Many-body calculation of the spatial extent of the wave-function of a non-magnetic impurity in a d-wave high-temperature superconductor using the t–J model

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Scanning tunneling microscopy (STM) by providing images of the effects of individual zinc impurities in cuprate superconductors with unprecedented atomic-resolution offers a stringent test to models of correlated fermions for high-temperature superconductors. Using a t–J model supplemented by Variational Monte Carlo many-body techniques, the static dependence of the hole density and of the valence bond and superconducting pairing amplitudes around the impurity are computed. A cross-shaped four-fold symmetric structure very similar to the observed STM observation is found, giving strong credit to the model.

**Introduction** – Cuprates superconductors can be considered as doped two-dimensional (2D) Mott insulators where electronic correlations play a dominant role¹². A number of exotic properties such as the pseudo-gap behavior reflect the complexity of the system. In a pioneering work, Anderson proposed the Resonating Valence Bond (RVB) Mott insulator as the relevant underlying parent state³ from which gapless d-wave superconductivity naturally emerges under doping. Within this scenario, the pseudo-gap naturally emerges as the energy scale associated to the formation of singlet electron pairs via the nearest-neighbor antiferromagnetic (AF) exchange. A mean-field version of the RVB theory using a t–J model could also explain a number of bulk experimental observations⁴.

Local probes of correlated materials with atomic resolution have recently become possible thanks to Scanning Tunneling Microscopy (STM)⁵ which provided unprecedented high-resolution maps of the surface of some undoped cuprate superconductors⁶. The measured space-resolved doped-hole charge density in the SC regime of Na-CCOC and Dy-Bi2212 cuprates revealed stripe patterns⁷. This discovery naturally raises the question whether such inhomogeneities are induced by impurities or whether they are intrinsic as the bulk static charge and spin stripe orders detected in Nd-LSCO⁸ and LBCO⁹ cuprates at doping δ ~ 1/8.

Substituting a single impurity atom for a copper atom indeed strongly affects its surrounding region. Therefore, it can serve as a local fine probe, providing important insights about the properties of the correlated medium itself¹⁰. Imaging the effects of individual zinc impurity atoms on superconducting Bi2212 performed by STM¹¹ showed clear real-space modulations which can be confronted to theoretical modeling. In other words, such observations offer a new stringent test to models of correlated fermions for high-temperature superconductors. It has been argued that a number of bulk properties of these materials can be explained within the correlated t–J model¹². However, local real-space responses have not yet been calculated reliably since, due to the short superconducting coherence length, a fully many-body approach is needed. In this Letter, we have carried out such a program of (i) computing within a many-body numerical technique the response induced by the introduction of a spinless impurity site within a bulk two-dimensional t–J model and (ii) confronting the theoretical results to the experimental observations to validate or invalidate the model.

The t–J Hamiltonian on a square lattice reads,

$$H_{t–J} = - \sum_{(i,j)\sigma} t_{ij} (c_{i\sigma}^\dagger c_{j\sigma} + h.c.) + \sum_{(i,j)} J_{ij} S_i \cdot S_j \cdot (1)$$

A zinc impurity is in the same 2+ oxidation state as the copper ion it is substituted for, so that it does not introduce extra charge. However, in contrast to the copper S=1/2 ion, the Zn²⁺ ion is in a spin-singlet state, inert magnetically. Hence, one can use a simple description: on the four bonds connected to the impurity site we set $t_{ij} = 0$ and $J_{ij} = 0$ as shown on Fig. 1. On all the other bonds, we set $t_{ij}$ and $J_{ij}$ to the same values $t$ and $J$, respectively. Although completely local such a “boundary” is expected to lead to a spatially-extended perturbation strongly affecting GS properties.

**Description of method** – Variational fully-projected fermionic wave-functions¹³ (WF) are known to incor-
porate very satisfactorily correlation effects of the t-J model. We have extended them to finite periodic \(L \times L\) clusters containing a single impurity (in practice, \(L = 8\) and \(L = 16\)). A Variational Monte Carlo (VMC) scheme is used to (i) realize a thorough optimization over the variational parameters \(P_i\) (see below) and (ii) to calculate the ground-state (GS) physical observables. The presence of the impurity on site \(i_0\) modifies the Hilbert space, i.e. \(c_{i_0\sigma}^\dagger|\Psi\rangle = 0\) and \(c_{i_0\sigma}|\Psi\rangle = 0\), where \(|\Psi\rangle\) is the GS of the system. In our Monte Carlo variational scheme an “impurity projector” \(P_{i_0} = (1 - n_{i_0})(1 - n_{i_0})\) is inserted, and the impurity variational wavefunction is defined as \(|\Psi_{VMC}\rangle = P_g P_{i_0}|D\rangle\), where \(P_g\) is the usual Gutzwiller projector enforcing the constraint of no-double occupancy on the remaining \(L^2 - 1\) sites.

