Collective modes and quasiparticle interference on the local density of states of cuprate superconductors

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We begin our model construction by noting that substantial quasiparticle gap inhomogeneities are observed in the low-temperature tunneling spectroscopy of underdoped and optimally doped Bi-2212 single crystals, suggesting at least two types of spatially separated regions, one with sharp quasiparticle coherence peaks at smaller energies $\Delta_q$ and the other with rounded hump-like features at larger energies $\Delta^*$. On the other hand, low-energy LDOS (for $E<0.5\Delta_d$) of Bi-2212 exhibit long-range spectral homogeneity. We therefore conjecture that dynamic SDW or CDW coexist with cuprate superconductivity and that they are only manifested in the quasiparticle LDOS when pinned by disorder. Thus, regions with rounded hump features in the quasiparticle spectra are manifestation of localized charge modulations due to pinning of collective modes by disorder, and the wave vector of the charge modulation is twice of that for the collinear SDW order, as proposed in Refs. 23, 24 and 32. In contrast, regions with sharp quasiparticle spectral peaks are representative of generic Bogoliubov quasiparticle spectra with a well-defined $d$-wave pairing order parameter $\Delta_k = \Delta_d \cos 2\theta_k$, where $\Delta_d$ is the maximum gap value and $\theta_k$ is the angle between the quasiparticle wave vector $k$ and the antinode direction. Our model therefore assumes “puddles” of spatially confined “pseudogap regions” with a quasiparticle scattering potential modulated at a periodicity of four lattice constants along the Cu-O bonding directions, and the spatial modulations can be of either the “checkerboard” pattern or “charge nematic” with short-range stripes. In the limit of weak perturbations, we employ the first-order $T$-matrix approximation and consider a (400x400) sample area with either 24 randomly distributed point impurities or 24 randomly distributed puddles of charge modulations that cover $\approx 6\%$ of the sample area. For simplicity, we do not consider the effect of disorder on either suppressing the local pairing potential $\Delta_d(r)$ or altering the nearest-neighbor hopping coefficient $t$ in the band structure of Bi-2212, although such effects reflect the internal structures of charge modulations.

Specifically, the Hamiltonian of the two-dimensional superconductor is given by $\mathcal{H} = \mathcal{H}_{BCS} + \mathcal{H}_{imp}$, where $\mathcal{H}_{BCS}$ denotes the unperturbed BCS Hamiltonian of the $d$-wave superconductor, $\mathcal{H}_{BCS} = \sum_{k \sigma \sigma'} (\epsilon_k - \mu) c_{k \sigma} c_{k \sigma'}^\dagger + \sum_k \Delta_k^* c_{k \uparrow} c_{-k \downarrow} + c_{-k \sigma} c_{k \sigma}^\dagger$, and $\mathcal{H}_{imp}$ is the perturbation Hamiltonian associated with impurity-induced quasiparticle scattering potential. Using the $T$-matrix method, the Green’s function $G$ associated with $\mathcal{H}$ is given by $G = G_0 + G_0 T G_0$, where $G_0$ is the Green’s function of $\mathcal{H}_{BCS}$ and $T = \mathcal{H}_{imp} / (1 - G_0 \mathcal{H}_{imp})$. The Hartree perturbation potential for single scattering events in the diagonal part of $G$ and for noninter-
acting identical point impurities at locations \( \mathbf{r}_j \) is \( V_\alpha(\mathbf{q}) = \sum_j V_{\alpha,m} e^{i \mathbf{q} \cdot \mathbf{r}_j} \) for nonmagnetic \( (V_\alpha) \) and magnetic \( (V_m) \) impurities, whereas that for puddles with short striplike modulations centering at \( \mathbf{r}_j \) is \(^3\)

\[
V_{\alpha}(\mathbf{q}) = \sum_j V_0 e^{i \mathbf{q} \cdot \mathbf{r}_j} \frac{2 \sin(q_{x,j} R_j) \sin(q_{x,j} R_j)}{q_{x,j} \sin(2 q_{x,j})},
\]

and that for checkerboard modulations is

\[
V_{\gamma}(\mathbf{q}) = \sum_j V_0 e^{i \mathbf{q} \cdot \mathbf{r}_j} \left[ \frac{2 \sin(q_{x,j} R_j) \sin(q_{x,j} R_j)}{q_{x,j} \sin(2 q_{x,j})} + (q_{x,j} \rightarrow q_{y,j}) \right].
\]

