

Spin collective mode and quasiparticle contributions to STM spectra of d -wave superconductors with pinning

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Abstract

We present additional details of the scanning tunneling microscopy (STM) spectra predicted by the model of pinning of dynamic spin collective modes in d -wave superconductor proposed by Polkovnikov *et al.* (Phys. Rev. B **65**, 220509 (2002)). Along with modulations at the twice the wavevector of the spin collective mode, the local density of states (LDOS) displays features linked to the spectrum of the Bogoliubov quasiparticles. The former is expected to depend more strongly on an applied magnetic field or the doping concentration. The spin collective mode and the quasiparticles are distinct, co-existing, low energy excitations of the d -wave superconductor (strongly coupled only in some sectors of the Brillouin zone), and should not be viewed as mutually exclusive sources of LDOS modulation.

Key words: spin density wave; superconductivity; pinning; quasiparticles

1. Introduction

The observation of a halo of checkerboard modulation in the local density of states (LDOS) around magnetic field-induced vortex cores by Hoffman *et al.* [1] in optimally doped $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$ has focused attention on the nature of the spin and charge collective modes in the cuprate superconductors. Charge order in this region was anticipated theoretically [2,3,4]. By ‘charge order’ we mean here periodic spatial modulations of all local observables invariant under spin rotations and time-reversal, such as the exchange and pairing energies, and the LDOS itself. If the modulation is primarily on quantities defined on a bond, rather than in the charge density on a site, then such order is better denoted as ‘bond order’; it was this bond order which was theoretically anticipated [2,4]. The general connection relating such charge/bond order to the ‘square’ of collinear, non-bipartite, spin correlations [5,6,7,8] (see Section 2 below) was used to develop a model [9,10,11]

relating the spatial structure and energy spectrum of the charge order to the *dynamic* spin fluctuation spectrum as measured by neutron scattering [12,13,14,15]. There have also been other discussions of competing order within vortex cores, including enhanced dynamic antiferromagnetism in a spin-gap state [16,17], static Néel order [18], and other models with static spin density wave order [19,20,21,22,23,24].

More recent measurements of Howald *et al.* [25] have shown that the LDOS modulations in the vortex halo also persists in zero magnetic field, albeit with a much weaker amplitude: here the pinning of the charge/bond order is presumably due to impurities and other imperfections in the $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$ crystal. Theoretical modeling of the STM spectrum has indicated [26,27] that the order is likely to be primarily on bond variables, as may be derived from a spin-Peierls state [28], *i.e.* a *bond order wave* [29]. This is in contrast to the prediction of a charge density modulation on the Cu sites in the anti-phase domain wall picture of ‘stripes’ [6,7,8], which is not observed [25].

Hoffman *et al.* [30] have also reported related mea-

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measurements in zero magnetic field, and have focused attention on modulations of the LDOS at wavevectors throughout the Brillouin zone, and on their dispersion as a function of energy. They have identified some wavevectors with quasiparticle excitations of the superconductor scattered by random impurities, as suggested in Refs.[31,32].

The purpose of the present paper is to discuss the relationship between the quasiparticle and collective mode contributions to the LDOS modulations in a d -wave superconductor. We will use precisely the model proposed earlier by Polkovnikov *et al.* [11] for the pinning of the spin collective mode: we show that the earlier expressions for the induced LDOS modulations also contain additional contributions which can be interpreted as those due to quasiparticle scattering, with a spectrum related to observations [30]. The relative strength of the collective and quasiparticle contributions can be varied by changing the gap to the spin collective mode: experimentally the gap can be reduced (and the collective mode contribution enhanced) by lowering the doping or by applying a magnetic field [3], and this should allow a test of our predictions. Some related observations have also been made independently by Han [33]. Our main conclusion is that the LDOS modulations observed by STM contain contributions from both the spin collective mode and the quasiparticles: as described in our simple model [11], these are relatively independent low energy excitations of the BCS superconductor, but they can become strongly coupled in some sectors of the Brillouin zone if permitted by energy and wavevector conservation [34]; they should not be viewed as mutually exclusive sources of LDOS modulations.