Motivated by the success of the R VB theory to explain bulk properties, the mean-field determinant \(|D\rangle\) is chosen to be the ground-state of a mean-field Hamiltonian of standard BCS-type,

\[
H_{MF} = \sum_{(i,j)\sigma} (\chi_{ij} c_{i\sigma}^\dagger c_{j\sigma} + h.c.) + \\
+ \sum_{(i,j)} (\Delta_{ij} c_{i\uparrow}^\dagger c_{j\downarrow} + h.c.) + \mu \sum_{\sigma} n_{i\sigma},
\]

deﬁned on all of the \(L \times L\) sites, including the \(i_0\) site (always occupied by a hole). We optimize all different non-equivalent bonds around the impurity, starting from an initial guess respecting or not the square lattice symmetry around \(i_0\). Since in principle the Hamiltonian \(C_{4v}\) symmetry around \(i_0\) (see Figure 1) could be spontaneously broken, we have performed a number of preliminary tests on small \(8 \times 8\) lattices, choosing the initial R VB bonds pattern with lower symmetries like e.g. \(C_4\) or \(C_s\) symmetries (the later allowing the formation of a domain wall). We have found that the full \(C_{4v}\) symmetry is systematically restored at the variational minimum. Therefore, to reduce the number of variational parameters and gain accuracy, the \(C_{4v}\) symmetry has been enforced on our largest \(16 \times 16\) cluster. As expected, all optimized WFs are found to show opposite signs of \(\Delta_{ij}\) on any site-sharing vertical and horizontal bonds, hence reﬂecting the expected orbital d-wave character of the superconducting order. Lastly, we note that allowing ﬁnite values of the parameters \(\Delta_{ij}\) and \(\chi_{ij}\) on the four bonds connected to the impurity is also important to gain energy as shown on Table I. The lowest-energy state (II) is obtained for a full optimization of the \(\Delta_{ij}\) and \(\chi_{ij}\) parameters over all bonds. Typically, \(\chi_{ij}\) has a signiﬁcant magnitude on the four bonds connected to the impurity site. Moreover, for decreasing doping, a sizable amplitude of \(\Delta_{ij}\) also appears on the later bonds.

Results on \(16 \times 16\) clusters - We now turn to the VMC calculations on the \(16 \times 16\) cluster with periodic-boundary conditions, assuming a physical value of \(t/J = 3\). Here, we consider a physical "core" \(8 \times 8\) region centered around the impurity (i.e. of the same size as our previous small cluster), where we impose a \(C_{4v}\) symmetry around the impurity state. Outside, we assume a uniform d-wave superconducting background (bg) whose parameters \(\chi_{i,i+\hat{x}} = \chi_{i,i+\hat{y}} = \chi_{bg}\) and \(\Delta_{i,i+\hat{x}} = -\Delta_{i,i+\hat{y}} = \Delta_{bg}\) are optimized simultaneously. This enables to reduce significantly the boundary effects and is justiﬁed since the spatial extension of the effect of the impurity rarely exceeds the assumed size of the core.

The spacial distribution of the local hole density \(\langle c_{i\sigma}^\dagger c_{i\sigma}\rangle\), the bond hole kinetic amplitudes \(K_{ij} = \langle c_{i\sigma}^\dagger c_{i\sigma} c_{j\sigma} c_{j\sigma}^\dagger + h.c.\rangle\) and the magnetic VB amplitudes \(S_{ij} = \langle \hat{S}_i \cdot \hat{S}_j \rangle\) are shown in Fig. 2(a) and in Fig. 3(a), respectively, for doping 1/8. Here, and throughout the paper, we only show the 6 \(\times\) 6 central region exhibiting the largest modulations. It turns out that the variational parameters \(\Delta_{ij}\) are suppressed on the four bonds connected to the impurity. This is compensated by an increase in \(\Delta_{ij}\) and hence of \(S_{ij}\) on the neighboring bonds, forming a cross-like structure (see thick blue bonds of Fig. 3(a)). Due to similarities with work done in a somewhat different context, we shall refer to these bonds as the four “dimer bonds”. These bonds are characterized by a simultaneous hole deﬁciency and a large gain in the magnetic energy (which can reach more than 40%), hence signaling a tendency towards singlet crystallization around the impurity. The distribution of \(K_{ij}\) in Fig. 2 shows also a remarkably strong modulation around the impurity.

