Conjectures for the microscopic theory of high temperature superconductivity

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Based on experimental results and our previous theoretical work, a microscopic theory of high temperature superconductivity is conjectured. In this conjecture, superconducting and antiferromagnetic long-range orders are driven by interlayer coupling. Strictly in two dimensions, the microscopic Hubbard model has an (resonating valence bond) insulator-to-metal transition at $x = x_c$ near optimal doping for zero temperature, leading to a quantum critical point, and one of the crossover lines is given by the pseudogap temperature $T^*$. We argue that various singular and non-Fermi liquid properties observed near optimal doping are due to the presence of this quantum critical point. In our conjecture, the crossover line $T^*$ also practically divides the superconducting region into two, depending on the doping level with respect to $x_c$. For $x \leq x_c$ the superconducting state has significant antiferromagnetic correlations, while for $x > x_c$ it has virtually no antiferromagnetic correlations, thus justifying the conventional BCS theory based on the noninteracting electrons. Inelastic neutron scattering resonance and systematically reduced superfluid density in the superconducting state below $x_c$ have their natural explanations in the present scenario. The present approach supports interlayer pair tunneling model where the superconducting condensation energy comes from the lowering of the $c$-axis kinetic energy in the superconducting state. Comparison of the present scenario with some of the leading theories based on the Hubbard and $t-J$ models is given. The generic features of both hole-doped and electron-doped cuprates as well as heavy-fermion superconductors may be understood in the unified framework within the present picture.

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I. INTRODUCTION

Since the discovery of high temperature superconductivity in copper oxide compounds, enormous experimental and theoretical effort has been made in order to understand various anomalous behaviors in normal and superconducting (SC) states of these materials. Right after its discovery, it was recognized that the high temperature cuprate superconductors have in common layered perovskite-like crystal structures which consist of conducting CuO$_2$ planes separated by layers of other elements. These latter layers function as charge reservoirs and mobile charge carriers (holes or electrons) supplied from them are believed to reside mainly within the CuO$_2$ planes. Through extensive worldwide effort as well as the improvement of sample quality over the years, many consensuses have been reached in experimental side. First, let us start by showing a generic phase diagram (Fig. 1(a)) of a hole-doped cuprate Ln$_{2−x}$Sr$_x$CuO$_4$ in the doping ($x = 1 − n$) and temperature ($T$) plane. Since this compound has only one CuO$_2$ layer in a unit cell, it is one of the best materials to study physics taking place in a two-dimensional CuO$_2$ plane. In other hole-doped compounds, the presence of multi-layers and CuO chains makes it more complicated to extract the intrinsic features associated with a single CuO$_2$ plane. But the CuO$_2$ plane in Ln$_{2−x}$Sr$_x$CuO$_4$ is still not totally isolated from other CuO$_2$ planes in different unit cells.

Near half-filling and at low temperature, antiferromagnetic (AF) long-range order appears with $T_N = 250-300$ K at $x = 0$. It is destroyed by 2% doping concentration. When $x$ reaches 0.06, SC long-range order starts to appear, and it is also destroyed by 30% doping. In between them, $T_c$ reaches a maximum value of 40 K at $x \simeq 0.16$. The SC gap was found to have mainly $d$-wave character with possibility of a small mixture of other angular momentum states in contrast to conventional BCS superconductors with an isotropic $s$-wave gap. The low temperature phase between $T_N$ and $T_c$ is often designated as spin glass (SG) phase.

Various recent experiments also show the existence of a crossover temperature $T^*$ larger than $T_c$ in a doping range of $x = 0$ to $x \simeq 0.18 − 0.19$. Below this pseudogap temperature $T^*$, the low frequency spectral weight begins to be strongly suppressed. Surprisingly the doping dependences of $T^*$ and $T_c$ are completely different in spite of their close relationship suggested by angle resolved photoemission (ARPES) and tunneling and NMR experiments. At optimal doping where $T_c$ is maximum, various non-Fermi liquid (NFL) properties are observed in the normal state. These include the linear temperature dependence of ab-plane resistivity, the
quadratic $T$ dependence of Hall angle and so on up to 1000 K. Far beyond optimal doping, the normal state properties are well described by the conventional Landau Fermi liquid. Several anomalous behaviors have been observed in the SC state as well. Near optimal doping and at underdoping, a sharp resonance (almost energy resolution limited) is observed in inelastic neutron scattering experiments. Furthermore in the same doping range, the superfluid density $n_s$ is systematically suppressed with decreasing doping in spite of increasing SC gap amplitude. In the overdoped regime, however, the SC properties appear to be well explained by the conventional weak coupling BCS theory.

Although they are not usually addressed in the context of a phase diagram, the following experiments deserve special attention in order to understand the complete picture of the physics. A recent ARPES experiment for an insulating cuprate Sr$_2$CuO$_2$Cl$_2$ showed nearly isotropic and quite similar band dispersions along $(\pi/2, \pi/2) - (\pi, 0)$ and $(\pi/2, \pi/2) - (0, 0)$ directions. Furthermore a $d$-wave-like modulation of the insulating gap in Ca$_2$CuO$_2$Cl$_2$ requires even at half-filling the presence of strong pairing fluctuations. In another important experiment, a 61 Tesla pulsed magnetic field suppressed superconductivity in Ln$_{2-x}$Sr$_x$CuO$_4$ single crystals and revealed an insulator-to-metal (IM) crossover for both ab-plane resistivity $\rho_{ab}$ and c-axis resistivity $\rho_c$ near optimal doping. The latter experiment may shed some insight into the underlying physics of normal state cuprates which is usually masked by the presence of SC long-range order. Any successful theory should explain all these features in a natural and yet unified way.

