Influence of Hole Doping on Antiferromagnetic Real-Space Approaches for the High-Tc Cuprates

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Recently proposed scenarios for the cuprates make extensive use of a “flat” quasiparticle (q.p.) dispersion and short-range hole-hole interactions in real-space, both caused by antiferromagnetic (AF) correlations. The density of states (DOS) at half-filling has a robust peak which boosts the superconducting critical temperature \( T_c \) to large values as holes are introduced into the (rigid) q.p. band. Here, the stability of such scenarios is studied after a finite but small hole density is introduced. The overall conclusion is that the main features of real-space AF-based approaches remain qualitatively similar, namely a large \( T_c \) is found and superconductivity (SC) appears in the \( d_{x^2-y^2} \) channel. As the hole density grows the chemical potential \( \mu \) crosses a broad peak in the DOS. We also observe that extended s-wave SC competes with d-wave in the overdoped regime.

The presence of “flat” regions in the normal-state q.p. dispersion is a remarkable feature of the phenomenology of hole-doped high temperature superconductors. \( \hfill [1] \)

These flat bands are located around momenta \( \mathbf{p} = (\pi, 0) \) and \( (0, \pi) \), and at optimal doping they are \( \sim 10 \text{meV} \) below the Fermi energy, according to angle-resolved photoemission (ARPES) studies. \( \hfill [2] \) Antiferromagnetic correlations may play an important role in the generation of these features, as has been suggested by studies of holes in the 2D t-J and Hubbard models at and away from half-filling. \( \hfill [2, 3] \) In addition, the flat regions induce a large peak in the DOS which can be used to boost \( T_c \). This leads to a natural explanation for the existence of an “optimal doping” which in this framework occurs when the flat regions are reached by \( \mu \). We will refer to these ideas as the “Antiferromagnetic van Hove” (AFVH) scenario. \( \hfill [3] \) Superconductivity in the \( d_{x^2-y^2} \) channel is natural in the AFVH scenario due to the strong AF correlations. \( \hfill [3] \) The interaction of holes is better visualized in real space i.e. with pairing occurring when dressed holes share a spin polaronic cloud, as in the spin-bag mechanism. \( \hfill [4] \) This real-space picture (see also Ref. \( \hfill [3] \)) holds even for a small AF correlation length, \( \xi_{AF} \), and in this approach there is no need to tune parameters to work very close to an AF instability. Previous scenarios have also used van Hove (vH) singularities in the band structure to increase \( T_c \), \( \hfill [10] \) but d-wave SC is not natural in this context unless AF correlations are included.

To obtain quantitative information from these intuitive ideas, holes moving with a dispersion calculated using one hole in an AF background, \( \epsilon_{AF}(\mathbf{p}) \), and interacting through a nearest-neighbors (NN) attractive potential, that mimics the sharing of spin polarons, have been previously analyzed. \( \hfill [2] \) Within a rigid band filling of \( \epsilon_{AF}(\mathbf{p}) \) and using a BCS formalism, \( d_{x^2-y^2} \) superconductivity dominates with \( T_c \sim 100K \) caused by the large DOS implicit in the hole dispersion. However, the accuracy of the rigid band approximation has not been studied before. In particular, the following questions arise: (i) does the q.p. peak in the DOS found at \( \langle n \rangle = 1 \) survive a finite hole density?; (ii) how does the q.p. dispersion change with hole doping, and to what extend does this affect previous calculations in this framework?; (iii) are the “shadow” regions generated by AF correlations important for real-space pairing approaches? In this paper all these issues are discussed. The overall conclusion is that as long as the hole density is such that the \( \xi_{AF} \) is at least of a couple of lattice spacings, the predictions of the original AFVH scenario \( \hfill [3] \) and other similar theories remain qualitatively the same.

