# Theory for electron-doped cuprate superconductors: *d*-wave symmetry order parameter

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Using as a model the Hubbard Hamiltonian we determine various basic properties of electron-doped cuprate superconductors like $Nd_{2-x}Ce_xCuO_4$ and $Pr_{2-x}Ce_xCuO_4$ for a spin-fluctuation-induced pairing mechanism. Most importantly we find a narrow range of superconductivity and, similar to hole-doped cuprates $d_{x^2-y^2}$, symmetry for the superconducting order parameter. The superconducting transition temperatures $T_c(x)$ for various electron doping concentrations $x$ are calculated to be much smaller than for hole-doped cuprates due to the different energy dispersion and a flat band well below the Fermi level. Lattice disorder may sensitively distort the symmetry $d_{x^2-y^2}$ via electron-phonon interaction.

It is of general interest to see whether the behavior of hole-doped and electron-doped cuprate superconductors can be explained within a unified physical picture, using for example the exchange of antiferromagnetic spin fluctuations as the relevant pairing mechanism. While hole-doped superconductors have been studied intensively[1] the analysis of electron-doped cuprates remained largely unclear. One expects on general physical grounds, if Cooper pairing is controlled by antiferromagnetic spin fluctuations, that *d*-wave symmetry pairing should also occur for electron-doped cuprates.[2,3] Previous experiments did not clearly support this and reported mainly *s*-wave pairing.[4–6] Perhaps as a result of this, so far electron-doped cuprates have received much less attention than hole-doped cuprates. However, phase-sensitive experiments[7] and magnetic penetration depth measurements[8,9] have recently exhibited *d*-wave symmetry Cooper pairing.

In order to obtain a unified theory for both hole-doped and electron-doped cuprates it is tempting to use the same Hubbard Hamiltonian taking into account, of course, the different dispersions for the carriers.[10] Note, in the case of electron doping the electrons occupy copper *d*-like states of the upper Hubbard band while the holes refer to oxygenlike *p* states yielding different energy dispersion as used in our calculations. Then, assuming similar itinerancy of the electrons and holes the mapping on an effective one-band model seems to be justified. We consider $U$ as an effective Coulomb interaction. Hence, for the theoretical analysis of the superconducting properties of electron-doped cuprates we use as a model the two-dimensional (2D) Hubbard Hamiltonian

$$H=-\sum_{\langle ij\rangle\sigma} t_{ij}(c^+_{i\sigma}c_{j\sigma}+c^+_{j\sigma}c_{i\sigma})+U\sum_i n_{i\uparrow}n_{i\downarrow}. \qquad (1)$$

Such a Hamiltonian has been successfully used for the hole-doped cuprates[11,12] in particular for the determination of the doping dependence of antiferromagnetic order for both electron and hole doping.[13] In Eq. (1) $c^+_{i\sigma}$ creates an electron with spin $\sigma$ on site $i$, $U$ denotes the on-site Coulomb interaction, and $t_{ij}$ is the hopping integral. For the optimally doped $Nd_{2-x}Ce_xCuO_4$ (NCCO) the Fermi surface and dispersion

$$\epsilon_k=-2t[\cos k_x+\cos k_y-2t'\cos k_x\cos k_y+\mu/2], \qquad (2)$$

are taken in accordance with photoemission [angle-resolved photoemission spectroscopy (ARPES)] experiments.[10] The chemical potential $\mu$ describes the band filling. Here and in the following we set the lattice constant $a=b$ equal to unity.

In Fig. 1 the results for $\epsilon_k$ of a tight-binding calculation are shown. We choose the parameters $t=138$ meV and $t'=0.3$. For comparison, we also show the results with $t=250$ meV and $t'=0$, which is often used to describe the hole-doped superconductors. One immediately sees the important difference: in the case of NCCO the flat band is approximately 300 meV *below* the Fermi level, whereas for the hole-doped case the flat band lies very close to it. Thus, using the resulting $\epsilon_k$ in a spin-fluctuation-induced pairing theory in the framework of the so-called FLEX approximation[14–16] we get a smaller $T_c$ for electron-doped cuprates than for the hole-doped ones. Furthermore, we also calculate the doping dependence $T_c(x)$, the symmetry of the order parameter $\phi(x)$, and some other basic properties like the dynamical spin susceptibility. Earlier calculations using the FLEX approximation, which were performed in the case