As to the theoretical side, right after the discovery of high temperature superconductors, Anderson first proposed the one-band Hubbard model as the simplest Hamiltonian which might capture the correct low energy physics of copper oxides. Zhang and Rice also derived an effective $t - J$ Hamiltonian from the more realistic three-band Hubbard model. The $t - J$ Hamiltonian was already known to be the large $U$ limit of the Hubbard Hamiltonian under certain assumptions. The Hubbard model is described by the Hamiltonian in which $c_{i,\sigma}$ destroys an electron at site $i$ with spin $\sigma$ on a two-dimensional square lattice

$$H = -t \sum_{\langle i,j \rangle, \sigma} c_{i,\sigma}^\dagger c_{j,\sigma} + U \sum_i c_{i,\uparrow}^\dagger c_{i,\uparrow} c_{i,\downarrow}^\dagger c_{i,\downarrow}.$$  \hspace{1cm} (1)$$

$t$ is a hopping parameter between nearest neighbors $(i, j)$ and $U$ denotes local Coulomb repulsion. It is believed that a realistic strength of the Coulomb repulsion lies in between the weak and strong coupling regimes, namely, $U \sim W - 2W$ where $W$ is the bandwidth of $8t$ in two dimensions. So far many theories have been proposed to understand the various anomalous properties of the cuprates by directly invoking the Hubbard model or its variants (one-band and three-band Hubbard, and $t - J$ models), or other phenomenological models. However, at present there is no consensus on which kind of approach is most appropriate for a given Hamiltonian or even on which Hamiltonian is most relevant for the cuprates. At the end of this paper, comparison of our approach with some leading theories based on the Hubbard and $t - J$ models will be given.

II. REVIEW OF OUR PREVIOUS WORK

First, let us begin by summarizing the main results of our previous work and presenting a proposed phase diagram in order to set the stage for the present study. As a first step to the microscopic theory of high-$T_c$ superconductivity, it is of great importance to identify pairing interaction which may eventually lead to a SC instability at low temperature, just like the Cooper problem in the development of the BCS theory. In a recent study, we examined the possibility of extracting pairing interaction directly from the Coulomb repulsion itself without the exchange of bosonic degrees of freedom such as spin fluctuations.

We found that among several gap symmetries pairing interaction with the $d_{x^2-y^2}$ ($\phi_d(\vec{k}) = \cos k_x - \cos k_y$) symmetry is most strongly induced from the local Coulomb repulsion $U$. It is consistent with a weak coupling renormalization group (RG) calculation. Due to its direct Coulombic origin, this mechanism for pairing correlations is similar to the lattice version of the Kohn-Luttinger theorem. However, the details are somewhat different. The Kohn-Luttinger theory requires a sharp Fermi surface and a resulting long-range oscillatory behavior in real space of the effective interaction, while our approach does not.

AF correlations are also induced from the local Coulomb repulsion at the same time as $d$-wave pairing correlations are. Both the induced pairing and AF correlations are found to increase with decreasing doping. The simultaneous induction of pairing and AF correlations from the same Coulomb repulsion may be understood in the context of the $t - J$ model. Projecting out the doubly occupied sites in the large $U$ limit of the Hubbard model generates or induces the Heisenberg term in the $t - J$ model. It has in general both pairing and AF correlations. The increasing pairing and AF correlations with decreasing doping found in our previous work is also realized in the $t - J$ model (in a relative sense) as decreasing hopping probability with decreasing doping. In that paper, we argued that the induced pairing correlations are the microscopic origin of pseudogap behavior in underdoped cuprates. This is because the pairing fluctuation origin of the pseudogap and its doping dependence are consistent with many experiments. This is also because of the excellent agreement of our calculations with
the observed energy dispersion of the insulating cuprates, Sr$_2$CuO$_2$Cl$_2$ \cite{[14]} and Ca$_2$CuO$_2$Cl$_2$. \cite{[15]} It is expected that the high energy pseudogap at half-filling continuously evolves into a relatively smaller pseudogap away from half-filling.

Based on the doping dependences of the induced pairing and AF correlations, a phase diagram was proposed for the high temperature superconductors, which is shown in Fig. [1](b). First, far away from half-filling the short-range correlations due to local Coulomb repulsion are very weak and don’t produce strong enough pairing interaction so that \( T_c \) vanishes. With decreasing doping, they start to induce both pairing and AF fluctuations, but the latter is probably not strong enough to compete with the former. Thus up to optimal doping level, local Coulomb repulsion plays as a driving force to superconductivity and \( T_c \) keeps growing. When electrons enter into the underdoping regime, the induced AF fluctuations start to play as a SC phase coherence-breaker by creating locally the spin density wave (SDW) state. It strongly breaks time-reversal symmetry and causes \( T_c \) to decrease. As far as \( T^* \) is concerned, beyond optimal doping, induced AF fluctuations are weak and thus the pseudogap temperature \( T^* \) closely follows \( T_c \). The strength of induced pairing interaction increases with decreasing doping. This makes \( T^* \) increase, creating a huge pseudogap region between \( T^* \) and \( T_c \).

Near half-filling and at low temperature, AF long-range order is stabilized by the three-dimensional effect. The AF spin fluctuations become strong more or less around the AF phase boundary, leading to another kind of a crossover temperature \( T_{RVB} \). \cite{[22]} Below \( T_{RVB} \) both AF and pairing fluctuations are weak and thus the pseudogap temperature \( T^* \) closely follows \( T_c \). The strength of induced pairing interaction increases with decreasing doping. This makes \( T^* \) increase, creating a huge pseudogap region between \( T^* \) and \( T_c \).

