Resonant Impurity Scattering in a Strongly Correlated Electron Model

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Scattering by a single impurity introduced in a strongly correlated electronic system is studied by exact diagonalization of small clusters. It is shown that an inert site which is spinless and unable to accommodate holes can give rise to strong resonant scattering. A calculation of the local density of state reveals that, for increasing antiferromagnetic exchange coupling, d-, s-, and p-wave symmetry bound states in which a mobile hole is trapped by the impurity potential induced by a local distortion of the antiferromagnetic background successively pull out from the continuum.

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The nature of impurity scattering in the high-T_c copper oxide superconductors is of particular interest for understanding their low-temperature transport properties. For example, recent experimental studies [1] have found that Zn impurities can change the low temperature dependence of the penetration depth from a linear to a quadratic temperature variation. A similar behavior is seen in the temperature dependence of the Knight shift [2]. In addition, the transport lifetime observed in microwave surface resistance measurements is impurity limited at low temperatures [3]. It is believed that Zn goes into a planar Cu(2) site suppressing the local moment on its site. Theoretical calculations of various transport properties [4–6] have found that models which assume a $d_{x^2-y^2}$ gap with strong resonant impurity scattering provide a possible explanation for the experimental data. However, the origin of this resonant scattering remains an open question. In particular, is such resonant scattering by local defects a consequence of the strong correlations in the host system? Here we report the results of numerical calculations on a t-J model with an inert impurity. We find that an added hole can have bound states of various symmetries as J/t increases. Thus as the host J/t ratio increases, a local inert impurity can give rise to strong resonant scattering.

Now, as one knows, a local impurity introduced into a noninteracting electron system can give rise to bound states [7]. In two dimensions on a tight-binding lattice even an infinitesimal local repulsive (attractive) impurity potential leads to a bound state located in energy above (below) the band (in higher dimension it occurs when the strength of the potential exceeds a critical value). In the calculations of transport properties, the effects of impurity scattering are often characterized by scattering phase shifts. For energies near a bound state the phase shift approaches $\pi/2$ [8] and one has strong resonant scattering. In this case the nature of the scattering is directly related to the one-body impurity potential. Here we are interested in the problem of an impurity in a strongly interacting host. The central idea we would like to put forward in this paper is the fact that an impurity introduced in a strongly correlated ground state (GS) could behave quite differently from an impurity in a weakly

interacting system. In the case of an on-site impurity potential in a tight-binding lattice mentioned above, the interaction is spatially located at the perturbed site, and the resultant bound states can have only s-wave symmetry. However, in a many-body ground state like an antiferromagnet (AF), the antiferromagnetic correlations are slightly enhanced in the vicinity of a vacancy [9], and thus the impurity produces a dynamic finite range potential. Bound states of various symmetries can then result as we shall show in this paper. Furthermore the occurrence of these states depends upon the strength of the correlations in the host.

An inert site introduced in a two-dimensional AF background can be described by the following Hamiltonian:

$$H = J\sum_{\langle ij \rangle}'(\mathbf{S_i} \cdot \mathbf{S_j} - \tfrac{1}{4}n_i n_j)$$
$$-t\sum_{\langle ij \rangle,s}' P_G(c_{i,s}^\dagger c_{j,s} + \text{H.c.})P_G, \qquad (1)$$

where the notations are standard and the prime means that the sum over the nearest neighbor links $\langle ij \rangle$ is restricted to the bonds *not* connected to the impurity site. The kinetic term of (1) describes the motion of extra empty or doubly occupied sites in the large-U limit of the Hubbard model. For simplicity, in the following we shall call "holes" either of these entities ($c_{i,s}^\dagger$ is the hole *creation* operator). The impurity model can be obtained
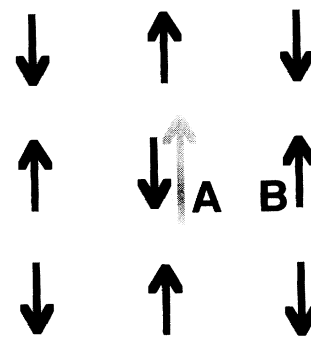

