States of Local Moment Induced by Nonmagnetic Impurities in Cuprate Superconductors

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By using a model Hamiltonian with d-wave superconductivity and competing antiferromagnetic (AF) orders, the local staggered magnetization distribution due to nonmagnetic impurities in cuprate superconductors is investigated. We show that the net moment induced by a single impurity corresponds to a local spin with $S_z = 0$ or $1/2$ depending on the strength of the AF interaction U and the impurity scattering strength ϵ. Phase diagram of ϵ versus U for the moment formation is presented. We discuss the connection of this result with the Kondo problem. When two impurities are placed at the nearest neighboring sites, the net moment is always zero, unusually robust to parameter changes. For two neighboring strong impurities, separated by a Cu-ion site, the induced net moment has $S_z = 0$, $1/2$, or 1.

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The nonmagnetic impurity effect in high temperature superconductors (HTS) has attracted significant interest both experimentally and theoretically for many years. The induction of a local magnetic moment would be expected due to the competition between spin magnetism and superconductivity in these systems. Nuclear magnetic resonance (NMR) measurements in $YBa_2Cu_3O_{7-x}$ have indicated that nonmagnetic Zn/Li impurities enhance the antiferromagnetic correlation and a staggered magnetic moment is induced on the Cu ions in the vicinity of the impurity sites [1–5]. Low-temperature scanning tunneling microscopy (STM) experiments [6] have directly observed a sharp near zero bias resonance peak around the Zn impurity atoms on the surface of superconducting $Bi_2Sr_2CaCu_2O_{8+x}$ (BSCCO). Both local potential scattering [7–11] and Kondo impurity scattering [12–14] in d-wave superconductors have been theoretically investigated. Recently Wang and Lee [15] tried to reconcile the local moment formation around a strong nonmagnetic impurity in HTS and a strong zero bias resonance in the local density of states (LDOS) spectrum by studying a renormalized mean-field theory of the t-J model.

On the other hand, the quantum interference effect among multiple impurities in HTS has drawn considerable attention in recent years [16–20]. The spatial distribution of the LDOS spectrum changes remarkably by varying the distance and orientation among the impurities. To our knowledge, so far there exists no study considering the local moment formation due to the quantum interference effect among multiple impurities in HTS. In this Letter, we apply an effective model Hamiltonian defined on a square lattice with a nearest neighboring (nn) interaction V_{DSC} to simulate the d-wave superconductivity (DSC) and an on site Coulomb interaction U to represent the competing antiferromagnetic (AF) order. The local magnetic moment distribution induced around a single impurity will be numerically studied. We show that the net moment induced around a single impurity can be attributed to a local spin with $S_z = 0$ or $1/2$ depending on the value of impurity scattering strength ϵ and U, and a phase diagram for the net moment formation is presented. The connection of this result with the Kondo problem is also discussed. With multiple impurities, we expect that a quantum interference effect should exhibit itself. When two impurities are placed at the nn sites, our numerical result indicates that the net induced moment is always zero, regardless of the value of U, ϵ, and doping. For two strong impurities at the next nn sites and at sites separated by a Cu-ion site, the net moment induced by them can be represented by a local spin with $S_z = 0$, $1/2$, or 1 depending on the U value and doping.

We begin with a phenomenological model Hamiltonian in a two-dimensional plane, in which both the DSC and the competing AF or the spin density wave (SDW) order are taken into account:

$$H = -\sum_{i,j,\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + \sum_{i,\sigma} (U n_{i\bar{\sigma}} + \epsilon \delta_{i_m,i} - \mu) c_{i\sigma}^\dagger c_{i\sigma} + \sum_{i,j} (\Delta_{ij} c_{i\uparrow}^\dagger c_{j\downarrow}^\dagger + \text{H.c.}), \quad (1)$$

where i_m is the impurity site; μ is the chemical potential. The hopping term includes the nn hopping t and the next nn hopping t'. The staggered magnetization and DSC order in cuprates are defined as $M_i^s = (-1)^i \langle c_{i\uparrow}^\dagger c_{i\uparrow} - c_{i\downarrow}^\dagger c_{i\downarrow} \rangle$ and $\Delta_{ij} = V_{DSC} \langle c_{i\uparrow} c_{j\downarrow} - c_{i\downarrow} c_{j\uparrow} \rangle / 2$. The mean-field Hamiltonian (1) can be diagonalized by solving the resulting Bogoliubov–de Gennes equations self-consistently

