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

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In the last decade, the Angle Resolved Photoemission Spectroscopy (ARPES) has achieved important advances in both energy and angular resolutions, which provide a direct measurement of the single-particle dispersion relation and superconducting gap. These dispersion relation data permit 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 within the mean-field approximation. In this work, we study the doping effects on the critical temperature (*Tc*), *d*-wave superconducting gap (Δ), and electronic specific heat of cuprate superconductors, such as $La_{2-x}Sr_xCuO_4$ and $Bi_2Sr_{2-x}La_xCuO_{6+\delta}$, by solving numerically two coupled integral equations for determining the chemical potential and the superconducting gap or *Tc*. Finally, the calculated electronic specific heat is compared with experimental results.

The Model

We use a Hubbard model where first- (Δ*t*) and second-neighbor (Δt_3) correlated-hoppings are considered in addition to the on-site (*U*) Coulombic interaction, which can be written as [1]

$$\hat{H} = \varepsilon_0 \sum_{i,\sigma} \hat{c}^{+}_{i,\sigma}\hat{c}_{i,\sigma} + t \sum_{\substack{<i,j>\\ \sigma}} \hat{c}^{+}_{i,\sigma}\hat{c}_{j,\sigma} + t' \sum_{\substack{i,j\\ \sigma}} \hat{c}^{+}_{i,\sigma}\hat{c}_{j,\sigma} + U\sum_i \hat{n}_{i,\uparrow}\hat{n}_{i,\downarrow}$$

$$+\Delta t \sum_{\substack{<i,j>\\ \sigma}} \hat{c}^{+}_{i,\sigma}\hat{c}_{j,\sigma}(\hat{n}_{i,-\sigma}+\hat{n}_{j,-\sigma}) + \Delta t_3 \sum_{\substack{i,j,\sigma\\ <i,l>,<j,l>}} \hat{c}^{+}_{i,\sigma}\hat{c}_{j,\sigma}\hat{n}_l$$

Mean-field dispersion relation

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

Mean-field parameters

Self energy: $\varepsilon_{eff} = \varepsilon_0 + nU/2$

First neighbor hopping parameter: $t_{eff} = t + n\Delta t$

Second neighbor hopping parameter: $t'_{eff} = t' + 2n\Delta t_3$

BCS Coupled Equations

For singlet Cooper pairs, the BCS coupled equations are given by

$$\begin{cases} \Delta(\mathbf{k}) = -\dfrac{1}{2N_s}\displaystyle\sum_{\mathbf{k}'} \frac{V_{\mathbf{k}\mathbf{k}'}\,\Delta(\mathbf{k}')}{E(\mathbf{k}')}\tanh\left(\frac{E(\mathbf{k}')}{2k_BT}\right) \\ n-1 = -\dfrac{1}{N_s}\displaystyle\sum_{\mathbf{k}'} \frac{\varepsilon(\mathbf{k}')-\mu}{E(\mathbf{k}')}\tanh\left(\frac{E(\mathbf{k}')}{2k_BT}\right) \end{cases}$$

where $E(\mathbf{k}) = \sqrt{(\varepsilon_{MF}(\mathbf{k})-\mu)^2 + \Delta^2(\mathbf{k})}$ and $V_{\mathbf{k},\mathbf{k}'\mathbf{q}} = U + 2\Delta t_3\gamma(\mathbf{k}+\mathbf{q},\mathbf{k}'+\mathbf{q}) + \Delta t\left[\beta(\mathbf{k}+\mathbf{q})+\beta(-\mathbf{k}+\mathbf{q})+\beta(\mathbf{k}'+\mathbf{q})+\beta(-\mathbf{k}'+\mathbf{q})\right]$

with $\beta(\mathbf{k}) = 2[\cos(k_x a)+\cos(k_y a)]$, and $\gamma(\mathbf{k},\mathbf{k}') = 4\cos(k_x a)\cos(k'_x a)+4\cos(k'_x a)\cos(k_y a)$

For a *d*-wave superconducting gap, the BCS coupled equations are given by

$$\begin{cases} 1 = \dfrac{4\Delta t_3}{2N_s}\displaystyle\sum_{\mathbf{k}'} \frac{\left[\cos(k_x a)-\cos(k_y a)\right]^2}{E(\mathbf{k}')}\tanh\left(\frac{E(\mathbf{k}')}{2k_BT}\right) \\ n-1 = -\dfrac{1}{N_s}\displaystyle\sum_{\mathbf{k}'} \frac{\varepsilon(\mathbf{k}')-\mu}{E(\mathbf{k}')}\tanh\left(\frac{E(\mathbf{k}')}{2k_BT}\right) \end{cases}$$

where $E(\mathbf{k}) = \sqrt{(\varepsilon_{MF}(\mathbf{k})-\mu)^2 + \Delta^2(\mathbf{k})}$ with $\Delta(\mathbf{k}) = \Delta\left[\cos(k_x a)-\cos(k_y a)\right]$.