2. Model

We assume the cuprate superconductor has a dominant spin collective mode near the wavevectors $\mathbf{K}_x = (3\pi/4, \pi)$ and $\mathbf{K}_y = (\pi, 3\pi/4)$, and so write for the spin operator on the lattice site \mathbf{r} at imaginary time τ

$$S_\alpha(\mathbf{r}, \tau) = \text{Re} \left[e^{i\mathbf{K}_x \cdot \mathbf{r}} \Phi_{x\alpha}(\mathbf{r}, \tau) + e^{i\mathbf{K}_y \cdot \mathbf{r}} \Phi_{y\alpha}(\mathbf{r}, \tau) \right], \quad (1)$$

where $\Phi_{x,y\alpha}$ are the spin density wave (SDW) order parameters which are assumed to be smooth functions of spacetime. As an aside, and for completeness, we mention that charge/bond order parameters can also be constructed out of the $\Phi_{x,y\alpha}$. We define

$$\begin{aligned} Q_{\mathbf{a}}(\mathbf{r}, \tau) &\equiv S_\alpha(\mathbf{r}, \tau) S_\alpha(\mathbf{r} + \mathbf{a}, \tau) \\ &\approx \text{Re} \left[e^{2i\mathbf{K}_x \cdot \mathbf{r} + i\mathbf{K}_x \cdot \mathbf{a}} \Phi_{x\alpha}^2(\mathbf{r}, \tau) \right] + \dots \end{aligned} \quad (2)$$

where \mathbf{a} is a vector representing a bond (say the nearest neighbor vector), we have assumed that $\Phi_{x\alpha}$ does

not vary significantly over the spatial distance \mathbf{a} , and the ellipses denote numerous other similar terms which can be deduced from (1). For \mathbf{a} a nearest-neighbor vector, $Q_{\mathbf{a}}$ measures the modulations in the exchange energy, while for $\mathbf{a} = 0$, $Q_{\mathbf{a}}$ measures the local charge density (for the t - J model the charge density is linearly related to the on-site S_α^2). Thus we see from (2) that, as noted earlier, the charge/bond order parameter is proportional to the square of the SDW order parameter. In a similar manner, we will see below that the LDOS modulations are also sensitive to the square of the SDW order and so occur at wavevectors $2\mathbf{K}_{x,y}$: however our computation will include retardation effects missing from a phenomenological correspondence analogous to (2). All our computations below will be in a regime where

$$\langle S_\alpha \rangle = \langle \Phi_{x\alpha} \rangle = \langle \Phi_{y\alpha} \rangle = 0 \quad (3)$$

(because spin rotation invariance is preserved), but we will nevertheless have the rotationally invariant

$$\sum_{\alpha} \langle \Phi_{x,y\alpha}^2 \rangle \neq 0, \quad (4)$$

because translational invariance is broken by a pinning potential. This should be contrasted with the distinct physical pictures of Refs. [18,19,20,21,22,23,24] all of which break spin rotation invariance with $\langle S_\alpha \rangle \neq 0$.

To keep this paper self-contained, we now briefly describe the model used to compute the LDOS modulations; for details see Ref. [11]. The effective action for the $\Phi_{x,y\alpha}$ fluctuations is assumed to be Gaussian:

$$S_\Phi = T \sum_{\mathbf{q}, \omega_n, \alpha} \chi_x^{-1}(\mathbf{q}, \omega_n) |\Phi_{x\alpha}(\mathbf{q}, \omega_n)|^2 + (x \rightarrow y) \quad (5)$$

where ω_n are Matsubara frequencies. The $\chi_{x,y}(\mathbf{q}, \omega)$ denote the dynamic spin susceptibility as a function of wavevector \mathbf{q} (measured from the ordering wavevectors $\mathbf{K}_{x,y}$) and frequency ω , which is measured by inelastic neutron scattering. In the absence of available experimental input for $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$, we will continue to use the simple phenomenological form [11] expected near a SDW ordering quantum phase transition in a superconductor[10]: $\chi^{-1}(\mathbf{q}, \omega_n) = \omega_n^2 + c^2 \mathbf{q}^2 + \Delta^2$, where c is a spin wave velocity, and Δ is the spin gap to collective excitations near the wavevectors $\mathbf{K}_{x,y}$ (we have assumed $\chi_x = \chi_y \equiv \chi$ for simplicity). Han [33] has used the same model, but with microscopic computations on the lattice t - J model as input for χ .