$$\sum_j \begin{pmatrix} \mathcal{H}_{ij,\sigma} & \Delta_{ij} \\ \Delta_{ij}^* & -\mathcal{H}_{ij,\bar{\sigma}}^* \end{pmatrix} \begin{pmatrix} u_{j,\sigma}^n \\ v_{j,\bar{\sigma}}^n \end{pmatrix} = E_n \begin{pmatrix} u_{i,\sigma}^n \\ v_{i,\bar{\sigma}}^n \end{pmatrix}, \quad (2)$$

where the single particle Hamiltonian $\mathcal{H}_{ij,\sigma} = -t_{ij} + (U n_{i\bar{\sigma}} + \epsilon \delta_{i_m,i} - \mu) \delta_{ij}$, $n_{i\uparrow} = \sum_n |u_{i\uparrow}^n|^2 f(E_n)$, $n_{i\downarrow} = \sum_n |v_{i\downarrow}^n|^2 [1 - f(E_n)]$, and $\Delta_{ij} = (V_{DSC}/4) \sum_n (u_{i\uparrow}^n v_{j\downarrow}^{n*} + v_{i\downarrow}^{*} u_{j\uparrow}^n) \tanh(E_n/2k_BT)$. The DSC order parameter at the ith site is $\Delta_i^D = (\Delta_{i+e_x,i} + \Delta_{i-e_x,i} - \Delta_{i,i+e_y} - \Delta_{i,i-e_y})/4$

where $\mathbf{e}_{x,y}$ denotes the unit vector along the (x, y) direction. Various doping concentrations can be tuned by varying the chemical potential. There will be no qualitative difference with the consideration of local distortion of hopping parameters around impurity. In the present calculation, we set the lattice constant a and hopping integral t as units, $t' = -0.2$ and $V_{\mathrm{DSC}} = 1.0$. Because of the localized nature of the impurity states, the order parameters around impurity are insensitive to the boundary conditions for large system sizes. The linear dimension of the unit cell is chosen as $N_x \times N_y = 32 \times 32$. The averaged electron density is fixed at $\bar{n} = 0.85$. The calculation is performed in a very low-temperature regime. The supercell techniques are employed to calculate the LDOS. The number of the unit cells is $M_x \times M_y = 20 \times 20$.

Our numerical results for a single impurity show that the local AF order may be absent around the impurity site for small ϵ and is present when impurity strength ϵ becomes larger. In Fig. 1, we plot three typical spatial distributions of the staggered magnetization and their corresponding LDOS spectra around the impurity site. The net local moment is defined as $S_z = \sum_i S_i^z$. The impurity is situated at (16, 16). The DSC order parameter is suppressed dramatically at the impurity site and recovers its bulk value at a few lattice constants away. Because the AF order and the DSC order are competing with each other, the local suppression of the DSC order may lead to the appearance of the local AF order. Both the induction of the local AF order and the local suppression of the DSC order around impurities are properly taken into account in the spatially unrestricted self-consistent calculation. Figures 1(a) and 1(b) correspond to $U = 2.0$ and $\epsilon = 3$. It is clear that no AF order induction is shown for such a weak impurity. In 1(b), the resonance energy at the impurity site (solid line) is less than zero while the resonance energy at the nn impurity site (dashed line) is greater than zero. The dotted line is for the site far from the impurity site. With the increasing of the impurity strength, the resonance peak height at the impurity site becomes weaker and its peak shifts to zero energy while the resonance peak height at the nn impurity site turns stronger and its peak also moves to zero energy. Figures 1(c) and 1(d) are for a strong impurity $\epsilon = 100$ and $U = 2.0$. We find that the induced staggered magnetization reaches a maximum value of 0.08 at the nn site of the impurity in 1(c), and the local static AF fluctuation extends over several lattice sites from the impurity but there is no net induced moment (or $S_z = 0$). The remarkable enhancement of the zero bias resonance peak at the nn sites is shown in panel Fig. 1(d), reflecting the characteristics of a strong impurity. The presence of weak local AF order results in a rather weak splitting of the resonance peak. In Figs. 1(e) and 1(f) we show the results for $U = 2.35$ and $\epsilon = 100$. A pronounced two-dimensional SDW order is clearly induced around this strong impurity in 1(e). The staggered magnetization at the nn site reaches to 0.33 and the net induced moment becomes $S_z = 1/2$. The zero bias resonance peak of the LDOS at a smaller U with $S_z = 0$ shown in 1(d) at the nn site is substantially suppressed and becomes two weak peaks in the larger U case with $S_z = 1/2$ [see Fig. 1(f)].