To study the presence of a large DOS peak away from half-filling, \( N(\omega)(= \sum_{\mathbf{p}} A(\mathbf{p}, \omega)) \) has been calculated numerically in systems with strong AF correlations. While accurate extrapolations to the bulk limit are difficult, the simple qualitative picture emerging from these studies seems robust. In Fig.1a, \( N(\omega) \) for the 2D t-J model obtained with exact diagonalization (ED) techniques is shown at several densities. \( \hfill [2] \) At half-filling, a large DOS peak caused by flat regions in the q.p. dispersion appears at the top of the valence band, as discussed before. \( \hfill [2] \) Weight exists at energies far from \( \mu \) i.e. the large peak carries only part of the total weight. As shown in Ref. \( \hfill [2] \) the maximum in the DOS is \textit{not} reached at the top of the valence band but at slightly smaller energies. As \( \langle n \rangle \) decreases, the peak is now much broader but it remains well-defined. At \( \langle n \rangle = 0.87 \), \( \mu \) is located close to the energy where \( N(\omega) \) is maximized. If a source of hole attraction exists in this system, a SC gap would open at \( \mu \) and the resulting \( T_c \) could be large. However, even with \( T_c \sim 100K \) the SC gap would not alter much the already robust peak in the DOS shown in Fig.1a. For \( \langle n \rangle \sim 0.75 \), \( \mu \) moves to the left of the peak, where \( T_c \) should become smaller. Then, as \( \langle n \rangle \) is reduced away from half-filling in the 2D t-J model Fig.1a suggests that \( \mu \) travels across a broad DOS peak providing a natural definition for the “underdoped, optimal and overdoped” densities. \( \hfill [2] \) Note that since the peak width increases substantially with hole density, strictly speaking the rigid
Quantum Monte Carlo (QMC) data for the 2D one-band Hubbard model in strong coupling indicate a qualitative behavior similar to that of the t-J model, i.e. \( \mu \) also crosses a peak as \( \langle n \rangle \) varies. This effect was observed in previous simulations, and also in our own studies (Fig.1b). However, note that QMC simulations must be supplemented by a Maximum Entropy (ME) analysis to obtain \( N(\omega) \). ME predictions are more accurate close to \( \omega \approx 0 \) than at finite frequency, and thus we here do not interpret Fig.1b as suggesting the “generation” by doping of a Kondo-like peak at the top of the valence band which does not exist at \( \langle n \rangle = 1 \). We believe that the absence of a sharp peak at half-filling is caused by the systematic errors of the ME procedure and the finite temperature of the simulation. Actually, a robust peak at \( \langle n \rangle = 1 \) appears in other computational studies, and in the t-J model (Fig.1a). Experimentally in the cuprates it has been already established that the states observed in PES upon doping are already present in the insulator and are not Kondo resonances. In the present calculation, Fig.1a suggests that the broad peak observed at \( \langle n \rangle < 1 \) in the t-J model is smoothly connected to the sharper peak found at half-filling.

Similar conclusions can be reached in geometries other than the 2D square lattice. In particular, we studied the DOS of the t-J model on a ladder, finding results very similar to those of Fig.1a, in agreement with previous calculations. Note that on ladders the presence of pairing at finite hole density has been predicted. Thus, a gap may open at \( \mu \) once couplings and lattice sizes are reached where pairing effects are important. We have observed such effects in our studies, but we also found that at \( \langle n \rangle = 1 \) the DOS has a sharp peak, as in Fig.1a. Then, the ladder DOS peak is not exclusively caused by a BCS-induced redistribution of spectral weight upon doping.

In all cases discussed here, calculations of the spin-spin correlations show that \( \xi_{AF} \) is approximately a couple of lattice spacings when \( \mu \) is located near the DOS peak, becoming negligible as the overdoped regime is reached. Thus, a nonzero \( \xi_{AF} \) and \( \mu \) near a large DOS peak are correlated features. It is in this respect that scenarios where AF correlations produce a large DOS that enhances \( T_c \) differ from \( vH \) theories where divergences in the DOS are caused by band effects already present before interactions are switch on.

While the existence of a robust peak in the DOS is in good agreement with ARPES data, it is in apparent disagreement with specific heat studies for YBCO which have been interpreted as corresponding to a flat DOS. The lack of \( p \)-resolution in the specific heat measurements may solve this puzzle. Actually, angle-integrated PES results for Bi2212 do not show the sharp flat features found in ARPES for the same material. Similar effects may affect the specific heat data.

