

Fourier Transformed Scanning Tunneling Peaks in the d -density wave phase

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In this brief note we repeat an earlier calculation of the Fourier transformed scanning tunneling spectra of the d -density wave (DDW) phase using a different band structure, which is more realistic and consistent with the angle resolved photoemission spectroscopy (ARPES) data. We note that four peaks, which used to be located at $(\pm\pi/4, 0)$ and $(0, \pm\pi/4)$, are still present, but at positive energies their wavevectors shift to the neighborhood of $(\pm 2\pi/5, 0)$, $(0, \pm 2\pi/5)$ and slowly disperse with energy. The implications for the sensitivity with respect to the band structure are discussed.

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Scanning tunneling microscopy (STM) experiments on the cuprate high-temperature superconductors give unique information about the local short-distance electronic structure of these materials. Careful analysis of this information can yield insights into the nature of the superconducting state^{1,2,3} (including, or perhaps especially, in the presence of vortices⁴) and also into the short and meso-scale structure that must develop as a precursor to superconductivity. Recently, it has even been possible to perform such experiments in the pseudogap regime above T_c ⁵ and also to study their doping dependence in the superconducting state.⁶ These experiments give us a window on the gap (or depletion of low-energy states) which is present in these materials and on its variation from place to place in a given sample. One striking aspect of all of these measurements is the presence of peaks in the Fourier transform of the local electronic density of states (LDOS) at wavevectors $(\pm 2\pi/\lambda, 0)$, and $(0, \pm 2\pi/\lambda)$, where the wavelength λ is between 4 and 7 lattice spacings.⁶ This problem has been analyzed from a variety of theoretical perspectives^{7,8,9,10,11,12,13,14,15,16,17,18}.

One class of proposed explanations of the pseudogap state of the cuprates is that it is due to spontaneous symmetry breaking which occurs below the pseudogap scale $T^*(x)$ so long as the doping is less than some critical value x_c (and, presumably, larger than some minimum value). According to one proposal²⁰, the broken-symmetry state has d -density wave (DDW) order and the pseudogap appears to be ‘pseudo’ only because this order parameter is difficult to observe directly. Nevertheless, some elastic polarized neutron scattering experiments²¹ seem to have observed this order directly in underdoped YBCO (although other similar experiments, but using unpolarized neutrons, have not found it²²). Furthermore, superfluid density, ARPES, Hall number, and infrared Hall angle measurements^{23,24} which are indirect tests of the order present in the pseudogap (if any) are consistent with DDW order. Can STM measurements settle this question by directly seeing the presence or absence of DDW order? Unfortunately, no. In the DDW state, there is a lattice scale pattern of currents which are staggered from one plaquette to another. Tunneling, on the

other hand, is sensitive to the local presence or absence of charge available for tunneling. It is not sensitive to currents unless they are accompanied by charge excesses or deficits. Since DDW order breaks time reversal symmetry, defects involving spin-orbit coupling can mix charge order, as “angular momentum” is not a good symmetry in this case.

However, STM measurements can be an indirect probe of DDW order. Observable variations of the charge density can be induced by impurities. They occur at wavevectors which connect points on the contour in momentum space at which the energy is equal to the applied voltage. The peaks are strongest when the joint density of states of the two \mathbf{k} -space points is greatest. According to this picture, Fourier-transformed LDOS peaks are due to the momentum-space structure of the single-particle gap. Such an explanation gives a compelling picture of the LDOS peaks seen in the superconducting state^{2,7,8,9}. As the voltage is increased, the Fermi points expand into ovals which stretch into banana-shaped loops. The corresponding wavevectors seen in STM measurements roughly follow the evolution of these energy contours. In the pseudogap state, however, the LDOS peaks hardly disperse with energy⁵. Is this indicative of some entirely different phenomenon which is causing the peaks in the pseudogap regime?

In this note, we argue that it is not. In a recent paper¹⁰, we examined the patterns resulting from quasi-particle scattering in the Fourier transform of the local density of states for a high T_c superconductor for which we assumed that the pseudogap is described by d -density wave order. We considered a $t-t'$ band structure, and in the spectra we found peaks in the LDOS centered about $(\pm\pi/4, 0)$, $(0, \pm\pi/4)$, which dispersed slowly with energy. Here, we show that their precise k -space location and dispersion with energy are dependent on the details of the band structure. In particular, if we use a more realistic band structure than we used previously, we find LDOS peaks at positive voltage bias which are located closer to where they have been observed experimentally – in the vicinity of $(\pm 2\pi/5, 0)$, $(0, \pm 2\pi/5)$ (although their location varies with doping⁶) as opposed to the wavevectors $(\pm\pi/4, 0)$, $(0, \pm\pi/4)$ with the previous band structure –

