Kosterlitz-Thouless Transition and Charge Redistribution in the Superconductivity of YBCO/PBCO Superlattices

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Recent experimental measurements of the resistive transition in $YBa_2Cu_3O_{7-x}/PrBa_2Cu_3O_{7-x}$ superlattices show a dramatic suppression in the resistive transition temperature T_c as the thickness of the Pr layer increases while the thickness of the Y layer decreases. We show that the qualitative features of these experiments (and in particular most of the suppression in T_c) can be accounted for within the Kosterlitz-Thouless theory. A small further suppression in T_c is shown to occur due to charge transfer from Y to the Pr layers.

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In recent experiments,[1-3] $YBa_2Cu_3O_{7-x}/PrBa_2Cu_3O_{7-x}$ (YBCO/PBCO) superlattices of varying layer thicknesses of both constituents were studied, with the intention of probing the effects of interlayer coupling by looking at how the intervening insulating Pr layers act in lowering the T_c. These experiments provide some very interesting possibilities. First, they obviously directly touch on the important question of whether the electron-electron interaction (lattice mediated or just due to some strong electron correlations[4] in the YBCO) has an important component of interplanar coupling. Second, and more indirectly, these experiments provide a three-dimensional system whose interlayer coupling can be weakened all the way to zero. An experimental crossover to a two-dimensional resistive transition must then occur, at some point, as a function of the Pr layer thickness, at a fixed but small superconducting current (see our concluding discussion). The third concerns the Kosterlitz-Thouless (KT) transition.[5-8] Studies of such films, for this KT transition, have been largely confined to the dirty limit.[6] For such films, however, the strong disorder combined with the low dimensionality leads to other possible interpretations than the KT one.[8] In high-T_c superlattices this transition width should be observable even in the clean limit and can, therefore, help resolve some of these subtle interpretations.[8]

In this Letter, we present a preliminary theoretical study of Refs. 1-3. We have two primary goals: (1) to correlate the experimentally measured critical temperatures with the measured resistive transition width, by combining the effects of both the KT suppression of T_c,[9] and the charge transfer from the YBCO layers; (2) to present a simple theoretical model for the superlattice, to solve it using the density-functional theory[10] (DFT), and to show that the corresponding charge transfers are consistent (in magnitude) with (1). To this end we start by reviewing some key points in the Landau-Ginzburg (LG) and KT theories.

The coupled layers, no matter how weakly coupled, have only one critical temperature (at zero uniform current flow; i.e., the thermodynamic transition) believed to be described by the LG form for the free energy:

$$F(\psi,A)=\int d^3r\left[\alpha|\psi|^2+\tfrac{1}{2}\beta|\psi|^4+\frac{\hbar^2}{2m^*}\left\{\left|\left(\frac{\partial}{\partial x}-\frac{2ie}{\hbar c}A_x\right)\psi\right|^2+\left|\left(\frac{\partial}{\partial y}-\frac{2ie}{\hbar c}A_y\right)\psi\right|^2+\gamma^{-1}\left|\left(\frac{\partial}{\partial z}-\frac{2ie}{\hbar c}A_z\right)\psi\right|^2\right\}\right]\quad(m^*\equiv 2m)\,, \tag{1}$$

where β depends on the microscopic parameters of the many-body Hamiltonian and is generally weakly temperature dependent, while $\alpha=\alpha' t^0$ with $t^0\equiv(T-T_c^0)/T_c^0$. The coupling between the layers in YBCO/PBCO can get very weak and this is reflected through $\gamma\equiv m_z/m$ with a large "mass" m_z perpendicular to the layers. The width of the critical region of Eq. (1) (with $A=0$) has been examined, for example, in Ref. 11 to linear order in $\epsilon=4-D$, with D the system's dimension. Now, when $\gamma=\infty$, fluctuations become so large that no long-range order can exist at any finite temperature. The loss of the three-dimensional long-range order implies the disappearance (at finite temperature) of the usual type of thermodynamic phase transition, e.g., a correlation length behaving like $\xi = |t|^{-\nu}$ close to the critical temperature, where $t = (T - T^*)/T^*$ with T^* the fluctuation-corrected T_c^0. However, the superfluid density (i.e., the helicity modulus)[12] can still remain finite for $t^0 < 0$, i.e., when $\gamma = \infty$ one needs to consider each two-dimensional plane independently. The appropriate free energy per plane is given by[7]

$$F = \tfrac{1}{2} K_0 \int d^2r |\nabla\phi|^2 + \frac{H_v}{k_B T}, \quad K_0 = \frac{\hbar^2 \rho_s^0(T)}{m^* k_B T}, \tag{2}$$

with H_v the contribution to the energy from the vortex-antivortex pairs of frugacity y_0, where $y_0 = e^{-E_c/k_B T}$ and E_c is the core vortex pair energy. In Eq. (2) we have assumed that $L_s \to \infty$ (see Ref. 5), and $\rho_s^0(T)$ is given by the uniform solution of Eq. (1) (with $A=0$), i.e., $\rho_s^0(T) = d|\psi|^2 = -d\alpha/\beta \equiv -\rho_0 t^0$, where d is the layer thickness.