Here all lengths are expressed in units of the lattice constant \( a \). \( R_j \) is the averaged radius of the \( j \)th puddle, and \( V_0 \) denotes the magnitude of the scattering potential by pinned collective modes. For simplicity, we neglect the energy dependence of \( V_{\alpha,\beta,\gamma} \) and assume that \( V_{\alpha}, V_{\alpha,m} \), and \( V_0 \) are sufficiently small so that no resonance occurs in the FT-LDOS. For sufficiently large scattering potentials, full \( T \)-matrix calculations become necessary as in Ref. 27. However, large \( V_{\alpha,m} \) would result in strong spectral asymmetry between positive and negative bias voltages, which differs from experimental observation. We also note that the energy dependence of \( V_{\beta,\gamma} \) reflects the spectral characteristics of the collective modes and their interaction with quasiparticles and impurities. For instance, we expect \( V_{\gamma} \neq \zeta \gamma \) for pinned SDW, where \( \zeta \) is the impurity pinning strength and \( \gamma \) is the coupling amplitude of quasiparticles with SDW fluctuations. Empirically for nearly optimally doped Bi-2212, \( R_j \) ranges from 5–10. Here we take different values for \( R_j \) with a mean value \( \langle R_j \rangle = 10 \).

Given the Hamiltonian and the scattering potentials \( V_{\alpha,\beta,\gamma}(\mathbf{q}) \), we find that for infinite quasiparticle lifetime and in the first-order \( T \)-matrix approximation, the FT of the LDOS \( \rho(\mathbf{r},E) \) involves elastic scattering of quasiparticles from momentum \( \mathbf{k} \) to \( \mathbf{k} + \mathbf{q} \) is

\[
\rho(\omega) = \frac{1}{\pi N^2} \lim_{\delta \to 0} \sum_{\mathbf{k}} V_{\alpha,\beta,\gamma}(\mathbf{q}) \left[ u_{\mathbf{k} + \mathbf{q} \mathbf{k}}^* u_{\mathbf{k} + \mathbf{q} \mathbf{k}} \right] \beta_{\mathbf{k} + \mathbf{q} \mathbf{k}} (\omega - E_{\mathbf{k} + \mathbf{q} \mathbf{k} + i \delta}) \\
+ u_{\mathbf{k} + \mathbf{q} \mathbf{k}} u_{\mathbf{k} + \mathbf{q} \mathbf{k}} \beta_{\mathbf{k} + \mathbf{q} \mathbf{k}} (\omega - E_{\mathbf{k} + \mathbf{q} \mathbf{k} + i \delta})^* \\
+ \frac{1}{\pi \beta_{\mathbf{k} + \mathbf{q} \mathbf{k}} (\omega + E_{\mathbf{k} + \mathbf{q} \mathbf{k} - 2 i \delta}) \\
+ \frac{1}{\pi \beta_{\mathbf{k} + \mathbf{q} \mathbf{k}} (\omega - E_{\mathbf{k} + \mathbf{q} \mathbf{k} + 2 i \delta}) \\
\right] \\
+ \frac{1}{\pi \beta_{\mathbf{k} + \mathbf{q} \mathbf{k}} (\omega + E_{\mathbf{k} + \mathbf{q} \mathbf{k} - 2 i \delta}) \\
+ \frac{1}{\pi \beta_{\mathbf{k} + \mathbf{q} \mathbf{k}} (\omega - E_{\mathbf{k} + \mathbf{q} \mathbf{k} + 2 i \delta}) \\
\right]
\]

\[
\epsilon_{\mathbf{k}} = \frac{1}{2} \left[ t_1 (\cos k_x + \cos k_y) + t_2 \cos k_x \cos k_y + t_3 (\cos 2 k_x + \cos 2 k_y) + t_4 (\cos k_x \cos k_y + \cos k_x \cos k_y) + t_5 \cos 2 k_x \cos 2 k_y \right],
\]

where \( t_{1-5} = -0.5951, 0.1636, -0.0519, -0.1117, 0.0510 \) eV, \( \mu \) is the chemical potential, and \( E_k = \sqrt{E_k^2 + \Delta_k^2} \). Using Eq. (3) and \( V_{\alpha,\beta,\gamma}(\mathbf{q}) \), we obtain the energy-dependent FT-LDOS maps in the first Brillouin zone for nonmagnetic point impurities in Fig. 1 with two different \( \Delta_d \) values and for pinned SDW (with spin-dependent coherence factor) in Fig. 2, whereas the corresponding LDOS modulations due to \( V_{\alpha,\beta,\gamma}(\mathbf{q}) \) in real space is shown in Figs. 3(a)–3(c). For nonmagnetic point impurity scattering at \( T \ll T_c \), the intensities associated with \( \mathbf{q}_A \) and \( \mathbf{q}_C \) are much stronger than those of \( \mathbf{q}_A \), as shown in Fig. 1 and also in Fig. 4(a). The results in Fig. 1 differ from the STM observation that reveals comparable intensities associated with \( \mathbf{q}_A \) and \( \mathbf{q}_B \), and weaker intensities with \( \mathbf{q}_C \). Interestingly, the intensities of \( \mathbf{q}_A \) and \( \mathbf{q}_{B,C} \) become reversed if one assumes mag
FIG. 2. Energy-dependent FT-LDOS maps with randomly distributed pinned SDW using Eq. (3) and $V_y$: (a) $\Delta_d=40$ meV and $(\omega/\Delta_d)=\pm0.15,\pm0.45,\pm75$, up and down from left to right; (b) $\Delta_d=20$ meV and $(\omega/\Delta_d)=0.15,0.45,0.75$, from left to right. The FT-LDOS does not exhibit discernible differences in the spectral characteristics except the total intensities if we simply replace $V_y$ by $V_y$ and assume nonmagnetic coherence factors in Eq. (3).