and which disperse less. The formalism and the method of calculation are identical to those in Ref. 10. So, we shall not repeat them here. The band structure which we use is flatter near the $(\pi, 0)$ point, consistent with ARPES measurements¹⁹. It is characterized by the energy dispersion (with the lattice spacing set to unity)

$$\begin{aligned} \epsilon_k = & t_0 + t_1(\cos k_x + \cos k_y)/2 + t_2 \cos k_x \cos k_y \\ & + t_3(\cos 2k_x + \cos 2k_y)/2 + t_5 \cos 2k_x \cos 2k_y \\ & + t_4(\cos 2k_x \cos k_y + \cos 2k_y \cos k_x)/2 \end{aligned} \quad (1)$$

and $t_{0-5} = 0.1305, -0.5951, 0.1636, -0.0519, -0.1117, 0.0510$ (eV). We also take the chemical potential shift (from the above dispersion) to be $\delta\mu = -0.034$ eV. The chemical potential is chosen such that, consistent with the ARPES measurements¹⁹, no electron pockets open in the band structure. The equal energy contours for this ARPES band structure as well as for the simpler band structure used in ref. 10 in which t_3, t_4, t_5 vanish are given for comparison in Fig. 1. We focus on the case of non-magnetic impurity scattering.

Our results are plotted in Fig. 2 for energies between -42 meV and 45 meV for a pure DDW state with a gap of $W_0 = 40$ meV. These calculations are identical to those of Ref. 10. We note the appearance of peaks corresponding to scattering between the tips of the ellipses, as indicated by arrows in Fig. 1. The position of the peaks is marked by circles in Fig. 2.

The dispersion of the wavevectors with energy is plotted in Fig.3. As indicated, for positive energies, the dispersion is quite small, and the magnitude of the wavevectors ranges from $(2\pi)/6.9$ at 3 meV to $(2\pi)/4.8$ at 39 meV. The dispersion is larger for negative energies, and the peaks are not as well-defined. We also note that if one does not shift the chemical potential, while electron pockets open, the dispersion of the peaks position with energy is much smaller and thus more in agreement with the experimental results. This indicates that both the position of the peaks and their energy dispersion are very sensitive to band structure parameters.

Thus, the position of the peaks resulting from quasi-particle interference in a pure DDW with an ARPES-

consistent band structure is similar to experimental observations, while the dispersion with energy is larger. However, this is a crude single impurity scattering T-matrix approximation calculation and other factors may need to be taken into account. Electron-electron interactions have been neglected, but are likely to be important for understanding ARPES experiments²⁴ in which they smear out antinodal quasiparticles. It is hard to imagine that this would not have an impact on LDOS measurements. Furthermore, the renormalization of the order parameter due to disorder in the presence of many impurities may need to be taken into account through a self consistent Bogoliubov-de Gennes calculation²⁵.

In conclusion, we obtained the quasiparticle interference spectra in a DDW state, which would correspond to the pseudogap phase of the cuprates. We used an ARPES consistent band structure. We observed the emergence of peaks with wavevectors of magnitude $2\pi/4 - 2\pi/7$ (at positive energies) along the $(\pi, 0)$ direction. The magnitude of the wavevectors is similar to those seen in recent STM experiments in the pseudogap phase^{4,5,6}. The energy dispersion of the peaks is larger than what was observed experimentally, though other theoretical and experimental factors may need to be taken into account when trying to connect our observations to the experimental data. However, the peaks seen in STM experiments will always disperse with energy – even in the case of charge order disrupted by impurities^{11,12}. The issue at hand is the quantitative one of how much.