The helicity modulus, per plane, can now be calculated.[7] One finds a finite renormalized superfluid density $\rho_s^R(T)$ [i.e., renormalized $\rho_s^0(T)$ due to H_v] below a new critical temperature T_c (the KT transition) which is different from the three-dimensional T^*. This $\rho_s^R(T)$ is given by[7]

$$K_R(T) \equiv \frac{\hbar^2}{m^*} \frac{\rho_s^R(T)}{k_B T} = \lim_{l \to \infty} K(l), \tag{3}$$

where $K(l)$ is given in terms of the KT recursion relations.[7] Above T_c free vortices are generated, leading to dephasing of $\psi(\mathbf{r})$ and to dissipation.[9]

From the above form for $\rho_s^R(T)$ the shift from T_c^0 to T_c is given by

$$\tau_c \equiv \frac{T_c^0 - T_c}{T_c} = \frac{4m^* k_B T_c^0}{\pi\hbar^2 \rho_0}. \tag{4}$$

In the clean limit, $\rho_0 = 3.3\rho$, where ρ is the electron density. In the dirty limit, $\rho_0 = 2.66\rho l/\xi_0$. In this limit, Eq. (4) can be written as[9] $g = 0.173\sigma_0/\sigma_n$, where $\sigma_0 = e^2/\hbar$ and σ_n is the sheet conductance. Finally, the form of the sheet resistance $R(T)$ around the resistive transition (i.e., close to T_c) is given by the number of unbound vortices[9] n_f as

$$R(T) \approx n_f \approx \xi(T)^{-2} \approx e^{-2(b\tau_c/\tau)^{+1/2}}, \tag{5}$$

where $\tau = (T - T_c)/T_c$. $R(T)$ will start showing strong deviation from Eq. (5) when T approaches T_c^0.

To relate b to some of the physical entries in Eq. (2), we can follow Ref. 7 and integrate the KT recursions. We write $E_c = -C_1(\hbar^2/2m^*)\rho_0 t^0$, where C_1 depends on the profile of $\psi(\mathbf{r})$ inside the core [i.e., $|\mathbf{r}| < (2m|\alpha|)^{-1/2}$] and whether the system is in the clean or dirty limit. The form of b we get is

$$b = C_2 z \frac{T_c^0}{T_c} e^{2z} \left[1 + C_1^{-1} \pi^{3/2} z^2 \frac{T_c^0}{T_c} e^{-z} \right]^{-1/2}, \tag{6}$$

where $z = C_1(\hbar^2/2m^*)\rho_0\tau_c/k_B T_c^0$. The coefficient C_2 is related to the somewhat arbitrary choice for the end point of $y(l)$. Assuming a linear dependence for $\psi(\mathbf{r})$ inside the core, we get in the clean limit, $z \approx 7m/\bar{m}$ and $C_1 \approx m/\bar{m}$, and in the dirty limit, $z \approx 1$ and $C_1 \approx 1$. ($\bar{m}$ is the effective mass in the YBCO plane.)