FIG. 1. Schematic picture of the A-B lattice around the impurity. A down spin removed at the impurity site leads to an excess 1/2 spin.

continuously from the uniform model (large-U Hubbard or t-J models) by gradually turning off the hoppings on the four bonds connected to a given site O. Eventually for vanishing couplings the impurity spin becomes frozen, e.g., $S_O^z = -1/2$ (formally, this can be achieved by adding an infinitesimal magnetic field). In other words, if a vacant site is introduced in a strongly correlated host by, let us say, removing a down spin at site O then an excess $S^z = 1/2$ is left over as depicted schematically in Fig. 1. In this case the scattering of an extra hole added to the system can occur in two different spin channels $S^z = 0$ or

$$N_{ii}^{\sigma,\sigma_0}(\omega) = -\frac{1}{\pi}\text{Im}\left\langle \Psi_{0,\sigma_0}^{imp} \mid c_{i,\sigma}\frac{1}{\omega + i\epsilon - H + E_0^{imp}}c_{i,\sigma}^{\dagger} \mid \Psi_{0,\sigma_0}^{imp} \right\rangle, \tag{2}$$

with $\mid \Psi_{0,\sigma_0}^{imp}\rangle$ the impurity GS. Note that the energies are measured with respect to the GS energy at half filling E_0^{imp}. An equivalent expression for the local density of the pure AF system is obtained by replacing "imp" by "pure" and omitting σ_0. In the pure case, an interesting structure appears at the bottom (top) of the upper (lower) Hubbard band with increasing coupling J. Indeed, recent exact calculations on various cluster sizes [10] have shown that a quasiparticle band of width $\sim J$ survives with increasing system size [see also Fig. 2(f)]. Our first motivation here is to investigate the influence of the impurity on this band structure.

At this stage it is useful to notice that the local density of states obeys the following sum rule,

$$\int_{-\infty}^{+\infty} N_{ii}^{\sigma,\sigma_0}(\omega)\,d\omega = \frac{1}{2} + \sigma\langle S_i^z\rangle_0, \tag{3}$$

where $\langle\cdots\rangle_0$ stands for the expectation value in the AF

$S^z = 1$. However, since the $S^z = 1$ sector involves triplet states of higher energies we shall restrict ourselves later on mainly to the $S_z = 0$ scattering channel. The following results are obtained by exactly diagonalizing small 4×4, $\sqrt{18}\times\sqrt{18}$, $\sqrt{20}\times\sqrt{20}$, and $\sqrt{26}\times\sqrt{26}$ clusters by a standard Lanczos method. We will measure energies in units of t.

Let us now formally construct the impurity state by removing a spin $-\sigma_0$ at site O from the AF and having the spin system relax around the impurity. The local hole density of states at a site i away from the impurity site is given by

