Superconducting Critical Temperature of Homologous Series of High-T_c Cuprates as a Function of Number of Layers

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We have considered a model of n-layer high-temperature cuprates of homologous series like $HgBa_2Ca_{n-1}Cu_nO_{2+2n+\delta}$ to determine the dependence of the critical temperature $T_c(n)$ on the number n of Cu–O planes in an elementary cell. Focusing on the description of the high-temperature superconducting system in terms of the collective phase variables, we have studied a semi-microscopic anisotropic three-dimensional vector XY model of stacked copper–oxide layers with adjustable parameters representing microscopic in-plane and out-of-plane phase stiffnesses. The model captures the layered composition and block structure along c-axis of superconducting homologous series. Implementing the spherical closure relation we have solved the phase XY model exactly with the help of transfer matrix method for vector variables. The calculated dependence of the critical temperature $T_c(n)$ on the block size n is monotonic with n.

PACS numbers: 74.20.–z, 74.72.–h, 74.50.+r

1. Introduction

High-temperature superconducting homologous series, like $HgBa_2Ca_{n-1}Cu_nO_{2+2n+\delta}$, are materials having the same charge reservoir, but differing by the number n of Cu–O planes in a unit cell [1, 2]. They also share the same characteristic dependence of the critical temperature as a function

of n with a maximum for $n = 3$ or $n = 4$. The origin of this extremum is still not fully understood, although, these groups of cuprates have been extensively studied [3–5]. The distances between copper–oxide planes or the content of the regions that separate them can be controlled (to some extent) in the process of synthesis of these materials. It allows us to study, how such changes influence the observed properties of these compounds like critical temperature or electrical resistivity and elucidate the role of the inter-layer coupling [6, 7].

It is well known that in spite of binding of electrons into pairs, which is essential in forming the superconducting state, however, its remarkable properties — zero resistance and Meissner effect — require the *phase coherence* among the pairs. Although, the phase order is unimportant for determining the value of the transition temperature T_c in conventional BCS superconductors, in materials with a low carrier density such as high-T_c oxide superconductors, phase fluctuations may have a profound influence on low temperature properties [8]. In particular, for cuprate superconductors, the conventional ordering of binding and phase stiffness energies appears to be reversed. Thus, a central problem of high-T_c superconductivity is the issue how pairing and phase correlations develop. The measurements of the frequency dependent conductivity, in the frequency range 100–600 GHz, show that phase correlations indeed persist above T_c, where the phase dynamics is governed by the bare microscopic phase stiffnesses [9].

In the present paper we propose a *semi-microscopic* model of n-layer cuprates, which is founded on *microscopic phase stiffnesses* that set the characteristic energy scales: in-plane $J_\parallel$, inter-plane (in-block) $J_\perp$, and inter-block $J'_\perp$ couplings (as opposed to recently presented mean-field approach for a single block of n superconducting layers, neglecting the *inter-block* coupling, see Ref. [10]). We employ an approach that goes beyond the mean field level and is able to capture both the effects of phase fluctuations and huge c-axis anisotropy on the superconducting phase transition.

2. The model

In underdoped high-temperature superconductors, two temperature scales of short-length pairing correlations and long-range superconducting order seem to be well separated [8]. We consider the situation, in which local superconducting pair correlations are established and the relevant degrees of freedom are represented by phase factors $0 \leq \varphi_\ell(\boldsymbol{r}_i) < 2\pi$, where $\boldsymbol{r}_i$ numbers lattice sites within ℓ-th ab plane. The system becomes superconducting once $U(1)$ symmetry group governing the $\varphi_\ell(\boldsymbol{r}_i)$ factors is spontaneously broken and the non-zero value of $\langle \exp[i\varphi_\ell(\boldsymbol{r}_i)] \rangle$ appears signaling the long-range phase order. The dependence of critical temperature on the c-axis block structure is of paramount importance for cuprate systems, in which two-dimensional physics predominates. We consider a multi-layer system described by the following Hamiltonian:

$$H = -J_\parallel \sum_\ell \sum_{i<j} \cos[\varphi_\ell(\boldsymbol{r}_i) - \varphi_\ell(\boldsymbol{r}_j)]$$

$$-J_\perp \sum_i \sum_m \sum_{\alpha \geq 0}^{n-2} \cos[\varphi_{mn+\alpha}(\boldsymbol{r}_i) - \varphi_{mn+\alpha+1}(\boldsymbol{r}_i)]$$

