Coulomb interaction-induced checkerboard patterns in disordered cuprates

Degang Zhang
Texas Center for Superconductivity and Department of Physics, University of Houston, Houston, TX 77204, USA
E-mail: dgzhang@mira.tcs.uh.edu

New Journal of Physics 9 (2007) 256
Received 11 April 2007
Published 10 August 2007
Online at http://www.njp.org/
doi:10.1088/1367-2630/9/8/256

Abstract. We study the effect of the Coulomb interaction on the local density of states (LDOS) and its Fourier component in disordered cuprates. It is shown that the Coulomb interaction suppresses strongly the maximum value of the LDOS induced by the dopant impurity at each energy value and expands significantly the Friedel oscillation in real space. The existence of the Coulomb interaction with a moderate strength yields an energy-dependent checkerboard LDOS modulation around the impurity, which is very different from that produced by pure quasiparticle interference. The orientation and transformation of the checkerboard pattern with energy and the relations among the modulation vectors, dopings and the bias voltages agree qualitatively with the recent scanning tunneling microscopy (STM) experiments.

It is well known that at half filling cuprates are the Mott insulators, where the on-site Coulomb interaction is larger than the kinetic energy of an electron. When oxygens (holes) are doped into cuprates, the electrons can move in the CuO$_2$ plane and cuprates become strange metals. In other words, the 'effective' on-site Coulomb interaction decreases. After further increasing the concentration of holes up to about 5%, cuprates become superconducting and have a d-wave symmetry gap. So cuprate superconductors inevitably possess disorder due to the oxygen doping. It is out of question that the electronic states in the CuO$_2$ plane are mainly determined by disorder and the Coulomb interaction.

Recently, a series of the STM experiments have revealed the electronic states in both real and momentum spaces for the superconductor Bi$_2$Sr$_2$CaCu$_2$O$_{8+δ}$ [1]–[3]. It was found that in real space, the local density of states (LDOS) has a weak energy-dependent checkerboard pattern. At low bias voltages, the charge modulation with a period $\frac{2\pi}{q_B}$ orients along 45° to the...
Figure 1. Schematic Fermi surface of high $T_C$ cuprate superconductors. The modulation wavevectors $q_A$ and $q_B$ connecting different points of the Fermi surface with the same energy are shown.

Cu–O bonds. At high bias voltages well below the superconducting gap, the charge modulation with a period $\frac{2\pi}{q_A}$ is parallel to the Cu–O bonds. We note that $q_B$ are the wavevectors connecting the end points of the same banana-like equal-energy contours while $q_A$ are the wavevectors connecting the nearest end points of the neighbor banana-like equal-energy contours (see figure 1). These two kinds of charge modulations coexist at intermediate voltages. With increasing the bias voltage or doping, $q_A$ becomes shorter while $q_B$ becomes longer [1, 2]. In [3], McElroy et al studied in detail the nanoscale electronic disorder induced by the oxygen dopant atoms. It was indeed verified that these dopant defects generate the LDOS modulations and also suppress superconducting coherence peaks in Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$. In contrast, a dispersionless LDOS was seen in the pseudogap region [4, 5].

A lot of theoretical investigations have been devoted to these fascinatingly experimental observations in the superconducting phase [6]–[16] and in the pseudogap region [17, 18]. In the superconducting phase, the relations among the modulation wavevectors, dopings and the bias voltages in momentum space, observed in these STM experiments, seem to be well explained by quasiparticle interference due to weak disorder, e.g. the impurity potential [6], the local modifications of hopping and superconducting order parameter [7], [11]–[13], short-range potential in or out of the Cu–O plane [10, 15], and so on. However, in order to determine whether or not these models can well describe these experimental phenomena, we must also calculate the LDOS in real space. Up to now, little work has been done in this direction. In [11], we investigated the LDOS modulations at different energies in the presence of a single extended impurity and randomly distributed impurities. It was shown that the LDOS near the impurity has a stripe-like structure along both $45^\circ$ to the Cu–O bonds and the Cu–O bonds rather than the checkerboard pattern at each energy. In addition, the Friedel oscillation only exists in a short distance ($\sim 10$ lattice constant) away from the impurity site. For many random impurities, a checkerboard pattern and its transformation with energy and doping have been observed theoretically. But the checkerboard pattern only covers a small indifective area and is different from that seen by the STM experiments, which expands into the bulk. Therefore, it is difficult to interpret the experimental phenomena in real space by using pure quasiparticle interference induced by weak disorder. What factor makes the LDOS at different energy values have the...
checkerboard patterns in the Cu–O plane? It is natural to consider the Coulomb interaction in the CuO$_2$ plane as a candidate because the undoped cuprates are the Mott insulators. In this paper, we investigate the influence of the Coulomb interaction on the Friedel oscillation in disordered cuprate superconductors. We shall see that the experimental phenomena are the results of disorder correlation mediated by the Coulomb interaction.

