The Energy-dependent Checkerboard Patterns in Cuprate Superconductors

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Motivated by the recent scanning tunneling microscopy (STM) experiments [J. E. Hoffman et al., Science 297, 1148 (2002); K. McElroy et al., Nature (to be published)], we investigate the real space local density of states (LDOS) induced by weak disorder in a d-wave superconductor. We first present the energy dependent LDOS images around a single weak defect at several energies, and then point out that the experimentally observed checkerboard pattern in the LDOS could be understood as a result of quasiparticle interferences by randomly distributed defects. It is also shown that the checkerboard pattern oriented along 45° to the Cu-O bonds at low energies would transform to that oriented parallel to the Cu-O bonds at higher energies. This result is consistent with the experiments.

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Recently the energy-dependent modulations of the local density of states (LDOS) in high temperature superconductors has attracted a lot of experimental and theoretical attentions[1-6]. By employing the high-resolution Fourier-transform scanning tunneling microscopy (STM), Hoffman et al. investigated the zero-field charge modulations in Bi$_2$Sr$_2$CaCu$_2$O$_{8+δ}$ [1] deduced from the checkerboard patterns in the real space LDOS. The charge modulation vectors near the origin of the momentum space were determined. They found that the period of the modulations depends on the energy and doping for energy below the maximum superconducting gap. With increasing energy (doping fixed) or doping (energy fixed), the LDOS modulation wave vectors oriented parallel to the Cu-O bonds become shorter while those along 45° to the Cu-O bonds become longer. They also observed that when energy increases, the charge modulation along 45° to the Cu-O bonds changes to that along the Cu-O bonds. Subsequently, McElroy et al. extended the previous measurements [1] to the second Brillouin zone and discovered the characteristic octet of quasiparticle states [2, 4].

A number of theoretical studies have devoted to the explanation of the STM experiments [3-6]. It has been proposed that the experimental phenomenon is due to the result of quasiparticle interference induced by disorder [1, 2]. Following this idea, Wang and Lee calculated the Fourier component of the LDOS produced by an single impurity with a moderate strength on-site potential [3]. They obtained the LDOS images in momentum space and compared them with those in Ref. [1], but didn’t examine the relations among the modulation wave vectors, dopings and the bias voltages. The present authors, on the other hand, investigated the effect of quasiparticle scatterings from a weak and extended impurity or defect [4]. The Fourier transform images of the LDOS and the relations among modulation wave vectors at different dopings and the bias voltages obtained by us [4] in the first Brillouin zone are consistent with the experimental observations [1, 2]. There exist also other works trying to understand the STM experiments [5, 6]. However, almost all the previous studies [3,4,5] were restricted to the discussion of the Fourier transform of the LDOS due to a single defect in the first Brillouin zone. So far there have existed no studies of the real space LDOS images at different energies, and the origin of the checkerboard patterns observed in the experiments. Thus it is necessary to do these calculations, and to compare the obtained results directly with the LDOS images in the STM experiments [1, 2].

In this paper, we base on the approach of our previous study [4] and examine the effect due to quasiparticle scattering from weak defects or impurities with both hopping and pairing modifications on the LDOS. The reason we choose weak defects as scatters is simply to eliminate the contribution from the resonant states. Using the T-matrix approach, We first calculate the energy dependent LDOS images due to a single extended defect and show how the pattern of the image changes as the energy varies. Then we demonstrate that the experimentally observed checkerboard pattern for the LDOS could be understood as a result of interferences among randomly distributed defects. Our results clearly indicate the dominant LDOS modulation along 45° to the Cu-O bonds at lower energy would transform to that oriented parallel to the Cu-O bonds at higher energy. This is also consistent with the STM experiments [1,2).