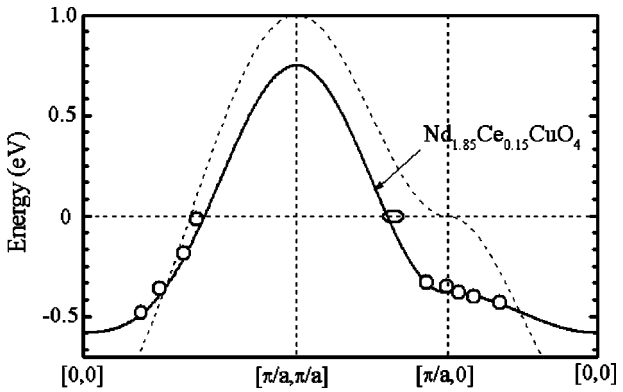


FIG. 1. Results of the energy dispersion $\epsilon_k$ of optimally electron-doped NCCO. The solid curve refers to our tight-binding calculation choosing $t=138$ meV and $t'=0.3$. Data (open dots) are taken from Ref. 10. The dashed curve corresponds to using $t=250$ meV and $t'=0$ and is typical for hole-doped cuprates.

 

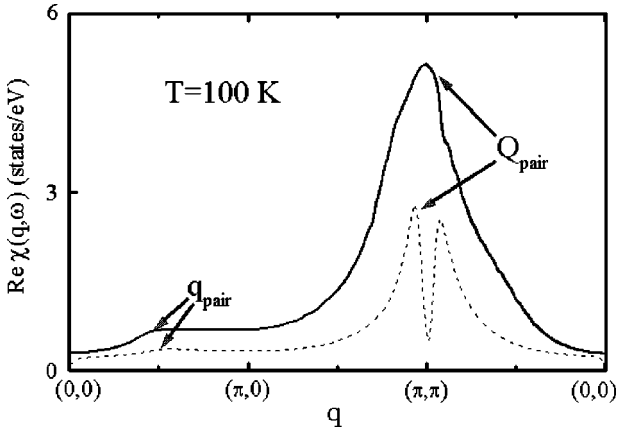


FIG. 2. Momentum dependence of the real part of the spin susceptibility along the Brillouin zone (BZ) route $(0,0)\rightarrow(\pi,0)\rightarrow(\pi,\pi)\rightarrow(0,0)$ at $T=100$ K for $\omega=0$ (solid curve) and $\omega=\omega_{sf}\approx 0.47t$ (dashed curve). The main contributions to the corresponding pairing interaction come from $\mathbf{q}_{pair}$ (along the antinodes) and $\mathbf{Q}_{pair}$ (along the ''hot spots'') as illustrated in Fig. 5.

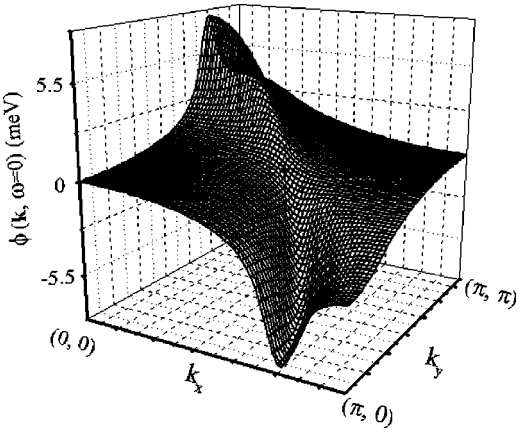


FIG. 3. Calculated $d_{x^2-y^2}$-wave symmetry of the superconducting order parameter at $T/T_c=0.8$ for $x=0.15$ in the first square of the BZ.

of hole-doped superconductors, were rather successful in determining many physical quantities.[1,14–16]

