c-axis resistivity in high-T_c superconductors

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The interactions between polarons and the anharmonic vibrations of the apical oxygen atoms in the normal state of $YBa_2Cu_3O_{7-\delta}$ superconductors have been studied by using a path integral formalism. The temperature effects in the distribution of double-well potentials associated with the anharmonic modes have been taken into account. It is shown that the c-axis electrical resistivity depends linearly on temperature for intermediate values of the overall electron-phonon coupling, whereas strong anharmonicity induces a nonmetallic behavior as a consequence of trapping of the charge carriers.
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During the last years, many theoretical and experimental investigations have been devoted to the physics of polarons in high-T_c superconductors (HTSC's). While experimental evidence has suggested that polarons are present in the normal state of some HTSC's,[1] it is still unclear whether and how condensation of polarons could take place in these systems.[2–6] Many puzzling physical properties of the HTSC's have been interpreted in terms of polaronic models.[7] Hall coefficient and T-linear electrical resistivity in $YBa_2Cu_3O_{7-\delta}$ have been quantitatively explained[8] by assuming that the normal state contains a nondegenerate gas of singlet bipolarons and that a fraction of them Anderson localizes because of disorder. The effects of interplanar disorder on the c-axis resistivity ρ_c have been discussed in the framework of a model[9] which assumes a metallic ground state for an anisotropic three-dimensional system. The magnitude of the negative $d\rho_c/dT$ has been correlated with the deviation from linearity in the planar resistivity as due to decreasing hole concentration. So far, the origins of the unusual c-axis transport properties of the cuprates are unknown, but the presence of the apical oxygen atoms is believed to play a role.[10] In a previous paper[11] I studied the conditions for localization of polarons in systems with structural lattice instabilities, focusing on the time-retarded nature of the interactions between a double-well potential (DWP) and the surrounding fermionic excitations. The model was applied to evaluate the electrical resistivity $\rho(T)$, and in particular it was shown that a negative $d\rho/dT$ can arise on the low-temperature side as a consequence of polaron trapping in the double-well potential associated with the lattice instability. However, our calculation did not include the effects of a distribution of DWP's, which, in fact, should be present in real systems. More specifically, the hopping time τ_0 between the minima of the DWP was treated as a phenomenological parameter and its temperature dependence was neglected. This paper is aimed at establishing that the procedure described in Ref. 11 is accurate at low temperatures (up to around 50 K), whereas, at higher temperatures, the phenomenological hopping time there considered is much longer than the correct one. The consequences on the high-temperature behavior of the electrical resistivity will be pointed out. First, let us sum up the main features of our model. The tightly bound electronic states of the system are described by the independent boson model in which one fixed electron is immersed in a cloud of phonons. This fermionic excitation (polaron) interacts with a double-well potential in a two-state configuration (two-level system), arising from an anharmonic vibrational mode. The interaction Hamiltonian $H_{\rm int}(\tau)$ between the DWP and the polaron is given by

$$H_{\rm int}(\tau) = -2\lambda Q(\tau)\tilde{c}^{\dagger}(\tau)\tilde{c}(\tau), \tag{1}$$

where λ is the electron-phonon coupling constant for the vibrational mode giving origin to the DWP. τ is the time in the Matsubara Green's function formalism and $Q(\tau)$ is the one-dimensional path for the atom which moves back and forth in the DWP. $\tilde{c}^{\dagger}(\tau)$ and $\tilde{c}(\tau)$ are the polaronic creation and annihilitation operators, respectively. The tightly bound electrons interact with a potential having an internal degree of freedom provided by the local lattice instability. This interaction is not magnetic in origin since the spin variables have not been considered. One hopping path for the atom is characterized by the number $2n$ of hops, by the set t_i of instants at which the ith hop takes place, and by the hopping time τ_0 between the minima of the DWP. The closure condition on the path is given by $(2n-1)\tau_s + 2n\tau_0 = \beta$, where β is the inverse temperature and τ_s is the time one atom is sitting in a well. The full partition function for the system is obtained by summing over all possible linear (in τ) paths for the atom. The result, to third order in λ, is