The Hamiltonian describing the scattering of quasiparticles from M impurities with local modifications of both hopping and pairing parameters in a d-wave superconductor can be written as

$$H = H_{BCS} + H_{imp},$$

(1)

where

$$H_{BCS} = \sum_{k\sigma}(\epsilon_k - \mu)c_{k\sigma}^c c_{k\sigma} + \sum_k \Delta_k (c_{k\uparrow}^c c_{-k\downarrow} + c_{-k\uparrow} c_{k\downarrow}),$$

$$H_{imp} = \sum_{k\sigma} \sum_{\mu\nu} T_{\mu\nu}^{imp} c_{k\sigma}^c (\mu) c_{\mu\nu} (\nu) c_{\nu\mu} (\nu) c_{\nu\sigma}.$$
\[ H_{\text{imp}} = \sum_{<i,j>,\sigma} \delta t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + \sum_{<i,j>} \delta \Delta_{ij} (c_{i\uparrow}^\dagger c_{j\downarrow}^\dagger + c_{j\downarrow} c_{i\uparrow}) \]

\[ + \sum_{i=1}^{M} [(V_{si} + V_{mi}) c_{\sigma R_i}^\dagger c_{R_i} + (V_{si} - V_{mi}) c_{\sigma R_i} c_{R_i}^\dagger]. \]

Here \( \mu \) is the chemical potential to be determined by doping, \( \epsilon_k = t_1 (\cos k_x + \cos k_y)/2 + t_2 \cos k_x \cos k_y + t_3 (\cos 2k_x + \cos 2k_y)/2 + t_4 (\cos 2k_x \cos k_y + \cos k_x \cos 2k_y)/2 + t_5 \cos k_x \cos 2k_y, \) where \( t_{1-5} = -0.5951, 0.1636, -0.0519, -0.1117, 0.0510 \) (eV). The band parameters are taken from those of Norman et al. [7] for Bi\textsubscript{2}Sr\textsubscript{2}CaCu\textsubscript{2}O\textsubscript{8+δ}, and the lattice constant \( a \) is set as \( a = 1 \). The order parameter away from the impurity is given by \( \Delta_k = \Delta_0 (\cos k_x - \cos k_y)/2 \).

Without loss of generality, at the impurity or defect site \( R_i \), we assume an on-site potential consisting of a nonmagnetic part, \( V_{si} \), and a magnetic part, \( V_{mi} \). The defect also induces a weak local modification in the hopping \( \delta t_i \), to the nearest neighbor sites, and a suppression of the superconductivity order parameter on the four bonds connected to the impurity site, \( \delta \Delta_1 \), and on the other twelve bonds connected to the nearest neighbor sites, \( \delta \Delta_2 \).

The Hamiltonian (1) with a single impurity has in fact been successfully applied by authors in Ref. 8 to explain the resonant STM spectra for Ni impurities in Bi\textsubscript{2}Sr\textsubscript{2}CaCu\textsubscript{2}O\textsubscript{8+δ}. However, in the present case, no resonances in LDOS have been observed in the recent STM experiments [1, 2]. So it is reasonable to assume that the on-site potentials (\( V_{si} \) and \( V_{mi} \)) and the modifications in hopping and pairing parameters \( (\delta t_i, \delta \Delta_1 \) and \( \delta \Delta_2 i) \) are all weak and have approximately the same order of magnitude. This model has been applied in Ref. 4 to explain the experimental observed Fourier transform of the LDOS at different energies and dopings in the first Brillouin zone [1, 2].

The Hamiltonian (1) can be solved by the standard Bogoliubov transformation plus Green’s function technique. When \( \delta t_i, \delta \Delta_1, \delta \Delta_2, V_{si} \) and \( V_{mi} \) are all small, keeping the leading term in the T-matrix approach should be good approximation. In such an approximation, the resonant states due to the impurity are eliminated and the LDOS change in real space due to these defects can be shown to have the following form

\[ \delta \rho(r, \omega) = -\frac{2}{\pi N^2} \sum_{i=1}^{M} \sum_{kk'} \sum_{\nu, \nu'=0,1} \cos [(k - k') \cdot (r - R_i)] \times \left[ 2\delta t_i A(k, k') + V_{si} \right] \alpha_{\nu \nu'}(k, k') \]