In order to investigate the pairing interaction we show in Fig. 2 results for the real part of the spin susceptibility at 100 K and $U=4t$ in the weak-coupling limit for $\omega=0$ (solid curve) and for $\omega=\omega_{sf}\approx 0.47t$ (dashed curve). $\omega_{sf}$ denotes the spin fluctuation (paramagnon) energy, where a peak in $\mathrm{Im}\,\chi(\mathbf{Q},\omega)$ occurs. The commensurate peak of Re $\chi(\mathbf{q},\omega=0)$ at $\mathbf{Q}=(\pi,\pi)$ is in accordance with recent calculations in Ref. 17, where it was pointed out that the exchange of spin fluctuations yields a good description of the normal state Hall coefficient $R_H$ for both hole- and electron-doped cuprates. Furthermore, we also find a linear temperature dependence of the in-plane resistivity $\rho_{ab}(T)$ if we do not take into account an additional electron-phonon coupling. This will be discussed later. Concerning the superconducting properties, note that the lower tiny peak would favor $d_{xy}$ pairing symmetry, but the dominating larger peak leads to $d_{x^2-y^2}$ symmetry and is also pair breaking for $d_{xy}$ symmetry. Evidently, the electron-doped cuprates are not close to $d_{xy}$ pairing symmetry as stated previously.[18] This explains why the resultant superconducting order parameter $\phi(\mathbf{k},\omega)$ exhibits almost pure $d_{x^2-y^2}$ symmetry.

In Fig. 3 we present our result for the superconducting order parameter $\phi(\mathbf{k},\omega)$ calculated from the generalized Eliashberg equations using the FLEX approximation. We show $\phi(\mathbf{k},\omega=0)$ for an electron doping $x=0.15$ at $T/T_c=0.8$, where the gap has just opened. The gap function clearly has $d_{x^2-y^2}$-wave symmetry. This is in agreement with the reported linear and quadratic temperature dependence of the in-plane magnetic penetration depth for low temperatures in the clean and dirty limit, respectively,[8,9] and with phase-sensitive measurements.[7] From our obtained result of a pure $d_{x^2-y^2}$-wave superconducting order parameter we expect a zero-bias conductance peak[19] (ZBCP) as recently observed in optimally doped NCCO (Ref. 20) and also in the hole-doped superconductors.[5] Note, its absence in some other experiments may be attributed to small changes in the surface quality and roughness[21] or to disorder.[22] The incommensurate structure in the order parameter close to $(\pi,0)$ results from the double-peak structure in Re $\chi$ at $\omega\approx\omega_{sf}=0.47t$ shown in Fig. 2. It means physically that the Cooper-pairing interaction occurs mainly not for a spin-fluctuation wave vector $\mathbf{Q}=(\pi,\pi)$ but mostly for $\omega=\omega_{sf}$ and for $\mathbf{Q}^*=(\pi-\delta,\pi+\delta)$. Furthermore, from Figs. 2, 3, and 5 we conclude that *no* $d_{xy}$-symmetry component is present in the superconducting order parameter, since the dominating $d_{x^2-y^2}$-type pairing suppresses $d_{xy}$ pairing. The ARPES study might test this.

In Fig. 4 we present our results for the phase diagram $T_c(x)$ and $T_N(x)$. We find in comparison to hole-doped superconductors smaller $T_c$ values and that superconductivity occurs in a narrower doping range as also observed in experiment.[23] Responsible for this are poorer nesting properties of the Fermi surface and the flat band around $(\pi,0)$ which lies well below the Fermi level. The narrow doping range for $T_c$ is due to antiferromagnetism up to $x=0.13$ and rapidly decreasing nesting properties for increasing $x$.

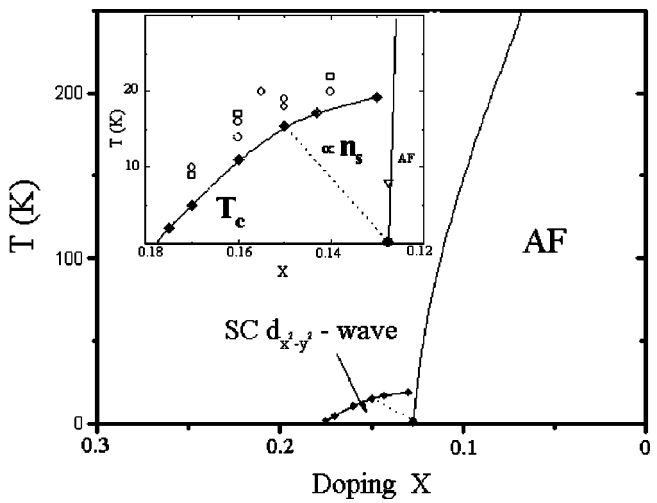


FIG. 4. Phase diagram $T(x)$ for electron-doped cuprates. The AF transition curve is taken from Ref. 13. The solid curve corresponds to our calculated $T_c$ values obtained from $\phi(\mathbf{k},\omega)=0$. The inset shows $T_c(x)$ for the doping region $0.18<x<0.12$ and experimental data (squares from Ref. 26, circles from Ref. 27, triangle from 28). The dotted curve refers to $T_s\propto n_s$.

