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ARPES-parameterized Hubbard approach to *d*-wave cuprate superconductors

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Abstract. In the last decade, the Angle Resolved Photoemission Spectroscopy (ARPES) has achieved important advances in both energy and angular resolutions, providing a direct measurement of the single-particle dispersion relation and superconducting gap. These dispersion relation data allow a full determination of the self-energy, first and second neighbor parameters in the Hubbard model. This model and its generalizations offer a simple and general way to describe the electronic correlation in solids. In particular, the parameters of correlated hopping interactions, responsible of the *d*-wave superconductivity in the generalized Hubbard model, are determined from ARPES data and the critical temperature within the mean-field approximation. In this work, we determine the model parameters for $Bi_2Sr_{2-x}La_xCuO_{6+\delta}$ and study its *d*-wave superconducting gap as a function of temperature by solving numerically two coupled integral equations. Finally, the calculated electronic specific heat is compared with experimental results.

Keywords: ARPES, *d*-wave superconductors, Hubbard model.
PACS: 74.20.-z, 74.20.Rp, 74.25.Jb

INTRODUCTION

Experimental evidence such as the spontaneous generation of a half-flux quantum at the meeting point of Josephson coupled superconducting crystals [1], as well as the corner superconducting quantum interference device (SQUID) made of a conventional superconductor and two orthogonally oriented plane faces of a single ceramic superconductor [2], strongly suggest the existence of a *d*-wave order parameter in many ceramic superconductors. In these cuprates, the charge carriers are confined to move mainly on the CuO_2 planes. Therefore, three-band Hubbard models have been proposed to describe the dynamics of the carriers on these planes [3], and the electronic states close to the Fermi energy can be well described by a single-band tight-binding model on a square lattice with a second-neighbor hopping [4]. Furthermore, it has been shown that the second-neighbor correlated-hopping interactions can lead to *d*-wave superconducting ground states [5]. Even in this single-band generalized Hubbard model there are several parameters that should be determined. In this article, we find out single- and correlated-electron-hopping parameters for $Bi_2Sr_{2-x}La_xCuO_{6+\delta}$ (BSLCO), within the mean-field approximation, from the angle-resolved photoemission spectroscopy (ARPES) experimental data [6]. We have previously applied this method to $La_{2-x}Sr_xCuO_4$ systems finding a good agreement between the theoretical results and experimental data of the critical temperature (T_c) as well as the electronic specific heat [7]. Once the model parameters are determined, the *d*-wave superconducting gap as a function of temperature can be obtained by solving two coupled integral equations [7]. Finally, the temperature behavior of the theoretical normalized electronic specific heat of $Bi_{1.74}Sr_{1.88}Pb_{0.38}CuO_{6+\delta}$ was obtained, observing a good agreement with experimental data [8].

THE MODEL

Let us consider a single-band square-lattice Hubbard model with on-site Coulombic interaction (U), first- (Δt) and second-neighbor (Δt_3) correlated-hopping interactions. Certainly, Δt and Δt_3 are always present in real materials and essential in the determination of the superconducting symmetry in spite of having small strengths. The corresponding Hamiltonian can be written as

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$$\hat{H} = \varepsilon_0 \sum_{i,\sigma} \hat{c}^{+}_{i,\sigma}\hat{c}_{i,\sigma} + t \sum_{\langle i,j\rangle,\sigma} \hat{c}^{+}_{i,\sigma}\hat{c}_{j,\sigma} + t' \sum_{\langle\langle i,j\rangle\rangle,\sigma} \hat{c}^{+}_{i,\sigma}\hat{c}_{j,\sigma} + U \sum_{i} \hat{n}_{i,\uparrow}\hat{n}_{i,\downarrow} + \Delta t \sum_{\langle i,j\rangle,\sigma} \hat{c}^{+}_{i,\sigma}\hat{c}_{j,\sigma}(\hat{n}_{i,-\sigma} + \hat{n}_{j,-\sigma}) + \Delta t_3 \sum_{\substack{\langle\langle i,j\rangle\rangle,\sigma \\ \langle i,l\rangle\langle j,l\rangle}} \hat{c}^{+}_{i,\sigma}\hat{c}_{j,\sigma}\hat{n}_{l} \qquad (1)$$

