Temperature × doping phase diagram of cuprate superconductors

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received 14 December 2014; accepted in final form 16 April 2015
published online 8 May 2015

PACS 74.72.-h – Cuprate superconductors
PACS 74.40.Kb – Quantum critical phenomena
PACS 74.62.Dh – Effects of crystal defects, doping and substitution

Abstract – Starting from a spin-fermion model for the cuprate superconductors, we obtain an effective interaction for the charge carriers by integrating out the spin degrees of freedom. Our model predicts a quantum critical point for the superconducting interaction coupling, which sets up a threshold for the onset of superconductivity in the system. We show that the physical value of this coupling is below this threshold, thus explaining why there is no superconducting phase for the undoped system. Then, by including doping, we find a dome-shaped dependence of the critical temperature as charge carriers are added to the system, in agreement with the experimental phase diagram. The superconducting critical temperature is calculated without adjusting any free parameter and yields, at optimal doping \( T_c \sim 45 \text{ K} \), which is comparable to the experimental data.

Introduction. – So far, there is no consensus concerning the microscopic mechanism which is responsible for the appearance of superconductivity in the cuprate superconductors. Yet, it is widely accepted that some sort of spin exchange mechanism should be responsible for the Cooper pair formation in the cuprates [1–4]. Following this path, in the present paper we obtain a novel superconducting interaction for the cuprates, which provides critical temperatures (high \( T_c \)) that are comparable to the ones experimentally observed, without resorting to any adjustment of free parameters.

We also obtain a dome-shaped superconducting phase diagram as charge carriers are added to the system, which reproduces qualitatively the experimental behaviour observed for the cuprates as the compound is doped. Indeed, the parent compounds of high-\( T_c \) superconductors are Mott insulators and the system becomes superconducting as holes are pumped into the \( \text{CuO}_2 \) planes while extra atoms (oxygen in YBCO, strontium in LSCO) are stoichiometrically added to the system. \( T_c \) increases up to an optimal value and then decreases forming the characteristic dome-shaped phase diagram [5,6].

Our starting point is the spin-fermion model, which has been extensively used to previously describe the cuprates [7–10]. The task of providing a minimal Hamiltonian, with only a few parameters, which captures the main physics presented by the cuprates can be rather elusive, because key issues may be lost in the attempt of simplifying the system description. As a matter of fact, there is no consensus whatsoever regarding the minimal model which entails the vast phenomenology presented by the cuprates, however the three-band Hubbard model proposed by Emery [11,12] is a good candidate to model the \( \text{CuO}_2 \) planes of the cuprates. It is well established that it is from these planes that superconductivity emerges in the cuprates. However, the three-band model is given in terms of several parameters and its analysis can be rather complicated. On the other hand, in the absence of doping the parent compound is reduced to a single-band Hubbard model with a strong on-site Coulomb repulsion at half-filling. For the square lattice, which is the appropriate lattice topology for the \( \text{CuO}_2 \) planes, the model is mapped into the antiferromagnetic spin-(1/2) Heisenberg model [13], which, indeed, describes well the dynamics of the spin degrees of freedom of undoped copper oxides [14]. Moreover, analytic calculations for the Heisenberg model provided the basis for understanding a range of experimental results for the undoped cuprates [15,16]. As the
system is doped, charge carriers are added to the \( p \) orbitals of the oxygen and we assume that the localized spins of Cu should interact with the spins of the itinerant fermionic charge carriers. This is the picture that we envision for the calculation of the superconducting phase diagram in the present paper. In fact, several authors have previously employed the same approach in order to model the cuprates superconductors [4,17–21].

Our approach is different from those previous attempts to describe the phenomenology of the cuprates because presently we employ the spin coherent states to integrate out the spin degrees of freedom in order to obtain the effective interaction for the charge carriers. It should be emphasized that we did not resort to any kind of perturbative method, diagrammatic expansion or auxiliary slave-boson technique in order to obtain our effective fermion theory.