$$-J'_\perp \sum_i \sum_m \cos[\varphi_{mn+n-1}(\boldsymbol{r}_i) - \varphi_{mn+n}(\boldsymbol{r}_i)], \tag{1}$$

where $J_\parallel > 0$, $J_\perp > 0$, and $J'_\perp > 0$ are in-plane, inter-plane (in-block) $J_\perp$, and inter-block $J'_\perp$ microscopic phase stiffnesses, respectively. The factors $\varphi_\ell(\boldsymbol{r}_i)$ are placed in sites of a three-dimensional cubic lattice, where indices i and j run over sites in the ab-planes of the ℓ-th layer, while α numbers the layers within the m-th block. The partition function of the system reads:

$$Z = \int_0^{2\pi} \prod_{\ell,i} \mathrm{d}\varphi_\ell(\boldsymbol{r}_i) \exp(-\beta H[\varphi]), \tag{2}$$

where $\beta = 1/(k_\mathrm{B}T)$ with T being the temperature. Introducing two-dimensional vectors $\boldsymbol{S}_\ell(\boldsymbol{r}_i) = [S_{x\ell}(\boldsymbol{r}_i), S_{y\ell}(\boldsymbol{r}_i)]$ of the unit length $\boldsymbol{S}_\ell^2(\boldsymbol{r}_i) = S_{x\ell}^2(\boldsymbol{r}_i) + S_{y\ell}^2(\boldsymbol{r}_i) = 1$ defined by

$$\boldsymbol{S}_\ell(\boldsymbol{r}_i) = [\cos\varphi_\ell(\boldsymbol{r}_i), \sin\varphi_\ell(\boldsymbol{r}_i)], \tag{3}$$

the Hamiltonian can be written in the XY-model form:

$$H = -J_\parallel \sum_\ell \sum_{i<j} \boldsymbol{S}_\ell(\boldsymbol{r}_i)\boldsymbol{S}_\ell(\boldsymbol{r}_j)$$

$$-J_\perp \sum_i \sum_m \sum_{\alpha \geq 0}^{n-2} \boldsymbol{S}_{mn+\alpha}(\boldsymbol{r}_i)\boldsymbol{S}_{mn+\alpha+1}(\boldsymbol{r}_i)$$

$$-J'_\perp \sum_i \sum_m \boldsymbol{S}_{mn+n-1}(\boldsymbol{r}_i)\boldsymbol{S}_{mn+n}(\boldsymbol{r}_i). \tag{4}$$

In terms of the vector variables the partition function in Eq. (2) becomes

$$Z = \int_{-\infty}^{+\infty} \prod_{i,\ell} \{\mathrm{d}^2\boldsymbol{S}_\ell(\boldsymbol{r}_i)\delta[\boldsymbol{S}_\ell^2(\boldsymbol{r}_i) - 1]\} \exp(-\beta H[\boldsymbol{S}]), \tag{5}$$

where $\mathrm{d}^2\boldsymbol{S}_\ell(\boldsymbol{r}_i) \equiv \mathrm{d}S_{x\ell}(\boldsymbol{r}_i)\mathrm{d}S_{y\ell}(\boldsymbol{r}_i)$ and the Dirac-δ function $\delta[\boldsymbol{S}_\ell^2(\boldsymbol{r}_i) - 1]$ assures that the integration over $\boldsymbol{S}_\ell(\boldsymbol{r}_i)$ variables runs only over the values, which satisfy the unit length condition $\boldsymbol{S}_\ell^2(\boldsymbol{r}_i) = 1$. Unfortunately, the partition function in Eq. (5) cannot be evaluated exactly. However, replacing the rigid length constraint in Eq. (5) by a weaker spherical closure relation [11, 12]

$$\delta\left[S_\ell^2(r_i) - 1\right] \rightarrow \delta\left[\frac{1}{N}\sum_{i,\ell} S_\ell^2(r_i) - 1\right] \tag{6}$$

renders the model in Eq. (1) exactly solvable. The relation in Eq. (6) means that the unit length of the $S_\ell(r_i)$ vectors is maintained on average. However, the direct implementation of Eq. (6) is obstructed by the lack of complete translational symmetry: grouping of layers within blocks breaks translational symmetry along c-axis, since the inter-plane coupling varies with a period of n, when moving from one plane to another. As a result, the three-dimensional Fourier transform of the $S_\ell(r_i)$ variables in Eq. (3) cannot be performed. To overcome this difficulty, we implement a combination of two-dimensional Fourier transform for in-plane vector variables

$$S_\ell(r_i) = \frac{1}{N_\|}\sum_{k} S_{k\ell}\exp(-ikr_i) \tag{7}$$

and transfer matrix method for one-dimensional decorated structure along c-axis [13]. This operation diagonalizes all terms in the Hamiltonian in Eq. (4) with respect to k, leaving the dependence on the layer index ℓ unchanged.