The all-important ingredient which produces an observable *static* modulation in the STM signal is the pinning of the sliding degree of freedom of the SDW fluctuations. This pinning is realized by any imperfection (impurity, vortex core, etc.) which breaks the lattice translational symmetry. We employ the simplest pos-

sible pinning term which is invariant under the SU(2) spin symmetry,

$$S_{\text{pin}} = - \sum_{\alpha} \int d\tau [\zeta_{\alpha} \Phi_{x\alpha}^2(\mathbf{r}_0, \tau) + (x \rightarrow y) + c.c.], \quad (6)$$

where $\zeta_{x,y}$ are complex coupling constants representing the pinning potential.

The electronic quasiparticles of the d -wave superconductor are described by a standard BCS model:

$$H_{\text{BCS}} = \sum_{\mathbf{k}} \Psi_{\mathbf{k}}^{\dagger} [(\varepsilon_{\mathbf{k}} - \mu)\tau^z + \Delta_{\mathbf{k}}\tau^x] \Psi_{\mathbf{k}}. \quad (7)$$

Here $\Psi_{\mathbf{k}} = (c_{\mathbf{k}\uparrow}, c_{-\mathbf{k}\downarrow}^{\dagger})$ is a Nambu spinor at momentum $\mathbf{k} = (k_x, k_y)$, $\tau^{x,y,z}$ are Pauli matrices in particle-hole space, and μ is a chemical potential. For the kinetic energy, $\varepsilon_{\mathbf{k}}$ we have first (t) and second (t') neighbor hopping, and the gap function is $\Delta_{\mathbf{k}} = (\Delta_0/2)(\cos k_x - \cos k_y)$. The full Hamiltonian for the conduction electrons includes a coupling to the collective SDW fluctuations:

$$H = H_{\text{BCS}} + \gamma \sum_{\mathbf{r}} c_{\mu}^{\dagger}(\mathbf{r}) \sigma_{\mu\nu}^{\alpha} c_{\nu}(\mathbf{r}) \times \\ \times (\Phi_{x\alpha}(\mathbf{r}) e^{i\mathbf{K}_x \cdot \mathbf{r}} + \Phi_{x\alpha}^*(\mathbf{r}) e^{-i\mathbf{K}_x \cdot \mathbf{r}} + (x \rightarrow y)), \quad (8)$$

where σ^{α} are the Pauli spin matrices, and γ describes the scattering of the Bogoliubov quasiparticles of the superconductor off the SDW fluctuations.

The predictions of this model [11] for the quasiparticle LDOS, to second order in the quasiparticle-collective mode coupling γ and to first order in the pinning strength ζ , can be written as

$$\delta\rho(\mathbf{r}, \omega) \approx \text{Im} \text{Tr} \frac{1 + \tau_z}{2} \times \\ \sum_{\mathbf{r}_1, \mathbf{r}_2} G_0(\mathbf{r} - \mathbf{r}_1, \omega) \Sigma(\mathbf{r}_1, \mathbf{r}_2, \omega) G_0(\mathbf{r}_2 - \mathbf{r}, \omega), \quad (9)$$

where G_0 is the electronic Green's function in the canonical translationally invariant BCS superconductor described by (7). There is a contribution to the self energy $\Sigma = \Sigma_{\text{sp}}$ from the coupling to the spin collective mode, and we focus only on the part which breaks translational invariance because of the pinning of the collective mode

$$\Sigma_{\text{sp}}(\mathbf{r}_1, \mathbf{r}_2, \omega) \approx 12\zeta\gamma^2 \int \frac{d\nu}{2\pi} \chi(\mathbf{r}_2, \nu) \chi(\mathbf{r}_1, \nu) \\ \times G_0(\mathbf{r}_2 - \mathbf{r}_1, \omega - \nu) \cos(\mathbf{K}_x \cdot (\mathbf{r}_1 + \mathbf{r}_2) - \delta) \\ + (x \rightarrow y). \quad (10)$$