To examine the local moment formation, we present the phase diagram of ϵ versus U in Fig. 2. It is obvious that the induced net moment ($S_z = 1/2$) should show up for larger impurity strength ϵ and stronger AF interaction U, while $S_z = 0$ tends to exist for smaller ϵ or weaker U. In fact, there exist three phase regimes depending on the magnitude of the U value or doping (not shown here). For small U, no AF order (nonmagnetic phase) is induced around the impurity [see Fig. 1(a)]. For intermediate U, weak local AF order (AF fluctuation phase) appears [see Fig. 1(c)], but the net induced magnetic moment vanishes corresponding to a local spin $S_z = 0$. Here the AF fluctuating phase could be correlated to the Kondo regime in which the moment of a spin $S_z = 1/2$ induced directly by the impurity is screened by the spins of the surrounding quasiparticles. As a result, the remnant-staggered magnetization around the impurity is still in presence while the net induced moment around the impurity becomes zero. As we increase U (or decrease the doping level), the induced SDW order near the impurity becomes stronger

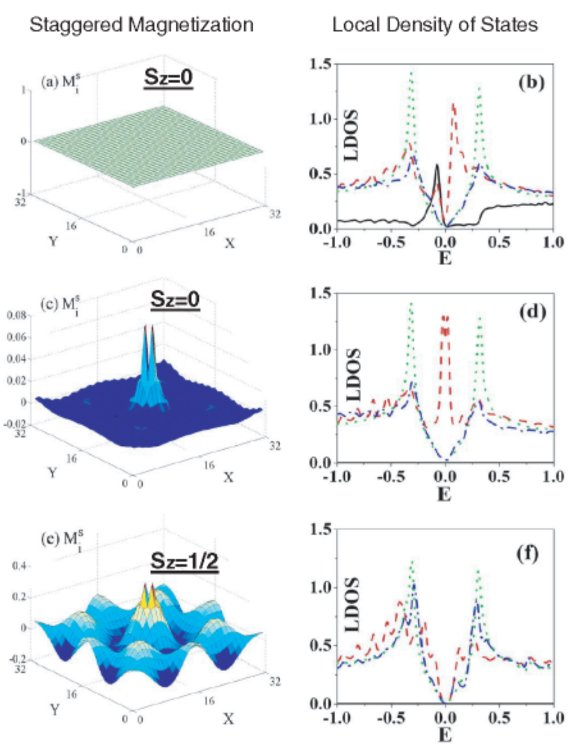

FIG. 1 (color online). Spatial variations of the staggered magnetization M_i^s [(a), (c), and (e)], and LDOS spectra [(b), (d), and (f)]. The impurity site is at (16,16). The solid lines in panels (b), (d), and (f) are for (16,16), dashed lines for (17,16), dashed-dotted lines for (17,17), and dotted lines for (16,1). The upper panels [(a),(b)], the central panels [(c),(d)], and the lower panels [(e),(f)] are for ($U = 2.0, \epsilon = 3$), ($U = 2.0, \epsilon = 100$), and ($U = 2.35, \epsilon = 100$), respectively.

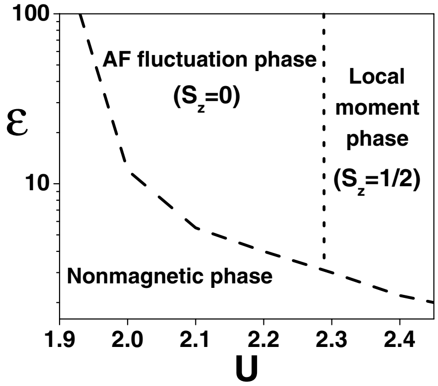

FIG. 2. Phase diagram of ϵ versus interaction strength U for various phases near the impurity.

