Spin-gap formation in cuprates: gauge theory

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(March 23, 2022)

Abstract

We analyze the phase diagram of single and bi-layer cuprates using the gauge-field description of the $t$-$J$ model. For $T > T_{BE}$ the in-plane fermion-pairing order parameter $\Delta_\parallel$ is eliminated by gauge field fluctuations, leading us to predict the absence of a spin-gap phase in single-layer cuprates. For bi-layer cuprates the inter-layer order parameter $\Delta_\perp$ is enhanced by spin correlations, and is less affected by gauge fluctuations. We believe that the spin gap in bi-layer materials is due to inter-layer fermion pairing, and that for these underdoped samples the superconducting gap may be nodeless.

PACS numbers: 74.20.Mn, 75.10.Jm, 74.25.Nf
It is widely accepted that the high-$T_c$ copper-oxide compounds are Mott-Hubbard insulators which become metallic and superconducting upon hole doping. Thus a useful starting point for describing the copper-oxides is the two-dimensional Hubbard model, and many workers have studied the strong-coupling limit which leads to the $t$-$J$ model. A common technique to incorporate the constraint of no double occupancy is to decompose the electron operator $c_{i\sigma}^\dagger$ as the product of a fermion operator $f_{i\sigma}^\dagger$ and a boson operator $b_i$, so that the constraint becomes $\sum_\sigma f_{i\sigma}^\dagger f_{i\sigma} + b_i^\dagger b_i = 1$. In this decomposition the fermions carry the spin, given by $\mathbf{S}_i = f_{i\sigma}^\dagger \mathbf{\sigma}_{\alpha\beta} f_{i\beta}$, and the bosons represent the empty sites. The exchange term can be written as

$$\mathbf{S}_i \cdot \mathbf{S}_j = -\frac{1}{2} (f_{i\sigma}^\dagger f_{j\sigma})(f_{j\sigma}^\dagger f_{i\sigma}) - \frac{1}{2} n_i n_j + \frac{1}{2} n_i$$

(1)

$$= -\frac{1}{2} (f_{i\uparrow}^\dagger f_{j\downarrow}^\dagger - f_{i\downarrow}^\dagger f_{j\uparrow}^\dagger)(f_{j\downarrow} f_{i\uparrow} - f_{j\uparrow} f_{i\downarrow})$$

(2)

which suggests two forms of mean-field decouplings $\Pi$: $\xi_{ij} = \sum_\sigma (f_{i\sigma}^\dagger f_{j\sigma})$ and $\Delta_{ij} = \langle f_{i\uparrow} f_{i\downarrow} - f_{i\downarrow} f_{i\uparrow} \rangle$. Let us briefly discuss the mean-field phase diagram, which is quite simple for intermediate doping $x \gtrsim 0.04$ [4]. It shows the onset of a nonzero $\xi_{ij}$ below a temperature $T \sim 0.2J$, and the onset of $d$-wave fermion pairing (i.e., $\Delta_{i,i+x} = -\Delta_{i,i+y}$) at a lower temperature shown by the dashed line in Fig. [1]. The physical interpretation of this state is the formation of a singlet ground state (the RVB state [1]), with a gap structure in the spin-excitation spectrum. In addition, the bosons are expected to effectively Bose condense, i.e. the diamagnetic susceptibility $\chi_B$ will diverge exponentially below a characteristic temperature, which in the mean-field approximation is given by $T_{BE}^{(0)} = 4\pi t \xi_x$. In the region bounded by $T_{BE}^{(0)}$ and the onset of fermion pairing, the pairing amplitude $\langle c_{i\uparrow} c_{j\downarrow} \rangle$ of the physical electrons is nonzero, and a $d$-wave superconductor is predicted. However, above $T_{BE}^{(0)}$ the holes are incoherent while the gap structure in the spin-excitation spectrum remains, and this region of the phase diagram has been called the spin-gap phase.

Experimentally there are clear signatures of spin-gap formation below $T \sim 150K$ in YBa$_2$Cu$_3$O$_{6+x}$ with $x = 0.6$ and in YBa$_2$Cu$_3$O$_8$. The signature is clearest in the copper and oxygen nuclear spin-relaxation rates $^{63/181}T_1^{-1}$ and $^{17}T_1^{-1}$, but it is also apparent in the Knight-shift data and in $T_2$ measurements [3]. Since the spin gap appears only in underdoped samples, one is naturally led to an explanation in terms of the fermion pairing discussed above. However, recently Millis and Monien re-examined the experimental evidence [4], and concluded that the spin-gap phase is absent in single-layer material such as La$_{2-x}$Sr$_x$CuO$_4$. They suggested that the inter-layer exchange coupling $J_\perp$ may be responsible for the spin-gap phase. However in the models they constructed, an unreasonably large exchange $J_\perp$, comparable to $J$, is required to explain the experimental data.