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

$$H = \sum_{\mathbf{k}\sigma} (\epsilon_{\mathbf{k}} - \mu) c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} + \sum_{\mathbf{k}} \Delta_{\mathbf{k}} (c_{\mathbf{k}\uparrow}^\dagger c_{\mathbf{k}\downarrow} + c_{\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow}) + \sum_{(i,j),\sigma} \delta t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + \sum_{(i,j)} \delta \Delta_{ij} (c_{i\uparrow}^\dagger c_{j\downarrow} + c_{j\downarrow} c_{i\uparrow}) + (V_s + V_m) c_{i\uparrow}^\dagger c_{0\uparrow} + (V_s - V_m) c_{i\downarrow}^\dagger c_{0\downarrow} + U \sum_i c_{i\sigma}^\dagger c_{i\sigma} c_{i\sigma}^\dagger c_{i\sigma},$$

(1)

where $(i,j)$ denotes that the sites $i$ and $j$ are the nearest neighbor sites, $\mu$ is the chemical potential to be determined by doping, $c_{i\sigma}^\dagger = \frac{1}{N} \sum_{\mathbf{k}} c_{\mathbf{k}\sigma}^\dagger e^{i\mathbf{k}\cdot\mathbf{r}}$, $N$ is the number of sites in the lattice, $\epsilon_{\mathbf{k}} = t_1 (\cos k_x + \cos k_y)/2 + t_2 \cos k_x \cos k_y + t_3 (\cos 2k_x + \cos 2k_y)/2 + t_4 (\cos 2k_x \cos k_y + \cos k_x \cos 2k_y)/2 + t_5 \cos 2k_x \cos 2k_y$ with $t_{1-5} = -0.5951, 0.1636, -0.0519, -0.1117, 0.0510$ (eV). The band parameters are taken from those of Norman et al. [19] for Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$, and the lattice constant $a$ is set as $a = 1$. The order parameter away from the impurity is given by $\Delta_{\mathbf{k}} = \Delta_0 (\cos k_x - \cos k_y)/2$. $\delta t_{ij} = \delta t$ for $i = 0$ or $j = 0$ and 0 for others. $\delta \Delta_{ij} = \delta \Delta_1$ for $i = 0$ or $j = 0$, $\delta \Delta_2$ for $i = 1$ or $j = 1$, and 0 for others. $U_s$ and $V_m$ are the nonmagnetic part and the magnetic part of an on-site potential, respectively. $U$ is the strength of the on-site Coulomb interaction while $V$ is that between the nearest neighbor sites.

The Hamiltonian (1) cannot be diagonalized exactly due to the presence of the Coulomb interaction. Because the cuprate superconductors are not antiferromagnetic or ferromagnetic and the charge modulations observed by the STM experiments are weak, here we are only interested in the case of weak to moderate $U$ and small $V$, where the charge density wave (CDW) and spin density wave (SDW) can be neglected [20]. In fact, the presence of weak CDW and SDW only produces an energy-independent peak at the modulation wavevectors in the Fourier component of the LDOS and does not affect the results in this paper because the interaction between the weak impurity and the weak CDW (SDW) is a second-order small quantity [17, 18], [21–27].

