Local density of states in a \textit{d}-wave superconductor with stripe-like modulations and a strong impurity

Hong-Yi Chen and C. S. Ting

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

Using an effective Hamiltonian with \textit{d}-wave superconductivity (dSC) and competing antiferromagnetic (AF) interactions, we show that weak and one-dimensionally modulated dSC, spin density wave (SDW) and charge density wave (CDW) could coexist in the ground state configuration. With proper parameters, the SDW order exhibits a period of 8a, while for dSC and CDW orders the period is 4a. The local density of states (LDOS), which probing the behavior of quasiparticle excitations, is found to have the identical stripe-like structure as those in dSC and CDW orders. The LDOS as a function of the bias voltage are showing two small bumps within the superconducting coherence peaks, a signature of the presence of stripes. When a strong impurity like Zn is placed in such a system, the LDOS at its nearest neighboring sites are suppressed at the zero bias by the local AF order and show a double-peak structure.

PACS numbers:

Many of the anomalous properties of high-$T_c$ superconductors (HTS) are believed to be related to the competition between the \textit{d}-wave superconductivity (dSC) and the hidden antiferromagnetic (AF) order, particularly in the underdoped HTS. Inelastic neutron scattering (INS) studies of the magnetic fluctuations in some of the HTS samples have provided important clues to the nature of the electronic correlations within the doped CuO$_2$ planes. In additon, the existence of one-dimensional charge density wave (CDW) and spin density wave (SDW) has also been reported on La$_{1.6-x}$Nd$_{0.4}$Sr$_x$CuO$_{4}$ and YBa$_2$Cu$_3$O$_{6.35}$-$\delta$. The elastic neutron scattering measurements on La$_{2-x}$Sr$_x$CuO$_4$ with $x=0.10$ sample by Lake et al. found that the signal got enhanced at $(\frac{1}{4}, \frac{1}{4} + \delta)(\frac{1}{2}, \frac{1}{2})$ at low temperature, indicating the presence of static AF order at least in some parts of the sample. The coexistence of the CDW and dSC in HTS in the absence of a magnetic field has attracted a lot of theoretical works. Recent progress in scanning tunneling microscopy (STM) on the surface of Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ (BSCCO) has given us a high resolution probe of its electronic correlations. The STM imaging by Hoffman et al., in the presence of a magnetic field revealed the quasiparticle states around the vortex cores in slightly overdoped BSCCO to exhibit a CDW of “checkerboard” pattern with 4a periodicity. Howald et al. reported that the four unit-lattice periodic charge modulation survives even at zero magnetic field and is energy independent. And it has been attributed to the superposition of stripe phases oriented along $x$- and $y$- directions in the sample. This issue has also been examined by several theoretical articles in the presence of a magnetic field, and in the absence of a magnetic field.

In case a stripe phase indeed exists in some of the HTS samples close to optimal doping as reported in the experiments, it should have important impact on the physics of HTS. We need to understand the origin of the stripe-like modulation observed in the local density of states (LDOS) and to examine its consequence on other experimentally measurable quantities, such as the LDOS near a unitary impurity in the absence of a magnetic field. In view of neutron scattering experiments mentioned above, we assume that the stripe phase observed in the STM experiments is originated in the competing AF interaction. In this paper and based upon a model Hamiltonian, we first construct a superconducting phase for a nearly optimal-doped or slightly underdoped HTS sample in which the dSC coexists with the SDW, and CDW orders. The parameters will be chosen in such a way that the dSC and CDW will have a weak one-dimensional modulation with period 4a while the period for the SDW is 8a. The superposition of the $x$- and $y$- oriented CDW stripes should yield the experimentally observed checkerboard patterns. Then we calculate the LDOS of the stripes and compare it with the pure \textit{d}-wave case. On the other hand, the low temperature STM experiments observed a sharp resonance peak near the zero bias at a nonmagnetic unitary impurity site, consistent with prediction for a pure dSC. In the presence of the stripe phase, we found that the LDOS is strongly suppressed by the AF order at the zero bias and a double-peak shows up. Hopefully, the obtained result could be used to compare with future STM experiments for samples with magnetic originated stripes.