FIG. 3. Real-space quasiparticle LDOS for a (400×400) area at $T=0$ due to scattering by (a) nonmagnetic point impurities, (b) pinned CDW, and (c) pinned SDW for $\Delta_d=40$ meV and $\omega=30$ meV.

FIG. 4. Evolution of the relative intensities of FT-LDOS with energy $(\omega)$ for $q_A$, $q_B$, and $q_C$ as defined in Fig. 1(c) and $V_y$, $V_m$, and $V_0$ all taken to be unity: quasiparticle scattering by (a) single nonmagnetic point impurity and (b) single magnetic point impurity.

FIG. 5. The FT-LDOS maps at $T=0$, 0.75$T_c$, and $T_c$ (from left to right) for (a) point impurities $V_{\bar{p}}(q)$ and (b) pinned SDW $V_{\bar{p}}(q)$. We assume $\Delta_d(T)=\Delta_d(0)[1-(T/T_c)^{1/2}]^{1/2}$, $\Delta_d(0)=40$ meV, tunneling biased voltage $=18$ mV, and $T_c=80$ K. Besides temperature-dependent coherence factors, the thermal smearing of quasiparticle tunneling conductance $(dI/dV)$ is obtained by using $(dI/dV)= \int f(E)(dI/dE)|_{E-V_m,dE}|$, where $f(E)$ denotes the Fermi function. (c) $|q_{\bar{A}}|$-vs-V (biased voltage) dispersion relation for pinned SDW at $T=0$ and $T_c$. The relevance of collective modes become indisputable when we consider the temperature dependence of the FT-LDOS. As shown in Fig. 5(a), in the limit of $T\rightarrow T_c^-$, the $q$ values contribute to the FT-LDOS map become significantly extended and smeared for point-impurity scattering. In contrast, pinned SDW yields strong intensities in the FT-LDOS map above $T_c$. Although our simplified model cannot exclude CDW, we note that pinned CDW would have coupled directly to the quasiparticle spectra and resulted in stripelike periodic local conductance modulation, which has not been observed in STM studies. On the other hand, various puzzling phenomena seem reconcilable with the SDW scenario. For instance, the nanoscale gap variations observed in Bi-2212 (Ref. 31) may be understood by noting that the LDOS in regions with disorder-pinned SDW con-
tains information of disorder potential coupled with quasiparticles and SDW, so that the humplike spectral features at \( \pm \Delta^* \) represent neither the SDW gap nor the superconducting gap \( \Delta_g \), and the values of \( \Delta^* \) vary in accordance with the disorder potential. The long-range spatial homogeneity of quasiparticle spectra in YBa\(_2\)Cu\(_3\)O\(_7\) (YBCO) (Ref. 35) as opposed to the strong spatial inhomogeneity in Bi-2212 can also be reconciled in a similar context. That is, SDW can be much better pinned in extreme two-dimensional cuprates like Bi-2212 than in more three-dimensional cuprates such as YBCO. Furthermore, SDW can be stabilized by magnetic fields,\(^{23,24,36}\) which naturally account for the checkerboard-like spectral modulations around the vortex cores of Bi-2212.\(^{19,37}\) Finally, the smooth evolution of the pseudogap phase with temperature through \( T_c \) may contribute to the anomalously large Nernst effect under a \( c \) axis magnetic field above \( T_c \),\(^{38}\) with spin fluctuations responsible for the excess entropy.

In summary, we employ first-order \( T \)-matrix approximation to study modulations in the quasiparticle FT-LDOS of cuprates as a function of energy, momentum, and temperature. Our results suggest that a full account for all aspects of experimental observation below \( T_c \) must include collective modes as relevant low-energy excitations besides quasiparticles, and that only collective modes can account for the observed FT-LDOS above \( T_c \).

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33 For coexisting superconductivity and CDW, \( V_\delta(q) \) represents the second-order effect of quasiparticle interference with pinned CDW. The first-order effect of CDW has been discussed in Ref. 25.