Tunable striped-patterns by lattice anisotropy and magnetic impurities in d-wave superconductors

Xian-Jun Zuo\textsuperscript{1}$^\star$, Yuan Zhou\textsuperscript{1}, and Chang-De Gong\textsuperscript{2,1}

\textsuperscript{1}National Laboratory of Solid State Microstructures and Department of Physics, Nanjing University, Nanjing 210093, People’s Republic of China
\textsuperscript{2}Center for Statistical and Theoretical Condensed Matter Physics, Zhejiang Normal University, Jinhua 321004, People’s Republic of China

(Dated: May 25, 2010)

Abstract

The pattern transition induced by lattice anisotropy (LA) and magnetic impurities is computationally observed in near-optimally doped d-wave superconductors (DSCs). For the single impurity case, a transition from the checkerboard to stripe pattern can be induced even with a very weak LA. Moreover, the modulation period of eight lattice constants ($8a$) in the spin order coincides with neutron scattering data. For the two-impurity case, an orientation transition from the longitudinal impurity-pinned stripe into the transverse pattern is observed when the LA ratio reaches some critical value. At the critical point, it is found that the structures around magnetic impurities could restore checkerboard patterns. These results indicate that the formation of stripes in DSCs might induced by various effects, and could be tunable experimentally.

PACS numbers: 74.20.-z, 74.62.Dh, 74.25.Jb

\textsuperscript{$\star$}xjzuo@yahoo.com.cn
The inhomogeneous phases in unconventional superconductors have attracted much attention recently. Various experiments reported the presence of stripe or checkerboard modulations in copper oxide-based compounds [1–12]. Neutron scattering (NS) measurements on cuprates such as La$_{2-x-y}$Nd$_y$Sr$_x$CuO$_4$ (LNSCO), La$_{2-x}$Sr$_x$CuO$_4$ (LSCO), La$_{2-x}$Ba$_x$CuO (LBCO), and Y-Ba-Cu-O (YBCO) family indicated the existence of incommensurate magnetic peaks, which has led to discussions of the existence of a stripe phase [1–3]. Several scanning tunneling microscopy (STM) experiments observed checkerboard-like charge-density wave (CDW) modulations with a period of roughly four lattice constants ($4\alpha$). Experimentally, both dispersive [5] and non-dispersive [6–8] modulated patterns have been observed in cuprates. The corresponding patterns were proposed to be understood in terms of quasiparticle interference (QPI) [13, 14], or in terms of static or fluctuating stripes [15], respectively. Currently, the issue of the nature of these modulated patterns is still under debate.

It is known that lattice anisotropy (LA) are ubiquitous in various cuprates. For instance, strong a-b axis asymmetry of both the normal and superconducting state electronic properties have been observed in the YBCO family [16–18]. Up to now, the relationship among lattice distortions, incommensurability and stripes has been intensively studied in cuprates [19–26]. Based on the anisotropic Hubbard ($t_x \neq t_y$) and $t_x - t_y - J_x - J_y$ models, Normand and Kampf et al. considered LA as a possible origin of the stripe formation in the cuprate superconductors [19]. Moreover, Becca et al. have shown that stripes and spin incommensurabilities are favored by LA [22]. In this work, we explore the effect of LA on the patterns around magnetic impurities in d-wave superconductors (DSCs). Including the competition and coexistence among the DSC, spin, and charge orders, we study the system by self-consistently solving the Bogoliubov - de Gennes (BdG) equations based on an anisotropic Hubbard-type model.

We start from the two dimensional $t_x - t_y - t' - U - V$ model, which consists of two parts, $H = H_0 + H_{imp}$. The Hamiltonian $H_0$ and $H_{imp}$ describe the superconductor and magnetic impurities, respectively, which is given by

$$H_0 = -\sum_{ij\sigma} t_{ij} (c_{i\sigma}^\dagger c_{j\sigma} + H.c.) + \sum_{ij} (\Delta_{ij} c_{i\uparrow}^\dagger c_{j\downarrow} + H.c.) + \sum_{i\sigma} (Un_{i,\sigma} - \mu) c_{i\sigma}^\dagger c_{i\sigma},$$

$$H_{imp} = \sum_{i}h_{eff}(i)(c_{i\uparrow}^\dagger c_{i\uparrow} - c_{i\downarrow}^\dagger c_{i\downarrow}),$$