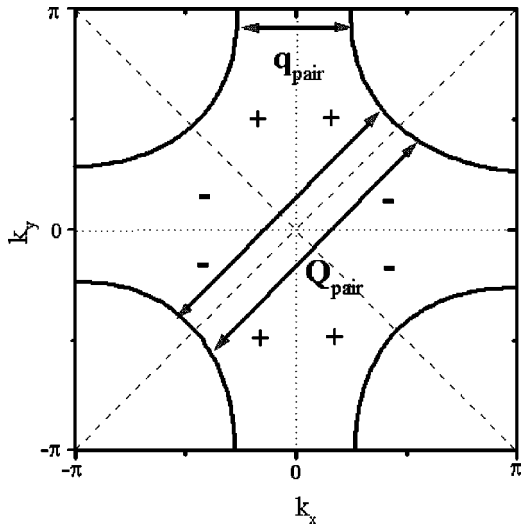


FIG. 5. Calculated Fermi surface for (optimally doped) NCCO. The + (−) and the dashed lines refer to the signs of calculated momentum dependence (see Fig. 3) of the $d_{x^2-y^2}$ gap function $\phi(k,\omega=0)$ and its nodes, respectively.

In order to understand the behavior of $T_c(x)$ in underdoped electron-doped cuprates we have calculated the Cooper-pair coherence length $\xi_0$, i.e., the size of a Cooper pair, and find similar values for electron-doped and hole-doped superconductors (from 6 Å to 9 Å). If due to strong-coupling lifetime effects the superfluid density $n_s$ becomes small, the distance $d$ between Cooper pairs increases. If for $0.15>x>0.13$ the Cooper pairs do not overlap significantly, i.e., $d/\xi_0>1$, then Cooper-pair phase fluctuations get important.[24,25,12] Thus we expect the same as for hole-doped superconductors $T_c \propto n_s$. Assuming that $n_s$ increases approximately linearly from $x\simeq 0.13$ to $x\simeq 0.15$ we estimate a $T_c$ which is smaller than that calculated from $\phi(\mathbf{k},\omega)=0$; see the dashed curve in Fig. 4. As a consequence, more experiments determining $T_c$ for $x\leqslant 0.15$ should be performed to check on the Uemura scaling $T_c \propto n_s$.

On general grounds we expect a weakening of the $d_{x^2-y^2}$-pairing symmetry if we include the electron-phonon interaction and if this plays a significant role. The absence of an isotope effect ($\alpha_0 = d\ln T_c/d\ln M \approx 0.05$) for doping $x=0.15$ (see Ref. 29) suggests the presence of a pure $d_{x^2-y^2}$ symmetry. We know from Fig. 2 that phonons connecting the Fermi surface with wave vector $\mathbf{Q}_{\rm pair}=(\pi,\pi)$ will add destructively to the spin fluctuation pairing.[30] If, due to the exchange of spin fluctuations a $d_{x^2-y^2}$-symmetry instability is the dominant contribution to the pairing interaction, an additional electron-phonon coupling with wave vector $\mathbf{q}_{\rm pair}=(0.5\pi,0)$ would be also pair building. Note, we generally expect that due to the poorer nesting the pairing instability due to electron-phonon and spin fluctuation interaction become more easily comparable. In this case the electron-phonon coupling would definitely favor *s*-wave symmetry of the underlying superconducting order parameter. This can be analyzed in detail by adding a term $\alpha^2F(\mathbf{q},\omega)$ to the pairing interaction.[30]