\[ + 2[\delta \Delta_1 B(k, k') + \delta \Delta_2 C(k, k')] \beta_{\nu \nu'}(k, k') \]

\[ \times \text{Im}[G_{k\nu}(i\omega_n)G_{k'\nu'}(i\omega_n)]|_{\omega_n \to \omega + i0^+}, \]  

where \( N \) is the number of sites in the lattice, \( A(k, k') = \cos k_x + \cos k_y + \cos k'_x + \cos k'_y, B(k, k') = \cos k_x - \cos k_y + \cos k'_x - \cos k'_y, C(k, k') = \cos (k_x - 2k'_x) - \cos (k_x - k'_x - k'_y) - \cos (k_x - k'_x) + \cos (k_y - k'_y), \) and \( \alpha_{\nu \nu'}(k, k') = (\xi_{k}\xi_{k'} - (1)^{\nu+\nu'}\xi_{k\nu+1}\xi_{k\nu'} + (1)^{\nu+\nu'}\xi_{k\nu'}\xi_{k\nu+1} + G_{k\nu}(i\omega_n)|_{\omega_n \to \omega + i0^+}. \) 

\[ \delta \Delta_1 = \Delta_0/(2E_k) \]

We note that \( V_{mi} \) is absent from Eq. (2) because there is no first order contribution from the magnetic potential. Obviously, the total LDOS change \( \delta \rho(r, \omega) \) is a summation of those due to individual impurity. In the present study, we base our numerical calculation on a finite lattice of 800 x 800 sites. For simplicity, we choose \( 2\delta t_i = V_{si} = -2\delta \Delta_1 = -4\delta \Delta_2, \) and assume that all these parameters are small such that the first order T-matrix approximation is valid. In our calculation, we also take the chemical potential \( \mu = -0.1238 \) corresponding to the optical doping (15%) and introduce a finite lifetime broadening \( \gamma = 2 \) meV to the quasiparticle Green’s function to smooth our data points by replacing \( \omega \) with \( \omega + i\gamma \) in Eq. (2).

According to Eq. (2), We plot the images of the LDOS change due to a single defect (\( M = 1 \)) located at the center of a 20 x 20 square lattice for different energies in Fig. 1. It is easy to see from the images at \( \omega = 0 \) and -12meV that the LDOS modulations orient parallel to (±1, ±1) directions (45° to Cu-O bonds). When the energy becomes more negative at \( \omega = -16, -20 \) and -25meV, the LDOS modulation clearly changes to (±1, 0) or (0, ±1) (along the Cu-O bonds) directions. At \( \omega = -16 \) and 16meV, the LDOS modulations are strongly aligned along the directions of 45° to Cu-O bonds. For higher energies at \( \omega = 20 \) and 25meV, the modulations along the Cu-O bonds begin to show up, and they may become dominant at higher energies. It is apparent that the LDOS images are asymmetric with respect to \( \omega = 0 \). We also note that with increasing energy \( |\omega| \), the region of the LDOS modulation along (±1, ±1) directions becomes smaller while that along (±1, 0) or (0, ±1) directions becomes larger.

In order to understand the LDOS modulations near a single impurity, we present the LDOS variations along (1, 0) and (1, 1) directions in Fig. 2. We can see that the LDOS on the impurity site has the maximum values at energy \( \omega < 12 \) meV. At and above 12meV, the LDOS near the nearest neighboring site to the impurity have the maximum values. Far away the impurity (about 20a), the LDOS modulations vanish. For \( \omega < -12 \) meV,
the LDOS along (1,0) direction show strong and long distance oscillations while those along (1,1) direction show rather week and short distance oscillations. This is the reason why the LDOS images shown in Fig.1 in this energy region have modulation vectors clearly along Cu-O bonds. At $\omega = -12, 0$ and $12 \text{meV}$, both modulations with approximately equal weight are present in the LDOS. As a result, the LDOS images with modulations along the directions of $45^\circ$ to Cu-O bonds can also be seen in this region. For $\omega > 12 \text{meV}$, the strength of the modulation along (1,0) direction begins to outgrow that along (1,1) direction. We expect that dominant modulation should be along (1,0) direction, as the energy gets even higher.