(1)
Here $c_{i\sigma}$ annihilates an electron of spin $\sigma$ at the $i$th site. The hopping integral $t_{ij}$ takes $t_x$ or $t_y$ between nearest neighbor (NN) pairs along $x$ or $y$ direction, and $t'$ between next-nearest neighbor (NNN) pairs. $U$ is the on-site Coulomb repulsion interaction. $\mu$ is the chemical potential, which is determined self-consistently in the calculation. The local effective field $h_{\text{eff}}(i)$ is introduced to model the exchange coupling between conducting electrons and the impurity spin, where we have treated the impurity spin as a Ising-like one. Some similar model had been employed to study the effects of magnetic impurities on cuprate superconductors, which can qualitatively explain the observed impurity states well. Therefore, we employed the above model in this work. Experimentally, the ratio of the lattice constants along $x$ and $y$ directions is $b/a \sim 1.01$ (Ref. [30]), thus the corresponding effective hopping integrals $t_x$ and $t_y$ are also anisotropic. According to the local-density approximation band calculation, the ratio of hopping integrals is estimated as $t_x/t_y \sim (b/a)^4 \sim 1.04$. In this work, we consider effects of LA on the patterns around magnetic impurities by tuning the ratio $\eta = t_y/t_x$, which is near the above estimated value, as shown below. The self-consistent mean-field parameters are given by $n_i = \sum_{\sigma} < c_{i\sigma}^\dagger c_{i\sigma} >$, the magnetization $m_i = (1/2)(< c_{i\uparrow}^\dagger c_{i\uparrow} > - < c_{i\downarrow}^\dagger c_{i\downarrow} >)$, and the DSC order parameter $\Delta_{ij} = (V/2) < c_{i\uparrow} c_{j\downarrow} - c_{i\downarrow} c_{j\uparrow} >$ with $V$ the phenomenological pairing interaction.

The Hamiltonian $H$ can be diagonalized by solving the following BdG equations,

$$
\begin{pmatrix}
H_{ij,\uparrow} & \Delta_{ij} \\
\Delta_{ij}^* & -H_{ij,\downarrow}^*
\end{pmatrix}
\Psi_j = E \Psi_i,
$$

where the quasiparticle wave function $\Psi_i = (u_{i\uparrow}, v_{i\downarrow})^T$. The spin-dependent single-particle Hamiltonian reads $H_{ij\sigma} = -t_x \delta_{i+x,j} - t_y \delta_{i+y,j} - t' \delta_{i+x',j} + [\sum_{i_m} \sigma h_{\text{eff}}(i) \delta_{i,i_m} + U n_{i,\sigma} - \mu] \delta_{ij}$. Here the subscripts $\hat{x}$ and $\hat{y}$ denote the unit vector directing along $x$- or $y$-direction NN bonds. $\tau'$ denotes the unit vector directing along four NNN bonds, and $i_m$ is the position of the impurity site. The self-consistent parameters are given by $n_{i\uparrow} = \sum_n |u_{i\uparrow}^n|^2 f(E_n)$, $n_{i\downarrow} = \sum_n |v_{i\downarrow}^n|^2 [1 - f(E_n)]$, and $\Delta_{ij} = \sum_n [u_{i\uparrow}^n v_{j\downarrow}^{n*} + v_{i\downarrow}^n u_{j\uparrow}^{n*}] \tanh(\beta E_n/2)$, where $f(E) = 1/(1 + e^{\beta E})$ is the Fermi-Dirac distribution function. Hereafter, the length is measured in units of the lattice constant $a$, and the energy in units of $t = t_x$. The pairing interaction is chosen as $V = 1.0$ to guarantee that the superconducting order $\Delta_0 \simeq 0.08t$, comparable with the observed $T_c$ in cuprate superconductors. The on-site Coulomb repulsion $U$ takes value $2.44$, which is the effective value near optimal doping in the hubbard-type model. We study LA effect on the patterns around impurities in DSCs near optimal doping with the filling factor.
\[ n_f = \sum_{i\sigma} c_{i\sigma}^\dagger c_{i\sigma} / (N_x N_y) = 0.85 \] (i.e., the hole doping \( x = 0.15 \)), where \( N_x, N_y \) are the linear dimension of the unit cell. The BdG equations are solved self-consistently for a square lattice of \( 24 \times 24 \) sites, and the periodic boundary conditions are adopted. The numerical calculation is performed at a very low temperature, \( T = 10^{-5} \)K, to extract the low-energy physics. The local effective field is taken to be \( h_{\text{eff}} \) at the impurity site and zero otherwise. The DSC order parameter at the \( i \)th site is defined as \( \Delta_i = (\Delta_{i,i+e_x} + \Delta_{i,i-e_x} - \Delta_{i,i+e_y} - \Delta_{i,i-e_y})/4 \), and the spin order parameter is \( M_i = (-1)^i m_i \).