$$Z_T = \sum_{n=0}^{\infty} \int_0^{\beta} \frac{dt_{2n}}{\tau_0} \cdots \int_0^{t_2-\tau_0} \frac{dt_1}{\tau_0} \exp[-\beta E(n,t_i,\tau_0)],$$

$$E(n,t_i,\tau_0) = \frac{1}{\beta}\Bigg[2\lambda Q_0 B e^{A\cosh(\omega_0\beta/2)}(4n\tau_0-\beta) + (\lambda Q_0)^2 B^2 e^{2A} g(n,\tau_0,\omega_0,\beta) + \frac{2}{3}(\lambda Q_0)^3 B^3 e^{3A} h(n,\tau_0,\omega_0,\beta) - (K^{(2)}+K^{(3)}) \sum_{i>j}^{2n} \left(\frac{t_i-t_j}{\tau_0}\right)^2 \Bigg], \tag{2}$$

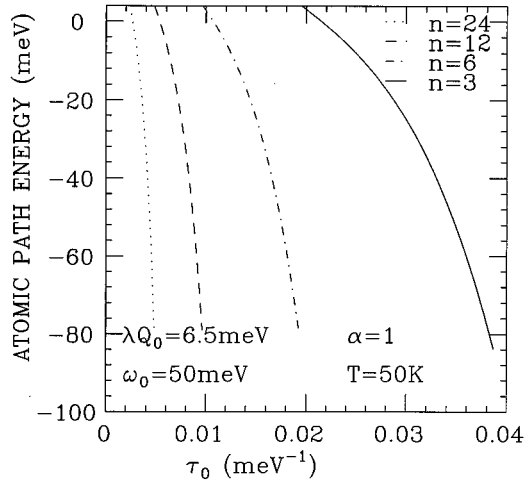

FIG. 1. Atomic path energies vs hopping time between the minima of the double-well potential for four linear hopping paths. The Einstein phonon frequency ω_0 is 50 meV. The tunneling energy λQ_0 between the minima is 6.5 meV. The temperature is set at 50 K, and the overall electron lattice coupling α is 1.

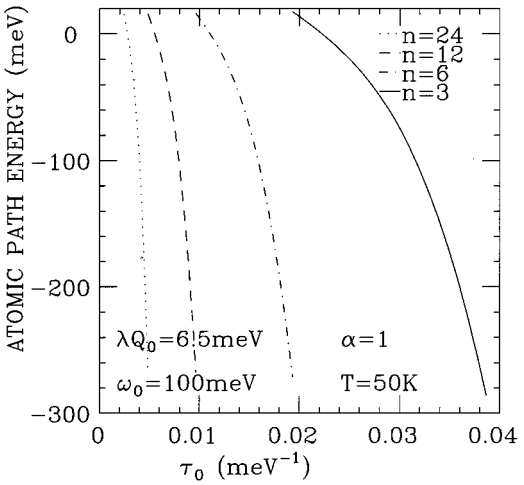

FIG. 2. As in Fig. 1, but with $\omega_0 = 100$ meV.

