States of Local Moment Induced by Nonmagnetic Impurities in Cuprate Superconductors

Yan Chen and C. S. Ting

Texas Center for Superconductivity and Department of Physics, University of Houston, Houston, TX 77204

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. From this, the net magnetic moment induced by a single or double impurities can be obtained. 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 and the impurity scattering. When two impurities are placed at the nearest neighboring sites, the net moment is always zero. For two unitary impurities at the next nearest neighboring sites, and at sites separated by a Cu-ion site, the induced net moment has $S_z =0$, or 1/2, or 1. The consequence of these results on experiments will be discussed.

PACS numbers: 75.20.Hr, 74.25.Jb, 72.10.Fk, 71.55.-i

The nonmagnetic impurity effect in high temperature superconductors (HTS) has attracted significant interest both experimentally and theoretically for many years. The induction of 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$_{7-x}$ have indicated that nonmagnetic Zn/Li impurities, enhance antiferromagnetic correlation and staggered magnetic moment is induced on the Cu ions in the vicinity of the impurity sites [1, 2, 3, 4, 5, 6, 7]. Low-temperature scanning tunneling microscopy (STM) experiments have directly observed a sharp near zero bias resonance peak around the Zn impurity atoms on the surface of superconducting Bi$_2$Sr$_2$CaCu$_2$O$_{8+x}$ (BSCCO). Both local potential scattering [8, 9, 10, 11, 12, 13] and Kondo impurity scattering [14, 15, 16] in d-wave superconductors have been theoretically investigated. Recently Wang and Lee [17] studied the formation of the local moment near a nonmagnetic impurity in HTS using a renormalized mean field theory of the $t-J$ model. They tried to reconcile quantum interference effect among multiple impurities in HTS draws considerable attention in recent years [11, 12, 14, 21, 22, 23]. The energy dependent of the spatial distribution of LDOS spectrum changes remarkably by varying the distance and orientations among the impurities. To our knowledge, so far there exists no study considering the local moment formation due to quantum interference effect among multiple impurities in HTS. In order to study this and related problems, we apply an effective model Hamiltonian defined on a square lattice with a nearest neighboring (n.n.) interaction $V_{DSC}$ to simulate the d-wave superconductivity (DSC) and an onsite Coulomb interaction $U$ to represent the competing antiferromagnetic (AF) order. In this paper, the local magnetic moment distribution induced around a single impurity will be numerically studied first.

We show that the net moment induced around the impurity can be attributed to a local spin with $S_z=0$, or 1/2 depending on the impurity strength and the value of $U$, and we shall also present a phase diagram for the net moment formation. With multiple impurities, we expect that quantum interference effect should exhibit itself. When two impurities are placed at the n.n. sites, our numerical result indicates that the net induced moment is always zero, regardless of the value of $U$, the impurity strength, and doping. For two unitary impurities at the next n.n. sites and at sites separated by a Cu-ion site, we demonstrate that the net moment induced by them can be represented by a local spin with $S_z=0$, or 1/2, or 1 depending on the strength of the AF interaction or 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:

$$H = -\sum_{i,j,\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + \sum_{i,\sigma} (Un_{i\sigma} + \epsilon \delta_{i,m,i} - \mu)c_{i\sigma}^\dagger c_{i\sigma}$$

$$+ \sum_{i,j} (\Delta_{ij} c_{i\uparrow}^\dagger c_{j\downarrow} + h.c.),$$

(1)

where $\epsilon$ is the on-site impurity strength, $i_m$ is the impurity site, $\mu$ is the chemical potential. The hopping term includes the n.n. hopping $t$ and the next n.n. hopping $t'$. The staggered magnetization and DSC order in cuprates are defined as $M_i^z = (-1)^i \langle c_{i\uparrow}^\dagger c_{i\uparrow} - c_{i\downarrow}^\dagger c_{i\downarrow} \rangle$ 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

$$\sum_j \left( \mathcal{H}_{ij,\sigma} - \Delta_{ij} \right) = E_n \left( u_i^{n,\sigma}, \bar{v}_j^{n,\sigma} \right),$$

(2)

where the single particle Hamiltonian $\mathcal{H}_{ij,\sigma} = -t_{ij} + (Un_{i\sigma} + \epsilon \delta_{i,m,i} - \mu)\delta_{ij}$, and $n_{i\uparrow} = \sum_n |u_{i\uparrow}^n|^2 f(E_n)$, $n_{i\downarrow} = \sum_n |\bar{v}_{i\downarrow}^n|^2 (1 - f(E_n))$, $\Delta_{ij} = \frac{V_{DSC}}{4} \sum_n (u_{i\uparrow}^n \bar{v}_{j\downarrow}^{n*} + \bar{v}_{i\uparrow}^n u_{j\downarrow}^{n*})$. 