III. RVB INSULATOR-TO-METAL TRANSITION NEAR OPTIMAL DOPING AT ZERO TEMPERATURE: QCP IN THE TWO-DIMENSIONAL HUBBARD MODEL

In principle, the above phase diagram resulting from the close competition between the induced pairing and AF correlations should be quantitatively similar for different cuprates with similar \( U \)'s. This is because these correlations are completely determined by the same Coulomb repulsion \( U \) at given \( x \) and \( T \). For most of the hole-doped cuprates, \( J = 4t^2/U \) lies in the range of 120-140 meV, indicating quite similar \( U \)'s with 20% variation at most. One the other hand, \( T_c \)'s, which are expected to be similar with 20% difference, widely vary from 40 K for Ln$_{2-x}$Sr$_x$CuO$_4$ to 133 K for HgBa$_2$Ca$_2$Cu$_3$O$_{8}$. This particular feature strongly suggests that the true SC long-range order is driven by interlayer coupling. It is consistent with the general trend that the cuprate compounds with more CuO$_2$ planes in a unit cell show higher \( T_c \). In the present paper, the interlayer coupling means not only the coupling between CuO$_2$ planes in a unit cell, but also between other CuO$_2$ planes in different unit cells. Strictly in two dimensions, AF long-range order cannot appear at finite temperature due to the Mermin-Wagner theorem \cite{[24]}, while SC long-range order can be stabilized at finite temperature by the Kosterlitz-Thouless phase transition. \cite{[25]}

However, there is possibility that SC long-range order is also destroyed at finite temperature mainly by the phase coherence-breaking effect of the induced AF fluctuations and partly by quantum fluctuations. This is consistent with the rigorous result by Su and Suzuki. \cite{[26]} These authors proved the nonexistence of \( d_{xy} \) ground state between the AF and SC phase boundaries (in a clean sample) is the RVB insulator in which an insulating gap is identified with the spin gap \( \Delta \). Note that \( T_c, T^*, T_N \) and \( T_{RVB} \) are determined as a result of close competition between the induced pairing and AF correlations and that any imbalance of the two correlations may drastically change the phase diagram. The pseudogap behavior in this scenario is as generic as AF correlations, because they are simultaneously induced from the same local Coulomb repulsion. In our picture \( T^* \) is different from a temperature below which the critical behavior (O(2) symmetry) of SC long-range order is found. In this previous work, however, interlayer coupling effect and the possibility of existence of a quantum critical point (QCP) were not considered.
slowly turning off the interlayer coupling. It is clear that slow turning off of the interlayer coupling reduces the AF and SC phase boundaries. At the same time the region of the RVB insulating ground state expands, as shown in Fig. 2(a). When the interlayer coupling is completely disconnected from neighboring CuO$_2$ planes in the same unit cell or in other unit cells, the AF and SC long-range orders totally disappear. And the RVB insulating ground state persists from half-filling all the way up to $x = x_c$ near optimal doping, as shown in Fig. 3(b). Considering $T^*$ meets $T_c$ at slightly overdoping region and its curvature, $x = x_c$ should be somewhat larger than optimal doping ($x_c \approx 0.18 - 0.19$). Since $T^*$ involves a short distance scale or rather a high energy scale, $T^*$ obtained in two dimensions is not expected to change substantially by a small interlayer coupling.

Thus in our second conjecture, the two-dimensional Hubbard model has an RVB insulator-to-metal transition at $x = x_c$ for $T = 0$, leading to a QCP, and one of the crossover lines is given by the pseudogap temperature $T^*$. This feature is presumably what Boebinger et al. found in their experiment of an insulator-to-metal crossover near optimal doping. As is well known from an extensive study of QCP by Sachdev, an immediate consequence from the presence of QCP is to create two crossover lines which occur at $T \sim |\Delta|^{1/z}$, where $z$ is the dynamical exponent and $\nu$ is the correlation length exponent (Fig. 2(c)). The crossover line above the RVB insulating ground state is identified with the pseudogap temperature $T^*$. The state above the QCP, sandwiched by the two crossover lines, is described by placing the $\Delta = 0$ scale-invariant critical theory at nonzero temperature. This is probably the region where various singular and NFL properties have been observed in the normal state and phenomenological marginal Fermi liquid (MFL) theory by Varma et al. works well. The fact that the pseudogap temperature $T^*$ naturally divides the pseudogap region and the NFL region, justifies a commonly used experimental method of determining the pseudogap temperature. For instance, in dc resistivity measurements, $T^*$ is a temperature where the resistivity starts to deviate from a linear temperature dependence.

Since we have identified strictly in two dimensions the QCP of the RVB insulator-to-metal and concomitant NFL behaviors in optimally doped cuprates, let us turn on the interlayer coupling in order to find the realistic phase diagram in quasi-two dimensions. Before doing that, it is important to point out the differences in electronic properties below and above $x_c$ at low temperature. In our third conjecture, at low temperature ($T^* \approx 0$), the crossover line $T^*$ roughly divides the doping-temperature plane into two regions, one with AF correlations and the other without them. The identification of $T^*$ at low temperature as a crossover of the AF correlations may be understood by the following two observations.

In our previous work, another crossover line $T_{RVB}$, which is not specifically addressed in this paper, was defined as a line where the AF correlations are just strong enough to destroy the SC long-range phase coherence, as shown in Fig. 1(b). When the interlayer coupling is completely turned off, it is easy to see $T_{RVB}$ approach $T^*$ at low temperature. As another supporting evidence, we and other groups found that most of the low temperature region including the SC state below $x \approx 0.2$ is inside of the AF phase in a mean-field study of the $t - J$ model. In a mean-field approximation, long-range order already sets in when the corresponding correlation length reaches roughly one lattice spacing. This dictates the above mean-field result to be interpreted as the presence of short-range AF correlations for $x \leq 0.2$ at low temperature. If this conjecture turns out to be correct, there is possibility that at low temperature and near $x \approx x_c$, a band Kondo effect is realized in finite dimensions, as is done in infinite dimensions. In the band Kondo effect, a nonvanishing local magnetic moment at site $i$, $\langle S_i^z \rangle$, due to local Coulomb repulsion is effectively screened out by surrounding (but the same kind of electrons at site $i$) itinerant electrons.