In FIG. 1, we plot the spatial distributions of the DSC, spin, and charge orders around the impurity site. As one can see [FIG. 1(a), (c), and (e)], all the three orders exhibit checkerboard modulations around the magnetic impurity. Similar to the nonmagnetic impurity case, a SDW with a period of \( 8a \) checkerboard pattern is observed around the magnetic impurity, which is in agreement with the NS experiment [4]. However, one notes that the checkerboard pattern of the DSC order can also be induced by the magnetic impurity, and a weak associated CDW pattern is observed, which is different from the nonmagnetic impurity case [13]. Moreover, the modulated DSC and CDW orders share the same periodicity \( 4a \). On the whole, the DSC order has a local minimum at the impurity site while the amplitudes of the CDW and SDW orders reach global maxima. This is the common feature of orders around the magnetic impurity despite various parameters. Therefore, in view of these features, we clearly see the relationship of competition and coexistence between antiferromagnetic and DSC orderings.

Figure 1: (color online) The surface plots of orders around the magnetic impurity on a unit cell of size \( 24 \times 24 \) sites with and without lattice anisotropy. (a), (c), and (e) are the spatial distributions of the DSC, spin and charge orders without LA. (b), (d), and (f) are the same plots but the lattice anisotropy ratio \( \eta = t_y/t_x = 0.99 \). Here we take \( U = 2.44, x = 0.15, t' = -0.25, \) and \( h_{\text{eff}} = 3 \).
Below we discuss the effect of LA on the pattern around a single impurity [See Fig. 1 (b), (d), and (f)]. As one can see, a symmetry-broken transition from the checkerboard to stripe pattern is induced. In this case, even if there is a very weak LA, this transition takes place. The reason lies in the fact that LA $t_y < t_x$ breaks the symmetry of the system, which leads to the formation of stripes along $y$ direction favorable. Therefore, we see that LA is favorable to the formation of stripes in DSCs. In addition, one notes that the anisotropy-induced SDW stripes also show a modulation with periodicity $8a$, which coexists with the DSC order. This indicates that the $8a$ modulations appearing in the SDW order is a robust feature in spite of different parameters. This conclusion is consistent with our previous study [28].

Now let us turn to consider the two-impurity case. Without LA, an $x$-orientated stripe structure can be induced due to the pinning effect of the magnetic impurities which have been placed along $x$ direction [Not shown but similar to FIG. 2 (a), (c), and (e)]. Similar to the single impurity case, the impurity-pinned SDW stripe also show a modulation with periodicity $8a$, while the coexisting DSC and CDW stripes share the same periodicity $4a$. For the case of two magnetic impurities with LA present, one could expect that the impurity-pinned effect would compete with LA effect, leading to orientation transition from the longitudinal ($x$ direction) impurity-pinned stripe into the transverse ($y$ direction) pattern when the LA ratio reaches some critical value. This speculation is confirmed by the following calculations, and the critical value is found to be $\eta^* \sim 0.982$, which is close to the above estimated value $t_y/t_x \sim (b/a)^{-4} \sim 0.9615$.

Accordingly, the ratio of lattice constants is estimated as $b/a \sim 1.005$. Thus, we see that only a weak LA is needed to observe this pattern transition in the disorder-pinned stripe

Figure 2: (color online) The surface plots of orders around two magnetic impurities in the presence of LA. (a), (c), and (e) are plots in the case with $\eta = 0.983$, while (b), (d), and (f) with $\eta = 0.981$. 
phase in DSCs experimentally. If adopting the estimated value by Normand and Kampf or by Citro and Marinaro \[19, 33\], one gets \(\eta = \frac{t_y}{t_x} = |\cos(\pi - 2\Phi)| \sim 0.9848\), with an angular distortion angle \(\Phi = 5^\circ\). As shown in FIG. 2 (a), (c) and (e), when the LA ratio is larger than the critical value (a weak anisotropy), \(\eta = 0.983 > \eta^*\), the x-orientated stripe structure is still stable. This case is very similar to the case without LA, except that the modulation amplitudes are slightly larger than those in the latter case. However, for the relatively strong anisotropy with \(\eta = 0.981 < \eta^*\), the orientation transition from x-stripe to y-stripe pattern takes place, as shown in FIG. 2 (b), (d), and (f). Clearly, in this case, LA effect dominates over the impurity pinning effect, and the y-stripe pattern is energetically more favorable. Also, as shown by all those stripe plots, the checkerboard-like modulations are still visible, especially in the DSC and SDW orders, which originate from the effect of QPI. Thus, we see that one can produce different modulated patterns by inserting magnetic impurities or tuning the LA in DSCs while the modulation periodicity holds the same.