The nonmagnetic impurity effect in high temperature superconductors (HTS) has attracted significant interest both experimentally and theoretically for many years. The induction of 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$_{7-x}$ have indicated that nonmagnetic Zn/Li impurities, enhance antiferromagnetic correlation and staggered magnetic moment is induced on the Cu ions in the vicinity of the impurity sites [1, 2, 3, 4, 5, 6, 7]. Low-temperature scanning tunneling microscopy (STM) experiments have directly observed a sharp near zero bias resonance peak around the Zn impurity atoms on the surface of superconducting Bi$_2$Sr$_2$CaCu$_2$O$_{8+x}$ (BSCCO). Both local potential scattering [8, 9, 10, 11, 12, 13] and Kondo impurity scattering [14, 15, 16] in d-wave superconductors have been theoretically investigated. Recently Wang and Lee [17] studied the formation of the local moment near a nonmagnetic impurity in HTS using a renormalized mean field theory of the $t-J$ model. They tried to reconcile quantum interference effect among multiple impurities in HTS.

On the other hand, quantum interference effect among multiple impurities in HTS draws considerable attention in recent years [11, 12, 14, 21, 22, 23]. The energy dependent of the spatial distribution of LDOS spectrum changes remarkably by varying the distance and orientations among the impurities. To our knowledge, so far there exists no study considering the local moment formation due to quantum interference effect among multiple impurities in HTS. In order to study this and related problems, we apply an effective model Hamiltonian defined on a square lattice with a nearest neighboring (n.n.) interaction $V_{DSC}$ to simulate the d-wave superconductivity (DSC) and an onsite Coulomb interaction $U$ to represent the competing antiferromagnetic (AF) order. In this paper, the local magnetic moment distribution induced around a single impurity will be numerically studied first.
of the vortex lattice is chosen as large system sizes. The linear dimension of the unit cell impurity are insensitive to the boundary conditions for large system sizes. The linear dimension of the unit cell of the vortex lattice 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 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 \( \epsilon \) and is present when impurity strength \( \epsilon \) 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 \((16,16)\). Panels (a) and (b) corresponds to \( U = 2.0 \) and \( \epsilon = 3.0 \). It is clear that no AF order induction is shown for such a weak impurity. In panel (b), the resonance energy at the impurity site (black line) is less than zero while the resonance energy at the n.n. impurity site (red line) is greater than zero. The green 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 n.n. impurity site turns stronger and its peak also moves to zero energy. Panels (c) and (d) are for a strong or unitary impurity \( \epsilon = 100 \) and \( U=2.0 \). We find the induced staggered magnetization reaches a maximum value of 0.08 at the n.n. site of the impurity in Fig. 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 zero bias resonance peak at the n.n. sites is shown in panel (d), reflecting the characteristics of a unitary impurity. The presence of weak local AF order results also a rather weak splitting of resonance peak. In Figs. 1(e) and 1(f) we show the our results for \( U = 2.35 \) and \( \epsilon = 100 \). A pronounced two-dimensional SDW order is clearly induced around this unitary impurity in Fig. 1(e). The staggered magnetization at the n.n. 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 Fig. 1(d) at the n.n. site is substantially suppressed and become two weak peaks in the larger \( U \) case with \( S_z = 1/2 \) (see Fig. 1(e)).