Taking the Bogoliubov transformation

$$c_{\mathbf{k}\uparrow} = \sum_{\nu=0,1} (-1)^\nu \xi_{\mathbf{k}\nu} \psi_{\mathbf{k}\nu}, \quad c_{\mathbf{k}\downarrow}^\dagger = \sum_{\nu=0,1} \xi_{\mathbf{k}\nu} \psi_{\mathbf{k}\nu+1},$$

(2)

where $\xi_{\mathbf{k}\nu}^2 = \frac{1}{2} \left(1 + (-1)^\nu \frac{\epsilon_{\mathbf{k}} - \mu}{E_k}\right)$, $\xi_{\mathbf{k}\nu} \psi_{\mathbf{k}\nu} = \frac{\Delta_k}{2E_k}$, and $E_k = \sqrt{(\epsilon_{\mathbf{k}} - \mu)^2 + \Delta_k^2}$, the Hamiltonian (1) can be re-expressed in terms of the fermionic creation and annihilation operators $\psi_{\mathbf{k}\nu}^\dagger$ and $\psi_{\mathbf{k}\nu}$.

Defining two-point Green’s functions

$$G_{\mathbf{k}\nu}(i\omega_n) = -\mathcal{F}\{T_z \psi_{\mathbf{k}\nu}(\tau) \psi_{\mathbf{k}\nu}^\dagger(0)\},$$

(3)

where $\mathcal{F}\phi(\tau)$ denote the Fourier transform of $\phi(\tau)$ in Matsubara frequencies, $\tau$ is the imaginary time, then the equations of motion for the Green’s functions $G_{\mathbf{k}\nu}(i\omega_n)$ can be easily derived by using the standard approach [28]. Neglecting the contributions of CDW and SDW in the
equations of motion and up to the first-order in $V_s$, $V_m$, $\delta t$, $\delta \Delta_1$ and $\delta \Delta_2$, the Green’s functions have the form

$$G^{\nu\nu'}_{kk}(i\omega_n) = G^0_{kk}(i\omega_n)\delta_{kk}\delta_{\nu\nu'} + G^0_{kk}(i\omega_n)\{\delta_{kk}\mathcal{D}_k[-1]^{\nu}\xi_{kk}\xi_{kk'}f_{kk'} + \xi_{kk'+1}g_{kk'}\}
$$

$$+ \alpha_{kk}[-1]^{nu'}\xi_{kk}\xi_{kk'}\xi_{kk'+1} + \beta_{kk}[-1]^{nu'}\xi_{kk}\xi_{kk'+1} + [-1]^{nu'}\xi_{kk}\xi_{kk'+1}]
$$

$$+ \mathcal{D}_k[-1]^{nu'}\xi_{kk}\xi_{kk'}(\alpha_{kk}A_k + \beta_{kk}C_k) + [-1]^{nu'}\xi_{kk}\xi_{kk'+1}(\alpha_{kk}B_k)
$$

$$+ [-1]^{nu'}\xi_{kk}\xi_{kk'+1}(\alpha_{kk}A_k - \beta_{kk}B_k)
$$

$$+ \mathcal{D}_k[(u_{kk'}\alpha_{kk} + v_{kk'}\beta_{kk})(f_{kk'}X_k + g_{kk'}Y_k) + (u_{kk'}\beta_{kk} - v_{kk'}\alpha_{kk})(f_{kk'}Y_k + g_{kk'}Z_k)]},$$

where

$$G^0_{kk}(i\omega_n) = \frac{1}{i\omega_n - [-1]^{nu'}E_k},$$

$$X_k = \sum_\nu \xi_{kk}^2G^0_{kk}(i\omega_n),$$

$$Y_k = \sum_\nu [-1]^{nu'}\xi_{kk}^2\xi_{kk'+1}G^0_{kk}(i\omega_n),$$

$$Z_k = \sum_\nu \xi_{kk'+1}^2G^0_{kk}(i\omega_n),$$

$$\alpha_{kk'} = \frac{V_s}{N} + \frac{2\delta t}{N}(\cos k_x + \cos k_y + \cos k_x' + \cos k_y'),$$

$$\beta_{kk'} = \frac{2\delta \Delta_1}{N}(\cos k_x - \cos k_y + \cos k_x' - \cos k_y'),$$