where Q_0 is the position of the minimum in the DWP, ω_0 is the typical phonon frequency in the Einstein model, and the functions A and B depend on temperature through the Bose distribution factor. Full expressions for the functions $h(n,\tau_0,\omega_0,\beta)$ and $g(n,\tau_0,\omega_0,\beta)$ are reported in Ref. 11 together with further details on the calculations. $K^{(2)}$ and $K^{(3)}$ are the effective couplings for the two physical processes (polaron-polaron attraction and DWP-polaron repulsion) which compete in the system. It is evident from Eq. (2) that the time-retarded nature of the interacting system is accounted for by the path integral method for any value of the coupling constants.[12] The one-path atomic energy function $E(n,\tau_0)$ should be minimized with respect to τ_0 in order to get the τ_0 value for the dominant path. I have carried out numerical calculations of $E(n,\tau_0)$ for several sets of the input parameters λ, Q_0, and ω_0 and the overall electron-lattice coupling α. In Fig. 1, $E(n,\tau_0)$ is reported on versus τ_0 for four values of n, at fixed temperature ($T=50$ K). The bare tunneling frequency λQ_0 is 6.5 meV, consistent with some experimental values on superconducting $YBa_2Cu_3O_{7-\delta}$ obtained by extended x-ray-absorption fine-structure techniques.[13] The Einstein phonon frequency ω_0 is set at 50 meV, a typical value for optical modes, as can be seen in experimental vibrational spectra.[14,15] α is taken equal to 1, thereby assuming that a relatively strong-coupling regime applies to the system. $E(n,\tau_0)$ gets the minimum value at the highest τ_0 value allowed by the boundary condition on the path, that is, at $(\tau_0)_{\max}=(2nK_BT)^{-1}$. This result, which is general, provides a criterion to determine the dominant path for the atom at any temperature. The dominant path is a sawtooth path, which is achieved once the sitting time τ_s tends to zero. Note that, at $T=10$ K, a path with $n=4$ hops would yield a $(\tau_0)^{-1}_{\max}\simeq 6.5$ meV, which is consistent with the phenomenological assumption made in Ref. 11, $(\tau_0)^{-1}\simeq\lambda Q_0$. By increasing temperature, the number of hops in the dominant path should decrease: At $T=50$ K, $(\tau_0)^{-1}_{\max}\simeq 6.5$ meV only if $n=1$. At $T>50$ K, no consistency can be achieved since the $(\tau_0)^{-1}_{\max}$, which minimizes the atomic path energy, is much bigger than λQ_0 for any number of hops. Then the phenomenological procedure we used in Ref. 11 is justified at low temperatures, whereas, at $T>50$ K, the correct hopping time (here determined) turns out to be shorter than the τ_0 value of Ref. 11. By increasing the number of hops, at fixed temperature, the range of allowed τ_0 values shrinks and the minimum atomic path energy becomes slightly less negative. Then the deepest bound states for the oscillating atom are associated with paths having a low number of hops. In Fig. 2, the one-path atomic energy is plotted versus τ_0 by assuming an Einstein frequency $\omega_0 = 100$ meV. The hardening of the phonon spectrum implies that polarons become heavier and their mobility is slowed down. As a consequence, polarons are less effective in inducing atomic scattering between the minima of the DWP, and accordingly the oscillating atom lowers its bound-state energy. Let us come now to the one-path coupling constants.[11] $K^{(2)}$, which is negative, describes the attractive part of the interaction between polarons arising in the system as a consequence of the self-trapping induced by the double-well potential. The sign of $K^{(3)}$ depends on the number of hops in the path: However, for the dominant path $\tau_0=(\tau_0)_{\max}$, the inequality $2n\tau_0>\beta/2$ is fulfilled and $K^{(3)}$ is repulsive at any T. The effective interaction strengths $\langle K^{(2)}\rangle$ and $\langle K^{(3)}\rangle$ can be obtained as a function of T by summing over n the dominant path contributions,

$$\langle K^{(2)}\rangle = -(\lambda Q_0)^2 B^2 e^{2A}\omega_0^2 \sum_{n=1}^{N} (\tau_0)^4_{\max},$$

$$\langle K^{(3)}\rangle = -2(\lambda Q_0)^3 B^3 e^{3A}\omega_0^2 \sum_{n=1}^{N} (\tau_0)^4_{\max}[2n(\tau_0)_{\max}-\beta/2], \tag{3}$$

and, using the result $\Sigma_{n=1}^{N} n^{-4}\simeq(1-N^{-3})/3$, we get

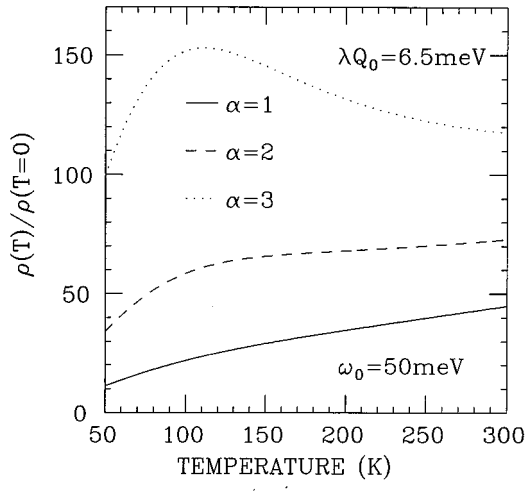

FIG. 3. Electrical resistivity vs temperature for three values of α. The other parameters are chosen as in Fig. 1.