3. Critical temperature

The partition function in Eq. (5) with help of the spherical closure relation in Eq. (6) can be determined exactly and consequently, one arrives to the equation binding the critical temperature ($k_B T_c = 1/\beta_c$) to the number of layers n and the phase stiffnesses $J_\|$, $J_\perp$, and $J_\perp'$:

$$1 = \frac{1}{n}\int_{-\frac{\pi}{a}}^{\frac{\pi}{a}}\frac{\mathrm{d}^2 k}{(2\pi/a)^2}\left.\frac{(\partial C_n(k)/\partial\zeta)\sqrt{D_n(k)} + (\frac{1}{2})(\partial D_n(k)/\partial\zeta)}{C_{n(k)}\sqrt{D_n(k)} + D_n(k)}\right|_{\zeta=\zeta_0}, \tag{8}$$

where we have defined:

$$C_n(k) = |B_n| - (\frac{\beta J_\perp'}{2})^2 |B_{n-2}|,$$

$$D_n(k) = \left[|B_n| + (\frac{\beta J_\perp'}{2})^2 |B_{n-2}|\right]^2 - (\beta J_\perp')^2 |B_{n-1}|^2, \tag{9}$$

and the Lagrange multiplier ζ results from representation of δ-function in a spectral form by the appropriate integral $\delta(x) = \int_{-i\infty}^{+i\infty}(\mathrm{d}\zeta/2\pi i)\exp(-\zeta x)$. The in-plane momentum dependence of $\lambda_1(k)$, $C_n(k)$, and $D_n(k)$ comes from $J_\|(k)$ dependence of $|B_n|$:

$$|B_n| = \frac{|B_2|}{2}(\lambda_+^{\frac{n}{2}} + \lambda_-^{\frac{n}{2}}) + \frac{|B_1|}{2}\frac{(\lambda_+^{\frac{n}{2}} - \lambda_-^{\frac{n}{2}})[2|B_2| - (\beta J_\perp)^2]}{\sqrt{\left[\zeta - \frac{\beta J_\|(k)}{2}\right]^2 - (\beta J_\perp)^2}}, \tag{10}$$

where

$$\lambda_{\pm} = \frac{1}{2}\left\{\left[\zeta - \frac{\beta J_{\parallel}(\boldsymbol{k})}{2}\right]^2 - \frac{\beta^2 J_{\perp}^2}{2} \pm \left[\zeta - \frac{\beta J_{\parallel}(\boldsymbol{k})}{2}\right]\right.$$

$$\left. \times \sqrt{\left[\zeta - \frac{\beta J_{\parallel}(\boldsymbol{k})}{2}\right]^2 - (\beta J_{\perp})^2}\right\}. \tag{11}$$

The saddle-point value ζ_0 can be determined from the condition that in criticality region order-parameter susceptibility becomes infinite

$$\left. \frac{C_n(\boldsymbol{k})\sqrt{D_n(\boldsymbol{k})} + D_n(\boldsymbol{k})}{(\partial C_n(\boldsymbol{k})/\partial\zeta)\sqrt{D_n(\boldsymbol{k})} + \frac{1}{2}\partial D_n(\boldsymbol{k})/\partial\zeta}\right|_{\boldsymbol{k}=0,\ \zeta=\zeta_0} = 0. \tag{12}$$

The closed formulae for the critical temperature can be easily obtained only for small values of n. However, for higher values of n we can resort to direct numerical evaluation of Eqs. (8) and (12) in order to compute $T_{\rm c}(n)$.