Next, we calculate the superconducting phase diagram using as input the physical values of parameters, which have been measured for the cuprates.

The paper is divided as follows: in the next section we introduce the model and briefly outline the derivation of the effective dynamics for the itinerant fermion fields. Then, we proceed by calculating the \( T_c \) \( \times \mu \) superconducting phase diagram obtaining the familiar dome-shaped diagram, which displays values that are comparable to the experimentally observed ones. However, for systems in a spatial dimension less than three the Coleman-Mermin-Wagner-Hohenberg theorem [22] forbids the occurrence of a phase transition at finite temperatures. Nonetheless, for two-dimensional systems, such as our case, there is an underlying Berezinskii-Kosterlitz-Thouless (BKT) transition [23] for \( T < T_{KT} \), below which phase coherence is found for a nonzero order parameter. The actual temperature for the appearance of superconductivity is set at

\[
T<T_{KT}
\]

where the spin stiffness is given by [29]:

\[
\bar{\chi} = \frac{\hbar v_f}{8} \sqrt{\rho_s} \left[ |S|^2 - 1 \right] - \frac{\rho_s}{2} |a\nabla| \nabla \cdot \psi + i \langle \nabla \psi \rangle
\]

with the itinerant spin operator as

\[
s = \psi_{\delta}^\dagger (\delta) \bar{\sigma} \psi_{\gamma}.
\]

The localized spins interact with the spin degrees of freedom of the charge carriers by a Kondo-like term, whereas the localized spins mutual interaction is described by an antiferromagnetic Heisenberg Hamiltonian. The complete Hamiltonian is

\[
H = -t \sum_{\langle i j \rangle} \left( c_{i \alpha}^\dagger c_{j \alpha} + c_{j \alpha}^\dagger c_{i \alpha} \right)
+ J_K \sum_i \langle c_{i \alpha}^\dagger \bar{\sigma} c_{i \beta} + \text{c.c.} \rangle
+ J_\theta \sum_{\langle i j \rangle} S_i \cdot S_j,
\]

where \( S_i \) is the localized spin operator and \( c_{i \alpha}^\dagger \) is the creation operator of a charge carrier with spin \( \alpha = \uparrow, \downarrow \), both at site \( i \). In terms of the three-band Hubbard model parameters, the Kondo coupling of an itinerant oxygen hole spin and the nearest local Cu spin is [19,26]

\[
J_k = t_{pd}^2 \left( \frac{1}{\Delta E} + \frac{1}{U_d + \Delta E} \right)
\]

and the exchange coupling between the Cu magnetic moments is given by [20,27]

\[
J_d = \frac{4t_{pd}^4}{(\Delta E + U_{pd})^2} \left( \frac{1}{U_d} + \frac{1}{2\Delta E + U_p} \right).
\]

Presently, in numerical calculation we employ the following values for the above parameters [27]: \( t_{pd} = 1.48 \), \( U_d = 8.5 \), \( U_p = 4.1 \), \( U_{pd} = 1.3 \) and the difference in energies [28] are \( \Delta E = U_d/4 - U_p/8 = 1.61 \), all given in units of eV.

Now, we express the partition function as a path integral in the complex time representation. In order to obtain the continuum limit of our model Hamiltonian in (1), we use spin coherent states. In the presence of these, we may replace the spin operators \( S_i \), by \( SN(x) \), where \( S \) is the spin quantum number and \( N(x) \) is a classical vector that is decomposed into two perpendicular components associated with ferromagnetic and antiferromagnetic fluctuations, respectively, \( L \) and \( n \). Moreover, we also replace the operator \( c_{i \alpha}^\dagger \) by the fermion field \( \psi_{\alpha}^\dagger (x) \), as usual. Hence, the partition function becomes

\[
Z = \int \mathcal{D}\psi \mathcal{D}\psi^\dagger \mathcal{D}L \mathcal{D}n \delta \left[ |n|^2 - 1 \right] \times \exp \left[ -\int_0^\beta d\tau \int d^2 x \left( \mathcal{H} - \psi^\dagger \partial_{\tau} \psi \right) \right],
\]

where the continuum Hamiltonian density reads

\[
\mathcal{H} = \psi^\dagger \left( i \hbar v_f \bar{\sigma} \cdot \nabla - \mu \right) \psi + \frac{\rho_s}{2} |a\nabla| \nabla \cdot \psi + \frac{\chi_\perp}{2} S^2 |L|^2 + SL \cdot [J_K S + i (n \times \partial_r n)]
+ (-1)^z |S| J_R n \cdot s,
\]