From a purely pairing correlation point of view, the pairing correlations become singular with decreasing temperature at any doping concentration. This makes the crossover region of the pairing correlations much wider than that of the AF correlations at low temperature near $x \approx x_c$. As another supporting evidence on this point, we again invoke our previous mean-field phase diagram. The mean-field $T_c$ line, which is interpreted as a crossover of short-range pairing correlations, extends up to $x \approx 0.35$ beyond $x = x_c$ where the mean-field AF order vanishes. It makes the crossover region of pairing correlations broad with respect to $x = x_c$ at low temperature.

In this situation, a potential location with the highest $T_c$, when the interlayer coupling turned on, is near $x = x_c$ in which the phase coherence-breaking AF correlations nearly vanish but the pairing correlations are still robust. The resulting phase diagram (Fig. 1(a)) will look like one where $T^*$ falls from a high value onto the $T_c$ line rather than the other where $T^*$ smoothly merges with $T_c$ in the slightly overdoped region, as recently argued by Tallon and Loram. In our scenario $T_c$ is never part of the $T^*$ line. For different compounds, different strength of interlayer pairing hopping drives SC long-ranger order in the same background of the two-dimensional electron system. This leads to a universal relation $T_c/T_{c, \max}^{RVB} = 1 - 82.6(x - 0.16)^2$ when $T_c$ is scaled by $T_{c, \max}^{RVB}$. Away from half-filling, the AF correlations manifest their existence most strongly in the SC state, because they easily destroy the SC long-range phase coherence. Our scenario also predicts that due to scatterings with AF fluctuations, quasiparticle scattering rate remains finite for $x \leq x_c$ even in a clean sample and at $T = 0$ and it is universal (up to the variation of $J$ or
with a spin-triplet, \( \langle c_{\bar{\mathbf{Q}}+\mathbf{Q},\uparrow}^\dagger c_{-\mathbf{Q},\downarrow} \rangle \), is dynamically generated. \( \bar{Q} \) is the AF wave vector \((\pi, \pi)\) in two dimensions. This is a generic feature for fermionic systems and cannot be obtained in a purely bosonic description of pairing and AF correlations. As long as the two correlations are strong (but both of them need not be in long-range ordered states), the spin-triplet correlations can be robust. Since both pairing and AF correlations are present below \( x_c \), as noted in the previous Section, in general the ground state has three different (pairing, AF and spin-triplet) correlations. To have a maximum transition amplitude \( |\langle n|S^+_{\bar{\mathbf{Q}}-\mathbf{Q}}^\dagger(0)\rangle| \), one finds two possible ways of transition between the three correlations, namely, AF ↔ AF and pairing ↔ spin-triplet. The former is most effective near half-filling, due to the presence of the AF long-range order in that region. On the other hand, the latter is most operative near \( x = x_c \), because the effective strength of SC long-range order is strongest there. \[1\] Between at half-filling and at \( x = x_c \), the two ways of transition compete.

Near \( x = x_c \) where a strong neutron resonance was observed and the second way of transition is most effective, the resonance energy is given by twice of the maximum gap energy, and its intensity by the product of superfluid density. This suggests that the sharp inelastic neutron resonance near optimal doping is a direct consequence of the collective excitations of the spin-triplet ground state. Observed incommensurate magnetic peaks may come from a band structure effect at the Fermi energy. There is also possibility that they are from the formation of inhomogeneous stripe structure. \[2\] It is important to note that the (energy resolution limited) collective mode nature of the neutron scattering resonance is best understood, when the pairing and AF correlations are treated on equal footing.

Recently Demler and Zhang \[43\] have reached a similar result to ours in the context of SO(5) symmetry, although details are somewhat different. In SO(5) theory, the spin-triplet amplitude is not an order parameter, but the generator of infinitesimal rotations between AF and SC order parameters. In the mixed AF+SC+spin-triplet phase that is discussed here, the spin-triplet state acquires a nonzero order parameter in the ground state. The above argument which is valid near \( x = x_c \) drastically changes...
with decreasing doping. In underdoping region where the first way of transition starts to become more operative, the resonance energy is no longer given by twice of the maximum gap energy. Otherwise, it would keep increasing with more underdoping, because the pseudogap size increases with decreasing doping. The intensity also does not behave like an order parameter any more, as it does near optimal doping. As the doping is decreased, the resonance energy becomes soft and becomes a Goldstone mode of the AF order near half-filling. To our opinion, there is no obvious reason for linear scaling of the resonance energy with $T_c$. At present it is uncertain whether this linear scaling is just a coincidence or comes from a deeper theoretical origin. It is expected that at optimal doping region or in slightly underdoping region two resonance peaks can appear in inelastic neutron scattering experiments, one from the first way of transition and the other from the second way.

With decreasing doping, the induced pairing correlations as well as the phase coherence-breaking AF correlations increase in underdoped and optimally doped samples. As a result, with decreasing doping, the SC gap amplitude increases but superfluid density or $\rho$ decreases. The resulting $\Delta (0)$max/$K_BT_c$ ratio is strongly doping dependent, monotonically increasing with decreasing doping below $x_c$. Above $x_c$ (overdoping), however, it is expected that the ratio approaches more or less the BCS mean-field value. This feature cannot be understood in the absence of AF correlations which are allowed in the model. The effective strength for the SC long-range order is also strongly doping dependent and is largest near $x_c$. It decreases below $x_c$ due to the increasing phase coherence-breaking AF correlations and also above $x_c$ owing to the decreasing pairing correlations, as discussed in the previous Section. In this respect, it is not surprising to find that the superfluid density and the SC condensation energy have their maximum values near $x_c$, and decrease below and above $x_c$. In the present scenario, the pseudogap is virtually unchanged by an applied magnetic field, because the characteristic energy scale for the pseudogap, $\Delta$, is much larger than the Zeeman energy. On the other hand, the SC long-range order is relatively easily destroyed by it because of its phase coherence-breaking nature.

