the order parameter are responsible for the observed linear temperature dependence of the \( ab \)-plane superfluid density at low \( T \) [1,5,7], then the experiments [8] on \( c \)-axis electrodynamics in YBCO are puzzling and have to be explained. Namely, it was found that the \( c \)-axis penetration depth \( \lambda_c(T) \) never has the linear temperature dependence observed in \( ab \)-plane. The best fit to the data up to about 40 K gives \( \Delta \lambda_c(T) \propto T^{2.1} \). If the phase fluctuations are predominantly classical down to low temperature one would expect the superfluid density to be linear at low \( T \) in all directions. Indeed, that is exactly what was obtained by Roddick and Stroud [5]
Anisotropy in the helicity modulus of a 3D XY-model: application to YBCO

in a simple model for an anisotropic superconductor using a variational self-consistent phase phonon (SCPP) approximation. Here we present a detailed Monte Carlo (MC) study of helicity moduli for an anisotropic 3D XY-model which incorporates the bilayer structure of YBa$_2$Cu$_3$O$_7$. As expected, we find the helicity moduli to decrease linearly at low temperatures in all directions. Thus the classical anisotropic 3D XY-model cannot account for the observed temperature dependence of the magnetic field penetration depth of YBa$_2$Cu$_3$O$_7$ along the c-axis.

The rest of the paper is organized as follows. In section 2 we discuss our model and some details of the MC calculation. Section 3 contains our numerical results for the helicity moduli and our conclusions.

2. The model and the simulation

We consider an anisotropic 3D XY-model for a system with bilayer structure described by the Hamiltonian

$$H = H_{ab} + H_c, \quad (1)$$

$$H_{ab} = \sum_{l,s,(i,j)} [-J_1 \cos(\phi_{i,l,s} - \phi_{j,l,s}) - J_2 \cos(2(\phi_{i,l,s} - \phi_{j,l,s}))], \quad (2)$$

$$H_c = \sum_{l,i} [-J_\perp \cos(\phi_{i,l,2} - \phi_{i,l,1}) - J'_\perp \cos(\phi_{i,l+1,1} - \phi_{i,l,2})]. \quad (3)$$

Here, the sum over $l$ runs over a stack of bilayers, the sum over $s = 1, 2$ runs over two layers in a given bilayer, $\langle i, j \rangle$ denotes the nearest neighbors within a single layer, the sum over $i$ runs over the sites in a given layer and $\phi_{i,l,s}$ is the phase of the order parameter on site $i$ of the layer $s$ in the bilayer $l$. The ab-plane Josephson couplings with constants $J_1$ and $J_2$ correspond to the transfer of one and two Cooper pairs [9], $J_\perp$ is the Josephson coupling constant between two layers within a given bilayer, and $J'_\perp$ is the Josephson coupling constant between layers in two adjacent bilayers. This Hamiltonian is obtained from the coarse-grained Ginzburg-Landau model for YBCO [10] by ignoring the temperature dependence of the amplitude of the order parameter.

The computation of the helicity modulus along direction perpendicular to the bilayers requires care as the separation between the layers in a bilayer, $c_b$, is, in general, different from the separation between the bilayers, $c'$. If a uniform vector potential $A$ is applied its effect on the Hamiltonian is to shift the phase difference between points $r_1$ and $r_2$ by $A_{1,2} = 2\pi A \cdot (r_2 - r_1)/\Phi_0$, where $\Phi_0 = hc/2e$ is the flux quantum: $\phi_{r_1} - \phi_{r_2} \rightarrow \phi_{r_1} - \phi_{r_2} + A_{1,2}$. The momentum conjugate to $\phi_{i,l,s}$ is the charge $n_{i,l,s}$ (in the units of $2e$) and its rate of change, given by $-\partial H/\partial \phi_{i,l,s}$, is the total current flowing into the site $(i, l, s)$. The resulting expression can be used to define the current along each bond connected to site $(i, l, s)$. In equilibrium $\langle n_{i,l,s} \rangle = 0$ and one obtains the average current conservation at each site $(i, l, s)$. For a uniform $A$ perpendicular to the layers, the average currents parallel to the bilayers vanish by symmetry and one has

$$\langle J_\perp \sin(\phi_{i,l,2} - \phi_{i,l,1} + \frac{2\pi}{\Phi_0} A c_b) \rangle = \langle J'_\perp \sin(\phi_{i,l+1,1} - \phi_{i,l,2} + \frac{2\pi}{\Phi_0} A c') \rangle, \quad (4)$$
Anisotropy in the helicity modulus of a 3D XY-model: application to YBCO

where the angular brackets denote the statistical average for the Hamiltonian $H(A)$:

$$\langle \cdots \rangle = \int \prod \phi_{i,l,s} \cdots \exp(-\beta H(A))/Z(A), \beta = 1/(k_B T), Z(A) = \int \prod \phi_{i,l,s} \exp(-\beta H(A)).$$

The expression on the left hand side of Eq. (4) gives the average current from the site $i$ in $s = 1$ layer of the bilayer $l$ into the site $i$ of $s = 2$ layer of the same bilayer. The expression on the right hand side of (4) gives the average current from the latter site into the site $i$ of $s = 1$ layer in the adjacent layer $l+1$.

