Phase diagram of the compounds $Ln_{2-x}Ce_xCuO_4$

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The concentration interval in which Cooper pairing occurs at $T = 0$ is calculated in a Hubbard model with an infinite repulsion. The results of calculations in the one-loop approximation agree qualitatively with experiment.

In accordance with calculations in crystal chemistry, we assume that the energy of one hole in the $2p^6$ shell of the O^{2-} ion is on the same order of magnitude as the Hubbard energy (U_d) of the copper $3d$ state. In compounds $Ln^{3+}_{2-x}M_xCuO_{4-\delta}$ doped with cations M^{4+}, in which the lower Hubbard subband is filled, we can thus ignore virtual $2p$ hole states and $3d^{10}(x^2-y^2)$ states of the upper Hubbard subband. From the condition of electrical neutrality we find n_d, the average number of holes in the $3d^{10}$ copper shell ($n_d < 1$):

$$n_d = 1 - x - 2\delta. \tag{1}$$

Assuming that the Hubbard energy is the largest energy parameter here ($U_d = \infty$), we write the Hamiltonian of $(x^2 - y^2)$ excitations first in terms of the Hubbard X operators and then in terms of products of ordinary creation operators $\hat{a}^{+}_{\vec{r}\sigma}$ and annihilation operators $\hat{a}_{\vec{r}\sigma}$:

$$\hat{H} = \sum_{\vec{r},\vec{r}'\sigma}' \hat{X}^{+}_{\vec{r}\sigma} t(\vec{r} - \vec{r}') X_{\vec{r}'\sigma} = \sum_{\vec{r},\vec{r}'\sigma}' (1 - \hat{n}_{\vec{r}\bar{\sigma}}) \hat{a}^{+}_{\vec{r}\sigma} t(\vec{r} - \vec{r}') \hat{a}_{\vec{r}'\sigma} (1 - \hat{n}_{\vec{r}'\bar{\sigma}}), \tag{2}$$

where $\hat{n}_{\vec{r}\sigma} = \hat{a}^{+}_{\vec{r}\sigma} \hat{a}_{\vec{r}\sigma}$ are the density operators in cell $\vec{r}$ with spin $\bar{\sigma} = -\sigma$.

By writing Hamiltonian (2) in terms of the Güzwiller factors $1 - \hat{n}_{\vec{r}\sigma}$, we can calculate the two-particle Born scattering amplitude (Fig. 1):

$$\Gamma_B(\vec{p}_1, \vec{p}_2; \vec{p}_3, \vec{p}_4) = -\frac{1}{2} \sum_{k=1}^{4} t(\vec{p}_k) - \sum_{\vec{p}} n_F(\xi_{\vec{p}}) [t(\vec{s} - \vec{p}) + t(\vec{p} + \vec{q})], \tag{3}$$

where $t_{\vec{p}} = \Sigma'_{\vec{r}} t(\vec{r}) e^{i\vec{p}\vec{r}}$, and $n_F(\xi)$ is a Fermi distribution. In the zeroth self-consistent-field approximation (Hubbard I),[1] we have $\xi_p = f t_{\vec{p}} - \mu$, and the average number of holes n_d is related to the chemical potential μ through the equation of state:

$$n_d = 2f \sum_{\vec{p}} n_F(\xi_{\vec{p}}), \quad f = 1 - \langle \hat{n}_{\vec{r}\sigma} \rangle = 1 - \frac{n_d}{2}. \tag{4}$$