On the theoretical side, there has been much effort on improving the mean-field theory by including fluctuation corrections. It has been recognized that the phase fluctuations of the field $\xi_{ij}$ are the most important, leading to a gauge theory in which the fermions and the bosons are coupled to a U(1) gauge field $a_{ij}$ [3][4]. Integration over the gauge field enforces the condition that a flow of fermions is accompanied by a backflow of bosons. Initially the gauge field has no dynamics, which it only acquires upon integrating out the fermions and bosons. We focus on the transverse gauge field because, unlike longitudinal fluctuations, transverse currents are not screened, giving rise to unusual infra-red singularities [4]. The transverse gauge-field propagator is given by $D(q,\omega) = \Pi(q,\omega)^{-1}$, where $\Pi = \Pi_F + \Pi_B$, where...
\[ \Pi_F(q, i\omega_n) = \chi_F q^2 + |\omega_n| k_F/q, \] and \[ \Pi_B(q, i\omega_n) = \chi_B q^2. \] Here \( \chi_F \) and \( \chi_B \) are the fermion and boson diamagnetic susceptibilities, and for free bosons \( \chi_B^0 = (\exp(T^{(0)}_{BE}/T) - 1)/24\pi m_B \), while the \( |\omega_n| k_F/q \) term represents Landau damping. Recently we found that gauge fluctuations modify the mean-field phase diagram in a significant way [3,4]. The Bose-condensation temperature is greatly suppressed, and the spin-gap phase is eliminated entirely. The former effect is due to thermal fluctuations of the gauge field, given by \( \langle |\omega_n| k_F/q \rangle \). Note that at sufficiently low temperatures the RMS flux per plaquette is small. Nevertheless, since the deBroglie wavelength \( \lambda_T \) of the bosons covers many lattice spacings, the effect on the random gauge flux is strong. Indeed we find that the dimensionless coupling constant is \( g = (T/\chi)_{\lambda_T}^2 \sim (m_B \chi)^{-1} \). At temperatures above Bose condensation we may ignore \( \chi_B^0 \) compared to \( \chi_F^0 \) and we find that \( g = 24\pi t/J \), i.e. the system is in the strong-coupling limit even for modest \( t/J \). In this limit the Feynman paths of the bosons are almost self-retracing. By taking only static gauge-field configurations and taking a quenched average, we find that \( \chi_B \) grows inversely with \( T \), but is suppressed compared to the high-temperature limit of \( \chi_B^0 \) by a factor \( (0.2g)^{-1} \). At sufficiently low temperatures, \( \chi_B \) becomes much larger than \( \chi_F^0 \) and can therefore no longer be ignored in the estimate of \( g \). We crossover to the weak-coupling limit and \( \chi_B \) self-consistently diverges exponentially below a temperature \( T_{BE} \) which we estimate to be \( T^{(0)}_{BE}/12 \). This suppression of the effective Bose condensation eliminates one of the most serious drawbacks of the mean-field phase diagram, where \( T^{(0)}_{BE} \) yields a temperature scale which is much too large.

We also examined the effect of gauge fluctuations on the fermion pairing. Here we find that it is the quantum fluctuations which are important, and the effect is strong enough to de-stabilize the mean-field transition until the temperature falls below \( T_{BE}[9] \). We computed the gauge field contribution to the free energy

\[
F_{\text{gauge}} = \sum_q \int_0^\infty \frac{d\omega}{2\pi} |2n_B(\omega) + 1| \arctan \left( \frac{\text{Im} \Pi(q, \omega + i\delta)}{\text{Re} \Pi(q, \omega + i\delta)} \right).
\]