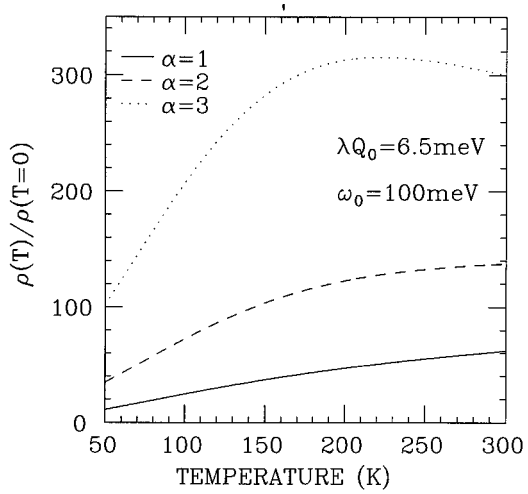

FIG. 4. Electrical resistivity vs temperature for three values of α. The other parameters are chosen as in Fig. 2.

$$\langle K^{(2)}\rangle = -\frac{(\lambda Q_0)^2 B^2 e^{2A}\omega_0^2}{3(2K_BT)^4}(1-N^{-3}),$$

$$\langle K^{(3)}\rangle = -\frac{2(\lambda Q_0)^3 B^3 e^{3A}\omega_0^2}{3(2K_BT)^5}(1-N^{-3}). \qquad (4)$$

The particular form of the maximum hopping time suggests that paths with a low number of hops provide the largest contribution to the effective interaction strengths in the temperature range (above 50 K) we are considering here. This observation allows one to choose a small cutoff ($N\simeq 4$) in the sum over n in Eqs. (3) and also in full partition function calculations [see Eq. (1)]. Instead, many hops paths should be considered at low temperatures where they provide the relevant excitations for the trapping of the charge carriers. The electrical resistivity can be calculated on the base of Eqs. (4) by assuming that polarons are scattered by the impurity potential due to the lattice instability. In Fig. 3, $\rho(T)$ normalized to the residual resistivity (which is 2.7 mΩ cm in our model) is reported for three values of α. The input parameters λQ_0 and ω_0 are chosen as in Fig. 1. Note that in a very-strong-coupling regime ($\alpha=3$), a negative $d\rho/dT$ arises in the system due to off diagonal scattering of the charge carriers by the DWP's distribution. It is remarkable that the resistivity upturn shows the maximum at around 100 K that is, in the range of the critical transition temperature of many HTSC compounds. In these systems structural lattice instabilities are believed to influence the out-of-plane electrical transport,[10] and in particular, the high c-axis scattering rate in $YBa_2Cu_3O_{7-\delta}$ is likely due to the c-axis vibrational mode associated with the apical oxygen atoms (two per unit cell in $YBa_2Cu_3O_{7-\delta}$). Recently, a careful Raman investigation[14] on superconducting $YBa_2Cu_3O_{7-\delta}$ has pointed out that the anharmonic character of the apex vibrations (and, more, of the plane oxygen in-phase modes) grows by decreasing the amount of oxygen in the sample. Underdoped $YBa_2Cu_3O_{7-\delta}$ shows a negative $d\rho_c/dT$ above T_c and high ρ_c values.[16] Then, structural defects at low hole concentration should increase α, hence the anharmonicity of the system, leading to the observed ρ_c behavior. By lowering α in Fig. 3, polarons increase their mobility, the absolute values of resistivity are strongly reduced (by a factor of 10 at 100 K), and the resistivity slope changes drastically. At $\alpha=1$ a linear-T resistivity emerges for $T>200$ K. This behavior can be understood as follows: By increasing T, paths with a decreasing number of hops become available to provide the relevant DWP excitations which act as scatterers for mobile polarons; on the other hand, the atomic hopping time between the minima of the DWP decreases as T^{-1}, and accordingly it becomes harder for polarons to see the internal degree of freedom in the scattering potential. By growing temperatures, trapping effects are less likely to occur, the mean free path for charge carriers does not saturate, and the resistivity grows. In this picture, the linear-T resistivity is essentially due to diagonal scattering of polarons in systems with intermediate values of electron-lattice coupling. By enhancing the phonon spectrum, $\omega_0=100$ meV in Fig. 4, the resistivity maximum, for $\alpha=3$, is shifted upwards in the temperature scale $T\simeq 200$ K, whereas saturation effects clearly appear at $T\geqslant 200$ K for $\alpha<3$. The bare tunneling frequency does not affect the $\rho(T)$ slope while the absolute values of ρ essentially scale as $\rho\propto 1/(\lambda Q_0)$. It is encouraging that our choice for λQ_0 leads to ρ values which are in the range of the experimental data for $YBa_2Cu_3O_{7-\delta}$ compounds.