Now let us discuss the \( p \)-dependence of the q.p. band obtained from \( A(p,\omega) \). Results are already available in the literature. In Fig.2a-b, the q.p. dispersion is shown at \( \langle n \rangle = 1 \), and at \( \langle n \rangle \sim 0.87 \) for the t-J model. Note that upon doping the small q.p. bandwidth and the flat regions remain well-defined, inducing a large DOS peak (Figs.1a). However, the region around \( p = (\pi, \pi) \) has changed substantially, i.e. the AF shadow region clearly observed at \( \langle n \rangle = 1 \) has reduced its intensity and considerable weight has been transferred to the inverse PES region (Fig.2b). Actually, the q.p. dispersion at \( \langle n \rangle \sim 0.87 \) can be fit by a tight-binding nearest-neighbors (NN) dispersion with a small effective hopping likely associated with \( J \). This effect was also noticed in studies of the Hubbard model.

The changes in the q.p. dispersion with hole doping can be interpreted in two ways: First, note that \( A(p,\omega) \) is influenced by matrix elements of bare fermionic operators connecting states with \( N \) and \( N \pm 1 \) particles. This is important when the q.p. weight is small i.e. when the state \( c_{p\sigma}|gs\rangle_N \) does not have a large overlap with the ground state of the \( N-1 \) particles subspace \( |gs\rangle_{N-1} \) (\( |gs\rangle_N \) being the ground state with \( N \) particles). It has been suggested that if the hole excitation is created by a new operator \( \gamma_{p\sigma} \) that incorporates the dressing of the hole by spin fluctuations, then \( \gamma_{p\sigma}|gs\rangle_N \) may now have a large overlap with \( |gs\rangle_{N-1} \). In other words, if the dressed hole state resembles an extended spin polaron, then the physics deduced from PES studies, which rely on the sudden removal of a bare electron from the
system, may be misleading. To the extent that spin polaron remains well-defined at finite density, the use of $\epsilon_{p\sigma}$ will induce spectral weight rearrangements between the PES and IPES regions, and Fig. 2b could resemble Fig. 2a after such spectral weight redistribution takes place, as some results already indicate. If this idea were correct, then the study of SC and transport, both regulated by dressed quasiparticles, could indeed be handled by filling a rigid band given by $\epsilon_{AF}(p)$.

However, an alternative is that the difference between Figs. 2a and 2b corresponds to an intrinsic change in the q.p. dispersion as $\xi_{AF}$ decreases. This is the less favorable case for the AFVH approach, and thus we analyze this possibility in detail here. For this purpose, we have applied the standard BCS formalism to a model with a low density of q.p.'s having a dispersion $\epsilon_{NN}(p)/eV = -0.2(cosp_x + cosp_y)$, which roughly reproduces the dominant features of Fig. 2b. As before, we include NN attraction between q.p.'s. While naively it may seem dubious to use the same interaction both at and away from half-filling, the hole-hole potential should not be much affected at distances shorter than $\xi_{AF}$. This can be illustrated by a real space analysis (Fig. 2c) of a smeared $\delta$-function potential of AF origin $V(q) = \xi_{AF}/[1 + \xi_{AF}^2(q - Q)^2]$, where the lattice spacing is set to 1, and $Q = (\pi, \pi)$. Fig. 2c shows that the NN potential ($x = 1$) does not change noticeably as $\xi_{AF}$ is reduced, while $V(x > 1)$ is rapidly suppressed. Then, using the same NN form of the potential for many densities is justified. Note also that the local character of the real-space potential does not imply small Cooper pairs. Their size can be regulated using both its range and intensity.

![Image](image_url)  
**FIG. 2.** (a) q.p. energy vs momentum obtained at half-filling.[2] The result shown, $\epsilon_{AF}(p)$, is a good fit of Monte Carlo data on a $12 \times 12$ cluster at $J/t = 0.4$; (b) q.p. dispersion vs momentum at $\langle n \rangle = 0.87$ and $J/t = 0.4$ using exact diagonalization of 16 and 18 sites clusters (from Ref.[19]). The open (full) circles are IPES (PES) results. Their size is proportional to the peak intensity. The solid line is the fit $\epsilon_{NN}(p)$; (d) $V(x)$ along the x-axis after Fourier transforming the smeared potential $V(p) = \delta(p - Q)$ (see text). $\xi_{AF}$ is given in lattice units.