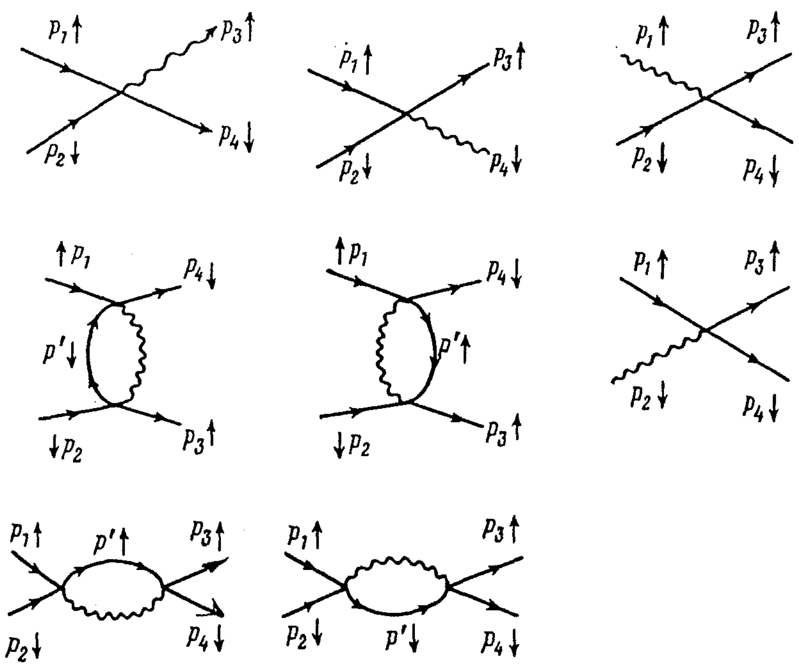

FIG. 1. Born scattering amplitudes. A wavy line shows the factor $t_{\vec{p}}$, and a solid line shows a one-particle Green's function $(i w_n - \xi_p)^{-1}$. Each four-vertex part makes its own contribution to the scattering amplitude with a factor of -1.

The momenta $\vec{p}_1$ and $\vec{p}_3$ correspond to incident and scattered waves with spin up, while $\vec{p}_2$ and $\vec{p}_4$ correspond to excitations with spin down. Here $\vec{s}=\vec{p}_1+\vec{p}_2=\vec{p}_3+\vec{p}_4$ is the resultant momentum, and $\vec{q}=\vec{p}_4-\vec{p}_1=\vec{p}_2-\vec{p}_3$ is the momentum transfer.

In the logarithmic approximation, and at $T=0$, a point at which the exact scattering amplitude (which cannot be drawn on the basis of two lines in the same direction) changes sign corresponds to the onset of superconductivity. This point has previously been calculated only in the Born approximation and for an "empty" lattice.[2] That case corresponds to the first sum in (3). The other sums should be thought of as the terms of the one-loop approximation, to which all the other one-loop corrections must be added (Fig. 2):

$$\Delta\Gamma(\vec{p},\vec{q}) = \sum_{\vec{p}'}\{ft_{\vec{p}}^2+[t(\vec{p}')+t(\vec{p}'+q)]t(\vec{p})+t(\vec{p}')t(\vec{p}'+\vec{q})\}$$
$$\times[n_F(\xi_{\vec{p}'+\vec{q}})-n_F(\xi_{\vec{p}'})][\xi_{\vec{p}'}-\xi_{\vec{p}'+\vec{q}}]^{-1} \qquad (5)$$

The largest contribution to (5) comes from fluctuations of the ferromagnetic type. Correspondingly, we set $\vec{s}=\vec{q}=0$ in all the equations. As a result, taking the limit $T\to 0$, we find the following condition for the occurrence of a superconductivity:

$$-2\epsilon_0-2\int_{-w}^{\epsilon} y\rho_0(y)dy+\epsilon_0^2(1+3f^{-1})\rho_0(\epsilon_0)\le 0. \qquad (6)$$

Here $\rho_0(\epsilon)$ is a seed density of states, and the parameter ϵ_0 determines the average density in terms of the equation of state in (4):