    The dependence of the critical temperature on the number of layers n in a block was presented in Fig. 1. Phase stiffnesses $J_{\parallel}$, $J_{\perp}$, and $J'_{\perp}$ were chosen to satisfy $J_{\parallel} \gg J_{\perp} > J'_{\perp}$, which is physically reasonable, since the interlayer couplings $J_{\perp}$ and $J'_{\perp}$ are much smaller than in-plane phase stiffness $J_{\parallel}$ and inter-layer (intra-block) phase stiffness $J_{\perp}$ is greater than inter-block coupling $J'_{\perp}$. We found that the critical temperature increases monotonically with n. This can be simply explained: for $n = 1$ (single-layer system) with the fixed phase stiffness $J_{\parallel}$, the critical temperature is determined by $J'_{\perp}$. On the other hand, in
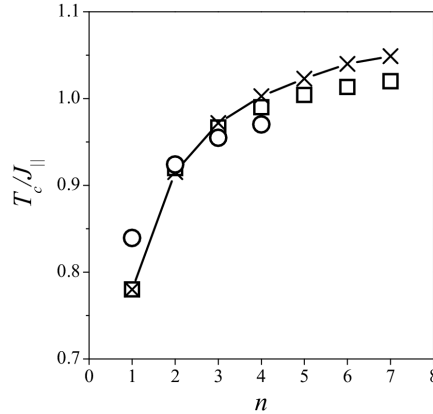

Fig. 1. Critical temperature vs. number of Cu–O layers within a block for $J_{\perp}/J_{\parallel} = 0.1$ and $J'_{\perp}/J_{\parallel} = 0.01$ (solid line with crosses). Empty squares denote the critical temperature dependence, $T_{\rm c}(n) = T_{\rm c}(1) + 0.28(1 - 1/n)$, from Ref. [4] (factor of 0.28 was chosen to fit the results of the present paper). Circles represent results from Monte-Carlo simulations of the classical XY model from Ref. [14] (the data is scaled by overall factor of 0.77).

the limit of $n \to \infty$, n-layer blocks are of infinite size and inter-block coupling $J'_\perp$ is effectively replaced by $J_\perp$ (as in the limit of infinite blocks, inter-block coupling is not important). Because $J_\perp > J'_\perp$, the critical temperature $T_c(n = \infty) > T_c(n = 1)$. For intermediate values of n, one can expect a monotonic increase in $T_c(n)$ with increasing n, as depicted in Fig. 1. In this respect, our findings are similar to the results from Ref. [4], where the increase in critical temperature of members of the same homologous series due to the interlayer Coulomb interaction was found to be $T_c(n) = T_c(1) + \text{const} \times (1 - 1/n)$. Similar results were obtained by Monte-Carlo simulations [14], where $T_c(n)$ was computed numerically by means of the Binder parameter for systems of a size up to $24 \times 24 \times 24$ [15].

We conclude that the change of the number n of layers within a block cannot alone lead to the appearance of the maximum in the critical temperature T_c as a function of n for fixed values of the microscopic phase stiffnesses. It is necessary to introduce another factor, which acts competitively to the effective increasing of inter-layer coupling (for $J_\perp > J'_\perp$) triggered by increasing n.

4. Summary and conclusions

We study a model of n-layer cuprates of homologous series like $HgBa_2Ca_{n-1}Cu_nO_{2+2n+\delta}$ to explain the dependence of the critical temperature $T_c(n)$ on the number n of Cu–O planes in the elementary cell. We focus on the "phase only" description of the high-temperature superconducting system motivated by the experimental evidence that the ordering of the phase degrees of freedom is responsible for the emergence of the superconducting state with long-range order. To this end, we have proposed a three-dimensional semi-microscopic XY model with two-component vectors that involve phase variables and adjustable parameters representing microscopic phase stiffnesses. The model fully implements the complicated stacked plane structure along c-axis to capture the layered composition of homologous series. We have solved the phase XY model exactly with the help of transfer matrix method implementing the spherical closure relation and with calculated $T_c(n)$ for chosen system parameters and arbitrary block size n. However, the obtained $T_c(n)$ dependence obtained is monotonic with n, as opposed to the experimentally observed bell-shape curve. As a result, we conclude that the change of the number n of layers within a block cannot alone lead to the appearance of the maximum in the critical temperature T_c as a function of n for fixed values of the microscopic phase stiffnesses. Since in homologous series with $n \geq 3$, Cu–O planes become inequivalent, charge rearrangement between layers within a block may occur, thus inflicting the values of in-plane phase stiffnesses and, consequently, the critical temperature. This issue will be addressed in our future works. Additionally, it would be interesting to relate the phase stiffnesses parameters used in the present paper with the microscopic material characteristics of the electronic system (like hopping parameters, antiferromagnetic exchange,

and Coulomb energy) to establish a link between our semi-microscopic approach and physics of strongly correlated systems.

Acknowledgment

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