In fact there are total six nonequivalent charge modulation vectors [2,4], not all of them can be clearly identified in our real space studies. We have discussed the LDOS modulations due to a single impurity. In fact, there should be randomly distributed defects in the experimental sample. In order to understand the effect of the disorder, we choose the defect concentration to be 1% and the defects are described by $H_{\text{imp}}$ in Eq.(1). In our simulation, we first produce a random distribution for the defects and then calculate the LDOS changes in a $20 \times 20$ square lattice similar to that of the experiments [1, 2].

Graphs in Fig. 3 show the LDOS images at 9 different energies for such a distribution of defects. As a consequence of quasiparticle interference by these defects, checkerboard patterns in the LDOS show up in our numerical simulations. It is evident from Fig. 3 that the LDOS modulation or the orientation of the checkerboard pattern is parallel to the $45^\circ$ direction from the Cu-O bonds at small $|\omega|$, while at larger $|\omega|$, the pattern tends to orient along the direction of the Cu-O bonds. The changing of the orientation is particularly apparent when $\omega$ becomes more negative. This conclusion is consistent with the STM experiments [1, 2].

In summary, we have studied the LDOS change induced by disordered and weak defects using Bogoliubov transformation and the the Green’s function technique. The obtained LDOS images due to randomly distributed defects exhibit checkerboard patterns which are similar to those observed in the STM experiments [1, 2]. With increasing energy $|\omega|$, the LDOS modulation along $(\pm 1, \pm 1)$ direction tends to orient itself in the $(\pm 1, 0)$ or $(0, \pm 1)$ direction. This modulation transformation has also been seen in these experiments. Combining our previous work [4], we conclude that the STM images [1, 2] can be qualitatively understood in the present theory. For the charge density wave order observed in Ref. [9], it is believed to be the dimerization hopping and transverse pairing modulations [10, 11, 12]. However, the origin of such a static order needs to be further studied.

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[1] J. E. Hoffman, K. McElroy, D.-H. Lee, K. M. Lang, H. Eisaki, S. Uchida, and J. C. Davis, Science 297, 1148 (2002).
[2] K. McElroy, R. W. Simmonds, J. E. Hoffman, D.-H. Lee, J. Orenstein, H. Eisaki, S. Uchida, and J. C. Davis, Nature (to be published).
[3] Qiang-Hua Wang and Dung-Hai Lee, Phys. Rev. B. 67, 020511(R) (2003).
[4] Degang Zhang and C. S. Ting, Phys. Rev. B. 67, 100506(R) (2003).
[5] J. H. Han, Phys. Rev. B. 67, 094506 (2003).
[6] A. Polkovnikov, S. Sachdev, and M. Vojta, cond-mat/0208334.
[7] M. R. Norman, M. Randeria, H. Ding, and J. C. Campuzano, Phys. Rev. B 52, 615 (1994).
[8] Jian-Ming Tang and M. E. Flatte, Phys. Rev. B 66, 060504(R) (2002).
[9] C. Howald, H. Eisaki, N. Kaneko, M. Greven, and A. Kapitulnik, Phys. Rev. B 67, 014533 (2003).
[10] D. Podolsky, E. Demler, K. Damle, and B. I. Halperin, Phys. Rev. B 67, 094514 (2003).
[11] M. Vojta, Phys. Rev. B 66, 104505 (2002).
[12] Degang Zhang, Phys. Rev. B 66, 214515 (2002).

FIG. 1. The LDOS change $\delta \rho(r, \omega)$ at different energy due to a single impurity at the center of a $20 \times 20$ square.

FIG. 2. The LDOS change $\delta \rho(r, \omega)$ versus the distance $|r|$ to the single impurity along (1,0) and (1,1) directions at different energy.

FIG. 3. The LDOS change $\delta \rho(r, \omega)$ at different energy due to the random impurities in a $20 \times 20$ square.
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