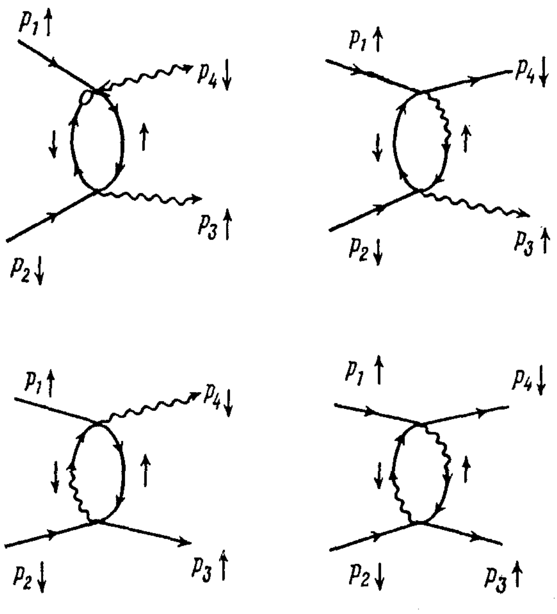

FIG. 2. One-loop paramagnetic corrections. All the diagrams have an extra factor of -1, since they contain a closed fermion loop. A circle represents the average Güzwiller factor $1-\langle n_{\vec{r}\sigma}\rangle=f$. The notation is otherwise the same as in Fig. 1.

$$\rho_0(\epsilon) = \sum_{\vec{p}} \delta(\epsilon - t_{\vec{p}}), \quad n_d = 2f \int_{-w}^{\epsilon} \rho_0(y) dy. \tag{7}$$

In the simple case of a so-called flat band, with $\rho_0(\epsilon) = \theta(w^2 - \epsilon^2)/2w$, $n_d = 2(1+\epsilon_0)/(3+\epsilon_0)$, the left side of (6) is always positive, and no Cooper singularity arises.

The case of greatest interest is that of a square lattice:

$$\rho_0(\epsilon) = 2K'(\epsilon)/\pi^2, \quad \int_{-1}^{\epsilon} y\rho_0(y) dy = -2[E'(\epsilon) - \epsilon^2 K'(\epsilon)]\pi^{-2}, \tag{8}$$

where $K'(\epsilon) = K(\sqrt{1-\epsilon^2})$ *and* $E'(\epsilon) = E(\sqrt{1-\epsilon^2})$ are the complete elliptic integrals of the first and second kinds. Condition (6) becomes

$$-\epsilon\pi^2 + 2E'(\epsilon) - \epsilon^2(1 - 3f^{-1})K'(\epsilon) \leq 0. \tag{9}$$

Equation of state (4) is determined by a numerical integration:

$$f = 1 - \frac{n_d}{2}; \quad n_d = 4f \int_{-1}^{\epsilon} K'(y) dy \pi^{-2}. \tag{10}$$

Eliminating f and n_d, we find the interval of values of the parameter ϵ for which condition (9) holds: $0.39 < \epsilon < 0.75$. According to the equation of state, this result corresponds to a fairly narrow concentration interval: $0.045 < 1 - n_d < 0.134$.

It can be seen from (9) that the logarithmic singularity in the density of states of the square lattice as $\epsilon \to 0$ is cancelled completely by the small values of the hopping integral.

A plane model with a triangular lattice also has a logarithmic singularity, but in this case at a finite energy, with the sign opposite that of the hopping integral. With $\epsilon \propto -t$, we have $\rho_0(\epsilon) \approx \ln|t/(\epsilon + t)|$. A study of the Cooper instability for negative hopping integrals and for $\epsilon \propto -t > 0$ reduces to a solution of the fast-parquet equations. In total analogy with Ref. 3, we have

$$-\dot{\Gamma}_1 = \Gamma_1^2 + \Gamma_2^2; \quad -\dot{\Gamma}_2 = 2\Gamma_2(\Gamma_1 - \Gamma_3); \quad \dot{\Gamma}_3 = \Gamma_2^2 + \Gamma_3^2. \tag{11}$$

The superior dot here means a differentiation with respect to the doubly logarithmic variable $s = |t|^{-1}\ln^2|t/T|$. We see that the amplitude Γ_2, which mixes the zero-sound channel (Γ_3) and the Cooper channel (Γ_1), disappears at a stable singular point:

$$\gamma_1 = 1, \quad \gamma_2 = \gamma_3 = 0, \quad \text{if} \quad \Gamma_K = \gamma_K/s. \tag{12}$$