For comparison, we also consider the cases with various strength of effective field, \(h_{\text{eff}} = 1\) or 10, and with a long distance between the two impurities. In these cases, we obtain similar results, and reach the same conclusion as discussed above, except that the critical value \(\eta^*\) changes more or less. For the cases with \(h_{\text{eff}} = 1\) and with a 8\(a\) distance between the two impurities, we happen to get the exact critical values of the LA ratio, i.e., \(\eta^* = 0.984\) and 0.998, which are both larger than the previous case with \(h_{\text{eff}} = 3\). Meanwhile, for the case with \(h_{\text{eff}} = 10\), the corresponding critical values is found to be \(\eta^* \sim 0.981\), which is smaller than the above cases. The reason lies in the fact that for a weaker effective field or a longer distance, the impurity pinning effect is reduced, while an opposite tendency is produced by a stronger effective field.

At the exact critical value of the LA, it is found that the structures around magnetic impurities restore checkerboard patterns because the competition between the impurity pinning effect and LA reaches the balance point, as shown in FIG. 3. In this case, it seems that the two impurities could induce their own checkerboard patterns independently, without interference with each other. These results indicate that one could observe the stripe-checkerboard-stripe transition under some conditions by tuning \(\eta\) in impurity-substituted DSCs.

In summary, we have studied the effect of LA on the patterns around magnetic impurities based on the \(t_x - t_y - t' - U - V\) model. It is demonstrated that LA could induce pattern
transition around impurities in near-optimally doped DSCs. In the single impurity case, it is found that even a very weak LA could induce a transition from the checkerboard to stripe pattern, because the symmetry of the system is broken. Modulated SDW pattern with $8a$ periodicity is observed, which coincides with the NS data. Meanwhile, the modulated DSC and CDW orders share the same periodicity $4a$. For the two-impurity case, a transition from the $x$-direction impurity-pinned stripe into the $y$-direction stripe pattern is observed as the LA ratio reaches the critical value $\eta^*$. At the exact critical values, it is found that the structures around magnetic impurities could restore checkerboard patterns. It is expected that these phenomena could be observed in the STM and NS experiments on DSCs under varying pressure or temperature.

This work is supported by the National Nature Science Foundation of China (Grants No. 10904063 and No. 10804047). CDG would also like to thank the 973 Project (Project No. 2006CB601002).

[1] J. M. Tranquada, B. J. Sternlieb, J. D. Axe, Y. Nakamura, and S. Uchida, Nature (London) 375, 561 (1995).
[2] H. A. Mook, Pengcheng Dai, F. Dogan, and R. D. Hunt, Nature 404, 729 (2000).
[3] M. Fujita, H. Goka, K. Yamada, J. M. Tranquada, and L.-P. Regnault, Phys. Rev. B 70,
[4] B. Lake, G. Aeppli, K. N. Clausen, D. F. McMorrow, K. Lefmann, N. E. Hussey, N. Mangkorntong, M. Nohara, H. Takagi, T. E. Mason, and A. Schroder, Science 291, 1759 (2001).

[5] J. E. Hoffman, E. W. Hudson, K. M. Lang, V. Madhavan, H. Eisaki, S. Uchida, and J. C. Davis, Science 295, 466 (2002).

[6] C. Howald, H. Eisaki, N. Kaneko, M. Greven, and A. Kapitulnik, Phys. Rev. B 67, 014533 (2003).

[7] M. Vershinin, S. Misra, S. Ono, Y. Abe, Y. Ando, and A. Yazdani, Science 303, 1995 (2004).

[8] T. Hanaguri, C. Lupien, Y. Kohsaka, D. H. Lee, M. Azuma, M. Takano, H. Takagi, and J. C. Davis, Nature (London) 430, 1001 (2004).

[9] K. McElroy, R. W. Simmonds, J. E. Hoffman, D.-H. Lee, J. Orenstein, H. Eisaki, S. Uchida, and J. C. Davis, Nature 422, 592 (2003).

[10] Y. Kohsaka, C. Taylor, P. Wahl, A. Schmidt, Jhinhwan Lee, K. Fujita, J. W. Alldredge, K. McElroy, Jinho Lee, H. Eisaki, S. Uchida, D.-H. Lee and J. C. Davis, Nature 454, 1072 (2008).

[11] B. Khaykovich, Y. S. Lee, R. Erwin, S.-H. Lee, S. Wakimoto, K. J. Thomas, M. A. Kastner and R. J. Birgeneau, Phys. Rev. B 66, 014528 (2002).