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We can perform the Gaussian integration over $L$ in (4) and rewrite the AF fluctuation field $n_i$ using the $CP^1$ formulation (Schwinger bosons) of the O(3) nonlinear sigma model, which is written in terms of the two complex fields $z_\alpha (\alpha = 1, 2)$, namely $n_i = z_\alpha^* (\sigma_i)_\alpha \bar{z}_\alpha$, $i = x, y, z$ [30]. We also perform the canonical transformation on the fermion field [31] $\psi_\alpha \rightarrow U_{\alpha \beta} \psi_\beta$, where the unitary matrix $U$ is given in terms of the $z_\alpha$-fields,

$$U = \begin{pmatrix}
    z_1 & -z_2^* \\
    z_2 & -z_1^*
\end{pmatrix}.$$  \hspace{1cm} (6)

Employing the polar representations of the bosonic fields, $z_\alpha = \rho_\alpha e^{i \theta_\alpha}/\sqrt{2}$, we can perform the functional integration over the Schwinger boson fields assuming constant $\rho_\alpha$ and we obtain the resulting effective Lagrangian density for the fermion fields associated to the charge carriers [32],

$$\mathcal{L}_{\text{eff}} = \bar{\psi} \left[ i\gamma^\mu \partial_\mu - \mu \right] \psi + g_1 \bar{\psi} \gamma^\mu \psi \partial_\mu + g_2 \bar{\psi} \gamma^\mu \psi \partial_\mu + g_3 s^2,$$  \hspace{1cm} (7)

where the above interaction strengths are $g_0 = (2\bar{\rho}_0)^{-1}$, $g_1 = (8\bar{\rho}_0)^{-1}$, $g_2 = (4\bar{\rho}_0)^{-1}$, and $g_3 = (4\bar{\rho}_0)^{-1}$, with $c^2 = \rho_\alpha \chi_\perp$ and $\bar{\rho}_0 = \rho_\alpha (a/\hbar \nu f)^2$. The first interaction term corresponds to a BCS-type superconducting interaction, with the singlet pair operator denoted by $p = \psi_{2\uparrow} \psi_{1\downarrow} + \psi_{1\uparrow} \psi_{2\downarrow}$, the second and third terms produce an insulating charge-gapped phase showing an excitonic condensate, a Nambu-Jona-Lasinio-type, the fourth term corresponds to an anisotropic spin-spin interaction. The couplings above are calculated taking the parameters from our model Hamiltonian, which yields $g_0^{\text{est}} = 0.21\text{eV}$, $g_1^{\text{est}} = 0.052\text{eV}$, $g_2^{\text{est}} = 0.34\text{eV}$, and $g_3^{\text{est}} = 0.045\text{eV}$, and we see that $g_1^{\text{est}}$ and $g_3^{\text{est}}$ are small compared to the superconducting interaction strength.