To examine the local moment formation, we present the phase diagram of \( \epsilon \) versus \( U \) in Fig. 2. It is obvious that the induced net moment \( S_z = 1/2 \) should show up for larger impurity strength \( \epsilon \) and stronger AF interaction \( U \), while \( S_z = 0 \) tends to exist for smaller \( \epsilon \) or weaker \( U \). In fact, there exist three phase regimes depending on the magnitude of \( U \) 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)). In both cases the net induced magnetic moment corresponds to a local spin with \( S_z = 0 \). For larger \( U \), a pronounced SDW order is induced (see Fig. 1(e)) and the net moment becomes \( S_z = 1/2 \) (local moment phase). In the nonmagnetic phase regime and for a unitary impurity, there is a sharp zero bias resonance peak in the LDOS without any splitting [9]. The splitting is gradually showing up in the AF fluctuation phase 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 AF fluctuation phase regime discussed here is absent in Ref. [17]. The staggered magnetization distribution around a unitary impurity like Zn obtained in this paper is in agreement with the results derived from the NMR experiments [1, 2, 3, 4, 5, 6]. The critical value of the \( U \) for inducing \( S_z = 1/2 \) is doping dependent. The underdoped case

\[ v_{ij} u_{ji} \tanh \left( \frac{E_{Fj}}{2k_B T} \right), \] with \( f(E) \) as the Fermi distribution function. The DSC order parameter at the \( i \)th site is \( \Delta^D = (\Delta_{i+e_x,i} + \Delta_{i-e_x,i} - \Delta_{i+e_y,i} - \Delta_{i-e_y,i})/4 \) where \( e_{x,y} \) denotes the unit vector along \((x, y)\) direction. Various doping concentrations can be tuned by varying the chemical potential. In the present calculation, we set the lattice constant \( a \) and hopping integral \( t \) as units, \( t' = -0.2 \) and \( V_{DSC} = 1.0 \). Due to the localized nature of the impurity states, the order parameters around the lattice constant \( 0 \) are insensitive to the boundary conditions for large system sizes. The linear dimension of the unit cell of the vortex lattice 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 very low temperature regime. The supercell techniques are employed to calculate the LDOS. The number of the unit cells is \( M_x \times M_y = 20 \times 20 \). 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 AF fluctuation phase regime discussed here is absent in Ref. [17]. The staggered magnetization distribution around a unitary impurity like Zn obtained in this paper is in agreement with the results derived from the NMR experiments [1, 2, 3, 4, 5, 6]. The critical value of the \( U \) for inducing \( S_z = 1/2 \) is doping dependent. The underdoped case
corresponds to smaller $U_c$. The $S_z = 1/2$ moment due to a unitary impurity is much easier to be induced in an underdoped sample than in optimally and overdoped samples, because the amplitude of the induced AF order becomes increasingly stronger as the hole doping is decreased. Since the existence of inhomogeneity in the HTS sample has been experimentally confirmed [24, 25], we also predict that the strong zero-bias-peak would be smaller than the number of unitary impurities as a result, the number of induced HTS sample has been experimentally confirmed [24, 25], since the existence of inhomogeneity in the HTS sample has been experimentally confirmed [24, 25], we also predict that the strong zero-bias-peak would be smaller than the number of unitary impurities like Zn. We also predict that the strong zero-bias-peak observed by Pan et al. at the Zn impurity site should be associated with $S_z = 0$ 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 unitary impurities. When they are placed at the n.n. 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 $U=2.2$ 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). Although it appears that the staggered magnetizations due to the two n.n. impurities have exact cancellation, their influence on the LDOS is still apparent and the result will not be present here. With $U=2.4$ and no impurities, one can numerically demonstrate that the staggered magnetization has a stripe like structure [26] with periodicity $8 \sigma$ which coexists with the DSC. The presence of the impurities could pin the stripes but does not modify the overall stripe-like 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 $U$, impurity strength $\epsilon$, and doping. For two unitary impurities placed at the next n.n. 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 stripe like 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 unitary impurities at sites separated by a Cu ion (see Fig. 4(a)). The distributions of the staggered magnetizations are shown in Figs. 4(b), 4(c) and 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 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 further 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 $S_z = 0$, or 1/2 or 1. In other words, quantum phase transitions may occur among different local moment phases by varying $U$ values or doping. The detailed study of various configurations of the impurities on the local moment formation and LDOS spectra will be presented as a future work.

In summary, we have investigated the induction of the local moment by a 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. The LDOS has been calculated for a single impurity. We show that the zero bias resonant peak obtained next to the unitary 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\cite{25}, 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 net magnetic moment around two n.n. 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 where the AF strength is appreciable. We demonstrate that net magnetic moment around two unitary impurities placed at the next n.n. sites and sites separated by a Cu ion could be either 0, 1/2 or 1 depending on the value of $U$. It is our hope that the present investigation on the local moment formation may provide useful information for future experimental test.

