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Angle-resolved photoemission spectra in the cuprates from the *d*-density wave theory

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Angle-resolved photoemission spectra present two challenges for the *d*-density wave theory of the pseudogap state of the cuprates: (1) Hole pockets near $(\pi/2,\pi/2)$ are not observed, in apparent contradiction with the assumption of translational symmetry breaking, and (2) There are no well-defined quasiparticles at the *antinodal* points, in contradiction with the predictions of mean-field theory of this broken-symmetry state. Here, we show how these puzzles can be resolved.

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At first glance, the *d*-density wave (DDW) proposal for the pseudogap state of the cuprates[1] seems to naturally explain the principal anomaly in photoemission spectra in this state: the existence of a gap with $d_{x^2-y^2}$ symmetry without superconductivity. However, since DDW order breaks translational symmetry, thereby splitting the Brillouin zone into two magnetic Brillouin zones, the Fermi surface in the first magnetic Brillouin zone should be duplicated in the second magnetic Brillouin zone. Thus, the Fermi surface consists of hole pockets, which is of importance in understanding a number of experiments, such as superfluid density,[2] Hall number,[3] etc. However, in angle-resolved photoemission spectroscopy (ARPES) in hole doped cuprates, Fermi arcs, not hole pockets, are observed.[4] There is spectral weight in the first, but not the second magnetic zone. In this paper, we show from a careful analysis that Fermi arcs rather than hole pockets are indeed the consequences of the DDW theory in ARPES.

A second important aspect of the proposal of a broken-symmetry state, even one of an unusual variety, is that it is expected to support electronic quasiparticles which are essentially Fermi-liquid-like, as they are in a BCS superconductor. However, from ARPES in underdoped samples no peak is observed at the antinodal points in the normal state, but one appears in the superconducting state upon cooling.[4] This observation also finds a natural explanation within our theory.[5] We show that the antinodal quasiparticles, being relatively high-energy excitations, decay by creating particle-hole pairs along the Fermi arcs in the DDW state. In contrast, in the *d*-wave superconducting (DSC) state, or in the coexisting DDW and DSC state, the Fermi arcs shrink to points, and the decay rate is considerably reduced, resulting in a peak in the spectral function. This reduction is bolstered by the suppression of the decay matrix element by the superconducting coherence factors.

The explanation discussed here involves interaction between quasiparticles, whose absolute magnitude is set by a reasonable Hubbard-like interaction of magnitude 1.5 eV, but the precise magnitude is of not much consequence. There may be other sources of broadening of the quasiparticle peak, including fluctuation effects, bilayer splitting, fractionalization, etc., which we do not address here. We merely wish to point out that within the simplest mean-field picture of DDW, there are *no* obvious puzzles.

In our mean-field analysis, and indeed in many theories, the nodal quasipartcles, or excitations at the Fermi arcs, should in principle be *sharp*, which is not entirely in keeping with ARPES, although a fairly well-defined peak is observed both above and below the superconducting transition temperature T_c. It remains to be seen if the present experimental situation changes with time or not.

To establish our notation, we begin with a brief summary of the mean-field theory of DDW. The Hamiltonian $\mathcal{H}$ can be simply written in the first magnetic zone by introducing the Pauli matrices σ_x and σ_z, the identity matrix $\mathbb{I}$, a row vector $\Psi^\dagger_{\mathbf{k},\alpha}\equiv(c^\dagger_{\mathbf{k},\alpha}, -ic^\dagger_{\mathbf{k}+\mathbf{Q},\alpha})$, and its Hermitian adjoint. The electron destruction operators of momentum $\mathbf{k}$ and spin α are $c_{\mathbf{k},\alpha}$ and the momentum $\mathbf{Q}=(\pi,\pi)$. Thus, $\mathcal{K}=\mathcal{H}-\mu\mathcal{N}$ is given by

$$\mathcal{K}=\sum_{\mathbf{k},\alpha}\Psi^\dagger_{\mathbf{k},\alpha}[(\epsilon^+_{\mathbf{k}}-\mu)\mathbb{I}+\epsilon^-_{\mathbf{k}}\sigma_z+W_{\mathbf{k}}\sigma_x]\Psi_{\mathbf{k},\alpha}. \quad (1)$$