$$\lambda_k = \sum_\nu \left\{ \frac{U + 8V}{N}\xi_{kk'}^2 - \frac{2V}{N}\xi_{kk'}^2[\cos(k_x' - k_x) + \cos(k_y' - k_y)] \right\},$$

$$\gamma_k = \frac{2V}{N}\sum_{kk'} \xi_{kk'}\xi_{kk'}[\cos(k_x' - k_x) + \cos(k_y' - k_y)],$$

$$a_k = \lambda_k X_k + \gamma_k Y_k, \quad b_k = -\lambda_k Y_k + \gamma_k X_k,$$

$$c_k = \lambda_k Y_k + \gamma_k Z_k, \quad d_k = -\lambda_k Z_k + \gamma_k Y_k,$$

$$f_{kk'} = [-1]^{nu'}\xi_{kk'}[\lambda_k + (\lambda_k^2 + \gamma_k^2)Z_k] + \xi_{kk'+1}[\gamma_k - (\lambda_k^2 + \gamma_k^2)Y_k].$$
\[
\begin{align*}
\delta_{k'} &= (-1)^V \xi_{k'} \left[ \gamma_k - (\lambda_k^2 + \gamma_k^2) Y_k \right] + \xi_{k'+1} \left[ -\lambda_k + (\lambda_k^2 + \gamma_k^2) X_k \right], \\
A_k &= a_k (1 - d_k) + b_k c_k, \\
B_k &= d_k (1 - a_k) + b_k c_k, \\
D_k &= \frac{1}{(1 - a_k)(1 - d_k) - b_k c_k}, \\
\mu_{k'} &= (-1)^V \xi_{k'} (1 + A_k D_k) + \xi_{k'+1} b_k D_k, \\
v_{k'} &= (-1)^V \xi_{k'} c_k D_k + \xi_{k'+1} (1 + B_k D_k). 
\end{align*}
\]

We note that Green’s functions have the symmetry \(G^{\nu\nu'}_{kk}(\pm i\omega_n) \equiv G^{\nu\nu'}_{kk}(i\omega_n)\). Obviously, the weak magnetic potential \(V_m\) does not appear in \(G^{\nu\nu'}_{kk}(i\omega_n)\) because it has only the higher-order contributions to Green’s functions.

The LDOS measured by the STM experiments reads [7, 11, 24]

\[
\rho(\mathbf{r}, \omega) = -\frac{1}{\pi} \Im \sum_{\sigma} \left[ -\mathcal{F}(c_{\nu\sigma}(\tau) c_{\nu\sigma}^\dagger(0)) \right] |_{i\omega_n \rightarrow \omega + i\delta}, \\
= -\frac{1}{N\pi} \Im \sum_{k,k',\nu,\nu'} \cos[(\mathbf{k} - \mathbf{k'}) \cdot \mathbf{r}] \\
\times \left[ (-1)^{\nu+\nu'} \xi_{kk'} \xi_{kk'}^{\dagger} G^{\nu\nu'}_{kk}(i\omega_n) - \xi_{k'+1} \xi_{k'+1}^{\dagger} G^{\nu\nu'}_{kk}(i\omega_n) \right] |_{i\omega_n \rightarrow \omega + i\delta}. 
\]

From equations (4)–(6), we can see that the Coulomb interaction itself does not produce the charge modulations in the present case. However, it has a strong impact on the LDOS induced by disorder. Substituting Green’s function \(G^{\nu\nu'}_{kk}(i\omega_n)\) into the formula (6), we can obtain the LDOS images at different energy values and doping. In our calculations, we have chosen \(N = 400 \times 400, \mu = -0.1246\) corresponding to about 15% doping, \(\Delta_0 = 44\text{ meV}\) and \(V_z = 2\delta t = -2\delta \Delta_1 = -4\delta \Delta_2\) for simplicity. We find that the other parameter options, including \(\delta \Delta_1\) and \(\delta \Delta_2\) to be positive and different doping, arrive at the similar conclusions.