In the parquet approximation,[3] a triangular lattice with an excitation energy

$$\epsilon_{\vec{p}} = -f|t|[\cos p_x + \cos p_y + \cos(p_x + p_y)] \tag{13}$$

leads to a superconductivity for a Fermi energy on the order of $f|t|$. As the Fermi level is raised, the density of state falls off rapidly, so we can again use "one-loop" approximation(6). Substituting the maximum value $\epsilon = 3|t|/2$ and $\epsilon\rho_0(\epsilon) = \sqrt{3}/\pi$ into (6), we find a positive value of the scattering amplitude. Consequently, again in the case of a triangular lattice with $t<0$, the superconductivity occurs in a fairly narrow concentration interval, corresponding to positive Fermi energies adjacent to the value $\mu \propto f|t|$.

A triangular lattice with a positive hopping integral is an exceptional case. For positive enegies in this case, the density of state is always finite, and it reaches its minimum as $\epsilon \to 3t$. In the same limit we have $\epsilon\rho_0(\epsilon) = \sqrt{3}/2\pi$, so the amplitude in (6) is extremely small in absolute value but negative.

For both simple lattices with a negative hopping integral, there thus exists a finite and fairly narrow concentration interval, for which there is a finite region in which a superconducting state exists even in the one-loop approximation, (6).

The result found here agrees only qualitatively with experimental data. According to Ref. 4, superconductivity occurs in the compound $Ln_{2-x}Ce_xCuO_{4-\delta}$ in the concentration interval $0.14 < x < 0.18$, and the value of δ is not known, beyond the fact that it is small. According to our analysis, superconductivity exists for a square lattice in a slightly broader region, shifted from the region given above: $0.045 < +2\delta < 0.134$.

This result is consistent with the numerical calculations by Scalapino *et al.*,[5] who found, even at $1 - n_d = 0.125$ a tendency for the repulsive scattering amplitude to decrease.

Large paramagnetic fluctuations thus cause a substantial shrinkage of the region in which a superconducting state exists. It is important to note that condition (6) incorporates fluctuations in an amplified form. All four sums in (5) can be thought of as the first term of an expansion of a generalized magnetic susceptibility. A ladder summation in the antiferromagnetic and zero-sound channels renormalizes the Born amplitude in (3). In the same approximation, it is possible to sum the contributions of the longitudinal and transverse paramagnetic fluctuations. As a result of this renormalization, relation (6) becomes

$$-\frac{2\epsilon_0}{[1+\epsilon_0(1+\Phi_0)\rho_0(\epsilon_0)]} + (1+\epsilon_0^2)\Phi_1(\epsilon_0) + \frac{3\epsilon_0^2\rho_0(\epsilon_0)}{2[1-\Phi_0+2\epsilon_0\rho_0(\epsilon_0)]} \leq 0, \qquad (14)$$

where $\Phi_K = \int_{-w}^{\epsilon_0} y^K \rho_0(y)dy$.

Analysis of (14) yields a region broader than that found from (6) for the existence of a superconducting state. In all three versions—for the square and triangular lattices with negative and positive hopping integrals—condition (14) holds beginning at some positive value and ending at some maximum possible value $\epsilon = w$, which corresponds to $n_d = 1$. An exceptional case is the model of a flat band, for which condition (14) holds in the interval $0.1838 < \epsilon < 0.827$ or for concentrations in the interval $0.256 > 1 - n_d > 0.045$.

In summary, conditions (6) and (14) both indicate that a superconductivity is possible in a Hubbard model with $U_d = \infty$. Numerical calculations[5] and experiments[4] agree qualitatively with this conclusion. The narrow dopant-concentration interval found in this manner lies outside the region in which antiferromagnetic fluctuations of nearly localized spins exist. According to Ref. 6, that interval is $|1-n_d|<t/U_d$, and with $U_d=\infty$ it lies outside the scope of the present paper.

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