[12] J. F. Ding, H. Liu, X. H. Huang, Y. W. Yin, Q. X. Yu, and X. G. Li, Appl. Phys. Lett. 94, 142508, (2009).

[13] Jian-Xin Zhu, Ivar Martin, and A. R. Bishop, Phys. Rev. Lett. 89, 067003 (2002); Yan Chen and C. S. Ting, Phys. Rev. Lett. 92, 077203 (2004).

[14] Q.-H. Wang, and D.-H. Lee, Phys. Rev. B 67, 020511 (2003).

[15] S. A. Kivelson, I. P. Bindloss, E. Fradkin, V. Oganesyan, J. M. Tranquada, A. Kapitulnik, and C. Howald, Rev. Mod. Phys. 75, 1201 (2003), and reference therein.

[16] D. N. Basov, R. Liang, D. A. Bonn, W. N. Hardy, B. Dabrowski, M. Quijada, D. B. Tanner, J. P. Rice, D. M. Ginsberg, and T. Timusk, Phys. Rev. Lett. 74, 598 (1995).

[17] D. H. Lu, D. L. Feng, N. P. Armitage, K. M. Shen, A. Damascelli, C. Kim, F. Ronning, Z. X. Shen, D. A. Bonn, R. Liang, W. N. Hardy, A. I. Rykov, and S. Tajima, Phys. Rev. Lett. 86, 4370 (2001).

[18] Takeshi Kondo, R. Khasanov, Y. Sassa, A. Bendounan, S. Pailhes, J. Chang, J. Mesot, H. Keller, N. D. Zhigadlo, M. Shi, Z. Bukowski, J. Karpinski, and A. Kaminski, Phys. Rev. B 80, 100505(R) (2009).
[19] B. Normand and A. P. Kampf, Phys. Rev. B 64, 024521 (2001); A. P. Kampf, D. J. Scalapino, and S. R. White, Phys. Rev. B 64, 052509 (2001).
[20] Kai-Yu Yang, Wei-Qiang Chen, T. M. Rice, and Fu-Chun Zhang, Phys. Rev. B 80, 174505 (2009).
[21] V. J. Emery, S. A. Kivelson, and J. M. Tranquada, Proc. Natl. Acad. Sci. U.S.A. 96, 8814 (1999).
[22] Federico Becca, Luca Capriotti, and Sandro Sorella, Phys. Rev. Lett. 87, 167005 (2001).
[23] M. Arai, T. Nishijima, Y. Endoh, T. Egami, S. Tajima, K. Tomimoto, Y. Shiohara, M. Takahashi, A. Garrett, and S. M. Bennington, Phy. Rev. Lett. 83, 608 (1999).
[24] X.-S. Ye and J.-X. Li, Phys. Rev. B 76, 174503 (2007); T. Zhou and Jian-Xin Li, Phys. Rev. B 69, 224514 (2004).
[25] I. Eremin and D. Manske, Phys. Rev. Lett. 94, 067006 (2005); 96, 059902(E) (2006).
[26] V. Hinkov, D. Haug, B. Fauqué, P. Bourges, Y. Sidis, A. Ivanov, C. Bernhard, C. T. Lin, and B. Keimer, Science 319, 597 (2008).
[27] A. V. Balatsky, I. Vekhter, and J. X. Zhu, Rev. Mod. Phys. 78, 373 (2006), and reference therein.
[28] Xian-Jun Zuo, Jin An, and Chang-De Gong, Phys. Rev. B 77, 212508 (2008); Xian-Jun Zuo, Chang-De Gong, and Yuan Zhou, (unpublished).
[29] E. W. Hudson, K. M. Lang, V. Madhavan, S. H. Pan, H. Eisaki, S. Uchida, and J. C. Davis, Nature (London) 411, 920 (2001).
[30] J. D. Jorgensen, B. W. Veal, A. P. Paulikas, L. J. Nowicki, G. W. Crabtree, H. Claus, and W. K. Kwok, Phys. Rev. B 41, 1863 (1990).
[31] O. K. Andersen, A. I. Liechtenstein, O. Jepsen, and F. Paulsen, J. Phys. Chem. Solids 56, 1573 (1995).
[32] C. Kusko, R. S. Markiewicz, M. Lindroos, and A. Bansil, Phys. Rev. B 66, 140513 (2002); Yuan Zhou, Hai-Qing Lin, and Chang-De Gong (unpublished).
[33] R. Citro and M. Marinaro, Physica C 408-410, 449 (2004), and reference therein.