We are grateful to Profs. T.K. Lee, S.H. Pan, Z.Q. Wang, G.-q. Zheng and Dr. J. X. Zhu for useful discussions. This work was supported by the Robert A. Welch Foundation, by the Texas Center for Superconductivity at the University of Houston through the State of Texas.

\begin{thebibliography}{99}
\bibitem{1} H. Alloul \textit{et al.}, Phys. Rev. Lett. \textbf{67}, 3140 (1991).
\bibitem{2} A.V. Mahajan \textit{et al.}, Phys. Rev. Lett. \textbf{72}, 3100 (1994); Eur. Phys. J. B \textbf{13}, 457 (2000).
\bibitem{3} J. Bobroff \textit{et al.}, Phys. Rev. Lett. \textbf{83}, 4381 (1999).
\bibitem{4} R. Kili\c{s}an, S. Krivenko, G. Khalilulin, and P. Fulde, Phys. Rev. B \textbf{59}, 14432 (1999).
\bibitem{5} W.A. MacFarlane \textit{et al.}, Phys. Rev. Lett. \textbf{85}, 1108 (2000).
\bibitem{6} M.-H. Julien \textit{et al.}, Phys. Rev. Lett. \textbf{84}, 3422 (2000).
\bibitem{7} J. Bobroff \textit{et al.}, Phys. Rev. Lett. \textbf{86}, 4116 (2001).
\bibitem{8} S.H. Pan \textit{et al.}, Nature \textbf{403}, 746 (2000).
\bibitem{9} M.I. Salkola, A.V. Balatsky, and D.J. Scalapino, Phys. Rev. Lett. \textbf{77}, 1841 (1996).
\bibitem{10} Jian-Xin Zhu, C.S. Ting, and C.R. Hu, Phys. Rev. B \textbf{61}, 8667 (2000).
\bibitem{11} M.E. Flatté, Phys. Rev. B \textbf{61}, 14920 (2000).
\bibitem{12} H. Tsuchiura, Y. Tanaka, M. Ogata, and S. Kashiwaya, Phys. Rev. B \textbf{64}, 140501 (2001).
\bibitem{13} Jian-Xin Zhu, Ivar Martin, and A.R. Bishop, Phys. Rev. Lett \textbf{89}, 067003 (2002).
\bibitem{14} Jian-Xin Zhu and C.S. Ting, Phys. Rev. B \textbf{63}, 020506(R) (2001); Phys. Rev. B \textbf{64}, 060501(R) (2001).
\bibitem{15} A. Polkovnikov, S. Sachdev, and M. Vojta, Phys. Rev. Lett. \textbf{86}, 296 (2001).
\bibitem{16} Xi Dai and Ziqiang Wang, cond-mat/0205498.
\bibitem{17} Ziqiang Wang and P.A. Lee, Phys. Rev. Lett. \textbf{89}, 217002 (2002).
\bibitem{18} M.E. Flatte and D.E. Reynolds, Phys. Rev. B \textbf{61}, 14810 (2000).
\bibitem{19} D.K. Morr and N. Stavropoulos, Phys. Rev. B \textbf{66}, 140508(R) (2002); Phys. Rev. B \textbf{67}, 020502(R) (2003).
\bibitem{20} D.K. Morr, and A.V. Balatsky, Phys. Rev. Lett. \textbf{90},
\end{thebibliography}
[21] Linyin Zhu, W.A. Atkinson, and P.J. Hirschfeld, Phys. Rev. B 67, 094508 (2003).
[22] B.M. Andersen, and P. Hegegard, cond-mat/0301225.
[23] W.A. Atkinson, P.J. Hirschfeld, and Linyin Zhu, cond-mat/0301630.

[24] S.H. Pan et al., Nature 413, 282 (2001).
[25] K.M. Lang et. al., Nature 415, 412 (2002); E. Hudson, Bull. Am. Phys. Soc. 47 (2), 1093 (2003) [March].
[26] Yan Chen, H.Y. Chen, and C.S. Ting, Phys. Rev. B 66, 104501 (2002).