GS. In the pure system, a small tunneling between the two Néel GS (for a finite system) leads to a zero expectation value of S_i^z for any site. However, the impurity breaks translation symmetry and the removal of a spin at site O imposes a local AF spin environment around it. In this sense the vacant site acts like a magnetic impurity of spin $-\sigma_0$. The local density of states $N_{ii}^{\sigma,\sigma}$ at all nonequivalent sites of a 20-site cluster at an intermediate coupling $J = 0.5$ is shown in Figs. 2(a)–2(e) and $\langle S_i^z\rangle_0$ is indicated for each case (assuming, e.g., $\sigma_0 = \sigma = \uparrow$ as in Fig. 1). The same quantities in the pure case are shown in Fig. 2(f) as a reference. If we assume that the "down spin" impurity lies, let us say, on the A sublattice then the total (integrated) density for the up spin is significantly larger on the B sublattice according to (3) and reflects the local AF spin environment. Specially interesting new features also appear on the B sites, namely
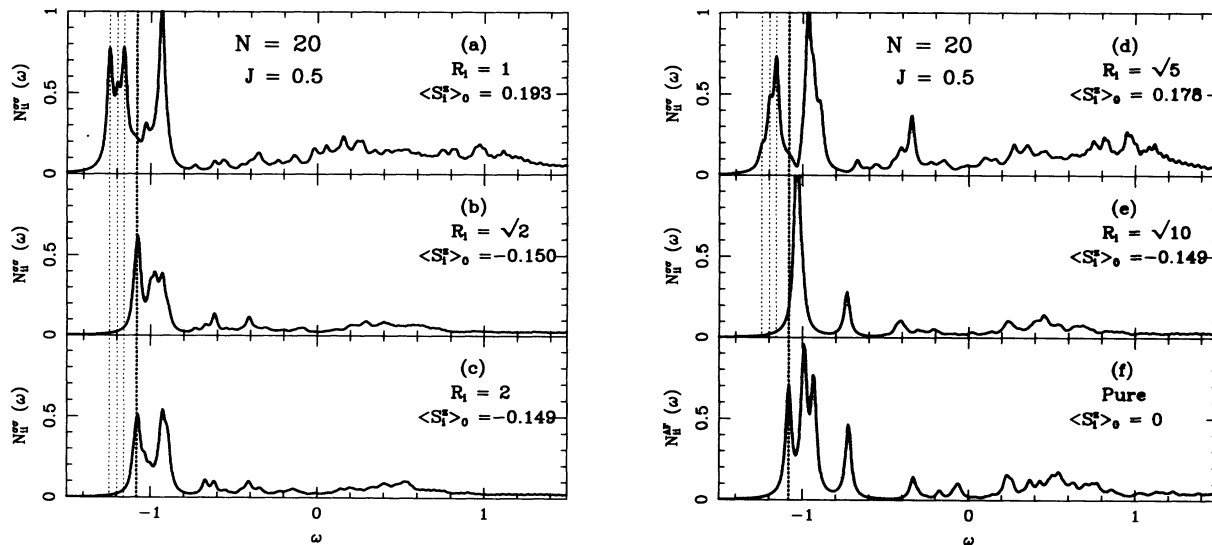

FIG. 2. Local density of states on various lattice sites at distances R_i from the impurity site on a $\sqrt{20}\times\sqrt{20}$ cluster for $J = 0.5$. The energies of the d-, s-, and p-wave bound states are indicated by thin dashed lines. The lower edge of the (upper) Hubbard band of the pure system is shown as a reference by a thicker dashed line. The expectation values of S_i^z on the sites are indicated on the plots.

sharp resonances reflecting the presence of bound states. Indeed, a comparison of Figs. 2(a) and 2(d) with Fig. 2(f) reveals that some peaks lie below the bottom of the quasiparticle band of the pure system and are somehow disconnected from the band (at higher energy). These features do not appear on the A sites since the density for the up spins is low on these sites. However, we note that these bound states are rather extended in space and clearly Fig. 2(d) shows that their wave functions are not just restricted to the nearest neighbor sites.

We have carefully studied the spin and the spatial symmetries of these bound states. Actually, the local density of states is obtained by decomposing the local hole operator into its symmetric components, $c_{i,\sigma} = \sum_\alpha (\mathcal{N}_i^\alpha)^{-1/2} c_{i,\sigma}^\alpha$ where α labels the irreducible point group representations [11] and $\mathcal{N}_i^\alpha$ are normalization factors such that $\sum_\alpha (\mathcal{N}_i^\alpha)^{-1} = 1$. The calculation of the density of states is then made separately in each symmetry sector and the various components added afterwards with the appropriate weights, $N_{ii}^{\sigma,\sigma_0} = \sum_\alpha (\mathcal{N}_i^\alpha)^{-1} N_{ii,\alpha}^{\sigma,\sigma_0}$, where $N_{ii,\alpha}^{\sigma,\sigma_0}$ is the density of states in the α-symmetry channel defined by substituting the new operators $c_{i,\sigma}^\alpha$ in (2). Note that each of these symmetry components independently satisfies the sum rule (3).