and locally we have a larger SDW gap near the chemical potential. Thus the number of quasiparticles may decrease which in turn would weaken their ability to screen the magnetic moment of $S_z = 1/2$. This also implies that the coupling between the induced moment and the DSC is reduced. When the coupling strength is less than a critical value, the local moment induced directly by the impurity decouples from the DSC. This is the reason why the net moment of $S_z = 1/2$ induced by the impurity is unscreened in Fig. 1(e) (local moment phase) when $U = 2.35$. In the nonmagnetic phase regime and for a strong impurity, there is a sharp zero bias resonance peak in the LDOS without any splitting [7]. The splitting is gradually showing up in the AF fluctuation phase regime at the Kondo regime. The LDOS could be substantially suppressed at zero bias and split into two weak peaks in the third regime with $S_z = 1/2$. It is important to notice that the Kondo regime discussed here is absent in Ref. [15]. However, this regime might be recovered in their calculation if the constraint on the number of local spin around the impurity is removed. The obtained staggered magnetization distribution around a strong impurity agrees with the NMR experimental results [1–5]. The critical value of U for inducing $S_z = 1/2$ is doping dependent. The $S_z = 1/2$ moment due to a strong impurity is much easier to be induced in an underdoped sample than in optimally and overdoped samples, because the induction of AF order becomes more prominent at the lower doping case. Since the existence of inhomogeneity in the HTS sample has been experimentally confirmed [21,22], as a result, the number of induced $S_z = 1/2$ moments would be smaller than the number of strong impurities like Zn. We also predict that the strong zero bias peak observed by Pan *et al.* [6] at the Zn impurity site should be associated with the $S_z = 0$ moment in the overdoped and possibly optimally doped regions. In the underdoped region, the induced moment would become $S_z = 1/2$ where the LDOS spectrum should be much suppressed by the induced SDW at zero bias.

We next study the quantum interference effect on the local moment formation due to two strong impurities. When they are placed at the nn sites [see Fig. 3(a)], our numerical results for the distribution of the induced magnetization around the impurities are shown in Figs. 3(b) and 3(c) with, respectively, $U = 2.0$ and 2.4. For $U = 2.0$ and 2.35 (not shown here), the induced staggered magnetizations are also uniformly zero and exactly identical to that in Fig. 3(b). It appears that the staggered magnetizations due to the two nn impurities have exact cancellation. With $U = 2.4$ and no impurities, one can numerically demonstrate that the staggered magnetization has a stripelike structure [23] with periodicity $8a$ which coexists with the DSC. The presence of the impurities could pin the stripes but does not modify the overall stripelike structure except the magnetizations at or very close to the impurity sites are altered [see Fig. 1(c)]. In all these cases, the net induced moment has $S_z = 0$. This result is very robust and independent of the value of U, ϵ, and doping. For two strong impurities placed at the next nn sites [see Fig. 3(d)], the induced spatial profiles of the staggered magnetization for $U = 2.0$ and 2.4 are, respectively, shown in Figs. 3(e) and 3(f). The net moment associated with Fig. 3(e) yields a local spin of $S_z = 1/2$, while that associated with Fig. 3(f) has $S_z = 1$. For $U = 2.35$, the induced SDW no longer has the stripelike structure and we still obtain $S_z = 1$. The induced net moment has been shown to have $S_z = 0$ when U is less than 1.9.

Finally, we place two strong impurities at sites separated by a Cu ion [see Fig. 4(a)]. The distributions of the

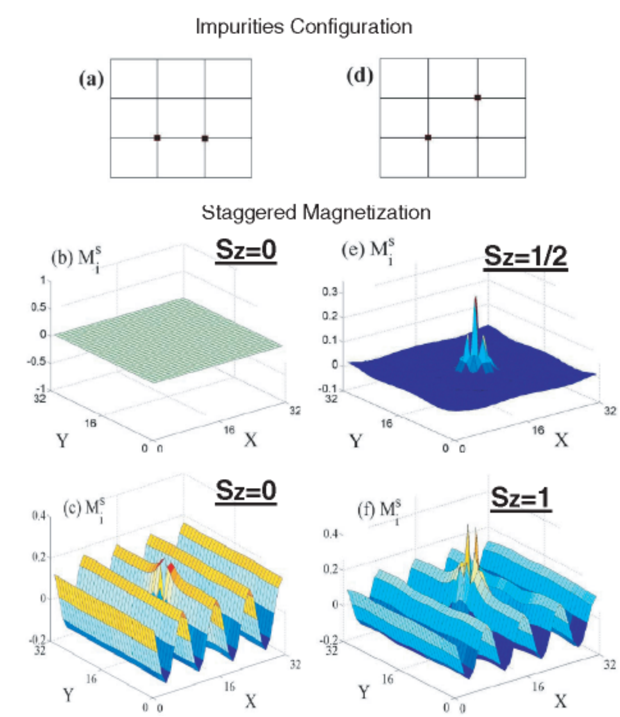

FIG. 3 (color online). Impurities configuration [(a),(d)] and staggered magnetization M_i^s [(b),(c) and (e),(f)]. The left panels [(a)–(c)] and the right panels [(d)–(f)] are for two nn impurities and two next nn impurities, respectively. Panels [(b),(c)] and [(e),(f)] correspond to $U = 2.0$ and $U = 2.4$, respectively.