Based on a square lattice with lattice constant $a(=1)$, we start from the effective mean-field Hamiltonian with $g$ as the nearest neighbor attractive \textit{d}-wave pairing potential, and $U$ as the on-site Coulomb interaction representing the competing AF order.

\begin{equation}
H = - \sum_{ij \sigma} t_{ij} c_{i \sigma}^\dagger c_{j \sigma} + \sum_{ij} (\Delta_{ij} c_{i \uparrow}^\dagger c_{j \downarrow} + \Delta_{ij}^* c_{i \downarrow} c_{j \uparrow}) + \sum_i (n_{i \sigma} - \mu + V_i) c_{i \sigma}^\dagger c_{i \sigma} \tag{1}
\end{equation}

where $t_{ij}$ is the hopping integral, $\Delta_{ij} = \frac{3}{2}(c_{i \uparrow} c_{j \downarrow} - c_{i \downarrow} c_{j \uparrow})$ is the spin-singlet \textit{d}-wave bond order parameter, $m_{i \sigma} = U \langle n_{i \sigma} \rangle$ is the AF order parameter, $\mu$ is the chemical
potential. In addition there is also a nonmagnetic impurity with $V_i = V_0 δ_{i0}$ as the single-site scattering potential at site $(0, 0)$. We shall diagonalize the above Hamiltonian by using Bogoliubov transformation, $c_i = \sum_n [u_{i\sigma} \gamma_n \sigma - \sigma v_{i\sigma}^n \gamma_n \sigma]$, and the equations of motion for $c_{1\sigma}$ and $c_{1\sigma}^\dagger$ will lead to usual Bogoliubov-de Gennes’ equations (BdG),

$$\sum_j \begin{pmatrix} \mathcal{H}_{ij} & \Delta_{ij} \end{pmatrix} \begin{pmatrix} u_{ij}^n \cr \bar{u}_{ij}^n \end{pmatrix} = E_n \begin{pmatrix} u_{ij}^n \cr \bar{u}_{ij}^n \end{pmatrix},$$

(2)

where $\mathcal{H}_{ij} = -t\hat{e}_{i+j} + (m_\sigma - \mu)δ_{ij} + V_0δ_{ij}$. The subscript $\hat{e}$ are the vectors $\hat{x}$, $\hat{y}$ and $\hat{x} + \hat{y}$ toward the nearest neighbor (NN) and next-nearest neighbor (NNN) sites, respectively. To self-consistently solve BdG equations we could get the $N$ positive eigenvalues $E_n$ ($n = 1 \cdots N$) and the $N$ negative eigenvalues $\bar{E}_n$ with corresponding eigenvectors $(u_{i1}^n, v_{i1}^n)$ and $(-\bar{v}_{i1}^n, u_{i1}^n)$, respectively. Using the following convenient notation $\bar{u}_{i1}^n = (-\bar{v}_{i1}^n, u_{i1}^n)$ and $\bar{v}_{i1}^n = (\bar{v}_{i1}^n, u_{i1}^n)$, the self-consistent conditions become,

$$\langle n_{1\uparrow} \rangle = \frac{2N}{\sum_{n=1}^{2N} \left| \bar{u}_{i1}^n \right|^2 f(E_n)}$$

$$\Delta_{ij} = \frac{2N}{\sum_{n=1}^{2N} \frac{g}{4} (\bar{v}_{i1}^n \bar{v}_{j1}^n + u_{i1}^n u_{j1}^n) \tanh(\frac{\beta E_n}{2})},$$

(3)

where $f(E) = 1/(e^{\beta E} + 1)$ is Fermi distribution function.