In conclusion, the path integral method here developed allows one to study the dynamical interactions between structural lattice instabilities and polaronic charge carriers as a function of temperature. I have carried out a numerical calculation for the energy of an atom moving in a double-well potential surrounded by polarons so that, at any temperature, we are able to determine the atomic paths which mostly contribute to the partition function of the interacting system. The theory has been applied to evaluate the out-of-plane electrical resistivity in high-T_c superconductors by choosing input parameters which are appropriate for those systems (markedly $YBa_2Cu_3O_{7-\delta}$). The superconducting transition is not accounted for by the present model. We find a negative $d\rho/dT$ (associated with high ρ values) for a strong-coupling regime in which off-diagonal polaron scat-

tering by double-well potentials is dominant. In this framework, the anharmonicity of some vibrational modes (enhanced in underdoped systems) is responsible for the negative resistivity slope. By reducing the strength of the overall electron-phonon coupling, polarons become more mobile, and by increasing the temperature, only paths with a small number of hops are available for polaron scattering. Then the charge carriers are unlikely trapped by the structural instabilities and the resistivity grows linearly with temperature.

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[1] See, e.g., *Proceedings of the International Workshop on Anharmonic Properties of High T_c Cuprates*, Slovenia, edited by D. Mihailovic, G. Ruani, E. Kaldis, and K. A. Müller (World Scientific, Singapore, 1995).

[2] A. S. Alexandrov and N. F. Mott, Supercond. Sci. Technol. **6**, 215 (1993).

[3] J. Ashkenazi, J. Supercond. **8**, 1 (1995).

[4] J. Mustre de Leon, I. Batistic, A. R. Bishop, S. D. Conradson, and S. A. Trugman, Phys. Rev. Lett. **68**, 3236 (1992).

[5] Chen Qinghu, Fang Minghu, Zhang Qirui, Wang Kelin, and Wan Shaolong, Phys. Rev. B **53**, 11 296 (1996).

[6] A. La Magna and R. Pucci, Phys. Rev. B **53**, 8449 (1996).

[7] D. Emin, Phys. Rev. B **45**, 5525 (1992).

[8] A. S. Alexandrov, A. M. Bratkovsky, and N. F. Mott, Phys. Rev. Lett. **72**, 1734 (1994).

[9] A. G. Rojo and K. Levin, Phys. Rev. B **48**, 16 861 (1993).

[10] Y. Zha, S. L. Cooper, and D. Pines, Phys. Rev. B **53**, 8253 (1996).

[11] M. Zoli, Phys. Rev. B **53**, 9074 (1996).

[12] R. P. Feynman, Phys. Rev. **97**, 660 (1955).

[13] J. Mustre de Leon, S. D. Conradson, I. Batistic, and A. R. Bishop, Phys. Rev. Lett. **65**, 1675 (1990); P. G. Allen, J. Mustre de Leon, S. D. Conradson, and A. R. Bishop, Phys. Rev. B **44**, 9480 (1991); E. A. Stern, M. Qian, Y. Yacoby, S. M. Heald, and H. Maeda, Physica C **209**, 331 (1993).

[14] D. Palles, N. Poulakis, E. Liarokapis, K. Conder, E. Kaldis, and K. A. Müller, Phys. Rev. B **54**, 6721 (1996).

[15] T. Egami and S. J. L. Billinge, *Progress in Materials Science* (Elsevier Science, New York, 1994), pp. 359–424.

[16] T. Ito, H. Takagi, S. Ishibashi, T. Ido, and S. Uchida, Nature (London) **350**, 596 (1991); M. Liu and D. Y. Xing, Phys. Rev. B **49**, 682 (1993).