Here μ is the chemical potential and $\mathcal{N}$ is the number operator. Note that $\mathcal{K}$ is complex Hermitian, reflecting broken time-reversal symmetry. In the first magnetic zone, it is convenient to define $\epsilon^\pm_{\mathbf{k}}=\frac{1}{2}[\epsilon_{\mathbf{k}}\pm\epsilon_{\mathbf{k}+\mathbf{Q}}]$, where $\epsilon_{\mathbf{k}}$ is the electronic band structure. A standard Bogoliubov transformation diagonalizes the Hamiltonian, but since $\mathbb{I}$ commutes with σ_x and σ_z, $(\epsilon^+_{\mathbf{k}}-\mu)$ cannot enter the coherence factors, which are

$$\left.\begin{matrix}u^2_{\mathbf{k}}\\ v^2_{\mathbf{k}}\end{matrix}\right\}=\frac{1}{2}\left(1\pm\frac{\epsilon^-_{\mathbf{k}}}{E_{\mathbf{k}}}\right), \quad (2)$$

where $E_{\mathbf{k}}=\sqrt{(\epsilon^-_{\mathbf{k}})^2+W^2_{\mathbf{k}}}$. The coherence factors must trade places as $\mathbf{k}\to\mathbf{k}+\mathbf{Q}$, which is a consistency check as to why they cannot be functions of $(\epsilon^+_{\mathbf{k}}-\mu)$. The energy eigenvalues are

$$E^\pm_{\mathbf{k}}=\epsilon^+_{\mathbf{k}}\pm E(\mathbf{k}). \quad (3)$$

The DDW gap is assumed to take the form

$$W_{\mathbf{k}}=\frac{W_0(T)}{2}(\cos k_x-\cos k_y) \quad (4)$$

The electron spectral function in a crystal need not be invariant under translation by a reciprocal lattice vector. In fact, it is weighted by the Fourier transform of the relevant

Wannier orbitals. If the Wannier orbitals are δ functions, the spectral weight is the same in all Brillouin zones. On the other hand, if the Wannier orbital is spread out spatially, then the spectral weight in higher Brillouin zones will be very small, and $I(\omega,\mathbf{k}+\mathbf{G})\ll I(\epsilon,\mathbf{k})$, where $I(\epsilon,\mathbf{k})$ is the angle-resolved photoemission intensity. In the DDW state, the unit cell has been doubled. The coherence factors $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ tell us how the two sites within the unit cell are superposed, so $v_{\mathbf{k}}/u_{\mathbf{k}}$ plays the role of the Wannier function. The corresponding spectral function in the DDW state is

$$\frac{A(\omega,\mathbf{k})}{2\pi}=u_{\mathbf{k}}^2\delta(\omega-E_{\mathbf{k}}^{+}+\mu)+v_{\mathbf{k}}^2\delta(\omega-E_{\mathbf{k}}^{-}+\mu). \quad (5)$$

Consider $\mu<0$, the case of hole doping, such that the chemical potential lies entirely in the valence band, so that $E_{\mathbf{k}}^{+}-\mu>0$. Then the ARPES intensity is

$$I(\omega,\mathbf{k})\propto n_F(\omega)v_{\mathbf{k}}^2\,\delta(\omega-E_{\mathbf{k}}^{-}+\mu). \quad (6)$$

Since $v_{\mathbf{k}+\mathbf{Q}}=u_{\mathbf{k}}$, the photoemission intensity in the first and second magnetic zones differ only by the following coherence factors:

$$I(\omega,\mathbf{k})\propto n_F(\omega)v_{\mathbf{k}}^2\,\delta(\omega-E_{\mathbf{k}}^{-}+\mu), \quad (7)$$

$$I(\omega,\mathbf{k}+\mathbf{Q})\propto n_F(\omega)u_{\mathbf{k}}^2\,\delta(\omega-E_{\mathbf{k}}^{-}+\mu). \quad (8)$$

For $\mathbf{k}$ in the first magnetic zone (i.e., for $\mathbf{k}+\mathbf{Q}$ in the second magnetic zone), $u_{\mathbf{k}}$ vanishes when $W_{\mathbf{k}}$ vanishes. In other words, the photoemission intensity in the second magnetic zone vanishes along the diagonals. For wave vectors close to the diagonals, the intensity goes as $W_{\mathbf{k}}^2$. Thus, the outer section of the hole pockets will have small or even vanishing spectral weight, and may not be detected in ARPES experiments. The spectral weight at a typical point on the outer part of a hole pocket will depend on various details, including the band structure, the precise angular dependence of the DDW gap, etc.