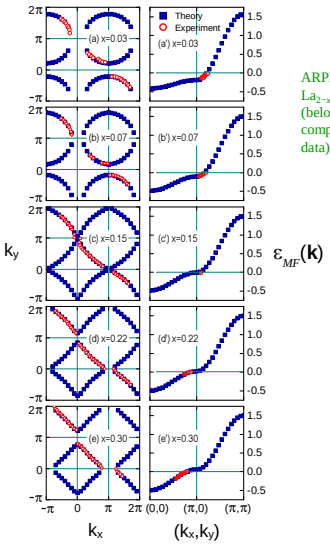
Electronic specific heat

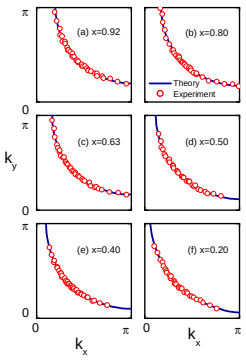
$$C_{el} = \frac{2k_B\beta^2 a^2}{4\pi^2}\iint_{1BZ} f[E(\mathbf{k})]\{1-f[E(\mathbf{k})]\}\left[E^2(\mathbf{k}) + \beta E(\mathbf{k})\frac{dE(\mathbf{k})}{d\beta}\right]dk_x dk_y$$

where $\beta = 1/k_BT$ and *f(E)* is the Fermi-Dirac distribution.

ARPES Data

ARPES data (red open circles) obtained from $La_{2-x}Sr_xCuO_4$ [2] (left figure) and $Bi_2Sr_{2-x}La_xCuO_{6+\delta}$ (below figure) [3] with different doping levels in comparison with the calculated dispersion relation (blue data).





Model parameters determined from ARPES data

$La_{2-x}Sr_xCuO_4$

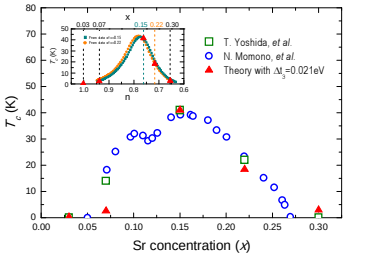
x	Tc [K]	t_{eff} [eV]	t'_{eff} [eV]	ε_{eff} [eV]	*n*	Δt_3[eV]
0.03	0	-0.25	0.097	0.199	1.002	0.021
0.07	14	-0.25	0.077	0.209	0.938	0.021
0.15	41	-0.25	0.064	0.260	0.761	0.021
0.22	22	-0.25	0.060	0.268	0.716	0.021
0.30	0	-0.25	0.056	0.290	0.655	0.021

$Bi_2Sr_{2-x}La_xCuO_{6+\delta}$

x	Tc [K]	t_{eff} [eV]	t'_{eff} [eV]	ε_{eff} [eV]	*n*	Δt_3[eV]
0.80	0	-0.25	0.095	0.252	0.916	0
0.63	14	-0.25	0.098	0.276	0.884	0.0267
0.50	24	-0.25	0.097	0.329	0.776	0.0234
0.40	34	-0.25	0.103	0.368	0.656	0.0227
0.20	25	-0.25	0.098	0.377	0.655	0.0173

$La_{2-x}Sr_xCuO_4$ Critical Temperature

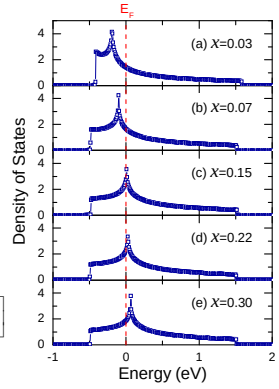
Theoretical (solid triangles) critical temperature (Tc) as a function of the Sr concentration (*x*) in comparison with experimental data of T. Yoshida *et al.* (open squares) [2] and N. Momono *et al.* (open circles) [4]. Inset: Tc versus electronic density (*n*) for the Hamiltonian parameters obtained from *x*=0.15 (solid squares) and *x*=0.22 (solid circles) with the values of *x* indicated by dashed lines.



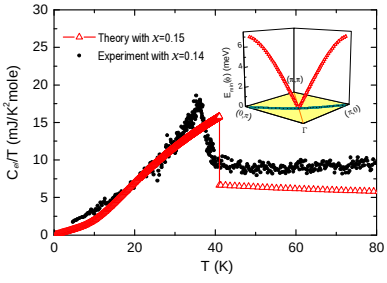
Density of States

Electronic density of states (DOS) for $La_{2-x}Sr_xCuO_4$. Notice that for *x*=0.15, the Fermi level (E_F) coincides with the van Hove singularity and then, the critical temperature is a maximum, as expected. By integrating *DOS(E)* up to E_F we obtain the electronic density (*n*).

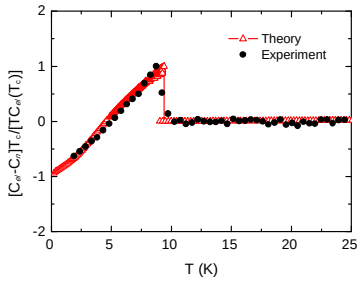
$$DOS(E) = -\frac{1}{\pi}\lim_{\eta\to 0^+}\mathrm{Im}\left[\sum_{\mathbf{k}}\frac{1}{E-\varepsilon_{MF}(\mathbf{k})+i\eta}\right]$$



Electronic Specific Heat



Theoretical (open triangles) electronic specific heat (C_{el}) versus temperature (T) for $La_{2-x}Sr_xCuO_4$ with x=0.15 in comparison with the experimental one (solid circles) for x=0.14 [5]. Inset: Single excitation energy gap (open triangles) in the first Brillouin zone.



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].

References

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[4] N. Momono, *et al.*, *Physica C* **233**, 395 (1994).
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