The parameter δ , which is the phase of the coupling ζ , distinguishes site centered SDWs ($\delta = 0$) and bond centered SDWs ($\delta = \pi/2$). Following the STM experiments [1,25,30], we will compute the Fourier transform of the LDOS:

$$\delta\rho_{\text{sp}}(\mathbf{q}, \omega) = \text{Tr} \frac{1 + \tau_z}{4} \left\{ \text{Im} \int \frac{d^2k}{(2\pi)^2} G_0(\mathbf{k}, \omega) \times \right. \\ \left. [\Sigma_{\text{sp}}(\mathbf{k}, \mathbf{k} + \mathbf{q}, \omega) + \Sigma_{\text{sp}}(-\mathbf{k}, -\mathbf{k} - \mathbf{q}, \omega)] G_0(\mathbf{k} + \mathbf{q}, \omega) \right. \\ \left. - i \text{Re} \int \frac{d^2k}{(2\pi)^2} G_0(\mathbf{k}, \omega) [\Sigma_{\text{sp}}(\mathbf{k}, \mathbf{k} + \mathbf{q}, \omega) - \right. \\ \left. - \Sigma_{\text{sp}}(-\mathbf{k}, -\mathbf{k} - \mathbf{q}, \omega)] G_0(\mathbf{k} + \mathbf{q}, \omega) \right\}. \quad (11)$$

Note that the imaginary part of this expression vanishes in the presence of inversion symmetry, $\delta\rho(\mathbf{r}, \omega) = \delta\rho(-\mathbf{r}, \omega)$. The results (10,11) are for a single pinning center, and the realistic many impurity case will be similar provided interference between impurities is small.

It is not difficult to see from (9-11) that in the limit of a large spin gap ($\Delta \rightarrow \infty$), the modulations in the LDOS predicted by (11) are identical to those predicted in a model of quasiparticle scattering off isolated, point-like static impurities or other imperfections considered in Ref. [32]. For a general scattering potential $u(\mathbf{q})$, and impurity-induced variation in the superconducting gap $v(\mathbf{q}_1, \mathbf{q}_2)$, the expression for the LDOS modulation due to *static* impurities in the Born approximation, $\delta\rho_{\text{imp}}(\mathbf{q}, \omega)$, is formally identical to Eq. (11) with Σ_{sp} replaced by

$$\Sigma_{\text{imp}}(\mathbf{k}, \mathbf{k} + \mathbf{q}, \omega) = u(\mathbf{q})\tau_z + v(\mathbf{k}, \mathbf{k} + \mathbf{q})\tau_x. \quad (12)$$

The following section will compare the predictions of (12) to those in (11) of a pinned dynamic SDW with a finite Δ .

It is interesting to note from (11,12) that for any real scattering potential, with $u^*(\mathbf{q}) = u(-\mathbf{q})$, the LDOS modulation at wavevector \mathbf{q} is determined by $\int d^2k \text{Im} [G_0(\mathbf{k}) G_0(\mathbf{k} + \mathbf{q}, \omega)]$. Contributions proportional to $\int d^2k \text{Im} [G_0(\mathbf{k})] \text{Im} [G_0(\mathbf{k} + \mathbf{q}, \omega)]$, which are used by Ref. [32] to explain the STM observations of Refs. [30,35], can only come from lifetime effects which produce a complex self energy.

3. Results

Sample results from the dynamic SDW model (11) are shown in Figs 1-3. For small spin gap Δ , the LDOS shows the expected [5,9] modulations near $\mathbf{q} = 2\mathbf{K}_{x,y}$. The magnitude of this modulation depends strongly on the value of Δ , and the strong expected dependence of Δ on doping and applied magnetic field [3] (Δ decreases with decreasing δ and increasing field) will lead to a corresponding variation in the LDOS peaks near $\mathbf{q} = 2\mathbf{K}_{x,y}$. This peak also disperses as a function of ω , with the dispersion being stronger for larger values of Δ as shown in Fig. 3; the decrease in the \mathbf{q} value of the peak with increasing ω is consistent with observations [30].