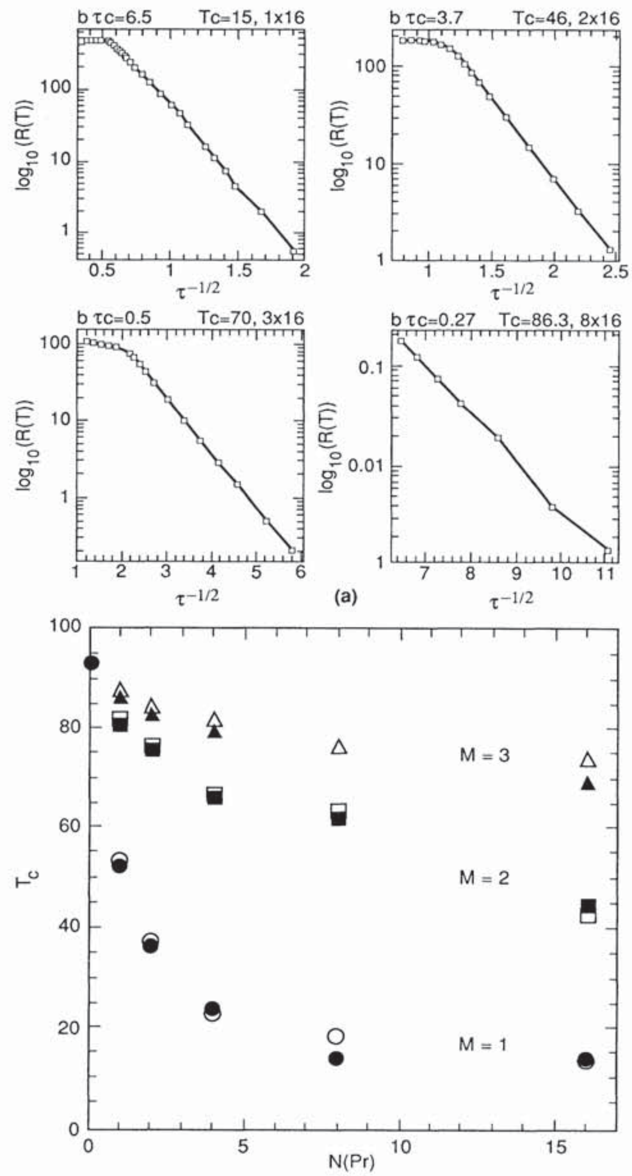

FIG. 1. (a) The linear region of $\log_{10}[R(T)]$ vs $\tau^{-1/2}$ representing the KT resistive transition region (see text). Four samples are displayed with $M = 1$, 2, 3, and 8 layers of YBCO and a fixed and very large ($N = 16$) number of intervening layers of PBCO. (b) Comparison of the measured T_c's, solid markers (from the position of the linear KT region, see text), and theoretically predicted values, open markers (from KT depression of T_c^0 and charge transfer, see text), for $M = 1$, 2, 3, and a range of layer thicknesses.

We next interpret the experimental result of Ref. 2 using the KT resistive transition. We are *assured* experimentally of a two-dimensional system when quantities within the YBCO *do not* change as a function of PBCO thickness. From Figs. 2 and 3 of Ref. 2 this occurs (to a high degree of accuracy) when the number of layers N of PBCO equals or exceeds 16. We therefore, primarily focus our attention on four samples: all with $N=16$ and $M=1$, 2, 3, and 8 layers of YBCO. These $\log_{10}[R(T)]$ are displayed in Fig. 1(a). Using Eq. (5) along with the experimental slopes in the linear region and the absolute position (in temperature) of this linear region, we get $b\tau_c \approx 6.5$ and $T_c \approx 15$ K, $b\tau_c \approx 3.7$ and $T_c \approx 46$ K, $b\tau_c \approx 0.5$ and $T_c \approx 70$, $b\tau_c = 0.27$ and $T_c = 86$ K for $M=1$, 2, 3, and 8 respectively. From the range of the linear region, we get $\tau_c \approx 3.8$, $\tau_c \approx 0.9$, $\tau_c \approx 0.24$, and $\tau_c \approx 0.02$ for $M=1$, 2, 3, and 8, respectively. Therefore, $b \approx 1.7$, $b \approx 4.1$, $b \approx 2.1$, and $b \approx 13.5$ for $M=1$, 2, 3, and 8, respectively. Finally, from these values of T_c and τ_c, we get $T_c^0 \approx 72$ K, $T_c^0 \approx 87$ K, $T_c^0 \approx 87$ K, and $T_c^0 \approx 88$ K for $M=1$, 2, 3, and 8, respectively. As we shall see below, these results imply a *close* consistency between the measured T_c's and the measured critical widths τ_c's (see Fig. 1) and lend strong support to the KT scenario. We finally note that as yet another support for the KT interpretation, we find that Eqs. (4) and (6) also provide a good qualitative description for the trends of both τ_c's and b's as a function of M.

We found that the mean-field (BCS) values for T_c^0 (at $N=16$) were close to their bulk YBCO values. Nevertheless, some suppression of T_c is evident; in particular for $M=1$. (The corresponding value of $T_c^0=72$ implies an additional suppression of ≈ 20 K.) We then next propose a theoretical model for this suppression, which is due to the variation of the hole concentration ρ, in the YBCO layers, as a function of the PBCO and YBCO layer thickness. Now this ρ is rigorously described by the DFT (Ref. 10) provided the exchange and correlation energy functional $E_{\rm xc}(\rho)$ is exactly known; it is not. This is particularly serious in the strongly correlated high-T_c perovskites. In fact, such a DFT (with best available $E_{\rm xc}$) for all the PBCO electrons does not even lead to the appropriate insulating ground state. We must then focus on the free carriers in the YBCO only and put in the insulting structure by hand; i.e., all the other electrons and lattice provide an appropriate effective potential (a "pseudo" potential) for the free hole carriers of density ρ.