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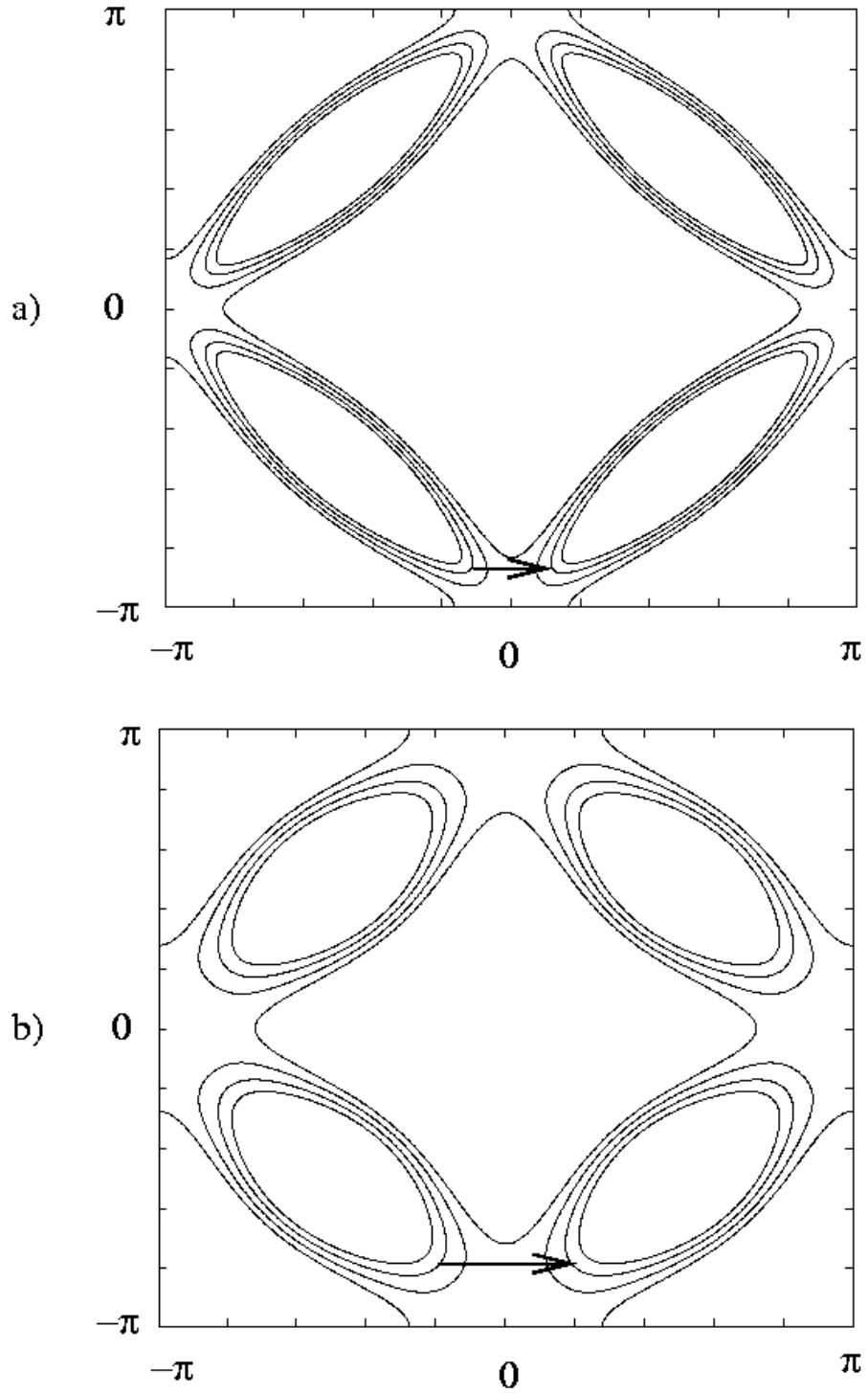


FIG. 1: Equal energy contours for the pure DDW state with a) $t-t'$ band structure b) ARPES consistent band structure. The magnitude of the DDW gap is taken to be 40meV. The innermost contour corresponds to +40meV energy, while the outermost contour corresponds to a -40meV energy. Scattering between regions of high density of states is indicated by the arrows.