For \( T > T_{BE} \), \( \Pi \) may be replaced by \( \Pi_F \), and Eq. (3) yields a large negative contribution to the free energy which is cutoff by \( T \), leading to a \( T^{5/3} \) correction term, and a specific heat of \( T^{2/3} \). Now we can ask what happens if the fermions form a \( d \)-wave pairing state with amplitude \( \Delta \). We can compute \( F_{\text{gauge}}(\Delta) \) by replacing \( \Pi \) in Eq. (3) by the corresponding polarization function \( \Pi(q, i\omega_n, \Delta) \) in the pairing state. Since a gap appears in \( \text{Im} \Pi(q, \omega) \), the \( \omega \) integral is cutoff by \( \Delta \) instead of \( T \), and we obtain \( F_{\text{gauge}} \sim \Delta^{5/3} \). This is to be added to the mean-field gain in free energy \( F_{\text{MF}} \sim -\Delta^2 \), which is overwhelmed by \( F_{\text{gauge}} \) for small \( \Delta \). However, a first-order transition is in principle still possible. We have carried out a detailed numerical computation of \( F_{\text{gauge}}(\Delta) \), and found that the pairing state is unstable for \( T > T_{BE} \). Below \( T_{BE} \), \( \chi_B(T) \) grows exponentially and consequently \( \text{Re} \Pi_B \) dominates over \( \text{Re} \Pi_F \). Thus \( F_{\text{gauge}}(\Delta) \) becomes less important and the cost of opening up a gap is correspondingly weaker. Our calculations show that a first-order transition to a \( d \)-wave superconductor. Our best estimate of the transition temperature is shown in Fig. [1]. We expect the first-order nature of the transition to be smoothened out once phase fluctuations of the superconducting order parameter are taken into account. An important consequence of this analysis is that the spin-gap phase is completely eliminated by gauge
fluctuations. This agrees with the absence of a spin-gap phase in single-layer materials such as La$_{2-x}$Sr$_x$CuO$_4$.

Now that we have de-stabilized the spin-gap phase in a single layer, we have to appeal to inter-layer coupling to explain the appearance of spin gaps \[4\]. In a bi-layer material it is natural to look for an order parameter \[10\]
\[
\Delta_{\perp}(\mathbf{r}_{ij}) = \langle f^{(1)}_i f^{(2)}_j - f^{(1)}_i f^{(2)}_j \rangle,
\]
by decoupling the inter-layer exchange term \(H_{\perp} = J_\perp \sum_i S_i^{(1)} S_i^{(2)}\). At present we only have a lower bound \(J_\perp \gtrsim 8\) meV from the absence of an optical mode in the neutron scattering from undoped YBCO \[11\], but we expect \(J_{\perp}\) to be much smaller than \(J_{\parallel}\). A conventional pairing theory would then predict a gap which is exponentially small in \(J/J_{\perp}\). To overcome this we note that the underdoped cuprates have a reasonable long antiferromagnetic correlation length in the plane. In a bi-layer it is then favorable to form singlets not only between spins which are directly on top of each other, but also between other pairs on the same sublattice. Thus we expect the inter-layer pairing gap to be enhanced by in-plane correlations. To analyze this we employ the random-phase approximation (RPA), which has been quite successful in reproducing the experimentally observed spin correlations \[12\]. The RPA approach corresponds to a decoupling of the exchange term \(S_i \cdot S_j\) in a third channel which differs from the decouplings in Eqs. \(1\) and \(3\). In order to avoid double counting we separate the Hamiltonian into two equal parts, decouple the first part using Eq. \(1\) and apply RPA on the second part. Our results should not be too sensitive to this admittedly \textit{ad hoc} procedure. Within this scheme we define \(J_{\perp}^{\text{eff}}(\mathbf{q})\) as the effective inter-layer exchange due to the summation of a series of RPA bubbles shown in Fig. 2. This analysis will be discussed in more detail in Ref. \[13\]. The result is
\[
J_{\perp}^{\text{eff}}(\mathbf{q}) = \frac{J_\perp}{(1 + \frac{1}{4} \chi^0 J_{\parallel}(\mathbf{q}))^2 - (\frac{1}{4} \chi^0 J_\perp)^2}, \tag{5}
\]
where \(\chi^0(\mathbf{q})\) is the free-fermion bubble for the two-dimensional band structure. The denominator vanishes at the onset of the Néel ordering, which occurs at \(x_c \simeq 0.08\) within our approximation. The numerical solution of \(J_{\perp}^{\text{eff}}(\mathbf{q})\) for \(x \gtrsim x_c\) is shown in Fig. 2 and we see that it is significantly enhanced near the incommensurate nesting vector \(Q_{\text{AF}} \simeq (\pi, \pi \pm 2x)\). We find that for \(x = 0.09\) the peak at \(Q_{\text{AF}}\) leads to an antiferromagnetic correlation length of approximately 3 lattice spacings. We next take the Fourier transform of \(J_{\perp}^{\text{eff}}(\mathbf{q})\) to obtain \(J_{\perp}^{\text{eff}}(\mathbf{r}_{ij})\) and consider the effective inter-layer exchange \(J_{\perp}^{\text{eff}}(\mathbf{r}_{ij}) S_i^{(1)} \cdot S_j^{(2)}\), which is decoupled using Eqs. \(2\) and \(4\). The gap equation for the order parameter \(\Delta_{\perp}(\mathbf{r}_{ij})\) is solved numerically in real space. We find that the pairing amplitude is especially large on the diagonal such that \(\Delta_{\perp}(\mathbf{r}_{ii}) \simeq |\Delta_i|(-1)^i\) decays slowly with \(i\). Transforming \(\Delta(\mathbf{r}_{ij})\) back to \(k\) space, we find a quasi-particle dispersion \(E(\mathbf{k}) = [\epsilon(\mathbf{k})^2 + \Delta_{\perp}(\mathbf{k})]^{1/2}\), where \(\Delta_{\perp}(\mathbf{k})\) is shown in Fig. 3. Notice that \(\Delta_{\perp}(\mathbf{k})\) exhibits some anisotropy but does not change sign. Thus the inter-layer pairing is \(s\)-wave in nature, with a full gap in the excitation spectrum.