Then, let us discuss the results obtained using the BCS formalism with an attractive NN potential $V = -0.6J$, with $J = 0.125eV$, for both dispersions $\epsilon_{AF}(p)$ and $\epsilon_{NN}(p)$. Solving numerically the gap equation, $T_c$ is shown in Fig. 3a. As reported before, SC at $T_c \sim 80 - 100K$ in the $d_{x^2-y^2}$ channel appears naturally if the AF-dispersion is used. If, instead, $\epsilon_{NN}(p)$ is used, the flat bands present in this narrow dispersion produce $T_c \sim 30K$ which is still large. Even more remarkable is the fact that the $d_{x^2-y^2}$ character of the SC state is maintained. This result can be understood noticing that a combination of $\epsilon_{NN}(p)$ with an attractive NN potential effectively locates us in the family of “t-U-V” models with U repulsive and V attractive, where it is known that for a “half-filled” electronic band the dominant SC state is $d_{x^2-y^2}$-wave. In other words, when $\mu$ is at the flat region in Fig. 2b it approximately corresponds to a “half-filled” q.p. band, leading to a $d_{x^2-y^2}$-wave SC state (Fig. 3a). Therefore, one of our main results is that even if the q.p. dispersion changes substantially with doping near the $Q$ point, such an effect does not alter the main qualitative features found in previous studies.
The present analysis also shows that the AF “shadow” regions of $\epsilon_{AF}(\mathbf{p})$ are not crucial for the success of the real-space approach. Actually, using $\epsilon_{NN}(\mathbf{p})$, which does not contain weight in PES near $(\pi, \pi)$, $T_c$ is still robust and the d-wave state remains stable. To make this point more clear, we analyzed $T_c$ using $\epsilon_{AF}(\mathbf{p})$ but modulating the contribution of each momentum with a $\mathbf{p}$-dependent weight $Z_p$ in the one particle Green’s function. We considered the special case where $Z_p$ is zero away from a window of total width $W$ centered at the saddle point, which is located in the flat bands region. Inside the window $W$, $Z_p = 1$. Such a calculation also addresses indirectly possible concerns associated with widths $\sim (\epsilon(\mathbf{p}) - \epsilon_F)^2$ that q.p. peaks would acquire away from half-filling in standard Fermi liquids. Results are shown in Fig.3b, for d-wave SC. Note that even in the case where $W$ is as small as just 5% of the total bandwidth (itself already small of order $2\Delta$), $T_c$ remains robust and close to 70K. Then, it is clear that the dominant contribution to $T_c$ comes from the flat regions and the shape of the q.p. dispersion away from them is not relevant for the success of the real-space approach.

We end this paper with novel predictions obtained from $\epsilon_{AF}(\mathbf{p})$ and $\epsilon_{NN}(\mathbf{p})$, when $\mu$ reaches the bottom of these bands (which should not be confused with the bottom of the full hole spectrum since a large amount of weight lies at energies lower than those of the q.p. band). In this regime, the BCS analysis applied to any of the two dispersions shows that extended s-wave SC dominates over $d_{x^2-y^2}$-wave SC in the “overdoped” regime (Fig.3a). This occurs when the q.p. band is nearly empty which, according to Fig.1a, corresponds to an overall density of $\langle n \rangle \sim 0.7$. This change in the symmetry of the SC state can be understood recalling again that $\epsilon_{NN}(\mathbf{p})$, supplemented by a NN attraction formally corresponds to an effective “t-U-V” model. It is well-known that in this model the SC state symmetry changes from d- to s-wave as the density is reduced away from half-filling to a nearly empty system. Actually the bound state of two particles with a NN tight binding dispersion and NN attraction is $s-wave$. To the extend that the AF- or NN-dispersions survive up to $\sim 25\%$ hole doping, as suggested by numerical data, scenarios based on the real-space interaction of q.p.’s predict a competition between extended s-wave and $d_{x^2-y^2}$-wave SC in the overdoped regime. It is remarkable that calculations based on the analysis of the low electronic density $\langle n \rangle \ll 1$ limit of the t-J model lead to analogous conclusions. Our approach is based on a very different formalism, but it arrives to similar results, and thus we believe that a crossover from d- to s-wave dominated SC in overdoped cuprates could occur. Recent ARPES data for overdoped Bi2212 have indeed been interpreted as corresponding to a mixing of s- and d-wave states.

Summarizing, the predictions of real-space theories based on dispersions and interactions calculated at half-filling are qualitatively stable upon the introduction of a finite hole density. These include a large $T_c$, within the BCS formalism, and SC in the $d_{x^2-y^2}$ channel. In the overdoped regime a possible crossover from d- to s-wave SC was discussed.

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