As is clear from Figs. 1 and 2, the LDOS also has peaks in its modulation at a number of other wavevec-

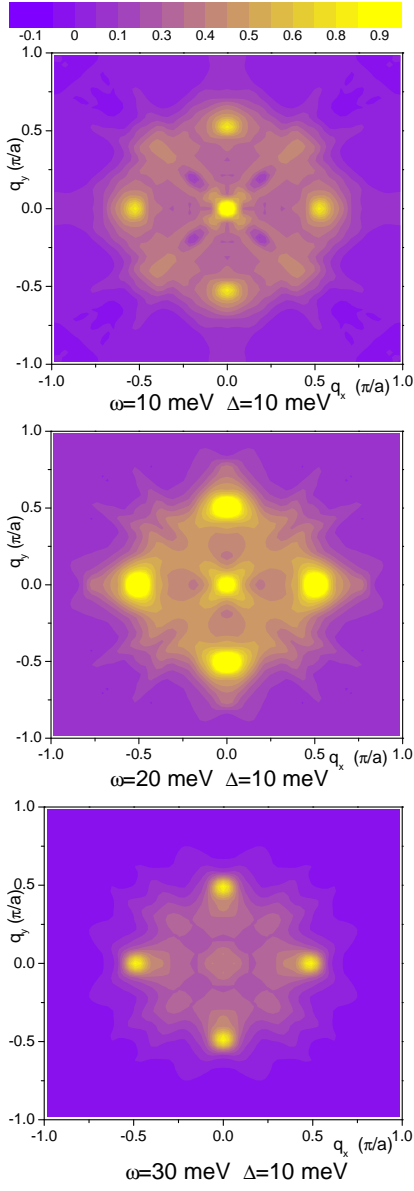


Fig. 1. Fourier map of the LDOS $\delta\rho_{sp}(\mathbf{q}, \omega)$ in (11) for $\Delta = 10$ meV and quasiparticle dispersion $\varepsilon_{\mathbf{k}}$ and pairing amplitude $\Delta_{\mathbf{k}}$ chosen as in Ref. [11]. The maxima around $(\pi/2, 0)$ come mainly from scattering off a pinned SDW. The other peaks are due to details of quasiparticle spectrum.

tors. These arise from the two flanking quasiparticle Green's functions in (11), and are consequently sensitive to all details of quasiparticle spectrum. These additional features are also present in the static impurity model (12) whose results are shown in Fig. 4. It is instructive to compare the static impurity scattering prediction in Fig 4 to the dynamic spin collective mode predictions in Figs. 1 and 2: apart from the strong contributions at $\mathbf{q} = \pm 2\mathbf{K}_{x,y}$ present in the latter, the for-