We now provide a quantitative analysis, using a generic band structure, of the qualitative arguments given after Eqs. (7) and (8). A commonly used model for the band structure is given by

$$\epsilon_{\mathbf{k}}^{+}=4t'\cos k_x\cos k_y, \quad (9)$$

$$\epsilon_{\mathbf{k}}^{-}=-2t(\cos k_x+\cos k_y). \quad (10)$$

A generic parameter set is $t=0.3$ eV, $t'/t=0.3$, and $\mu=-0.3$ eV; with this set of parameters, the doping level is 14.3%. The Fermi surface with a typical value of $W_0(0)=0.06$ eV consists of four hole pockets as shown in Fig. 1. The corresponding $v_{\mathbf{k}}^2$ appearing in the photoemission intensity is shown Fig. 2. It is clear that only half of each hole pockets will be visible in the ARPES spectra, resulting in Fermi arcs, despite the fact that the actual Fermi surface consists of hole pockets.[6]

We now turn to a discussion of the lifetime of a quasiparticle at the antinodal region $\mathbf{k}^*$ close to $(\pi,0)$, where the free-electron Fermi surface crosses the band edge. The equation that determines $\mathbf{k}^*$ is obtained by solving

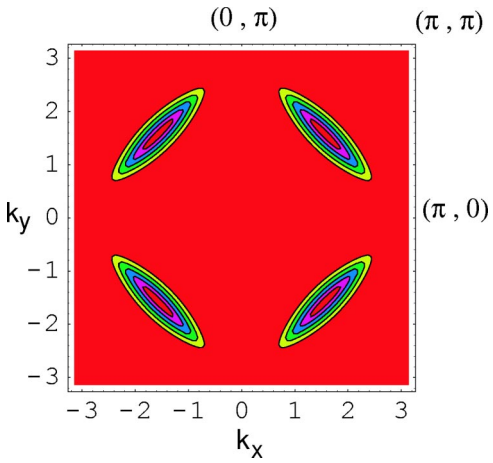

FIG. 1. (Color online) The Fermi surface for $W_0(0)=0.06$ eV. The band-structure parameters are defined in the text.

$$\epsilon_{\mathbf{k}^*}\equiv\epsilon_{\pi,k_y}^{+}+\epsilon_{\pi,k_y}^{-}=\mu \quad (11)$$

for k_y. Antinodal quasiparticles at $\mathbf{k}^*$ have an energy very close to W_0, the maximum of the DDW gap. Hence, they can scatter into a nearby wave vector while creating a particle-hole pair near the Fermi arcs (the inner section of the hole pockets). This is very different from the situation in the *d*-wave superconducting state, where there are only Fermi points, not arcs, as a result of which there is very little phase space for low-energy particle-hole pairs. Second, the density of states is enhanced at the gap edge, resulting in an abundance of available phase space into which the quasiparticle can be scattered. In the superconducting state, this density-of-states enhancement is canceled by coherence factors. These coherence factors reflect the fact that the quasiparticles are neutral, so they are only weakly scattered by interactions which are coupled to charge.

We will set up the lifetime calculation in full generality, assuming that both DDW and DSC order parameters are present, and then vary the size of the DSC order parameter. In order to more easily compare with experimental results, we will assume mean-field-like temperature dependence for the DSC gap so that we can display our results as a temperature-dependent decay rate.

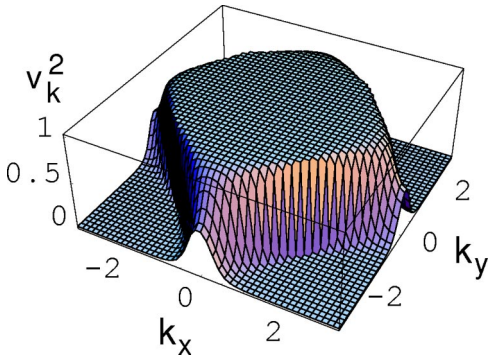

FIG. 2. (Color online) The coherence factor $v_{\mathbf{k}}^2$. The parameters are the same as in Fig. 1.

Consider an initial quasiparticle state of momentum $\mathbf{k}_1$ in the antinodal region (to be precise, $\mathbf{k}^*$ defined above) and of energy $\mathcal{E}_{\mathbf{k}_1}$, where $\mathcal{E}_{\mathbf{k}}=\sqrt{(E_-(\mathbf{k})-\mu)^2+|\Delta(\mathbf{k})|^2}$. In the pseudogap state, where the *d*-wave superconducting order parameter $\Delta=0$, $\mathcal{E}_{\mathbf{k}}=E_-(\mathbf{k})-\mu$. Suppose that this initial state decays into a final state of energy $\mathcal{E}_{\mathbf{k}_2}+\mathcal{E}_{\mathbf{k}_3}+\mathcal{E}_{\mathbf{k}_4}$. In lowest-order perturbation theory, the decay rate for such a process is