The low energy peaks observed in Fig. 2 correspond to bound states of different spatial symmetries as we shall discuss here. However, as mentioned above, they all appear in the singlet sector, i.e., for $\sigma = \sigma_0$. For a more quantitative analysis we define the binding energy by, $\Delta_B = (E_{1h,0}^{imp} - E_0^{imp}) - (E_{1h,0}^{pure} - E_0^{pure})$, where the subscript "$1h$" refers to the single hole GS (with or without the impurity). Δ_B corresponds to the difference between the energy of an impurity and a mobile hole confined in the same cluster and their energy when they are separated in two different clusters. The GS energies $E_{1h,0}^{pure} - E_0^{pure}$ of a single hole moving in a pure AF background have been calculated elsewhere [12] for the same clusters. As seen in Fig. 2 the various resonances are located within Δ_B from the bottom of the pure quasiparticle band. Since $\Delta_B < 0$ these peaks emerge *below* the continuum in the gap and hence correspond to actual bound states. In other words, an added hole can gain energy by binding to the impurity in order to reduce the magnetic energy loss.

Since the phenomenon of binding is a fine balance between delocalization energy and magnetic energy there is naturally a critical value J_c of J above which it sets in. In Fig. 3(a) we show Δ_B vs J for various cluster sizes for the d-wave channel. The values of J_c for our clusters are quite small, between 0.1 and 0.2. However, J_c slightly increases (almost uniformly) with system size and we expect the actual value to be of the order of 0.3. It is interesting to notice that the binding energy of a single hole to the impurity is significantly smaller than the binding energy of a moving pair of holes [13] as seen in Fig. 3(a). Hence, a collective delocalization of both
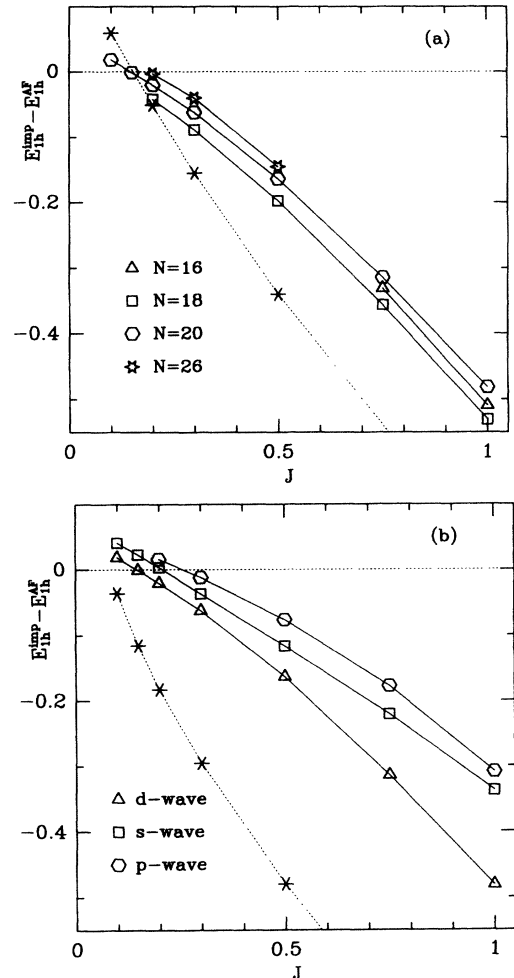

FIG. 3. (a) Binding energy of the d-wave bound state for several cluster sizes vs J. The dashed curve corresponds to the binding energy of a pair of mobile holes on a 26-site cluster in an AF background (see Ref. [13]). (b) Binding energy of the d-, s-, and p-wave bound states on a 20-site cluster vs J. The dashed curve corresponds to the binding energy of a pair of mobile holes on the same cluster (see Ref. [13]).

objects can strengthen even more the attractive effective potential. In addition, for a *finite* hole density, i.e., in the metallic state, we expect that the critical value of J_c will be increased and that resonant scattering will occur in place of bound states at lower J.