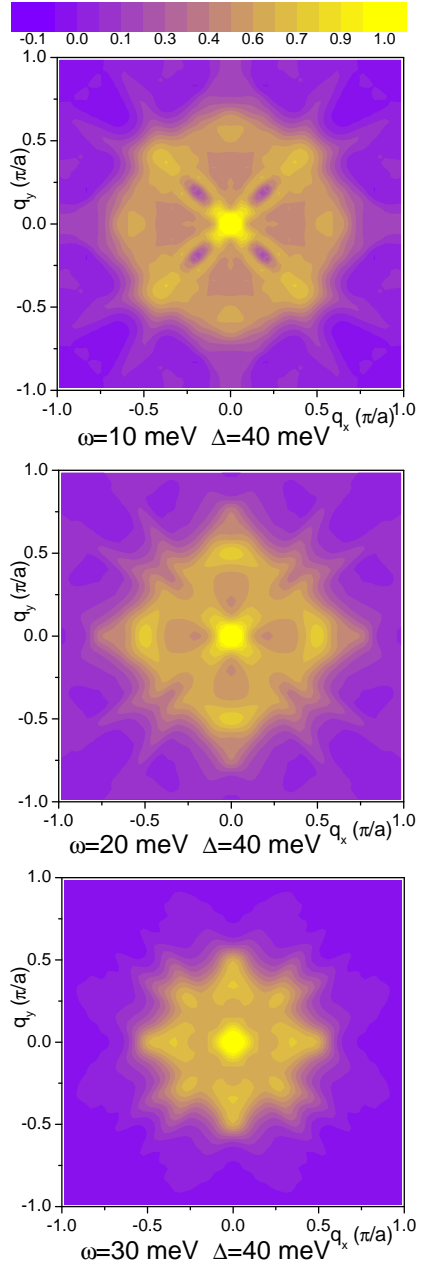


Fig. 2. As in fig. 1 for $\Delta = 40$ meV.

mer has the same general features as the large Δ cases of the latter. This is one of the main points of this paper.

The physics of the structure in the static impurity scattering LDOS modulation, $\delta\rho_{imp}(\mathbf{q}, \omega)$ in (12), has already been discussed by Wang and Lee [32]. Assuming spatial inversion symmetry, the expression (12) can be rewritten as:

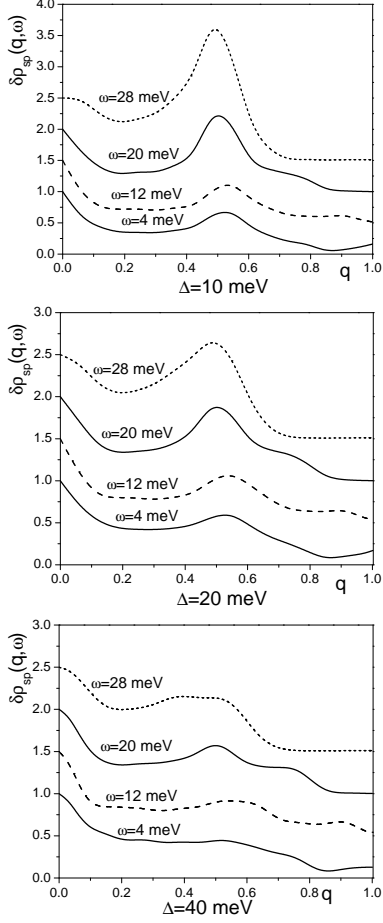


Fig. 3. Fourier component of the LDOS, $\delta\rho_{sp}(\mathbf{q}, 0)$, for $\mathbf{q} = (q\pi/a, 0)$; a large contribution near $q = 0$ is not shown.

$$\delta\rho_{imp}(\mathbf{q}, \omega) = 2 \int \frac{d^2k}{(2\pi)^2} \delta(-\omega^2 + \varepsilon_{\mathbf{k}}^2 + \Delta_{\mathbf{k}}^2) \times \left(u(\mathbf{q}) \frac{(\omega - \varepsilon_{\mathbf{k}})(\omega - \varepsilon_{\mathbf{k}+\mathbf{q}}) - \Delta_{\mathbf{k}}\Delta_{\mathbf{k}+\mathbf{q}}}{-\omega^2 + \varepsilon_{\mathbf{k}+\mathbf{q}}^2 + \Delta_{\mathbf{k}+\mathbf{q}}^2} - v(\mathbf{k}, \mathbf{k} + \mathbf{q}) \frac{(\omega - \varepsilon_{\mathbf{k}})\Delta_{\mathbf{k}+\mathbf{q}} + \Delta_{\mathbf{k}}(\omega - \varepsilon_{\mathbf{k}+\mathbf{q}})}{-\omega^2 + \varepsilon_{\mathbf{k}+\mathbf{q}}^2 + \Delta_{\mathbf{k}+\mathbf{q}}^2} \right). \quad (13)$$