where $\hat{c}^{+}_{i,\sigma}$ ($\hat{c}_{i,\sigma}$) is the creation (annihilation) operator with spin σ = ↓ or ↑ at site i, $\hat{n}_{i,\sigma} = \hat{c}^{+}_{i,\sigma}\hat{c}_{i,\sigma}$, $\hat{n}_i = \hat{n}_{i,\uparrow} + \hat{n}_{i,\downarrow}$, $\langle i,j\rangle$ and $\langle\langle i,j\rangle\rangle$ respectively denote first- and second-neighbor sites. In fact, in the last term of Eq. (1), l is a first-neighbor site of both i and j, which are second neighbors. The interaction terms of Eq. (1) are schematically illustrated in Figures 1(a) for onsite Coulomb interaction (U), 1(b) for first-neighbor correlated hopping (Δt), and 1(c) for second-neighbor correlated hopping (Δt_3) involving three sites. This model can lead to s- and d-wave superconducting ground states without negative U [5].

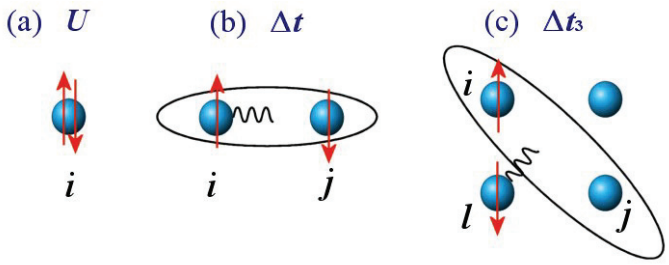

FIGURE 1. Illustration of (a) onsite Coulomb interaction (U) between electrons with opposite spins (red arrows), (b) first-neighbor correlated hopping (Δt), and (c) second-neighbor correlated hopping (Δt_3) involving three sites, where the ellipses indicate the bond associated to the electron hopping and the wavy line represents the interaction between electron and the bond charge.

Performing a Fourier transform, this Hamiltonian in the momentum space becomes

$$\hat{H} = \sum_{\mathbf{k},\sigma} \varepsilon(\mathbf{k}) \hat{c}^{+}_{\mathbf{k},\sigma}\hat{c}_{\mathbf{k},\sigma} + \frac{1}{N_S} \sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} V_{\mathbf{k},\mathbf{k}',\mathbf{q}} \hat{c}^{+}_{\mathbf{k}+\mathbf{q},\uparrow}\hat{c}^{+}_{-\mathbf{k}'+\mathbf{q},\downarrow}\hat{c}_{-\mathbf{k}'+\mathbf{q},\downarrow}\hat{c}_{\mathbf{k}+\mathbf{q},\uparrow} + \frac{1}{N_S} \sum_{\mathbf{k},\mathbf{k}',\mathbf{q},\sigma} W_{\mathbf{k},\mathbf{k}',\mathbf{q}} \hat{c}^{+}_{\mathbf{k}+\mathbf{q},\sigma}\hat{c}^{+}_{-\mathbf{k}'+\mathbf{q},\sigma}\hat{c}_{-\mathbf{k}'+\mathbf{q},\sigma}\hat{c}_{\mathbf{k}+\mathbf{q},\sigma} \qquad (2)$$

where N_s is the total number of sites,

$$\varepsilon(\mathbf{k}) = \varepsilon_0 + 2t\left[\cos(k_x a) + \cos(k_y a)\right] + 4t' \cos(k_x a)\cos(k_y a)\,, \qquad (3)$$

$$V_{\mathbf{k},\mathbf{k}',\mathbf{q}} = U + \Delta t\left[\beta(\mathbf{q}+\mathbf{k}) + \beta(\mathbf{q}-\mathbf{k}) + \beta(\mathbf{q}+\mathbf{k}') + \beta(\mathbf{q}-\mathbf{k}')\right] + \Delta t_3\left[\gamma(\mathbf{q}+\mathbf{k},\mathbf{q}+\mathbf{k}') + \gamma(\mathbf{q}-\mathbf{k},\mathbf{q}-\mathbf{k}')\right], \qquad (4)$$

and

$$W_{\mathbf{k},\mathbf{k}',\mathbf{q}} = \Delta t_3\, \gamma(\mathbf{q}+\mathbf{k},\mathbf{q}+\mathbf{k}')\,, \qquad (5)$$

being

$$\beta(\mathbf{k}) = 2[\cos(k_x a) + \cos(k_y a)]\,, \qquad (6)$$

$$\gamma(\mathbf{k},\mathbf{k}') = 4\cos(k_x a)\cos(k'_y a) + 4\cos(k'_x a)\cos(k_y a)\,, \qquad (7)$$