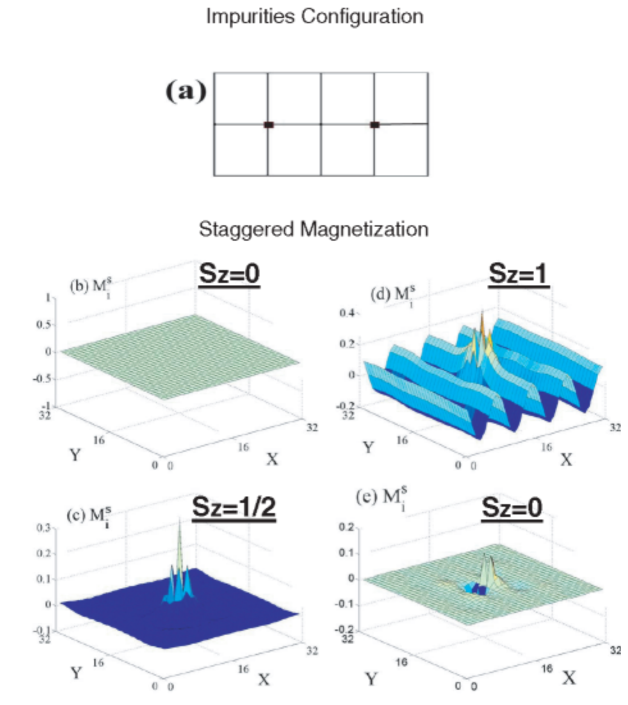

FIG. 4 (color online). Impurities configuration (a) and spatial profiles of staggered magnetization M_i^s [(b)–(e)] in a 32×32 lattice. Their corresponding parameters are (b) ($U = 1.9$), (c) ($U = 2.0$), (d) ($U = 2.4$), and (e) ($U = 2.2$, $t' = -0.3$).

staggered magnetizations are shown in Figs. 4(b)–4(d) for $U = 1.9$, 2.0, and 2.4, and the induced net moments have, respectively, $S_z = 0$, 1/2, and 1. In Fig. 4(b), no induced AF order is present for small U. The net moment has $S_z = 0$. In Fig. 4(c), a remarkable enhancement of the local AF order is shown at the central Cu site and the DSC order at this site is suppressed to almost zero. This is a kind of *constructive* interference effect. Its net moment has $S_z = 1/2$. In Fig. 4(d), one can clearly observe the pinning of SDW stripes by impurities. The local magnetization at the central Cu site is also enhanced. The net moment has $S_z = 1$. As shown in Fig. 4(e), if we choose $U = 2.2$ and a different band parameter $t' = -0.3$, the induced local moment associated with two individual impurities would have opposite polarity and yield a net $S_z = 0$. The *destructive* interference effect is shown at the center site where local AF order is equal to zero. This type of opposite polarities occurs when two impurities separated farther apart even with $t' = -0.2$ as used in the present paper. The net local moment induced by two impurities spaced by one Cu ion could result in $S_z = 0$, 1/2, or 1. In other words, quantum phase transitions may occur among different local moment phases by varying U values or doping.

In summary, we have investigated the induction of the local moment by single and double impurities in HTS based on a phenomenological model with DSC and competing AF orders. By tuning the impurity potential and the value of U, a transition between various net magnetic moment states may appear. We show that the zero bias resonant peak obtained next to the strong impurity site is always associated with weak U and $S_z = 0$. When $S_z = 1/2$, the LDOS at zero bias is suppressed by the gap of the locally induced SDW. This is consistent with the recent STM experiments [22], where the zero bias resonant peaks due to Zn impurities are observed only in the hole rich region, not in the hole poor region in BSCCO. In addition, the quantum interference effect by two nonmagnetic impurities has also been studied. Our calculation predicts the absence of the net magnetic moment around two nn impurities, regardless of the values of the impurity strength, doping, and U. This result indicates that the number of induced $S_z = 1/2$ moments is always smaller than the number of Zn impurities even in an underdoped sample. The present investigation on the local moment formation may provide useful information for future experimental tests.

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