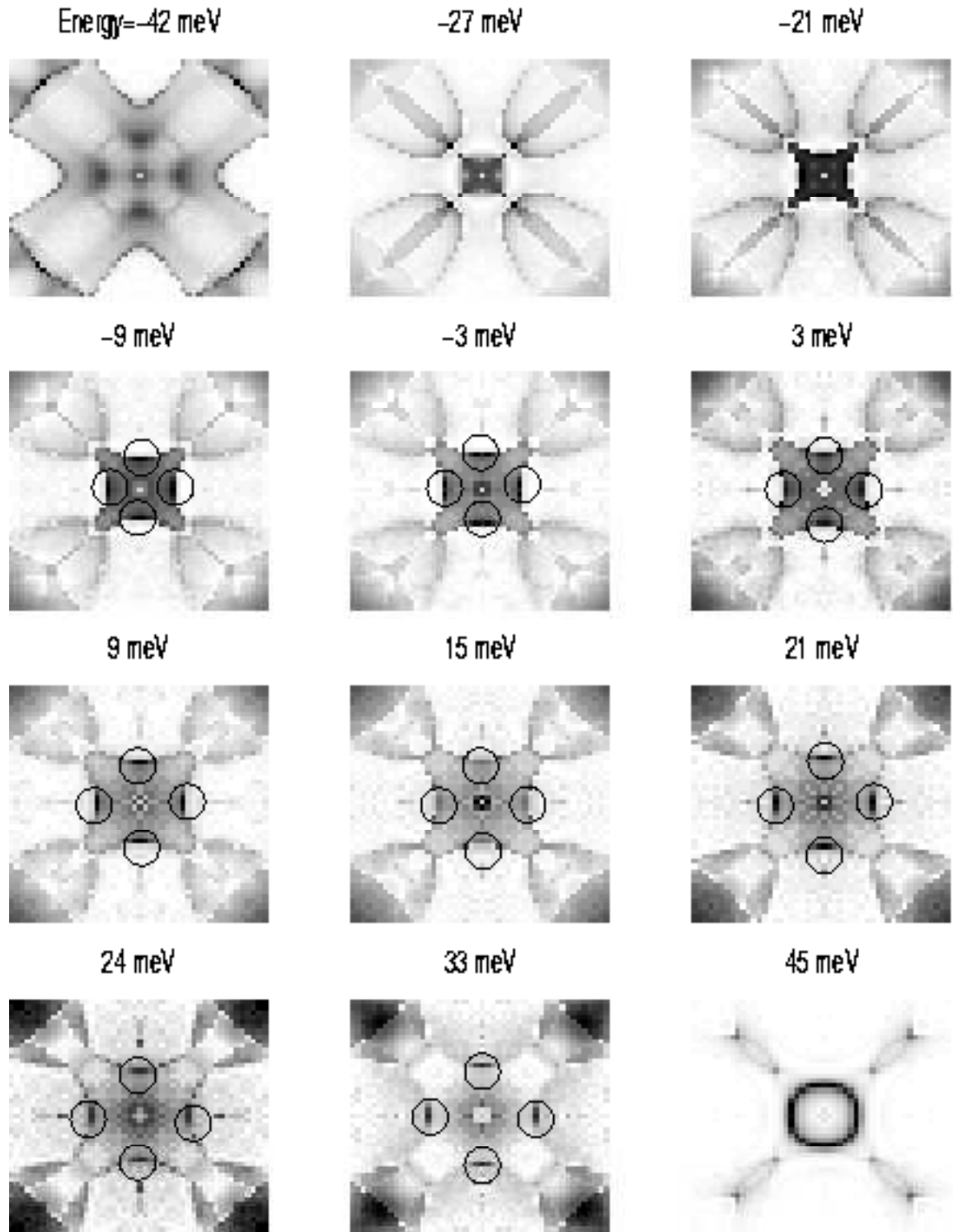


FIG. 2: Quasiparticle interference spectra for a DDW state with DDW gap of 40meV for non-magnetic impurity scattering $V = 0.1eV$. The results are displayed for energies ranging from -42meV to 45meV on a linear gray scale. Each plot represents the spectral intensity as a function of momentum in the 1st BZ, for $|q_x|, |q_y| < \pi$. The positions of the peaks are indicated by circles

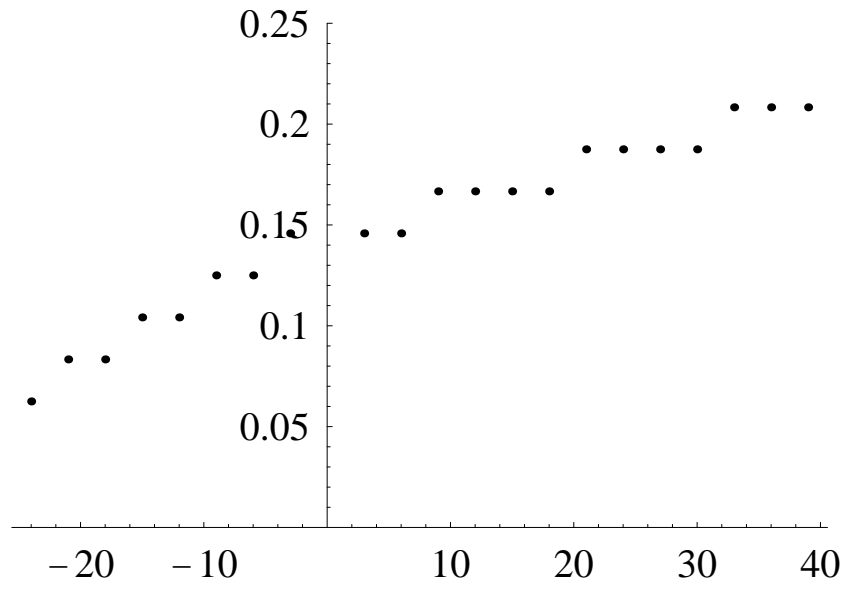


FIG. 3: The energy dispersion of the wavevectors of the observed peaks. The magnitude of the wavevectors is plotted in units of 2π , and the energy is measured in meV . The magnitude of the DDW gap is $40meV$.