Since the calculation will be performed near the optimal-doped or slightly underdoped regime, we choose the filling factor, which is defined as $n_f = \sum_\sigma \langle c_{i\sigma}^\dagger c_{i\sigma} \rangle / N_x N_y$ with the summation over one unit cell, is fixed to be 0.85 (i.e. the hole doping $x_h = 0.15$), where $N_x$, $N_y$ are the linear dimension of the unit cell under consideration. The chemical potential $\mu$, therefore, needs to be adjusted each time when the on-site repulsion $U$ is varied. The NNN hopping integral is chosen to be $t' = -0.2$, as relevant to the hole-doped cuprate, to fit the hole-like Fermi surface. Through out this paper, we are going to use the same value of $U$, $g$, $t'$, and $n_f$.

Once the self-consistent solution is obtained, we calculate the staggered magnetization and the electron density defined as $M_x = (-1)^i (n_{\uparrow i} - n_{\downarrow i})$ and $n_i = (n_{\uparrow i} + n_{\downarrow i})$, respectively. Furthermore, the LDOS of the energy $E$ at the positon $i$ can be written as

$$\rho_i(E) = \frac{1}{M_x M_y} \sum_{n, k} \left| \bar{u}_{i1}^n \right|^2 f'(E_{n,k} - E) + \left| \bar{v}_{i1}^n \right|^2 f'(E_{n,k} + E),$$

(4)

where $\rho_i(E)$ is proportional to the local differential tunneling conductance as measured by STM experiment, and the summation is averaged over a $M_x \times M_y$ wavevectors in first Brillouin Zone. In addition, the LDOS spatial maps observed in STM experiment at a fixed bias voltage $E$ could be obtained by calculating $\rho_i(E)$ at each site of the lattice.

In the absence of the magnetic field, $t_{ij} = t$ and $t'$ are the NN and NNN hopping integrals, respectively. Since the strength of the onsite repulsion, $U$, required to generate AF order has to be fine tuned to study the interplay of the two competing orders. The non-zero AF order appears only for certain range of $U$ and $g$, and larger $U/g$ is able to produce stronger antiferromagnetism. With our chosen parameters $U = 2.05$ and $g = 0.71$, weak stripe modulations can be generated in the dSC order parameter, the staggered magnetization and electron density. Here we set $t = 1$.

In Figure 1(a), our numerical result for the spatial distribution of the dSC order, which is defined as $\Delta_1 = (\Delta_{1+x} + \Delta_{1-x} - \Delta_{1+y} - \Delta_{1-y})/4$, exhibits the stripe behavior along $y$-direction with the period $4a$. The staggered magnetization (Fig. 1(b)) shows stripe like SDW along $y$-direction. Its period is $8a$ and its amplitude is less than 0.1. The electron density (Fig. 1(c)) has one-dimensional CDW modulation with $4a$ as its period and a very weak amplitude (less than 0.001). The origin of such static stripes could be understood in terms of the existence of a nesting wave vector $q_A \sim 0.25 \pi/a$ connecting the upper and lower pieces of the Fermi surface near $(\pi, 0)$ along $k_y$-direction [See Fig. 1 in Refs. 24]. For proper values of $U$ and doping, this wave vector would modulate the staggered magnetization with SDW stripes along $x$-direction with period $2\pi/4a = 8a$. Accompanying the SDW stripes we have the charge stripes with period $4a$. If we choose a larger $U (> 2.05)$ here, the effect...
is to enhance the amplitudes of the SDW/CDW stripes, not to change its period. For smaller $U (= 2.0)$, only dSC without stripes is obtained. The stripe configurations discussed above are associated with the ground state of the system. What have been observed by STM experiments are related to quasiparticle excitations. In Fig. 1(c) we present the spatial map of the LDOS at energy $E = 0.04$, and it exhibits the same stripe like modulation with period $4a$ as that appeared in CDW shown in Fig 1(c). We have checked the LDOS at several different bias energies, and found that the same stripe like structure still prevails and the modulation period or wavevector is energy independent. This result can be regarded as a necessary condition for existing a static-stripe CDW order in the sample. Since the $y$- and $x$- oriented stripes are degenerated in energy. The observed checkerboard pattern in the STM experiments could be understood by a superposition of these two perpendicularly oriented LDOS maps. Part of the modulation wavevectors observed in the experiments are also dispersive or energy dependent, this behavior should be related to the scattering of quasiparticles from defects including the randomly distributed stripes which break the translational invariance. Here we would like to emphasize that our quasiparticles are excitations from the SDW/CDW (stripes) + dSC ground state. The information of the stripes is nonpertubatively included in wave functions of the quasiparticles. After the Hamiltonian is diagonalized, there exists no extra term which couples the quasiparticle with the stripes. It should also be interesting to calculate the energy-dependent LDOS in the presence of stripes and to see its difference as compared with the case for a pure dSC. In Fig. 2, we show the energy dependence of the LDOS at one of the hole (electron) accumulated stripes, namely at one of the minima (maxima) in Fig. 1(c). It appears that there exist two small bumps within the superconducting coherence peaks, a signature of the presence of weak SDW and CDW orders. At the different sites, the LDOS also can be shown to have the similar features.