It is important to note that it is crucial in this approach that the in-plane \(d\)-wave pairing is suppressed by gauge fluctuations. One might ask whether gauge fluctuations will destroy the inter-plane pairing as well. We believe that this does not happen for the following
reason. There are two gauge fields modes $a_1$ and $a_2$ in the two layers, which are split into $a_{\perp} \equiv (a_1 \pm a_2)/\sqrt{2}$ at the onset of inter-layer pairing. The gauge propagators are given by $\Pi_{\perp}^\pm$ where

$$\Pi_{\pm}(q, i\nu_n) = C + 2T \sum_{\omega_n} \int \frac{d^2k}{(2\pi)^2} \left( \hat{q} \times \frac{\partial \epsilon}{\partial k} \right) \left( \hat{q} \times \frac{\partial \epsilon'}{\partial k} \right) \frac{\epsilon' - \omega_n\omega'_n \pm \Delta\Delta'}{(\omega_n^2 + E^2)(\omega'_n^2 + E'^2)},$$

where $i\omega'_n = i\omega_n - i\nu_n$; $\epsilon, \epsilon' = \epsilon(k \pm q/2)$; $\Delta, \Delta' = \Delta_{\perp}(k \pm q/2)$; and $E = \sqrt{\epsilon^2 + \Delta^2}$. For $\Delta = 0$, the constant $C$ exactly cancels the second term for $q \to 0$ and $\nu_n = 0$, so that the gauge field is massless in the normal state. In the pairing state a gap opens up in $\Pi_+(0,0) \sim \Delta_{\perp}^2$, but $\Pi_-$ remains massless. Furthermore, when we substitute $\Pi_{\perp}$ into Eq. (4), we find that while the $\Pi_+$ propagator introduces an energy cost and is pair-breaking as before, the $\Pi_-$ propagator is actually pair-enhancing. This is because even though an energy gap is introduced into Im $\Pi_-$, the coherence factor in Eq. (4) is such that $-\text{Im} \Pi_{\perp}/\text{Re} \Pi_{\perp}$ is enhanced for $\omega > 2\Delta_{\perp}$ compared to its normal state value, and this overwhelms the loss of the contribution from $\omega < 2\Delta_{\perp}$. This pair-enhancing nature of the $a_-$ mode can also be understood in another way [14]. The fermions on the two planes couple to the $a_-$ mode with opposite charge, so that the exchange of an $a_-$ mode leads to an attraction, analogous to what happens in the $t^*t'-J$ model [13]. In our case we expect that the effects of the $a_+$ and $a_-$ gauge fluctuations largely cancel each other, leaving the mean-field transition intact.

Since we are unable to compute $\Delta_{\perp}$ quantitatively, in the remainder of the paper we will use $\Delta_{\perp}$ as a parameter to compute various physical quantities, which we compare with experiments. We calculated the nuclear-relaxation rate $1/T_1$ for the copper and the oxygen sites, and we immediately encountered the problem that for $s$-wave pairing the Hebel-Slichter peak appears below $T_c$. We circumvented this by arguing that since the order parameter is not invariant under the local gauge transformation $f^{(1,2)}_{\sigma} \to e^{i\theta_{\sigma}} f^{(1,2)}_{\sigma}$ the transition should be broadened into a crossover behavior, and a BCS-type gap should be replaced by a pseudo gap as shown in the inset in Fig. [4]. With this and a modest broadening $\Gamma = 0.1T_1$, we eliminated much of the Hebel-Slichter peak, and the results are shown in Fig. [4]. Notice that above the crossover transition, $(63T_1T)^{-1}$ increases upon lowering $T$, which is due to antiferromagnetic correlations. We do not see this increase in $(63T_1T)^{-1}$, because the form factor $17F(q)$ for the oxygen site vanishes at the antiferromagnetic nesting vector $Q_{AF}$ [3]. We also computed $1/T_2$ and the uniform susceptibility $\chi(q = 0)$, shown in the second panel of Fig. [4]. The results compare reasonably well with experiments provided we choose $\Delta_{\perp} \approx 150K \approx 0.1J$. We believe that this is not an unreasonable value if $J_{\perp} \approx 0.2J$.