This expression is not a convolution of the product of the density of states of quasiparticles at energy ω with momenta differing by \mathbf{q} , but rather the product of the density of states of one quasiparticle with the real part of the Green function of the other. It contains weak logarithmic divergences at special nesting wavevectors, but this is barely visible in our plots; it has been claimed [32] that the structure at these wavevectors could be enhanced for strong impurity scattering in a description beyond the Born approximation. Instead, in Fig 4, the main contributions for \mathbf{q} along the Brillouin zone diagonals come from values of \mathbf{k} and $\mathbf{k} + \mathbf{q}$ near the nodal points and the underlying Fermi

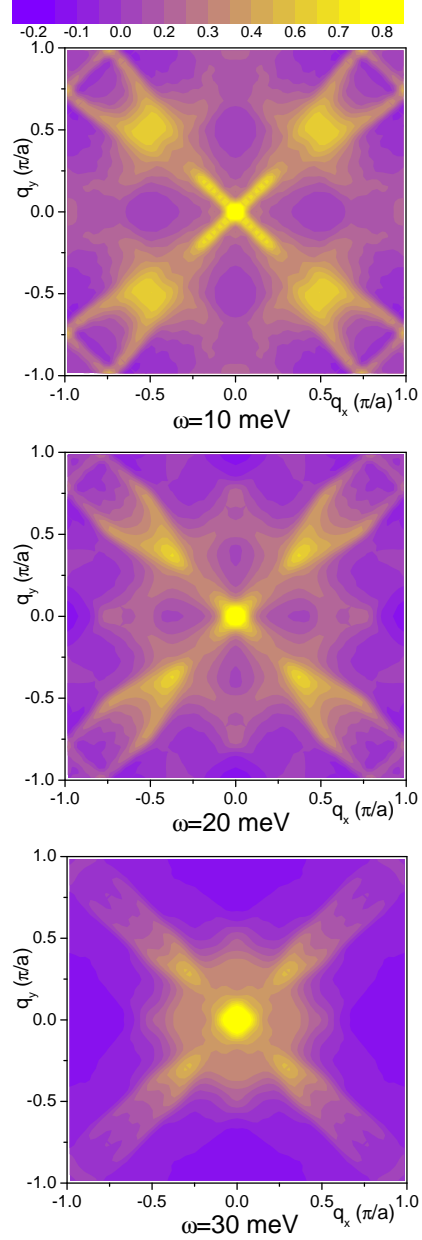


Fig. 4. Fourier map of LDOS for scattering off a single localized defect, $\delta\rho_{imp}(\mathbf{q}, \omega)$ in (12). We used a localized defect with $u(\mathbf{q}) = 1$, $v(\mathbf{k}, \mathbf{k} + \mathbf{q}) = 2 \cos(k_x + q_x) - 2 \cos(k_y + q_y)$.

surface near $\pm(\pi, 0), \pm(0, \pi)$ respectively. We emphasize that both these features of quasiparticle-scattering induced LDOS modulations also appear in our model [11] of a pinned dynamic spin collective mode. In particular, as we noted earlier, if Δ is large, then the pinned SDW model is equivalent to an effective short-range static quasiparticle potential, along with additional weak modulations at $\pm 2\mathbf{K}_{x,y}$ (compare Figs 2, and 4). For smaller Δ , the effective quasiparticle poten-

tial created by the SDW fluctuations is dynamic, but the qualitative picture at wavevectors different from $\pm 2\mathbf{K}_{x,y}$ remains the same.

In conclusion, we have shown that the model of Ref [11] displays many of the features observed in recent STM experiments. Besides the modulations of the LDOS at wavevectors $\pm 2\mathbf{K}_{x,y}$ arising from the spin collective mode, we find other features related to the spectrum of the fermionic Bogoliubov quasiparticles (similar physics is also expected from a possible charge/bond order collective mode). The positions of the maxima at $\pm 2\mathbf{K}_{x,y}$ have a relatively small (but not negligible) dependence on the tunnelling energy ω , while other features are more strongly dependent on ω and the details of the quasiparticle spectrum. We have also made predictions on the doping and magnetic field dependence of the relative contributions of the quasiparticle and spin-collective mode induced modulations.

Note added: Some related points and observations appear in [36].

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