Figure 2 shows the LDOS patterns with a moderate \(U = 0.25\text{ eV}\) and a small \(V = 0.01\text{ eV}\) at different energy values due to a single impurity at the center of a \(40 \times 40\) square. In this case, the ratio of the on-site Coulomb interaction to the nearest neighbor hopping \(\frac{U}{t} \approx 1.7\). Because \(U \gg V\), the model (1) falls into the local antiferromagnetic phase where spontaneous staggered moments form around a single potential scatterer (see figure 1 in [20]). It is expected that the local staggered moments induced by the weak impurities are too weak and their contributions to the LDOS can be omitted. Obviously, the LDOS patterns for \(\omega > 0\) have similar periodic structures with those for \(\omega < 0\). At \(\omega = \pm 12\text{ meV}\), the LDOS has a checkerboard modulation with a period \(\sim 5a\). Its orientation is along 45° to the Cu–O bonds. With increasing energy to \(\pm 18\text{ meV}\), the modulation period becomes shorter to \(\sim 4a\). We note that there also exists about a \(20 \times 20\) checkerboard modulation along the Cu–O bonds around the impurity at \(\pm 18\text{ meV}\). At high energy, e.g. \(\omega = \pm 30\text{ meV}\), the LDOS shows a checkerboard pattern along the Cu–O bonds, which possesses a multi-period structure. Obviously, there does not exist the long-wavelength modulations. When \(\omega = \pm 24\text{ meV}\), two kinds of the checkerboard patterns along both 45° to the Cu–O bonds and the Cu–O bonds coexist. The charge modulation and its transformation with energy agree qualitatively with the STM experiments. Obviously, the Coulomb interaction suppresses the maximum LDOS on or near the impurity sites and magnifies the Friedel oscillation in a large area at each energy, comparing with the results in [11].
Figure 2. The LDOS $\rho(\mathbf{r}, \omega)$ at different energy values due to a single impurity at the center of a $40 \times 40$ square. $U = 0.25$ eV and $V = 0.01$ eV.
In order to further understand the influence of the Coulomb interaction on the electronic states in the CuO$_2$ plane, we study the Fourier component of the LDOS, i.e. $\rho_q(\omega) = \frac{1}{\pi} \sum_r e^{-i\mathbf{q} \cdot \mathbf{r}} \rho(\mathbf{r}, \omega)$. In figure 3, we present $\rho_q(\omega)$ along $(\pi, 0)$ direction at different energy values. Obviously, $\rho_q(\omega)$ has a peak at the modulation wavevector $q_A$, which changes with $\omega$, $U$ and $V$. With increasing $U$ and $V$ ($\omega$ fixed) or $\omega$ ($U$ and $V$ fixed), the peak moves to the origin and $|q_A|$ becomes shorter. If $U$ or $V$ has a large enough value, the peak will disappear at high energy below the superconducting gap. This seems to be consistent with the STM experiments [1, 2]. In contrast, the peak at $q_A$ produced by the pure quasiparticle interference never disappears when energy approaches the superconducting gap. Figure 4 shows $\rho_q(\omega)$ along $(\pi, \pi)$ direction at different energy values. We can see that when $U < \sim 0.1$ eV and $V = 0$ eV, the peak at the modulation wave vector $q_B$ does not move with $U$ at each energy. However, $q_B$ becomes longer if $U > \sim 0.1$ eV or a small $V$ is presented. Therefore, when $U$ and $V$ are fixed, the peaks at $q_A$ and $q_B$ have an opposite shift with increasing energy. In other words, $q_A$ becomes shorter while $q_B$ becomes longer. The relation between

Figure 3. The Fourier component $\rho_q(\omega)$ of the LDOS along the antinodal direction at different energy values and Coulomb interaction.

Figure 4. The Fourier component $\rho_q(\omega)$ of the LDOS along the nodal direction at different energy values and Coulomb interaction.
$q_A(q_B)$ and $\omega$ has been observed by the STM experiments [1, 2]. Note that both $q_A$ and $q_B$ are very sensitive to the presence of $V$ while a small $U$ term has a large impact on $q_A$. If $U \gg 0.3$ eV or $V \gg 0.02$ eV, the theoretical curves for the Fourier component of LDOS along both $(\pi, 0)$ and $(\pi, \pi)$ directions at each energy completely deviate from the STM experiments.