and $2\mathbf{q}$ is the wave vector of the pair center of mass. After a standard Hartree-Fock decoupling of the interaction terms with $\mathbf{q}\neq\mathbf{0}$ [9] applied to Eq. (2), the reduced Hamiltonian for $\mathbf{q}=\mathbf{0}$ is

$$\hat{H} = \sum_{\mathbf{k},\sigma} \varepsilon_{MF}(\mathbf{k}) \hat{c}^{+}_{\mathbf{k},\sigma}\hat{c}_{\mathbf{k},\sigma} + \frac{1}{N_S} \sum_{\mathbf{k},\mathbf{k}'} V_{\mathbf{k},\mathbf{k}',\mathbf{0}} \hat{c}^{+}_{\mathbf{k},\uparrow}\hat{c}^{+}_{-\mathbf{k}',\downarrow}\hat{c}_{-\mathbf{k}',\downarrow}\hat{c}_{\mathbf{k},\uparrow} + \frac{1}{N_S} \sum_{\mathbf{k},\mathbf{k}',\sigma} W_{\mathbf{k},\mathbf{k}',\mathbf{0}} \hat{c}^{+}_{\mathbf{k},\sigma}\hat{c}^{+}_{-\mathbf{k}',\sigma}\hat{c}_{-\mathbf{k}',\sigma}\hat{c}_{\mathbf{k},\sigma}\,, \qquad (8)$$

where the mean-field dispersion relation of an effective square lattice with a lattice parameter a is given by

$$\varepsilon_{MF}(\mathbf{k}) = \varepsilon_{eff} + 2t_{eff}[\cos(k_x a) + \cos(k_y a)] + 4t'_{eff}\cos(k_x a)\cos(k_y a)\,, \qquad (9)$$

where $\varepsilon_{eff} = \varepsilon_0 + nU/2$, $t_{eff} = t + n\Delta t$, and $t'_{eff} = t' + 2n\Delta t_3$.

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By applying the BCS formalism to Eq. (8), we found the following two coupled integral equations [5,7], which determine the *d*-wave superconducting gap [$\Delta(\mathbf{k})$] and the chemical potential (μ) for a given temperature (T) and electron density (n),

$$\Delta(\mathbf{k}) = -\frac{1}{2N_S}\sum_{\mathbf{k}'}\frac{V_{\mathbf{k},\mathbf{k}',0}\Delta(\mathbf{k}')}{E(\mathbf{k}')}\tanh\left(\frac{E(\mathbf{k}')}{2k_BT}\right) \tag{10}$$

and

$$n-1 = -\frac{1}{N_S}\sum_{\mathbf{k}'}\frac{\varepsilon_{MF}(\mathbf{k}')-\mu}{E(\mathbf{k}')}\tanh\left(\frac{E(\mathbf{k}')}{2k_BT}\right), \tag{11}$$

where the single-particle excitation energy is given by

$$E(\mathbf{k}) = \sqrt{(\varepsilon_{MF}(\mathbf{k})-\mu)^2+\Delta^2(\mathbf{k})} \tag{12}$$

and $\Delta(\mathbf{k}) = \Delta_d\left[\cos(k_xa)-\cos(k_ya)\right]$. Eq. (11) can be rewritten as [6]

$$1 = \frac{\Delta t_3 a^2}{2\pi^2}\int_{-\pi/a}^{\pi/a}\int_{-\pi/a}^{\pi/a}dk_xdk_y\frac{\left[\cos(k_xa)-\cos(k_ya)\right]^2}{E(\mathbf{k})}\tanh\left(\frac{E(\mathbf{k})}{2k_BT}\right). \tag{13}$$

where the double integral is always positive and then $\Delta t_3 > 0$ has a key participation in the formation of *d*-wave superconducting state within this model, in spite of its small strength. The critical temperature (T_c) can be obtained from the condition $\Delta_d(T_c) = 0$.

PARAMETER DETERMINATION FROM ARPES DATA

Angular resolution photoelectron spectroscopy (ARPES) has been used to find out the electronic dispersion relation, as well as to quantify the anisotropy of superconducting gaps in cuprate superconductors [10]. In particular, such dispersion relationship around the Fermi energy for $Bi_2Sr_{2-x}La_xCuO_{6+\delta}$ (BSLCO), with different chemical compositions x, has been measured by extrapolating the peaks of momentum distribution curves up to the Fermi energy (E_F) even when the spectral weight is suppressed in going towards E_F due to the presence of an energy gap or pseudogap [6]. Notice that in BSLCO, as the La concentration x increases, the hole concentration p decreases, as determined by the room-temperature Hall coefficient [11].

