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Anisotropy in the helicity modulus of a three-dimensional 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 XY-model of YBCO in the 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.

1. Introduction

Emery and Kivelson presented [1, 2] very strong physical arguments for the fluctuations in phase of the superconducting order parameter playing a significant role in systems with low superfluid density n_s (e.g., high-T_c copper oxide superconductors and the organic superconductors). 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_ϕ. If T_ϕ 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 Δn_s, which in turn enhances the phase fluctuations $\Delta\phi$ ($\Delta n_s\,\Delta\phi \geqslant 1/2$). 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 $\lambda(T)$ ($\lambda^{-2} \propto n_s$) for $YBa_2Cu_3O_{6.95}$ [4] gave unambiguous evidence for three-dimensional (3D) XY critical

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scaling behaviour in a temperature interval of about 10 K below $T_c = 92.74$ 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 3D 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 λ^{-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 λ^{-2} in YBCO at low temperatures.

If the phase fluctuations in the order parameter are, indeed, 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. That is, it was found that the c-axis penetration depth $\lambda_c(T)$ never has the linear temperature dependence observed in the 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] 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 $YBa_2Cu_3O_7$. 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 $YBa_2Cu_3O_7$ 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

$$H = H_{ab} + H_c, \tag{1}$$

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

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

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 neighbours 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 the 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 $\boldsymbol{A}$ is applied, its effect on the Hamiltonian is to shift the phase difference between points $\boldsymbol{r}_1$ and $\boldsymbol{r}_2$ by $A_{1,2} = 2\pi\,\boldsymbol{A}\cdot(\boldsymbol{r}_2 - \boldsymbol{r}_1)/\Phi_0$, where $\Phi_0 = hc/2e$ is the flux quantum: $\phi_{\boldsymbol{r}_1} - \phi_{\boldsymbol{r}_2} \longrightarrow \phi_{\boldsymbol{r}_1} - \phi_{\boldsymbol{r}_2} + A_{1,2}$. The momentum conjugate to $\phi_{i,l,s}$ is the charge $n_{i,l,s}$ (in 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, $\langle\dot{n}_{i,l,s}\rangle = 0$, and one obtains the *average* current conservation at each site (i,l,s). For a uniform $\boldsymbol{A}$ perpendicular to the layers, the average currents parallel to the bilayers vanish by symmetry and one has

$$\left\langle J_\perp \sin\left(\phi_{i,l,2} - \phi_{i,l,1} + \frac{2\pi}{\Phi_0}Ac_b\right)\right\rangle = \left\langle J'_\perp \sin\left(\phi_{i,l+1,1} - \phi_{i,l,2} + \frac{2\pi}{\Phi_0}Ac'\right)\right\rangle, \tag{4}$$

where the angular brackets denote the statistical average for the Hamiltonian $H(A)$: $\langle\cdots\rangle = \int\prod \mathrm{d}\phi_{i,l,s}\ \cdots\exp(-\beta H(A))/Z(A)$, $\beta = 1/(k_BT)$, $Z(A) = \int\prod \mathrm{d}\phi_{i,l,s}\exp(-\beta H(A))$. The expression on the left-hand side of equation (4) gives the average current from the site i in the $s = 1$ layer of the bilayer l into the site i of the $s = 2$ 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 the $s = 1$ layer in the adjacent bilayer $l + 1$.

Since the average currents along bonds parallel to $\boldsymbol{A}$ 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 MC method, we evaluate the average helicity modulus over all bonds parallel to $\boldsymbol{A}$:

$$\begin{aligned}\gamma_{zz} = \frac{2\pi}{\Phi_0}\Bigg\{&\frac{1}{N^3}\sum_{l,i}[J_\perp c_b\langle\cos(\phi_{i,l,2} - \phi_{i,l,1})\rangle + J'_\perp c'\langle\cos(\phi_{i,l+1,1} - \phi_{i,l,2})\rangle]\\
&- \frac{1}{k_BT}\Bigg\langle\frac{1}{N^3}\sum_{l,i}[J_\perp\sin(\phi_{i,l,2} - \phi_{i,l,1}) + J'_\perp\sin(\phi_{i,l+1,1} - \phi_{i,l,2})]\\
&\times\sum_{l,i}[J_\perp c_b\sin(\phi_{i,l,2} - \phi_{i,l,1}) + J'_\perp c'\sin(\phi_{i,l+1,1} - \phi_{i,l,2})]\Bigg\rangle\\
&+ \frac{1}{k_BT}\frac{1}{N^3}\sum_{l,i}[J_\perp\langle\sin(\phi_{i,l,2} - \phi_{i,l,1})\rangle + J'_\perp\langle\sin(\phi_{i,l+1,1} - \phi_{i,l,2})\rangle]\\
&\times\sum_{l,i}[J_\perp c_b\langle\sin(\phi_{i,l,2} - \phi_{i,l,1})\rangle + J'_\perp c'\langle\sin(\phi_{i,l+1,1} - \phi_{i,l,2})\rangle]\Bigg\}.\end{aligned} \tag{5}$$

Here, N^3 is the number of bonds parallel to $\boldsymbol{A}$. We note that computing γ_{zz} as $\partial^2F/\partial A_z^2$, 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 γ_{xx} along the x- (i.e. a-) direction is derived in an 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 γ_{zz} and γ_{xx} obtained from the spin-wave expansion in the zero-temperature limit as a check on the MC results at low temperatures. We find (in 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)

$$\gamma_{zz}(T) = \tfrac{1}{2}[(J_\perp c_b + J'_\perp c') - (J_\perp - J'_\perp)(J_\perp c_b - J'_\perp c')/(J_\perp + J'_\perp)] - \alpha_z k_b T, \tag{6}$$

where

$$\alpha_z = \frac{1}{4N}\sum_{\boldsymbol{k}}\Bigg[(J_\perp c_b + J'_\perp c')\left(\frac{1}{\omega_1(\boldsymbol{k})} + \frac{1}{\omega_2(\boldsymbol{k})}\right) - (J_\perp c_b \kappa(\boldsymbol{k}) + J'_\perp c'\kappa'(\boldsymbol{k}))\left(\frac{1}{\omega_1(\boldsymbol{k})} - \frac{1}{\omega_2(\boldsymbol{k})}\right)\Bigg], \tag{7}$$

$$\kappa(\boldsymbol{k}) = (J_\perp + J'_\perp \cos(k_z c))/\sqrt{(J_\perp + J'_\perp)^2 - 4J_\perp J'_\perp \sin^2(k_z c/2)}, \tag{8}$$

$$\kappa'(\boldsymbol{k}) = (J_\perp \cos(k_z c) + J'_\perp)/\sqrt{(J_\perp + J'_\perp)^2 - 4J_\perp J'_\perp \sin^2(k_z c/2)}, \tag{9}$$

$$\omega_{1,2}(\boldsymbol{k}) = 2J_1\left(\sin^2\frac{k_x a}{2} + \sin^2\frac{k_y a}{2}\right) + (J_\perp + J'_\perp)/2 \mp \tfrac{1}{2}\sqrt{(J_\perp + J'_\perp)^2 - 4J_\perp J'_\perp \sin^2(k_z c/2)}. \tag{10}$$

In equation (7) the sum over $\boldsymbol{k}$ runs over the $k_z \geqslant 0$ half of the Brillouin zone: $-\pi \leqslant k_x a, k_y a, k_z c \leqslant \pi$ and $c = c_b + c'$. The analytic expression for γ_{xx} is much simpler due to homogeneity of in-plane couplings and bond lengths:

$$\gamma_{xx} = J_1 a\left[1 - \frac{k_B T}{2N}\sum_{\boldsymbol{k}} \sin^2\frac{k_x a}{2}\left(\frac{1}{\omega_1(\boldsymbol{k})} + \frac{1}{\omega_2(\boldsymbol{k})}\right)\right]. \tag{11}$$

To study the helicity moduli of the model described by the Hamiltonian (1)–(3), we have used MC 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 an MC acceptance rate of about 50%. The errors were calculated by breaking up each link into five blocks of 50 000 MC sps, then calculating the average values for each of 35 blocks and finally taking the standard deviation σ 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 such that their ratio reflects the structure of $YBa_2Cu_3O_{7-\delta}$ [14]. The value of the 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 the Josephson coupling between bilayers $J'_\perp$ was chosen such that $J_\perp c_b = J'_\perp c'$. Since the helicity modulus is proportional to the inverse square of the magnetic field penetration depth $\lambda(T)$ [5], we present our results for the helicity moduli in figure 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 figure 1 we obtained $k_B T_c = 1.265$ (in units of J_1). This value