Superconducting properties of R VB states are characterized by the singlet-pair correlations at distance \(r\), \(\langle \Psi_{VMC}|\tilde{S}_{s+r}^\dagger \tilde{S}_s^\dagger \Psi_{VMC}\rangle/\langle \Psi_{VMC}|\Psi_{VMC}\rangle\), where the operator \(\tilde{S}_{s} = c_{i(s),\uparrow}^\dagger c_{i(s),\downarrow} + c_{i(s),\downarrow}^\dagger c_{i(s),\uparrow}\) creates a singlet-pair of electrons on the bond between locations \(s\) and \(s + \hat{a}\) on the lattice, \(\hat{a}\) being the unit vector that speciﬁes the bond direction (along \(x\) or \(y\)). On the \(8 \times 8\) cluster, we have computed pairing correlations between separate bonds for increasing bond separation. However, at the largest distance available on this cluster, the correlations have not completely reached saturation. To get a better estimation of the superconducting order parameter we have considered the \(16 \times 16\) cluster and computed the pairing amplitudes \(\Delta_{ij}\) for all bonds (\(i, j\)) within the "core" region,

\[
\Delta_{(s),j(s+\hat{a})} = \frac{\langle \tilde{S}_{s}^\dagger \tilde{S}_{s+\hat{a}}^\dagger \rangle}{\langle \tilde{S}_{s}^\dagger \tilde{S}_{s} \rangle},
\]
where $\Delta_{bg}$ is a pair operator on the most remote bond in the homogeneous background. As shown in Fig. 2(a), pairing is enhanced on the dimer bonds, and is depleted around the impurity, where holes are less present.

The 16×16 cluster also allows to reduce the doping content, e.g. to 20 holes, going further into the underdoped region. Interestingly, the hole distribution around the defect is very sensitive to the doping ratio. Indeed, for doping around 12.5% (32 holes) we found that holes are slightly repelled from the bonds around the impurity. In contrast, for 7.8% doping, holes tend to concentrate more around the impurity site as shown in Fig. 2(b).

Let us now compare our findings to prior theoretical approaches. The first investigation of a single impurity immersed in a correlated host has been performed using Lanczos exact diagonalization of small clusters. A calculation of the local density of states revealed bound-states (of different orbital symmetries) in which a mobile hole is trapped by the induced impurity potential. Here, a unique mobile hole was assumed in the cluster, hence preventing real bulk pairing and giving rise to a very small doping $\sim 5\%$ in the surrounding region.

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**FIG. 2:** (Color online.) VMC results for the GS on-site hole densities (circles) and kinetic bond amplitudes (colored segments) obtained on a 16×16 cluster. Only the central region around the impurity is shown. Diameters of circles and widths of segments scale with the absolute value of the relative differences w.r.t. the impurity-free homogenous state at the same $\delta_{ave}$ hole density (whose reference values are estimated by interpolating pure clusters with available flanking hole densities). Higher (lower) hole densities and bond magnitudes w.r.t. the homogeneous case are shown by open (filled) circles and blue (green) bonds respectively. For completeness, we also show on the plot the (bare) numerical values of the non-equivalent sites/bonds. (a) and (b) corresponds to 32 ($\delta_{ave} \simeq 0.1255$) and 20 ($\delta_{ave} \simeq 0.0784$) doped holes giving rise for an homogeneous background to $E_{\text{homog}}/t = -0.1487$ and $E_{\text{homog}}/t = -0.0941$ per bond, respectively.

**FIG. 3:** (Color online.) VMC results for the GS magnetic bond amplitudes obtained on a 16×16 cluster. Same conventions and parameters as in Fig. 2. (a) and (b) corresponds to 32 ($\delta_{ave} \simeq 0.1255$) and 20 ($\delta_{ave} \simeq 0.0784$) doped holes giving rise for an homogeneous background to $E_{\text{homog}}/J = -0.074$ and $E_{\text{homog}}/J = -0.084$ per bond, respectively.

Discussions – Let us now compare our findings to prior theoretical approaches. The first investigation of a single impurity immersed in a correlated host has been performed using Lanczos exact diagonalization of small clusters. A calculation of the local density of states revealed bound-states (of different orbital symmetries) in which a mobile hole is trapped by the induced impurity potential. Here, a unique mobile hole was assumed in the cluster, hence preventing real bulk pairing and giving rise to a very small doping $\sim 5\%$ in the surrounding region. Although our VMC calculations are done in a different physical range (and on much larger clusters), we find, for decreasing doping, the emergence of excess hole density around the impurity, which possibly could be consistent with a bound-state formation when $\delta \to 0$.

Metlitski and Sachdev have introduced a theory of valence bond solid (VBS) correlations near a single impu-
FIG. 4: (Color online.) VMC results for the pairing bond amplitudes $\Delta_{ij}$ obtained on a 16 $\times$ 16 cluster. Same conventions and parameters as in Fig.2 (a) and (b) corresponds to 32 ($\delta_{\text{ave}} \approx 0.1255$) and 20 ($\delta_{\text{ave}} \approx 0.0784$) doped holes giving rise, for an homogeneous background, to $\Delta_{bg} \approx 0.0787$ and $\Delta_{bg} \approx 0.0626$, respectively.

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