To continue the discussion why the symmetry of the order parameter depends for electron-doped cuprates more sensitively on electron-phonon interaction, we show in Fig. 5 the calculated Fermi surface for optimally doped NCCO. Note, the topology of the Fermi surface for the electron-doped cuprates is very similar to optimally hole-doped $Bi_2Sr_2CaCu_2O_{8+\delta}$ (BI2212), as was also pointed out recently in Ref. 31. We estimate that mainly no phonons are present along the edges $(-0.25\pi,\pi)\rightarrow(0.25\pi,\pi)$ bridging Brillouin zone (BZ) areas, where the superconducting order parameter, $\phi(\mathbf{k},\omega)$, is always positive (denoted by +/+). Note, attractive electron-phonon coupling bridging +/− areas $(-0.5\pi,-0.5\pi)\rightarrow(0.5\pi,0.5\pi)$ is *destructive* for $d_{x^2-y^2}$-symmetry Cooper pairing. However, due to poorer nesting conditions, pairing transitions of the type +/+ are somewhat contributing and then a mixed symmetry $\{d_{x^2-y^2}+\alpha s\}$ may occur.[32]

Further experimental study of the doping dependence of the oxygen-isotope effect are necessary for a better understanding of the role played by the electron-phonon interaction. For example, if due to structural distortion and oxygen deficiency in the $CuO_2$ plane the phonon spectrum $F(\mathbf{q},\omega)$ changes significantly, then this affects the isotope coefficient $\alpha_0$ and reduces $T_c$. Possibly the reported large isotope effect of $\alpha_0=0.15$ for slightly changed oxygen content, i.e., $Nd_{1.85}Ce_{0.15}CuO_{3.8}$, could be related to this.[33,34] As an example, one might think of the oxygen out-of-plane $B_{2u}$ mode, which becomes active if $O_4$ is replaced by $O_{3.8}$.[35] A further signal of a significant electron-phonon coupling might be the quadratic temperature dependence of the resistivity.[36]

In summary, our unified model for cuprate superconductivity yields for electron-doped cuprates, as for hole-doped ones, pure $d_{x^2-y^2}$ symmetry pairing in a good agreement with recent experiments.[7–9] In contrast to hole-doped superconductors we find for electron-doped cuprates smaller $T_c$ values due to a flat dispersion $\epsilon_k$ around $(\pi,0)$ well below the Fermi level. Futhermore, superconductivity only occurs for a narrow doping range $0.18>x>0.13$, because of the onset of antiferromagnetism and, on the other side, due to poorer nesting conditions. We get $2\Delta/k_BT_c=5.3$ for $x=0.15$ in reasonable agreement with experiment.[4] We argue that if the electron-phonon coupling becomes important, for example due to oxygen deficiency, then the *s*-wave pairing instability competes with $d_{x^2-y^2}$-wave symmetry. This might explain a possible *s*-wave symmetry order parameter as reported in earlier measurements.

Our results seem physically clear in view of the discussion presented in connection with Figs. 2 and 5, in particular. Moreover, the important input of the calculation, namely the dispersion $\epsilon_{\mathbf{k}}$, was taken in agreement with ARPES measurements. The canonical value used for the strength of the effective Coulomb interaction $U$ is in accordance with this. Thus, it is no surprise that by also calculating $\mathrm{Im}\,\chi(\mathbf{q},\omega)$ we obtain reasonable agreement with inelastic-neutron scattering measurements.[37] This sheds light on the general validity of our results.

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[1] See, for example D.J. Scalapino, Phys. Rep. **250**, 329 (1995).
[2] If the dominant *repulsive* pairing contribution in high-$T_c$ superconductors can be mainly described by their spin susceptibility, then the underlying order parameter must change its sign. From group theory we know (Ref. 3) that for a nested Fermi surface described by $\mathbf{Q}=(\pi,\pi)$, i.e., $\epsilon_{\mathbf{k}+\mathbf{Q}}=-\epsilon_{\mathbf{k}}$, the $d_{x^2-y^2}$-symmetry order parameter is the simplest possibility.
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[32] Due to our tetragonal ansatz, one component of the resulting order parameter must be imaginary, e.g., $\{d_{x^2-y^2}+i\alpha s\}$. However, a slight orthorhombic distortion would allow our proposed $\{d_{x^2-y^2}+\alpha s\}$ symmetry.
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