One can now introduce the Hubbard-Stratonovich (HS) auxiliary fields in (7),

$$\Delta = g_0 (\psi_{2\uparrow} \psi_{1\downarrow} + \psi_{1\uparrow} \psi_{2\downarrow}),$$  \hspace{1cm} (8)

$$M = g_1 \bar{\psi} \gamma^\mu \psi \partial_\mu,$$  \hspace{1cm} (9)

$$N = g_2 \bar{\psi} \gamma^\mu \psi \partial_\mu,$$  \hspace{1cm} (10)

$$s_z = g_3 \bar{\psi} \gamma^2 \bar{\psi} \gamma^3,$$  \hspace{1cm} (11)

in order to rewrite the effective Lagrangian density as

$$\mathcal{L}_{\text{eff, HS}} = -\frac{g^2 \hbar}{(2\pi)^2} \Phi^I(k) A \Phi(k),$$  \hspace{1cm} (12)

where the Nambu field is given by

$$\Phi^I(k) = \begin{pmatrix}
    \psi_{1\downarrow}^I(k) & \psi_{2\uparrow}^I(k) & \psi_{1\downarrow}(-k) & \psi_{2\uparrow}(-k)
\end{pmatrix}^T.$$  \hspace{1cm} (13)

and the matrix $A$ is

$$A = \begin{pmatrix}
    -\mu_+ + N_- & -h \nu f k_- & 0 & -\Delta \\
    -h \nu f k_+ & -\mu_- + N_+ & -\Delta & 0 \\
    0 & -\Delta^* & \mu_+ - N_+ & h \nu f k_+ \\
    -\Delta^* & 0 & h \nu f k_- & -\mu_- - N_+
\end{pmatrix}.$$  \hspace{1cm} (14)

such that $k_\pm = k_y \pm ik_z$, $\mu_\pm = \mu \pm M$, and $N_\pm = N \pm s_z$, since we have Fourier transformed $\mathcal{L}_{\text{eff, HS}}$, and the standard quadratic terms of the HS fields have been omitted in (12) for the sake of simplicity. This transformation is exact and no approximation has been performed to the theory up to this point. Notice that we have eliminated the quartic fermionic interactions in (12) at the expenses of having introduced the scalar fields (8)–(11). But now we can perform the Gaussian integration over the fermionic fields exactly, since the partition function can be expressed as a path integral in the complex time representation.

Replacing the HS fields for their expected values, the auxiliary field $N$ in (10) only introduces a trivial shift of the chemical potential and therefore shall be omitted from now on. The case for $g_0, g_3 \neq 0$ has been previously reported [33]. However, in the present paper, we shall neglect the $g_3$ interaction term, since its coupling is small compared to $g_0$ and we are not interested in the magnetic ordering of the itinerant fermion fields for the cuprates, only the superconducting phase is considered in the present paper. Furthermore, to our best knowledge, the case $g_0, g_1, g_3 \neq 0$ has never been investigated, but the case for $g_0 = g_1 = 0$ has been previously reported [34] and it was shown that, as long as $g_0 > g_1$, such as the case for our parameter values, the system does not present the excitonic gap and becomes superconducting as charge carrier are added to the system, $\mu > 0$ increases.

**The superconducting phase diagram.** – We start our analysis calculating the free energy (effective potential) as a function of the order parameters. We proceed to the evaluation of the partition function as a path integral in the complex time representation and integrate it over the fermionic fields. Thereby, the effective potential becomes

$$V_{\text{eff}} = -\frac{1}{\beta} \sum_{n = -\infty}^{\infty} \frac{a_D}{2\pi}^2 \int d^2 k \log \left( \frac{\prod_{j=1}^3 [i \omega_n - E_j]}{\prod_{j=1}^3 [i \omega_n - E_j (M = 0, \Delta = 0)]} \right)$$  \hspace{1cm} (15)

where $\omega_n = (2n + 1)\pi T$ are the Matsubara frequencies for fermions, $a_D$ is the lattice spacing for dopants, and

$$E_j = \pm \left[ M^2 + |\Delta|^2 + \mu^2 + (h \nu f |k|^2) \right]$$

$$\pm 2 \sqrt{M^2 (|\Delta|^2 + \mu^2) + \mu^2 (h \nu f |k|^2)}^{1/2}.$$  \hspace{1cm} (16)
The above expression corresponds to the first term of a large-$N$ expansion. Any improvements to the critical temperature calculated here can be done employing standard diagrammatic techniques. However, our results are exact in the $N \to \infty$ limit.

