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) order, 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 \( \epsilon \). Phase diagram of \( \epsilon \) 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.

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\(_2\)Cu\(_3\)O\(_x\)-e 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 an impurity site [1–5]. Low-temperature scanning tunneling microscopy (STM) experiments [6] have directly observed a sharp near zero bias resonance peak around an impurity site [1–5]. However, Wang and Lee [15] tried to reconcile the observed a sharp near zero bias resonance peak around an impurity site [1–5].

The net induced moment is always zero, regardless of the value of \( U, \epsilon, \) and doping. For two strong impurities at the next nn sites and at sites separated by a Cu-ion site, the net induced moment 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:

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

where \( i_n \) is the impurity site; \( \mu \) 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 \( M_i^z = (-1)^i (c_{i\uparrow}^\dagger c_{i\downarrow} - c_{i\downarrow}^\dagger c_{i\uparrow}) \) and \( \Delta_{ij} = V_{\text{DSC}} (c_{i\uparrow}^\dagger c_{j\downarrow}^\dagger - c_{i\downarrow}^\dagger c_{j\uparrow})/2. \) The mean-field Hamiltonian (1) can be diagonalized by solving the resulting Bogoliubov–de Gennes equations self-consistently:

\[
\sum_j \left( \frac{\mathcal{H}_{ij,\sigma}}{\Delta_{ij}^D} - \mathcal{H}_{ij,\sigma}^D \right) \left( \frac{u_{i,\sigma}^0}{v_{i,\sigma}^0} \right) = E_\sigma \left( \frac{u_{i,\sigma}^0}{v_{i,\sigma}^0} \right),
\]

where the single particle Hamiltonian \( \mathcal{H}_{ij,\sigma} = -t_{ij} + (U n_{i\sigma} + \epsilon \delta_{n_{i\sigma}} - \mu) \delta_{ij}, \) \( n_{i\sigma} = \sum_{\sigma} |u_{i\sigma}|^2 f(E_{n_{i\sigma}}), \) \( n_{ij} = \sum_{\sigma} |v_{i\sigma}^0|^2 (1 - f(E_{n_{i\sigma}})), \) and \( \Delta_{ij} = (V_{\text{DSC}}/4) \sum_{\sigma} (u_{i\sigma}^0 v_{j\sigma}^0 + v_{i\sigma}^0 u_{j\sigma}^0) \tanh (E_{j\sigma}/k_B T). \) The DSC order parameter at the \( i \)th site is \( \Delta_{ij}^D = (\Delta_{i+\sigma,i} + \Delta_{i+\sigma,i} - \Delta_{i+\sigma,i} - \Delta_{i-i+\sigma})/4. \)
The averaged electron density is fixed at .0022. The calculation is performed in a very low-temperature regime for small . The local AF order may be absent around the impurity site . The net local moment is defined as 

\[ M_r = \sum_{\mu} M_{\mu} \]

where \( M_{\mu} \) represents the staggered magnetization and their distributions of the staggered magnetization and their corresponding LDOS spectra around the impurity site. 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 \( N_x \times N_y = 20 \times 20 \).

Our numerical results for a single impurity show that the local AF order may be absent around the impurity site for small \( \varepsilon \) and is present when impurity strength \( \varepsilon \) 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 \( S_z = \sum_{\mu} S_{\mu z} \). The impurity is situated at (16, 16). The DSC order parameter is induced directly by the induced staggered magnetization 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 \( \varepsilon \) versus \( U \) in Fig. 2. It is obvious that the induced net moment \( S_z = 1/2 \) should show up for larger impurity strength \( \varepsilon \) and stronger AF interaction \( U \), while \( S_z = 0 \) tends to exist for smaller \( \varepsilon \) 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.
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 $U$, $\epsilon$, 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 $M_{Sz}$ [(b),(c) and (e),(f)]. The left panels [(a)–(c)] and the right panels [(d)–(f)] are for two nn impurities and two nn impurities, respectively. Panels [(b),(c)] and [(e),(f)] correspond to $U = 2.0$ and $U = 2.4$, respectively.

![FIG. 2](Phase diagram of $\epsilon$ versus interaction strength $U$ for various phases near the impurity.)
of opposite polarities occurs when two impurities 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 $S_z \neq 1/2$, 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 non-magnetic 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.

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

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**References**