Next let us introduce a nonmagnetic strong impurity like Zn into our system at site $(0,0)$ and investigate its effect. Here the on-site impurity potential is taken to be $V_0 = 100$. From Fig. 3(a), one can easily see that the dSC order is suppressed and recovers to its bulk value at a length scale of $\xi_0$, the superconducting coherence length ($\sim 5a$), away from the impurity. Beyond this range, the weak stripe-modulation in the dSC order parameter still remains. In Fig. 3(b) we show that the impurity induced staggered-moment of the SDW is zero at the impurity site and reach the maximum value at its four NN sites. The net induced local moment by the impurity corresponds to a local spin with $S_z=1/2$ when $U$ becomes stronger. From Fig. 3(b), the SDW is clearly pinned at the impurity site with one of its ridges. The spatial profile of the electron density change is presented in Fig.3(c), and it exhibits a Freidel-like oscillation around the impurity. It is easy to see that the electron number reaches to zero or $\delta n_i = -0.85$ at the impurity site, which is much larger than the amplitude (0.001) of the CDW stripes. This is the reason why the stripes in Fig. 1(c) are too faint to see in Fig 1(c). Fig. 3(d) displays the LDOS map at energy $E = 0.04$. The intensity is zero at the impurity site and there are four peaks appear on the four NN sites around the impurity. The intensities of the two peaks at the site $(0, \pm 1)$ are less than those at the site $(\pm 1, 0)$. The stripe structure in Fig. 1(d) still prevails, but it is again too weak to see here.

It is well known that a sharp single resonance peak at zero bias in the LDOS at the NN sites of a unitary impurity appears for a pure dSC. In the presence of weak stripes, the LDOS as a function of energy at the NN site, $(0,1)$ and $(1,0)$ around the impurity are respec-
Fig. 1, and the impurity scattering potential \( \rho_0 \). The parameter values are the same as the Fig. 1, and the impurity scattering potential \( \rho_0 = 100 \).

Effectively displaced in Fig. 4(a) and (b). The zero bias peak previously obtained for \( U = 0 \) is dramatically depressed by \( U \neq 0 \) and splits into two distinct peaks. This is because stronger local AF order is induced near the strong impurity site and a larger SDW gap opens up locally that suppresses the LDOS close to the impurity. This makes the LDOS in the present case very different from that of a pure d-wave (or \( U = 0 \)) case. The oscillation in the LDOS at negative bias below the left peak is originated from the energy-dependent modulations induced by the impurity, and the large amplitude seems to come from the size effect. When \( U/g \) is not large enough to generate extended SDW, the weak and local AF order induced by the impurity may force the resonance peak just to split a little.\(^{25,26}\) The shapes of split peaks at site \((0, 1)\) and \((1, 0)\) are slightly different. This indicates that the fourfold symmetry for a pure dSC changes to twofold symmetry when the stripe phase is in presence. If the experimentally observed\(^{13,14}\) stripe structure is of magnetic origin, we predict that the LDOS should exhibit a double-peak feature near the zero bias.