In summary, we have investigated in detail the effect of the Coulomb interaction on sites and between the nearest neighbor sites on the electronic states in disordered cuprate superconductors. It is shown that the Coulomb interaction plays an important role in forming the checkerboard patterns of the LDOS modulations induced by the impurity. Our model (1) produces the essential features of the energy-dependent LDOS modulations as observed in the STM experiments [1]–[3]. In fact, cuprate superconductors contain a lot of random oxygen-dopant impurities. However, all the impurities correlate with each other through the Coulomb interaction. We conclude that it is nothing but this kind of correlation that leads to the energy-dependent checkerboard patterns of the LDOS modulations in cuprate superconductors.

Acknowledgments

I thank Professors C S Ting and S H Pan for useful discussions. This work was supported by the Texas Center for Superconductivity at the University of Houston and by the Robert A Welch Foundation under grant no E-1146.

References

[1] Hoffman J E, McElroy K, Lee D-H, Lang K M, Eisaki H, Uchida S and Davis J C 2002 Science 297 1148
[2] McElroy K, Simmonds R W, Hoffman J E, Lee D-H, Orenstein J, Eisaki H, Uchida S and Davis J C 2003 Nature 422 592
[3] McElroy K, Lee J, Slezak J A, Lee D-H, Eisaki H, Uchida S and Davis J C 2005 Science 309 1048
[4] Vershinin M et al 2004 Science 303 1995
[5] Hanaguri T et al 2004 Nature 430 1001
[6] Wang Q-H and Lee D-H 2003 Phys. Rev. B 67 020511(R)
[7] Zhang D and Ting C S 2003 Phys. Rev. B 67 100506(R)
[8] Han J H 2003 Phys. Rev. B 67 094506
[9] Polkovnikov A, Sachdev S and Vojta M 2003 Physica C 388 19
[10] Zhu L, Atkinson W A and Hirschfeld P J 2004 Phys. Rev. B 69 060503(R)
[11] Zhang D and Ting C S 2004 Phys. Rev. B 69 012501
[12] Dell’Anna L, Lorenzana J, Capone M, Castellani C and Grilli M 2005 Phys. Rev. B 71 064518
[13] Cheng M and Su W-P 2005 Phys. Rev. B 72 094512
[14] Zhu J-X, Balatsky A V, Devereaux T P, Qimiao Si, Lee J, McElroy K and Davis J C 2006 Phys. Rev. B 73 014511
[15] Nunner T S, Chen W, Andersen B M, Melikyan A and Hirschfeld P J 2006 Phys. Rev. B 73 104511
[16] Balatsky A V, Vekhter I and Zhu J-X 2006 Rev. Mod. Phys. 78 373
[17] Chen H D, Vafek O, Yazdani A and Zhang S C 2004 Phys. Rev. Lett. 93 187002
[18] Tesanovic Z 2004 Phys. Rev. Lett. 93 217004
[19] Norman M R, Randeria M, Ding H and Campuzano J C 1994 Phys. Rev. B 52 615
[20] Harter J W et al 2007 Phys. Rev. B 75 054520
[21] Howald C, Eisaki H, Kaneko N, Greven M and Kapitulnik A 2003 Phys. Rev. B 67 014533
[22] Podolsky D, Demler E, Damle K and Halperin B I 2003 Phys. Rev. B 67 094514
[23] Vojta M 2002 Phys. Rev. B 66 104505
[24] Zhang D 2002 Phys. Rev. B 66 214515
[25] Ichioka M and Machida K 2002 J. Phys. Soc. Japan 71 1836
[26] Sachdev S 2003 Rev. Mod. Phys. 75 913
[27] Kivelson S A, Fradkin E, Oganesyan V, Bindloss I P, Tranquada J M, Kapitulnik A and Howald C 2006 Rev. Mod. Phys. 75 1201
[28] Mahan G D 2000 Many-Particle Physics (New York: Kluwer)