Finally it is worthwhile to comment on the SC condensation energy. In the present scenario the SC long-range order is stabilized only through a pair hopping process along the $c$-axis (due to the interlayer coupling). It forces the SC condensation energy to come from the lowering of the $c$-axis kinetic energy in the SC state. This interlayer coupling theory was already proposed by Anderson and others. Many features are consistent with $c$-axis optical measurements. Recently some significant discrepancies found in the measured $c$-axis penetration depth in $\text{Tl}_2\text{Ba}_2\text{CuO}_6+\delta$ and in the prediction from the interlayer tunneling model, were resolved by Chakravarty et al. by subtracting fluctuation effects in the electronic specific heat data.

V. GAP SYMMETRY IN THE SC STATE

In this Section, we discuss the gap symmetry of the SC order parameter for cuprates. In the previous study, for several $d$-wave type symmetries the effective strength of pairing correlations, $(\Delta^+_g(0)\Delta^-_g(0))$, was found as

$$\frac{n}{4N} \sum_{\vec{k}} \phi^2_g(\vec{k}) [f(E_-(\vec{k})) + f(E_+(\vec{k}))] - \text{sign} \left( \frac{\phi_g(\vec{k} + \vec{Q})}{\phi_g(\vec{k})} \right) \times \frac{\Delta_{sdw}}{2U N} \sum_{\vec{k}} \phi^2_g(\vec{k}) \frac{\Delta_{sdw}}{\lambda(\vec{k})} [f(E_-(\vec{k})) - f(E_+(\vec{k}))],$$

(3)

where $\lambda(\vec{k}) = \sqrt{((\varepsilon(\vec{k}) - \varepsilon(\vec{k} + \vec{Q}))/2)^2 + \Lambda_{sdw}^2}$ and $E_{\pm}(\vec{k}) = (\varepsilon(\vec{k}) + \varepsilon(\vec{k} + \vec{Q})/2 \pm \lambda(\vec{k}))$. Generally $\Delta_\delta(i)$ is defined as $\Delta_\delta(i) = \frac{1}{2} \sum_{\vec{k}} g(\delta) (c_{i+\delta,\uparrow} c_{i+\delta,\downarrow} - c_{i+\delta,\downarrow} c_{i+\delta,\uparrow})$, where $g(\delta)$ is an appropriate gap structure factor in real space. $\varepsilon(\vec{k}) = -2t(\cos k_x + \cos k_y) - \mu$ for nearest neighbor hopping, $\mu$ is the chemical potential controlling the particle density $n$, $N$ the total number of lattice sites, $f(E)$ the Fermi-Dirac distribution function, $\phi_g(\vec{k})$ the Fourier transform of $g(\delta)$, and the summation accompanied by the prime symbol is over wave vectors in half of the first Brillouin zone. For local $s$-wave and extended $s$-wave symmetries, there are additional contributions to the above equation. But the second term in Eq. is still the major factor determining whether or not $(\Delta^+_g(0)\Delta^-_g(0)) > (\Delta^+_g(0)\Delta^-_g(0))_0$.

Purely from a symmetry reason are ruled out several gap symmetries such as local $s$-wave ($\phi(\vec{k}) = 1$) and $d_{xy}$ ($\phi(\vec{k}) = 2\sin k_x \sin k_y$), both of which have $\phi(\vec{k} + \vec{Q}) = \phi(\vec{k})$. In the real space representation, a pair with a local $s$-wave symmetry involves an upspin (downspin) electron and a downspin (upspin) electron at the same site $i$. A pair with a $d_{xy}$ symmetry the combination of an upspin (downspin) electron in site $i$ and the downspin (upspin) electrons in the next-nearest neighbors with an appropriate sign. Thus the pair configurations of the above two symmetries are directly against that dictated by the strong local Coulomb repulsion $U$. Eventually the most stable gap symmetry among various possible types with $\phi(\vec{k} + \vec{Q}) = -\phi(\vec{k})$, is determined by the band structure near the Fermi surface. Near half-filling $|\phi(\vec{k})|$ of $d_{x^2-y^2}$ symmetry $(\phi(\vec{k}) = \cos k_x - \cos k_y)$ is much larger than, for instance, that of extended $s$-wave $(\phi(\vec{k}) = \cos k_x + \cos k_y)$ near the Fermi surface. It enables $d_{x^2-y^2}$ gap symmetry to be realized in most cases. Far away from half-filling, however, the extended $s$-wave form factor becomes important and there is possibility
that the SC gap contains a substantial fraction of extended s-wave component, leading to a $d_{x^2-y^2} + is$ gap symmetry.

Recently there is some controversy over the gap symmetry in electron-doped cuprates Nd$_{2−x}$Ce$_x$CuO$_{4−δ}$ and Pr$_{2−x}$Ce$_x$CuO$_{4−δ}$, namely, isotropic s-wave against anisotropic d-wave.\[\text{\textsuperscript{17}}\] According to the above principle of finding the most stable gap symmetry, local (or isotropic in momentum space) s-wave is ruled out from the beginning. It is due to its incompatibility with the underlying strong local Coulomb repulsion. The correct gap symmetry for electron doped cuprates should be extended s-wave or $d_{x^2-y^2}$ or a mixture of these symmetries, depending on the projected density of states at the Fermi energy for a given symmetry. The gap of an extended s-wave symmetry vanishes only at the AF zone boundary. According to ARPES experiments\[\text{\textsuperscript{18}}\] and band structure calculations,\[\text{\textsuperscript{19}}\] however, the Fermi surface of electron doped cuprates is likely to be circular near the zone center. In this situation a gap node of the extended s-wave symmetry does not appear in the Fermi surface. Consequently this symmetry, if it is correct, might have been interpreted as the isotropic s-wave in previous experiments. This feature may imply that the observed pairing symmetry itself does not tell us any crucial information about the mechanism of superconductivity.