For increasing coupling J-, d-, s-, and p-wave bound states successively appear [14] (negative value of Δ_B) in the range $0.15 < J < 0.25$ as seen in Fig. 3(b). The largest (absolute) value of the binding energy is always obtained in the d-wave channel. However, note that above a rather *small* critical value of 0.25 (for 20 sites) all bound states of d, s, and p symmetry coexist. As mentioned previously, we expect the actual critical value of J for the onset of binding to be slightly larger in the thermodynamic limit.
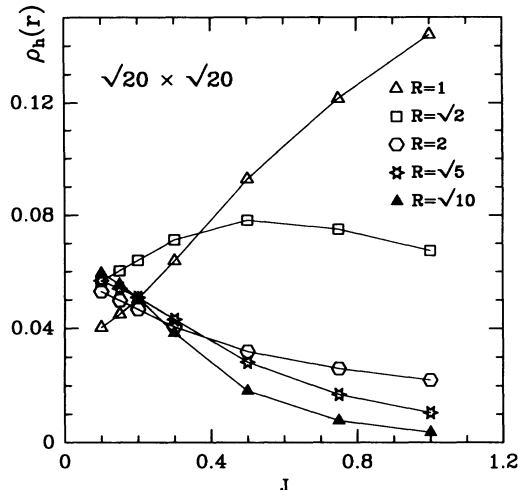
FIG. 4. Hole density on the different nonequivalent 20-site cluster sites vs J. An extra hole has been introduced into the cluster in addition to the impurity.

The distribution of the hole charge density around the impurity gives useful insights about the bound state wave function. The charge density on some nonequivalent sites is shown in Fig. 4 for the lowest energy d-wave bound state as a function of J. Above $\sim J_c$, when binding sets in, the charge density becomes maximum on the nearest neighbor sites of the impurity. Hence, the hole wave function becomes localized around the impurity site. We also note that a significant hole density is present on the 4 sites at distance $\sqrt{2}$ although this amplitude is not as big as in the case of a moving hole pair [15]. A priori, this could seem surprising since the density of states in Fig. 2(b) does not show any significant weight at the d-wave bound state energy. In fact, this simply means that adding the extra hole to the impurity GS on these particular sites produces a very small overlap with the actual d-wave bound state. Such a large amplitude on the next nearest neighbor sites can only be obtained by adding the hole at distance 1 from the impurity and by having the system relax to its GS configuration. Such retardation effects were also observed in the case of a bound pair of holes propagating on the lattice [15].

We conclude by summarizing our findings. In the presence of an inert site, the extra spin $1/2$ created by removing a down spin at site O is distributed. As seen from the values of $\langle S_i^z \rangle_0$ listed in Fig. 2 for $J = 0.5$, the total lattice spin deviation of $1/2$ spreads largely over the sites of the $\sqrt{20} \times \sqrt{20}$ cluster. The notion that the introduction of a nonmagnetic Zn site can induce moments on the surrounding Cu sites has been discussed by Finkel'stein et al. [16], who used a holon-spinon description. When a hole is added to the system containing an impurity, d-, s-, and p-wave bound states successively appear as

J increases. The largest binding energy is obtained in the d-wave channel. The dynamic nature of this strongly interacting system provides a collective potential which depends not just on the impurity potential and the band-structure hopping parameter t, but rather in an essential way on the exchange correlations determined by J. This suggests that the postulated resonant scattering from Zn impurities introduced in the CuO_2 plane of the cuprates may arise in a natural way from the strong correlations of the host.

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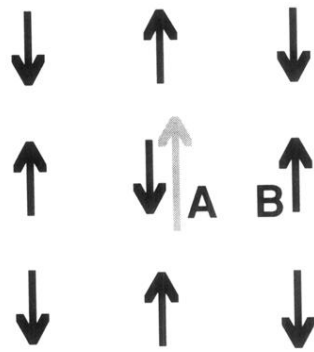[16] A.M. Finkel'stein et al., Physica (Amsterdam) 168C, 370–380 (1990).

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