Since the average currents along bonds parallel to $A$ are equal, one can calculate the $z$-axis helicity modulus (the $z$-axis is perpendicular to the layers, i.e. it is along the crystallographic $c$-axis) by computing the derivative of any one of those average currents with respect to $A$ at $A = 0$. For computational purposes using the Monte Carlo method we evaluate the average helicity modulus over all bonds parallel to $A$

$$\gamma_{zz} = \frac{2\pi}{\Phi_0} \left\{ \frac{1}{N^3} \sum_{l,i} \left[ J_\perp c_b (\cos(\phi_{i,l,2} - \phi_{i,l,1}) + J_\perp c' (\cos(\phi_{i,l+1,1} - \phi_{i,l,2})) \right] 
- \frac{1}{k_B T} \left( \frac{1}{N^3} \sum_{l,i} \left[ J_\perp \sin(\phi_{i,l,2} - \phi_{i,l,1}) + J_\perp c' \sin(\phi_{i,l+1,1} - \phi_{i,l,2}) \right] \right) \right.$$ 

$$\times \sum_{l,i} \left[ J_\perp c_b \sin(\phi_{i,l,2} - \phi_{i,l,1}) + J_\perp c' \sin(\phi_{i,l+1,1} - \phi_{i,l,2}) \right] \right)$$

$$+ \frac{1}{k_B T} \frac{1}{N^3} \sum_{l,i} \left[ J_\perp (\sin(\phi_{i,l,2} - \phi_{i,l,1})) + J_\perp c' (\sin(\phi_{i,l+1,1} - \phi_{i,l,2})) \right]$$

$$\times \sum_{l,i} \left[ J_\perp c_b (\sin(\phi_{i,l,2} - \phi_{i,l,1})) + J_\perp c' (\sin(\phi_{i,l+1,1} - \phi_{i,l,2})) \right] \right\}.$$  

(5)

Here, $N^3$ is the number of bonds parallel to $A$. We note that computing $\gamma_{zz}$ as $\partial^2 F/\partial A_z^2$, where $F$ is the Helmholtz free energy, which is valid (up to a multiplicative constant) for orthorhombic lattices without a basis, would give a wrong result in our case. The in-plane helicity modulus $\gamma_{xx}$ along $x$- (i.e. $a$-) direction is derived in analogous way.

The elementary excitations of the XY-model are spin-waves and vortices [3], but in the zero temperature limit only the spin-waves are statistically relevant. It is useful to have the analytic expressions for $\gamma_{zz}$ and $\gamma_{xx}$ obtained from the spin-wave expansion in the zero temperature limit as a check on the Monte Carlo results at low temperatures. We find (in the units of $(2\pi/\Phi_0)2N$, where $N$ is the number of tetragonal unit cells, and taking $J_2 = 0$ for the sake of simplicity)

$$\gamma_{zz}(T) = \frac{1}{2} \left[ (J_\perp c_b + J_\perp c') - (J_\perp - J_\perp) (J_\perp c_b - J_\perp c')/(J_\perp + J_\perp) \right] - \alpha_2 k_B T,$$

(6)

where

$$\alpha_2 = \frac{1}{4N} \sum_k \left[ (J_\perp c_b + J_\perp c') \left( \frac{1}{\omega_1(k)} + \frac{1}{\omega_2(k)} \right) \right.\left. - (J_\perp c_b \kappa(k) + J_\perp c' \kappa(k)) \left( \frac{1}{\omega_1(k)} - \frac{1}{\omega_2(k)} \right) \right].$$

(7)

$$\kappa(k) = (J_\perp + J_\perp \cos(k_z c))/\sqrt{(J_\perp + J_\perp)^2 - 4J_\perp J_\perp \sin^2(k_z c/2)},$$

(8)
Anisotropy in the helicity modulus of a 3D XY-model: application to YBCO

\[ \kappa'(k) = \frac{(J_\perp \cos(k_z c) + J'_\perp)}{\sqrt{(J_\perp + J'_\perp)^2 - 4J_\perp J'_\perp \sin^2(k_z c/2) \cdot (J_\perp + J'_\perp)^2 - 4J_\perp J'_\perp \sin^2(k_z c/2)}} \]  

(9)

\[ \omega_{1,2}(k) = 2J_1 \left( \frac{\sin^2 k_x a}{2} + \frac{\sin^2 k_y a}{2} \right) + \frac{(J_\perp + J'_\perp)}{2} \right) \pm \frac{1}{2} \sqrt{(J_\perp + J'_\perp)^2 - 4J_\perp J'_\perp \sin^2(k_z c/2) \cdot (J_\perp + J'_\perp)^2 - 4J_\perp J'_\perp \sin^2(k_z c/2)}} \]  