We start our analysis showing that at zero temperature and $\mu = 0$ there is a critical coupling $g_c$ for the superconducting interaction strength which is required for the system to become superconducting. Indeed, we integrate eq. (15) over $k$ in the first Brillouin zone at $T = 0$ in order to obtain the effective potential in terms of $\Delta$, with $M = \mu = 0$,

\[
V_{\text{eff}}(\Delta) = \frac{|\Delta|^2}{g_0} + \frac{a_D^2}{3\pi(hv_f)^2} \left[ |\Delta|^2 + \left( \frac{h v_f \pi}{a_D} \right)^2 \right]^2
- |\Delta|^3 \left( \frac{h v_f \pi}{a_D} \right)^3.
\] (17)

The minima condition requires $V_{\text{eff}}'(\Delta) = 0$ and $V_{\text{eff}}''(\Delta) > 0$. Thus, $\Delta_0 = 0$ is a minimum only for $g_0 \leq g_c$, while, on the other hand,

\[
\Delta_0 = \left( \frac{g_0 a_D}{h v_f} \right)^2 - 4 \left( \frac{4 g_0 a_D}{\pi (h v_f)^2} \right).
\] (18)

is a minimum only for $g_0 > g_c$, with $g_c = 2 h v_f / a_D = 0.86 \text{ eV}$. Comparing $g_0$ and $g_0'_{\text{est}}$, we see that $g_0'_{\text{est}} < g_c$, explaining why the system is not superconducting in the absence of doping (or $\mu = 0$), as indeed observed experimentally.

We now turn to the finite temperature analysis. Since we are looking for the condition of minima for the free energy, we take the derivative of $V_{\text{eff}}$ with respect to $\Delta$ and $M$ after the summation over the Matsubara frequencies, the nonzero solutions of the order parameters provide the following two coupled equations:

\[
\frac{1}{g_0} = \sum_{j=\pm 1} \left( \frac{a_D}{2\pi} \right)^2 \int dk^2 \frac{1}{2\Delta} \frac{\partial \Delta}{\partial \epsilon_j} \tanh \left( \frac{\beta \epsilon_j}{2} \right),
\] (19)

\[
\frac{1}{g_1} = \sum_{j=\pm 1} \left( \frac{a_D}{2\pi} \right)^2 \int dk^2 \frac{1}{2M} \frac{\partial M}{\partial \epsilon_j} \tanh \left( \frac{\beta \epsilon_j}{2} \right).
\] (20)

The numerical solutions for the superconducting critical temperature $T_c$, as a function of the chemical potential $\mu$ can be seen in fig. 1. Since $g_0 > g_1$, we find only superconductivity for the system, as we have already stated above, and at $\mu = 0$ the system is in the normal state. As $\mu$ increases a Fermi surface builds up and the system asymptotically becomes superconducting, in agreement with Cooper’s theorem; as $\mu$ increases even further, $T_c$ reaches a maximum value at an optimal chemical potential and it decreases as charge carriers are added to the system. A dome-shaped plot is consistent to previous results for two-color and two-flavor QCD [35] and also strongly interacting two-dimensional Dirac fermions [36]. Those results and the phase diagram presently calculated suggest that Dirac fermions may play a relevant role in the description of systems containing Dirac fermions. Moreover, we see that we have obtained a high value for $T_c \sim 45 \text{ K}$, which is comparable to the experimental data for a single CuO$_2$ plane. Notice that the high value of the critical temperature was obtained simply employing the model parameters given above, without resorting to any adjustment of free parameters.

Conclusions. – Starting from the spin-fermion model we have obtained an effective model for charge carriers by integrating out the spin degrees of freedom. Our model predicts a critical interaction for the superconducting interaction which sets a quantum critical point for the appearance of superconductivity in the system. We have shown that the interaction strength is smaller than this threshold explaining why there is no superconductivity in the absence of doping. As charge carriers are added to the system, a Fermi surface builds up and the quantum phase transition is washed out, in agreement with Cooper’s theorem.