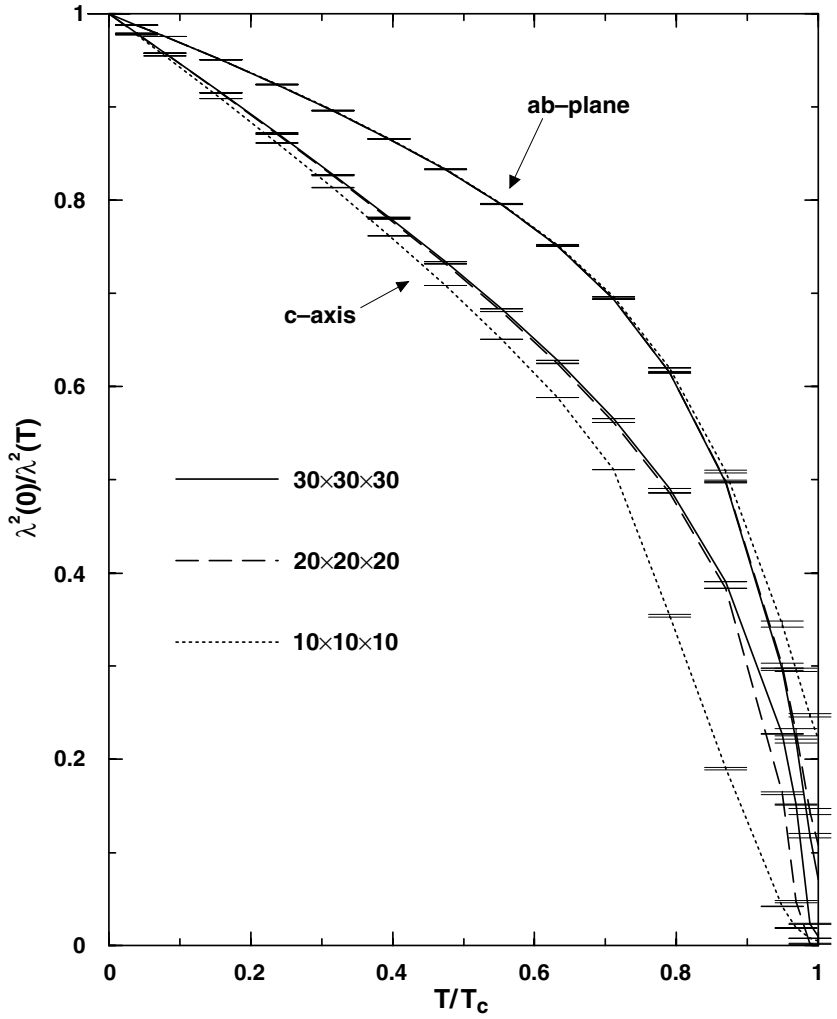

Figure 1. The temperature dependence of the helicity moduli for three different lattice sizes.

should be compared to 0.89–0.95 for a two-dimensional square lattice [15–17] and 2.2 for a 3D cubic lattice [18–20] (which we have also reproduced with our code) in units of the coupling constant.

As anticipated, $\lambda^2(0)/\lambda^2(T)$ decays linearly at low T both along the ab-plane and along the c-axis with the slopes of -0.2366 ± 0.0001 and -0.415 ± 0.001, respectively, as determined by the linear fits to the low-temperature data ($T \leqslant 0.01 T_c$). These values should be compared with $-0.166\,67 \pm 0.000\,05$ 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 the ab-plane, -0.404 along the c-axis for our anisotropic 3D XY-model, and $-1/(6J_1) = -0.166\,6\dot{6}/J_1$ for the isotropic 3D XY-model, in excellent agreement with our MC result. Note that our results for the ab-plane helicity modulus are somewhat lower than the spin-wave result $0.25/J_1$ for the two-dimensional square lattice, which is easily understood from equations (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 the ab-plane, -0.52 along the 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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