Two features are particularly important. (a) The h-h interaction is screened by the very large dielectric constant ϵ of the background (see, e.g., Ref. 13) in these perovskites. (b) The relatively low ρ implies a small Fermi momentum k_F.

The Thomas-Fermi screening length $\lambda_{\rm TF} = [\hbar^2 \pi\epsilon/(4m_e k_F e^2)]^{1/2}$ is then quite large (≈ 20 Å); i.e., the screening is ineffective and is the reason for the variation in ρ at large YBCO and PBCO thickness (see Fig. 3 of Ref. 2).

In our model, then, the superlattice is treated as being composed of an infinite sequence of M Y layers followed by N Pr, where each layer is treated as a plane with a distance of $d=12$ Å to its neighbors. Thus, the Cu-O plane-chain-plane structure (PCP) in each of these layers is assumed to be represented by a single conducting plane. The M Y layers each possess a "background" charge distribution of -1, and a compensating "free" two-dimensional charge of $+1$ (representing an extra hole per PCP characteristic of a bulk 1-2-3 superconductor) is also placed on these planes. In contrast, the background charge on the Pr layers is assumed to be zero and there are no carriers induced on the PCP associated with Pr layers. This corresponds to the assumption that all Pr is in the 4^+ state which seems to be the case experimentally. (This, however, is not necessary and our model would apply equally for intermediate valence.)

Writing the many-body ground-state energy of the above system as a functional of the density $\rho(\mathbf{r})$, we minimize the energy to obtain the charge distributions ρ_i on the Y and Pr layers. In 2D, $\rho = \hbar^2 k_F^2/2\pi$, and the average energy $E_{\rm av} = \frac{1}{2} E_F$ for a free-electron gas. This leads to $T = \pi\hbar^2\rho/2m_e$ per particle. Similarly, $E_{\rm xc}$ is approximated by exchange alone $E_{\rm ex}$.[14] Including the Coulomb term we get

$$\frac{\pi\hbar^2}{m_e}\rho_i - \frac{4e^2}{\sqrt{2\pi}\epsilon}\rho_i^{1/2} + \frac{e^2}{\epsilon}\sum_j (\rho_j - \bar{\rho}_j)\int d^2 r_j \frac{e^{-k_0 r_{ij}}}{r_{ij}} - \lambda = 0 \quad (k_0 \to 0)\,, \tag{7}$$

with ρ_i the discrete values of $\rho(\mathbf{r})$ per layer and λ a Lagrange multiplyer from the requirement of overall charge neutrality. Equation (7) is then solved numerically for the ρ_i's using $\epsilon=25$ and $m_e=0.55$.[15] With these results for ρ_i the suppression in T_c^0 is evaluated using the experimentally measured relation between the bulk hole density, in the YBCO, and the critical temperature.[16] The additional suppression in the T_c^0 is very well accounted for [see Fig. 1(b)]. This relatively small additional suppression in T_c is supported by recent exciting experiments[17] where the PBCO is doped with hole donors (with Ca). *The additional donor density can be made to restore the bulk YBCO density, yet it is found that it only elevates T_c (e.g., for $M=1$) by ≈ 20 K.*[17]

We conclude with final remarks on the crossover from 2D to 3D. For any finite interlayer coupling (i.e., $\gamma^{-1} \neq 0$), the 2D vortex pairs must be replaced by vortex loops. Such vortex loop excitations should not modify the nature of the thermodynamic phase transition at T^* (see above). In addition, in the limit of zero supercurrent flow j_s, such vortex loops cannot dephase $\psi(\mathbf{r})$, i.e., produce dissipation. Below T^*, coherence between the YBCO layers exists; above T^* this coherence is lost, but still for $j_s \rightarrow 0$ and $\gamma^{-1} \neq 0$ only weak dissipation can exist below T_c^0. For larger j_s (sufficiently large to tear the vortex loop) dissipation starts above T_c, i.e., the resistive transition. We believe that this certainly occurs for the very large PBCO widths. Furthermore, the theoretical understanding of the exciting and subtle crossover behaviors for thinner PBCO layers can be guided by such experiments on perovskite superlattices.[1-3]

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