In conclusion, we have studied a cuprate superconductor with weak stripe-like modulations in the dSC, SDW and CDW order parameters without and with a strong nonmagnetic impurity. In the absence of the impurity, the LDOS exhibits two small bumps within the superconducting coherence peaks, a signature of the presence of the competing AF order. The LDOS maps displays the same stripe modulation as the CDW along y-direction with periodicity \( 4a \) which is nondispersive or energy independent. The components of the modulation wavevectors observed by the experiments which are energy dependent or dispersive should be attributed to the effect due to scatterings of quasiparticles from defects\(^{23,24}\). In the presence of a strong impurity, we predict that the LDOS at the NN sites of the impurity are strongly suppressed by the AF order and reveal a double peak structure. Hopefully our theoretical results could be useful to future STM experiments performed on samples with weak stripe-like structures.

Acknowledgements: We thank Profs. S.H. Pan and N. C. Yeh for the useful discussions. This work is supported by The Texas Center for Superconductivity at University of Houston and by a grant Robert A. Welch Foundation.

---

1. K. Yamada, et al., Phys. Rev. B 57, 6165 (1998).
2. J.M. Tranquada, et al., Nature 375, 561 (1995).
3. H.A. Mook, et al., Nature 404, 729 (2000).
4. J.M. Tranquada, et al., Phys. Rev. Lett. 78, 338 (1997).
5. H.A. Mook, P. Dai, and F. Dogan, Phys. Rev. Lett. 88, 97004 (2002).
6. B. Luke, et al., Nature 415, 299 (2002).
7. M.I. Salkola, V.J. Emery, and S.A. Kivelson, Phys. Rev. Lett. 77, 155 (1996).
8. I. Martin, G. Ortiz, A.V. Balatsky, and A.R Bishop, Int. J. Mod. Phys. B 14, 3567 (2000).
9. Y. Chen, Hong-Yi Chen, and C.S. Ting, Phys. Rev. B 66, 104501 (2002).
10. M. Ichikawa and K. Machida, cond-mat/0205501.
11. D. Podolsky, E. Demler, K. Damle, and B. I. Halperin, Phys. Rev. B 67, 094514 (2003); D. Zhang, Phys. Rev. B 66, 214515 (2002).
12. J.E. Hoffman, et al., Science 295, 466 (2002).
13. C. Howald, et al., cond-mat/0201546.
14. C. Howald, et al., Phys. Rev. B 67, 014533 (2003).
15. S.A. Kivelson, et al., cond-mat/0210683.
16. Y. Zhang, E. Demler, and S. Sachdev, Phys. Rev. B 66, 094501 (2002).
17. Jian-Xin Zhu, Ivar Martin, and A.R. Bishop, Phys. Rev. Lett. 89, 067003 (2002).
18. H.D. Chen, et al., Phys. Rev. Lett. 89, 137004 (2002).
19. A. Polkovnikov, M. Vojta, and S. Sachdev, Phys. Rev. B 65, 220509 (2002).
20. S.H. Pan, et al., Nature 403, 746 (2000).
21. A.V. Balatsky, M.I. Salkola, and A. Rosengren, Phys. Rev. B 51, 15547 (1995); M.I. Salkola, A.V. Balatsky, and D.J. Scalapino, Phys. Rev. Lett. 77, 1841 (1996).
22. J.E. Hoffman, et al., Science 297, 1148 (2002).
23. Q.H. Wang and D.-H. Lee, Phys. Rev. B 67, 020511 (2003).
24. D.G. Zhang, and C.S. Ting, Phys. Rev. B 67, 100506 (2003).
25. Ziqiang Wang and Patrick A. Lee, Phys. Rev. Lett. 89, 217002 (2002); Y. Chen and C.S. Ting, cond-mat/0304646.
26. H. Tsuchiura, et al., Phys. Rev. B 64, R140501 (2001).