For the model parameters appropriate for the cuprates compounds, we have calculated the superconducting phase diagram, by means of the BKT mechanism, and we have found a dome-shaped dependence of the temperature on the chemical potential, which is in agreement with the well-known results for the cuprates. Without resorting to any adjustment of free parameters, we have found an optimal $T_c$ which is high and comparable to the experimental data, $T_c \sim 45 \text{ K}$. Superconductivity arises from a novel mechanism, which originates from the purely magnetic interactions involving the localized spins and itinerant electrons of the original system. This result is also consistent with DMRG calculations for the 1d Heisenberg-Kondo model [37], which shows the development of a superconducting phase mediated by antiferromagnetic fluctuations. On the same token, mean-field calculations for the 2d Kondo lattice [38], shows that, as an AFM Heisenberg exchange coupling
is taken into account, singlet Cooper pair occurs among conduction electrons, leading to heavy fermion superconductivity. Hence, our derivation may provide an analytical explanation for those results without the resort of any approximation, which is a very interesting result.

The singlet pairing that we have obtained here emerges from the interaction of local magnetic moments with the spins of a conduction band. Several compounds like pnictides, heavy fermion compounds, chalcogenides (and cuprates as well) may be described by multi-orbital models with interactions between magnetic moments and the spins of conduction bands. Their structure, phase diagrams and experimental data provide a phenomenological evidence relating these compounds [39]. Therefore, the approach employed here is not just restrained to the cuprates, but might be applied to several other compounds, providing a framework for the underlying microscopic mechanism which is responsible for the appearance of superconductivity in several unconventional superconductors.

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ECM has been supported in part by CNPq and FAPERJ.

APPENDIX

In this appendix we discuss how $d$-wave superconductivity can be obtained from the approach employed above. We start pointing out that we have assumed a constant contact point exchange coupling among local magnetic moments, as seen in (3). Instead, let us take, for instance, the following exchange interaction [9]:

$$H_{\text{exc}} = g \sum_{\mathbf{q}} \chi_0^{-1}(\mathbf{q}) \mathbf{S}_\mathbf{q} \mathbf{S}_{-\mathbf{q}},$$

(A.1)

where $g$ is some constant value and the spin susceptibility was proposed by Millis, Monien and Pines [40], which has been shown to provide a quantitative fit to the NMR experiments in YBCO,

$$\chi_0(\mathbf{q}, \omega) = \frac{\chi_0}{1 + \xi^2 (\mathbf{q} - \mathbf{Q})^2 - i\omega/\omega_{\text{SF}}},$$

(A.2)

with $\chi_0$ as the static susceptibility peaked at wave vector $\mathbf{Q} = (\pi/a, \pi/a)$, $\xi$ as the antiferromagnetic correlation length and $\omega_{\text{SF}}$ as the paramagnon energy. This spin susceptibility has a regular Ornstein-Zernike form and RPA calculations for nearly half-filled Hubbard model also provide the same overall form [39].

Following our approach, we argue that the superconducting coupling becomes $g_0 \rightarrow g_0 \chi(\mathbf{q})$ in momentum space and the new gap equation in the singlet channel becomes [3]

$$\Delta(k) = -\tilde{g} \int d^2k \chi(k - p) \Delta(p) \tanh(\beta E/2),$$

(A.3)

where $\tilde{g} > 0$. Except for the extra minus sign on the right-hand side of the above equation, this is essentially the self-consistent gap equation from the BCS theory. Because of the sign change, an isotropic $s$-wave solution is impossible, since the gap equation is not convergent. However, since $\chi(q)$ is peaked near $Q = (\pi/a, \pi/a)$, pairing interaction relates the gap at momenta $k$ and $k + Q$. In this situation, we use the ansatz $\Delta(k) = -\Delta(k + Q)$ therefore eliminating the minus sign. For tetragonal lattice, this ansatz implies $d_{x^2-y^2}$ symmetry of the pairing gap [41].

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