\section*{VI. COMPARISON WITH SOME LEADING THEORIES BASED ON THE HUBBARD AND $T−J$ MODELS}

In this Section we compare the present approach with some leading theories for the high-T$_c$ superconductivity. Perhaps the closest theories to our approach are those based on the Anderson’s RVB state in one way or another. Anderson and his co-workers first applied a mean-field approximation\[\text{\textsuperscript{20}}\] to the $t–J$ model. The mean-field theory studied by these authors and by others\[\text{\textsuperscript{21,24}}\] has been a starting point for further development of the theory such as $1/N$ expansion theory\[\text{\textsuperscript{57}}\] and gauge theory\[\text{\textsuperscript{28,59}}\] of the $t–J$ model. In slave boson theory of the $t–J$ model, typically two mean-field order parameters are considered

$$\chi_{ij} = \langle f_{i,\uparrow}^\dagger f_{j,\sigma} \rangle,$$

$$\Delta_{ij} = \langle f_{j,\uparrow}^\dagger f_{i,\downarrow} - f_{j,\downarrow}^\dagger f_{i,\uparrow} \rangle,$$

(4)

together with $\langle b_i \rangle$ In the slave boson representation, a physical electron is decomposed into a spinon (fermion) and a holon (boson), $c_{i,\sigma}^\dagger = f_{i,\sigma}^\dagger b_i$.

Depending on the vanishing or nonvanishing of $\Delta_{ij}$ and $\langle b_i \rangle$, the doping and temperature plane is divided into four regions.\[\text{\textsuperscript{20}}\] Region I with $\Delta_{ij} = 0$ and $\langle b_i \rangle \neq 0$ is a Fermi liquid phase. Region II with $\Delta_{ij} \neq 0$ and $\langle b_i \rangle = 0$ is the spingap phase, in which a $d$-wave gap appears in the fermion spectrum without Bose condensation of holons. Region III with $\Delta_{ij} \neq 0$ and $\langle b_i \rangle \neq 0$ indicates SC long-range order in physical electrons. Region IV with $\Delta_{ij} = 0$ and $\langle b_i \rangle = 0$ is designated as the strange metal phase, because it shows various non-Fermi liquid features.

In many respects, the slave boson mean-field theory of the $t–J$ model\[\text{\textsuperscript{50,59}}\] has shed some important insight into the microscopic understanding of the cuprate superconductors. This is because the predicted phase diagram is, at least, qualitatively consistent with experiments, and the pseudogap is closely related to a spingap, and furthermore it starts from the microscopic model as opposed to other phenomenological models. However, there are also some serious problems with the slave boson mean-field theory, as noted by Ubbens and Lee.\[\text{\textsuperscript{50}}\]

One of them is that the temperature scale for Bose condensation of holons is too high. Furthermore the maximum $T_c$, which is determined by the two lines $\Delta_{ij} \neq 0$ and $\langle b_i \rangle \neq 0$, occurs at too small doping concentration ($x < 0.06$). At this doping level, the SC long-range order even does not appear in cuprate superconductors. Close to half-filling, several exotic phases have been reported to be stable such as mixed phases\[\text{\textsuperscript{52}}\] (equivalently $\pi$-flux phases\[\text{\textsuperscript{53}}\]), dimerized phases,\[\text{\textsuperscript{53,54}}\] and staggered flux phases.\[\text{\textsuperscript{53,56}}\] It is unclear whether these states are realized or not in cuprates. In a recent paper\[\text{\textsuperscript{53}}\] we argued that these problems can be naturally resolved, when AF correlations, the weaknesses of a mean-field approximation, and the limitation of the $t–J$ model near half-filling are properly taken into account.

In the original RVB theory,\[\text{\textsuperscript{15}}\] Anderson suggested that the RVB ground state may be obtained by Gutzwiller projection on the BCS ground state. As shown in the previous study,\[\text{\textsuperscript{19}}\] however, strong local Coulomb repulsion $U$ induces the AF and pairing correlations\ at the same time. This makes one Gutzwiller projection on the noninteracting electrons enough to yield the RVB ground state. Unless the interlayer coupling is introduced in the RVB based theories, they suffer from having only one energy scale $\Delta$ which has to explain $T^*$ and $T_c$ at the same time. Some studies on the $t–J$ model at half-filling or the Heisenberg model showed that a mixed phase\[\text{\textsuperscript{24}}\] (equivalently a $\pi$-flux phases\[\text{\textsuperscript{53}}\]) is the ground state of the model. However, the observed energy dispersion in the insulating cuprates Sr$_2$CuO$_2$Cl$_2$\[\text{\textsuperscript{14}}\] and Ca$_2$CuO$_2$Cl$_2$,\[\text{\textsuperscript{17}}\] is different from what the flux phase predicts. The observed band dispersions along $(\pi/2, \pi/2)$ and $T_c$ at the same time. This makes one Gutzwiller projection on the noninteracting electrons enough to yield the RVB ground state. Unless the interlayer coupling is introduced in the RVB based theories, they suffer from having only one energy scale $\Delta$ which has to explain $T^*$ and $T_c$ at the same time. Some studies on the $t–J$ model at half-filling or the Heisenberg model showed that a mixed phase\[\text{\textsuperscript{24}}\] (equivalently a $\pi$-flux phases\[\text{\textsuperscript{53}}\]) is the ground state of the model. However, the observed energy dispersion in the insulating cuprates Sr$_2$CuO$_2$Cl$_2$\[\text{\textsuperscript{14}}\] and Ca$_2$CuO$_2$Cl$_2$,\[\text{\textsuperscript{17}}\] is different from what the flux phase predicts. The observed band dispersions along $(\pi/2, \pi/2)$ point instead of linear. In fact the experiments are more consistent with our calculations based on the Hubbard Hamiltonian\[\text{\textsuperscript{19}}\]. Although these differences (the Hubbard vs. $t–J$ Hamiltonians) are rather quantitative, it is not clear whether in some subtle issues associated with our conjectures these Hamiltonians give
the same answer or not.