So far we have ignored any inter-layer hopping of the form $t_{\perp}c^{(1)}_{\sigma}c^{(2)}_{\sigma'}$ which is reasonable provided $xt_{\perp} < J_{\perp}$. If this is violated we expect inter-layer pairing to be suppressed, but we have not studied this quantitatively. Not enough is known about $t_{\perp}$ and $J_{\perp}$, but our guess is that $xt_{\perp}$ and $J_{\perp}$ are comparable. However, even a small $t_{\perp}$ will lead to coherence between bosons on the two planes immediately below $T_{BE}$, so that the fermion pairing becomes genuine superconducting pairing between electrons on the two layers. At low temperatures the in-plane $s$-wave and the inter-plane $d$-wave pairing will co-exist, giving rise to a quasi-particle dispersion $E(k) = (\epsilon(k)^2 + \Delta_{\perp}(k)^2)^{1/2}$, where $\Delta_{\perp}(k) = \Delta_{\perp}(k) \pm \Delta_{||}(k)$. If $\Delta_{\perp}$
is indeed as large as 150 K, as the experiments seem to indicate, comparison with Fig. 1 indicates that for underdoped materials it is likely that $\Delta_\perp > |\Delta_\parallel|$ for all $\mathbf{k}$, so that the superconducting gap is nodeless. As doping is increased, $\Delta_\perp$ decreases rapidly with the loss of antiferromagnetic correlations, which was essential for the enhancement of $J_\perp$, and we crossover to a superconducting state with nodes. As long as $\Delta_\perp$ remains finite we expect that there are eight nodes along the Fermi surface instead of the four nodes for a conventional $d$-wave superconductor. This new phase diagram is shown schematically in the insert in Fig. 1. Finally we note that Chakravarty et al. have shown that inter-layer pair tunneling leads to an anisotropic $s$-wave gap function. We emphasize that in our theory the order-parameter symmetry is always $d$-wave in the plane, even in the nodeless state. Furthermore, to the extent that our nodeless pairing state is always preceded by a spin-gap phase, we believe that the origin of superconductivity in our treatment is closer to the original RVB picture of pre-formed spin-singlet pairs than the more recent inter-layer pair-tunneling model.

We acknowledge helpful conversations with A.J. Millis. This work was supported by the NSF through the Material Research Laboratory under Grant No. DMR-90-22933.
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FIGURES

FIG. 1. The phase diagram for single-layer cuprates. The dashed line is the mean-field pairing transition. The solid line takes gauge fluctuations into account, so that fermion pairing only survives for $T < T_{BE}$, resulting in a $d$-wave superconductor. The inset is a schematic phase diagram for bi-layer materials. The spin-gap phase is due to inter-layer pairing. The superconducting state has $d$ symmetry in the plane with nodes in the gap function, but there may be a region indicated by the shaded area where the gap is nodeless.

FIG. 2. The effective interlayer coupling $J_{\perp}^{\text{eff}}(q)$ for various values of the doping $x$, using $J_{\perp} = 0.2J$. This is obtained by summing over RPA bubbles (inset). For $x \to 0.08$ there are strong incommensurate peaks at the nesting vector $Q_{AF}$.

FIG. 3. The gap $\Delta_{\perp}(k)$ for $x = 0.085$ and $J_{\perp}^{0} = 0.2J$. The gap has an extended $s$-wave symmetry, and is enhanced close to the Fermi surface (dotted line), especially at the corners.

FIG. 4. The first panel shows the nuclear-relaxation rates $(T_{1}T)^{-1}$ on the $^{63}\text{Cu}$ and the $^{17}\text{O}$ sites. The rise is $(^{63}T_{1}T)^{-1}$ is due to antiferromagnetic correlations, which is absent in $(^{17}T_{1}T)^{-1}$. The second panel shows $1/T_{2}$ and $\chi(0,0)$. The opening of a pseudo-gap (see inset) causes a rapid decrease in $(T_{1}T)^{-1}$, $1/T_{2}$, and $\chi(0,0)$ for $T \lesssim 0.1J$. 

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