(10)

In Eq. (7) the sum over \( \mathbf{k} \) runs over \((k_z \geq 0)\)-half of the Brillouin zone \(-\pi \leq k_x, k_y, k_z \leq \pi \) and \( c = c_b + c' \). The analytic expression for \( \gamma_{xx} \) is much simpler due to homogeneity of in-plane couplings and bond lengths

\[ \gamma_{xx} = J_1 a \left[ 1 - \frac{k_B T}{2N} \sum_{\mathbf{k}} \sin^2 k_x a \left( \frac{1}{\omega_1(\mathbf{k})} + \frac{1}{\omega_2(\mathbf{k})} \right) \right] \]  

(11)

To study the helicity moduli of the model described by the Hamiltonian (1-3) we have used Monte Carlo simulations based on the Metropolis algorithm [12]. In our finite-lattice MC simulations we have used periodic boundary conditions on lattices with \( 10 \times 10 \times 10, 20 \times 20 \times 20 \) and \( 30 \times 30 \times 30 \) sites. For a given set of parameters \( J_1, J_2, J_\perp, c_b, J'_\perp, c' \), the simulation would start at a low temperature with all phases aligned. The first 250 000 MC steps per site (sps) were thrown away followed by seven MC links of 250 000 MC sps each. At each temperature the range over which the phase angle was varied [13] was adjusted to ensure the MC acceptance rate of about 50%. The errors were calculated by breaking up each link into 5 blocks of 50 000 MC sps, then calculating the average values for each of 35 blocks and finally taking the standard deviation \( \sigma \) of these 35 average values as an estimate of the error. The final configuration of the phase angles at a given temperature was used as a starting configuration for the next higher temperature. The cumulant analysis [13] was performed using the results for the three lattice sizes to determine the value of the transition temperature \( T_c \).

3. Numerical results and conclusions

We have performed MC simulations for different choices of parameters and since they give qualitatively similar results we present here only the data for a single set of parameters \( J_1 = 1, J_2 = 0, J_\perp = 0.1, J'_\perp = 0.04, c_b = 0.4, c' = 1 \). The values of \( c_b \) and \( c' \) were chosen so that their ratio reflects the structure of YBa\(_2\)Cu\(_3\)O\(_{7-\delta}\) [14]. The value of Josephson coupling between the layers of a bilayer is taken to be one order of magnitude smaller than the in-plane Josephson coupling and the value of Josephson coupling between bilayers \( J'_\perp \) was chosen such that \( J_\perp c_b = J'_\perp c' \). Since the helicity modulus is proportional to inverse square of the magnetic field penetration depth \( \lambda(T) \) [5], we present our results for the helicity moduli in Fig. 1 as \( \lambda^2(0)/\lambda^2(T) \) as a function of \( T/T_c \). From the cumulant analysis of the numerical results for the three lattice sizes in in Fig. 1 we obtained \( k_B T_c = 1.265 \) (in the units of \( J_1 \)). This value should be compared to 0.89 – 0.95 for a two-dimensional square lattice [15-17] and 2.2 for a three-dimensional cubic lattice [18-20] (which we have also reproduced with our code) in the units of the coupling constant.
As anticipated, $\lambda^2(0)/\lambda^2(T)$ is decaying linearly at low $T$ both along the $ab$-plane and along the $c$-axis with the slopes of $-0.2366 \pm 0.0001$ and $-0.415 \pm 0.001$, respectively, as determined by the linear fits to the low-temperature data ($T \leq 0.01T_c$). These values should be compared with $-0.16667 \pm 0.00005$ which we found for our isotropic $30 \times 30 \times 30$ lattice with the periodic boundary conditions. We note that the spin-wave expansion formulae (5-11) give the slopes of 0.2367 along $ab$-plane, -0.404 along $c$-axis for our anisotropic 3D XY-model, and $-1/(6J_1) = -0.16666/J_1$ for the isotropic 3D XY-model,
in excellent agreement with our Monte Carlo result. Note that our results for the $ab$-plane helicity modulus are somewhat lower than the spin-wave result $0.25/J_1$ for two-dimensional square lattice, which is easily understood from Eqs. (10-11) when $J_\perp$ and $J'_\perp$ are one to two orders of magnitude smaller than $J_1$.

In terms of the superfluid density fraction $\rho_s = \lambda^2(0)/\lambda^2(T)$ as a function of $t = T/T_c$ the slopes are -0.30 along $ab$-plane, -0.52 along $c$-axis for our anisotropic 3D XY-model, and -0.37 for the isotropic 3D XY-model (compare with the value -0.4 reported in [7]).

Our calculations clearly demonstrate that classical phase fluctuations cannot explain the observed nonlinear temperature dependence of the $c$-axis magnetic field penetration depth for high-$T_c$ samples of YBCO [8].

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