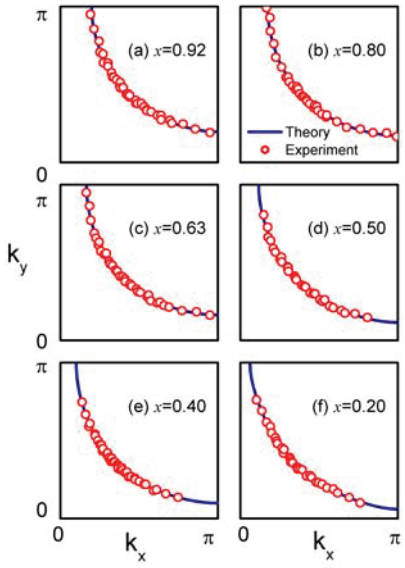

FIGURE 2. (a–f) ARPES data (open circles) obtained from $Bi_2Sr_{2-x}La_xCuO_{6+\delta}$ with different chemical compositions (x) indicated inside in comparison with the calculated dispersion relation (solid lines) at the Fermi energy.

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In figures 2(a-f), the calculated Fermi surfaces (blue lines) for x = 0.92, 0.80, 0.63, 0.50, 0.40 and 0.20 are respectively shown and compared with ARPES experimental data (red open circles). The theoretical results of Fig. 2 have been obtained from Eq. (9) and the fitted values of ε_{eff}, t_{eff} and t'_{eff} are summarized in Table 1, where the last two columns n and Δt_3 are explained below. We have taken a constant value of t_{eff} = -0.25 eV as in the Ref. [12], since only the relative magnitudes of t'_{eff}/t_{eff} and $\varepsilon_{eff}/t_{eff}$ can be determined by ARPES data. Once the effective hopping and self-energy parameters are obtained, the electronic density of states (*DOS*) can be calculated from [13]

$$DOS(E) = \frac{1}{\pi} \lim_{\eta \to 0^+} \mathrm{Im} \left[\sum_{\mathbf{k}} \frac{1}{E + \varepsilon_{MF}(\mathbf{k}) + i\eta} \right] \tag{14}$$

where $\varepsilon_{MF}(\mathbf{k})$ is the mean-field dispersion relation given by Eq. (9). By integrating $DOS(E)$ up to E_F we obtain the electronic density (n), whose numerical values for samples with different La concentrations x, are listed in Table1, where we observe an increase of the hole concentration (1-n) from a half-filling electronic band when x diminishes. This approach could be used to calculate the hole doping p for each x, instead of utilizing the temperature-dependent Hall coefficient and its comparison with other cuprates, as a guide to estimate p [11].

TABLE 1. Model parameters determined from ARPES data of $Bi_2Sr_{2-x}La_xCuO_{6+\delta}$ together with the experimental T_c and Hall-effect estimated hole doping p [6].

x	p	T_c [K]	t'_{eff} [eV]	ε_{eff} [eV]	n	Δt_3 [eV]
0.92	0.07	0	0.087	0.189	0.993	-
0.80	0.10	0	0.095	0.252	0.916	-
0.63	0.12	14	0.098	0.276	0.884	0.0267
0.50	0.14	24	0.097	0.329	0.776	0.0234
0.40	0.16	34	0.103	0.368	0.656	0.0227
0.20	0.18	25	0.098	0.377	0.655	0.0173

Finally, for $Bi_2Sr_{2-x}La_xCuO_{6+\delta}$, the experimental data of T_c from M. Hashimoto, *et al*. [6] allow the determination of the correlated hopping parameters Δt_3 for each doping concentration, whose values are presented in Table 1.