The mechanism to superconductivity proposed in our previous and this papers is fundamentally different from the conventional one in which superconductivity is driven by exchange of some bosonic degrees of freedom such as phonons, spin and charge fluctuations and so on. It suggests that the exchange of spin fluctuations cannot be the leading mechanism to high temperature superconductivity, at least, in the Hubbard type model. This is because this approach completely neglects the leading pairing interaction directly induced from the local Coulomb repulsion. But instead it depends on the residual pairing interaction from the AF correlations which were already induced (simultaneously with the pairing correlations) from the Coulomb repulsion.

VII. NUMERICAL STUDIES FOR THE HUBBARD AND T−J MODELS

There have been several numerical studies on the Hubbard and t − J models in two dimensions. Among many important issues, the existence of pairing correlation which may lead to a SC instability at low temperature is of particular importance. Several methods including exact diagonalization (ED), quantum Monte Carlo (QMC) and density matrix renormalization group (DMRG) support with decreasing temperature growing d-wave pairing correlations away from half-filling. This is consistent with a weak coupling RG study of the Hubbard model. We believe what many numerical methods such as ED, QMC and DMRG find is the pairing correlations induced from the local Coulomb repulsion in the presence of the induced AF correlations. However, the fact that in the numerical calculations the pairing strength increases with decreasing doping just as the AF correlations do, might have given a misleading impression that the pairing correlations come from the exchange of spin fluctuations.

On the other hand, a constrained path quantum Monte Carlo (CPQMC) method appears to show a negative answer to the existence of pairing correlations in the Hubbard model. This result is in direct conflict with that of the RG study. Although it is valid in the weak coupling limit, the RG result cannot be qualitatively wrong. It is because of its systematic nature and the general experience that many weakly interacting systems are more or less smoothly connected to corresponding strong coupling systems. Thus in the CPQMC method, there is possibility that away from half-filling their ill-suited trial wave function (SDW solution) generates mainly the states with AF correlations but neglects those with pairing correlations. Or in the process of constraining paths to avoid the fermion sign problem, the d-wave pairing correlations are strongly suppressed. Indeed Zhang’s calculations may suggest the fate of those theories based on purely magnetic correlations such as the exchange of spin fluctuations, magnetic polarons and so on.

VIII. HOLE-DOPED CUPRATES AND HEAVY-FERMION SUPERCONDUCTORS

The present scenario may also apply without any drastic modification to electron-doped high-$T_c$ superconductors as well as heavy-fermion superconductors. The main qualitative difference between hole-doped cuprates and the above compounds is that for the latter local magnetic moments from Ce or U atoms residing between conducting planes play an important role in determining the phase diagram and electronic properties. Electrons in the CuO$_2$ plane interact with local magnetic moments from Ce or U atoms. This enables the AF correlations in the CuO$_2$ plane to easily induce AF correlations in those atoms, enhancing the overall AF fluctuations in the CuO$_2$ plane. Then the close balance between the pairing and AF correlations is broken in favor of the latter in the conducting electrons. As a result, AF long-range phase significantly increases, and accordingly SC phase shrinks and remains at the edge of the AF phase boundary. Because of the resulting imbalance of the two correlations in the conducting plane, there is possibility that the pseudogap state is completely destroyed or remains at most in a narrow region of the $x-T$ plane. The corresponding SC gap symmetry is determined by the relative sign of $\phi_g(\vec{k}+\vec{Q})$ vs. $\phi_g(\vec{k})$ and the shape of the Fermi surface. In general it can be other than a $d$-wave symmetry. Thus, high temperature superconductors for both hole-doped and electron-doped cuprates as well as heavy-fermion superconductors may be understood in the unified framework within the present scenario. We also argue that differences observed in hole-doped and electron-doped cuprates do not come from the different signs of charge carriers. They are from the presence of magnetically active atoms (Ce) between CuO$_2$ planes in the latter. If this turns out to be correct, the correct model Hamiltonian for the heavy-fermion superconductors would be the periodic Anderson model or the Kondo lattice model with strongly correlated conducting electrons instead of with the noninteracting electrons. Various studies of the superconductivity on the basis of spin fluctuations in these compounds and even in organic superconductors should be reconsidered for their validity.

IX. MAXIMIZING THE SC CRITICAL TEMPERATURE $T_c$

It is also interesting to discuss the issue of maximizing the SC critical temperature $T_c$ on the basis of the present scenario. There are roughly three ways of increasing $T_c$. 