SPECIFIC HEAT RESULTS

The energy spectrum of elementary excitations in solids determines the temperature dependence of their specific heat. In particular, for a superconductor it gives information regarding to the symmetry of its superconducting state. An *s*-wave superconductor has an exponentially temperature dependent electronic specific heat (C_{el}), while an anisotropic nodal superconducting gap leads to a power-law C_{el}, as occur in the cuprate superconductors [1]. The electronic specific heat (C_{el}), can be calculated as [14]

$$C_{el} = \frac{2k_B\beta^2 a^2}{4\pi^2} \int_{-\pi/a}^{\pi/a} \int_{-\pi/a}^{\pi/a} f[E(\mathbf{k})]\{1 - f[E(\mathbf{k})]\} \left[E^2(\mathbf{k}) + \beta E(\mathbf{k}) \frac{dE(\mathbf{k})}{d\beta} \right] dk_x dk_y \,, \tag{15}$$

where $\beta = 1/(k_B T)$ and $f(E)$ is the Fermi-Dirac distribution. The specific heat of the normal state can be obtained by taking $\Delta(\mathbf{k})$ equal to zero in Eqs. (12) and (15). In Fig. 3, the calculated C_{el} (open triangles) for the compound $Bi_{1.74}Sr_{1.88}Pb_{0.38}CuO_{6+\delta}$, with an estimated p=0.21 is shown and compared with the available experimental C_{el} data [8]. The model parameters for this compound, ε_{eff} = 0.398 eV and t'_{eff} =0.094 eV, were obtained by extrapolating those obtained from the ARPES data of M. Hashimoto *et al*. [6]. Moreover, by integrating the corresponding *DOS(E)*, a value of n=0.547 was obtained and the experimental T_c =9.4K leads to a value of Δt_3=0.016 eV. Notice that the dimensionless electronic specific heat (C_{el}) is presented in Fig. 3 by subtracting the normal-state one (C_n) and dividing by $TC_{el}(T_c)/T_c$. The theoretical results reveal an almost second-degree power-law behavior, in agreement with the experimental data, because the low-temperature behavior of C_{el} is very sensitive to the existence of nodes in the gap. In spite of the simplicity of the model, the linear behavior of C_{el} in the normal state and the discontinuity between the normal and superconducting C_{el} are well reproduced.

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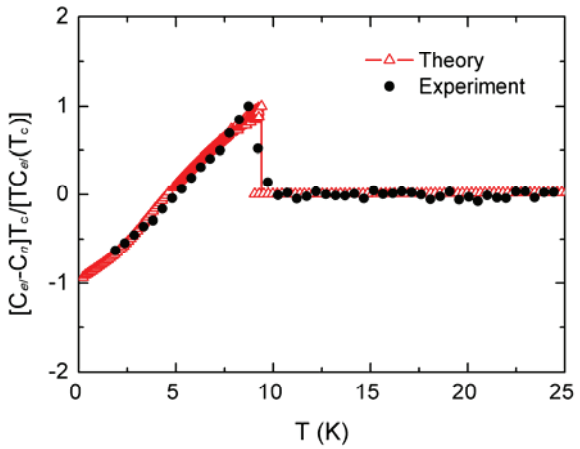

FIGURE 3. Theoretical (open triangles) normalized electronic specific heat (C_{el}) versus temperature (T) for $Bi_{1.74}Sr_{1.88}Pb_{0.38}CuO_{6+\delta}$ in comparison with the experimental one (solid circles) [6].

CONCLUSIONS

We have determined, by using ARPES data, the parameters of a generalized Hubbard model for samples of $Bi_2Sr_{2-x}La_xCuO_{6+\delta}$ with different values of x. From these data, we extrapolated the model parameters for a sample of $Bi_{1.74}Sr_{1.88}Pb_{0.38}CuO_{6+\delta}$, whose electronic specific heat has been measured as a function of the temperature. The normalized electronic specific heat calculated without adjustable parameters is compared to experimental data and a good agreement is observed. Furthermore, this model correctly gives the diminution of the electronic density (n) from half-filling ($n = 1$) when the lanthanum concentration diminishes in $Bi_2Sr_{2-x}La_xCuO_{6+\delta}$. The presented approach could be used to determine the hole doping (p) instead of using the temperature-dependent Hall coefficient, especially in those materials where the relation between p and the doping concentration (x) is not straightforward. It is worth mentioning that a single-band Hubbard model can reproduce the experimental dispersion relation and the second-neighbor correlated hopping could lead to a d-wave superconducting ground state with a second-degree power-law temperature dependence of the electronic specific heat.

Finally, it would be worth mentioning that for the values of Δt_3 used in this work, the superconducting ground state has d-wave symmetry, since the s-wave superconductivity requires a larger value of Δt_3 or a negative U, as discussed in Ref. [5]. The interaction term $W_{\mathbf{k},\mathbf{k}',\mathbf{0}}$ has no effect on the singlet d-wave superconducting ground state and it could lead to spin-triplet p-wave superconductivity if a small lattice distortion is considered [15].

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