First, $T_c$ can be increased by a stronger interlayer coupling. In the family of Bi$_2$Sr$_2$Ca$_{n-1}$Cu$_n$O$_{2n+4}$ (BSCCO), TIBa$_2$Ca$_{n-1}$Cu$_n$O$_{2n+3}$ (T1BCCO), Tl$_2$Ba$_2$Ca$_{n-1}$Cu$_n$O$_{2n+4}$ (T2BCCO), and HgBa$_2$Ca$_{n-1}$Cu$_n$O$_{2n+2}$ (HBCCO) where $n = 1, 2, 3$ and 4, $T_c$ for larger $n$ is higher than that of smaller $n$. Except for T1BCCO, however, all the others show their highest $T_c$'s at $n = 3$. It indicates the saturation of the interlayer coupling strength with increasing the number of layers in a unit cell. Making the interlayer region more metallic is also suggestive to enhance the interlayer coupling. Second, $T_c$ can be increased by decreasing the local Coulomb repulsion $U$. When HBCCO compound is subjected to a high pressure of 30 GPa, $T_c$ increases from 133 K to 164 K. Applying pressure causes the increase of hopping integral between nearest neighbors, effectively decreasing $U$. Thus, the local Coulomb repulsion is also a driving force to the pairing correlations, $U$ cannot be arbitrarily small to achieve the highest $T_c$. There must be an optimal strength $U$ (presumably $U \sim W$) in which $T_c$ is maximized. Third, $T_c$ can be also increased by breaking the close balance between the pairing and AF correlations in favor of the former. In principle this can be achieved by putting some atoms between the CuO$_2$ planes, which respond diamagnetically to the phase coherence-breaking AF fluctuations in such a way that the overall strength of AF correlations are reduced in the CuO$_2$ planes. It is exactly opposite to what happens in electron-doped cuprates. Although the implementation of this possibility is uncertain in a real situation, this last way can be most effective to maximize $T_c$.

**X. CONCLUSION**

Before closing we comment on a few points. Since the conclusion of the present paper crucially depends on the three conjectures, it is important to prove or disprove them, of course, on the basis of fully systematic or rigorous calculations. It is believed that the mechanism to superconductivity and the interplay between antiferromagnetism and superconductivity expounded in this paper can be applicable to heavy-fermion superconductors as well as organic superconductors. A stripe issue has not been specifically addressed in this paper. Through the microscopic separation of hole-rich regions from antiferromagnetically correlated regions, the stripe structure tends to maintain the AF correlations more effectively than the other case in which they are uniformly suppressed by doped holes. Then it is not difficult to expect that in the stripe state $T_c$ and $T^*$ are suppressed by some amount from those values in the uniform state. We believe that the differences in the stripe state and in the uniform state are mainly quantitative. The conclusion reached in this paper is not expected to qualitatively change in the presence of stripe structure. However, stripe-type structure can be important in the low doping region to stabilize both pairing and AF correlations at the same time.

In some of magnetic experiments such as NMR, another crossover temperature $T^0$ (larger than $T^*$) is often identified, at which Knight shift shows its maximum. This feature can be easily understood on the basis of the competing nature of pairing and AF correlations as well as of the phase diagram obtained in Ref. The obtained mean-field phase diagram shows that the mean-field AF phase line stays above the mean-field SC phase line for $x \leq x_c$. As was discussed in Section these AF and SC mean-field phase lines should be interpreted as the onset ($T^0$) of short-range AF correlations and as the onset ($T^*$) of short-range pairing correlations (pseudogap), respectively. For $T^* < T < T^0$, the two correlations compete, while they grow with decreasing temperature. In spin-lattice relaxation rate which picks up strongly the $\tilde{q} = \tilde{Q}$ component, for $T^* < T < T^0$ the contribution from the AF correlations dominates that from the pairing correlations so that $1/T_1T$ keeps increasing until it starts to decrease at $T^*$. On the other hand, Knight shift which picks up the $\tilde{q} = 0$ component and thus is unaware of the growing AF correlations, is more strongly influenced by the increasing pairing correlations. Consequently Knight shift reaches its maximum at $T^0$, and starts to slowly decrease below it and then rapidly decrease below $T^*$.

Based on experimental results and our previous theoretical work, we have conjectured a microscopic theory of high temperature superconductivity. In this conjecture, SC and AF long-range orders are driven by interlayer coupling. Strictly in two dimensions, the microscopic Hubbard model has an RVB insulator-to-metal transition at $x = x_c$ near optimal doping for zero temperature, leading to a QCP, and one of the crossover lines is given by the pseudogap temperature $T^*$. We argued that various singular and non-Fermi liquid properties observed near optimal doping are due to the presence of this QCP. In our conjecture, the crossover line $T^*$ also practically divides the SC region into two, depending on the doping level with respect to $x_c$. For $x \leq x_c$ the SC state has significant AF correlations, while for $x > x_c$ it has virtually no AF correlations, thus justifying the conventional BCS theory based on the noninteracting electrons. Inelastic neutron scattering resonance and systematically reduced superfluid density in the SC state below $x_c$ have their natural explanations in the present scenario. The present approach supports interlayer pair tunneling model in which the SC condensation energy comes from the lowering of the c-axis kinetic energy in the SC state. Comparison of the present scenario with some of the leading theories based on the Hubbard and $t - J$ models was given. The generic features of both hole-doped and electron-doped cuprates as well as heavy-fermion superconductors may be understood in the unified framework within the
present picture.

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In the previous study we did not realize that the local Coulomb repulsion can also induce the $d$-wave pairing correlations. But the conclusion equally applies to the present problem.
FIG. 1. Schematic phase diagrams in doping ($x = 1 - n$) and temperature ($T$) plane based on (a) experiments and (b) our previous work, in the presence of the interlayer coupling. $T_c$ and $T_N$ denote the SC and AF transition temperatures, respectively. $T^*$ is the pseudogap temperature, while $T_{RVB}$ in (b) is a temperature where the AF correlations become strong. The thick solid line in (b) denotes the insulating RVB ground state with a spingap.

FIG. 2. Schematic phase diagrams in doping ($x = 1 - n$) and temperature ($T$) plane (a) with a reduced interlayer coupling, and (b) and (c) without it. $T_c$, $T_N$, and $T^*$ are the same as in Fig. 1. The thick solid lines denote the insulating RVB ground state with a spingap $\Delta$, and without the interlayer coupling these lines terminate at $x = x_c$ for $T = 0$ shown as a black dot in (b) and (c).