$$\frac{1}{\tau_1}=2\pi\int_{\mathbf{k}_2\mathbf{k}_3\mathbf{k}_4}|M_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3\mathbf{k}_4}|^2(2\pi)^2\delta(\mathbf{k}_1-\mathbf{k}_2-\mathbf{k}_3-\mathbf{k}_4)\times\delta(\mathcal{E}_{\mathbf{k}_1}-\mathcal{E}_{\mathbf{k}_2}-\mathcal{E}_{\mathbf{k}_3}-\mathcal{E}_{\mathbf{k}_4})[1-f(\mathcal{E}_{\mathbf{k}_2})]\times[1-f(\mathcal{E}_{\mathbf{k}_3})][1-f(\mathcal{E}_{\mathbf{k}_4})], \quad (12)$$

where $\int_{\mathbf{k}_2\mathbf{k}_3\mathbf{k}_4}=\int[d^2k_2/(2\pi)^2][d^2k_3/(2\pi)^2]\times[d^2k_4/(2\pi)^2]$; $M_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3\mathbf{k}_4}$ is a matrix element, and $f(\mathcal{E}_{\mathbf{k}})$ is the Fermi function. We have in mind a situation in which $\mathbf{k}_2$ is close to $\mathbf{k}_1$, and $\mathbf{k}_3$ and $\mathbf{k}_4$ are close to the zone diagonal, but we will perform the integrals over the full Brillouin zone.

There is a second contribution to the decay rate, $1/\tau_2$, resulting from scattering off thermally excited quasiparticles. The corresponding expression involves a different matrix element $N_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3\mathbf{k}_4}$ and the quasiparticle at momentum $\mathbf{k}_2$ is thermally excited with probability $f(\mathcal{E}_{\mathbf{k}_2})$. In all other respects the equation is the same as Eq. (12) except that the energy and momentum conserving δ functions must be changed accordingly.The total decay rate is the sum $1/\tau=1/\tau_1+1/\tau_2$.

The matrix elements $M_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3\mathbf{k}_4}$ and $N_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3\mathbf{k}_4}$ will depend on the form of the interaction between quasiparticles and also on the coherence factors. If we choose a Hubbard-like density-density interaction $\lambda\rho_\uparrow(\mathbf{q})\rho_\downarrow(-\mathbf{q})$ between the original electrons, the coherence factors are extremely complicated in the coexisting DDW and DSC state, and the multidimensional numerical integrations involved in calculating the scattering rates become next to impossible to carry out. To obtain upper bounds, we replace them by their maximum values. In the DDW state, we expect the coherence factors to be rather tame, but in the state with both DSC and DDW orders, they will suppress the decay rate as in a pure superconducting state. Thus, such an approximation will *underestimate* the difference between the decay rates in the pseudogap and the underdoped superconducting states. We call this interaction, treated with this approximation, model *A*.

In order to capture the effect of the coherence factors in the mixed DDW and DSC state, we consider a model interaction. Since we are only concerned with the interaction between the quasiparticles in the valence band, we choose the interaction to be (Ω is the volume of the system.)

$$\mathcal{V}=\frac{\lambda}{\Omega}\sum_{\mathbf{q},\mathbf{k},\mathbf{k}'}\psi^{v\dagger}_{\mathbf{k}\uparrow}\psi^{v}_{\mathbf{k}+\mathbf{q}\uparrow}\psi^{v\dagger}_{\mathbf{k}'\downarrow}\psi^{v}_{\mathbf{k}'-\mathbf{q}\downarrow}, \quad (13)$$

where $\psi^{v\dagger}_{\mathbf{k},\alpha}$ creates a quasiparticle in the valence band of the DDW state. We have ignored the temperature and momentum dependence of the interaction, because we are primarily interested in temperatures much lower than the DDW transition temperature, where the temperature dependence of the DDW gap should be weak. Moreover, we merely wish to demonstrate how the development of superconductivity affects the lifetime, so we also neglect the momentum space structure of the interaction. For this interaction, which we call model *B*, the coherence factors are equal to unity for the DDW order alone, but are nontrivial in the state with both orders as a result of the coherence factors associated with superconductivity in the mixed state. We can view the mixed state as DSC developing on top of DDW. Thus, the coherence factors for this interaction can be read off from the BCS theory and the matrix elements are

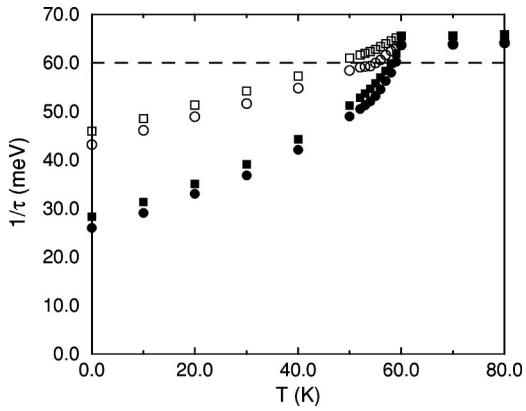

FIG. 3. The lifetime of a quasipartcle in the antinodal region at wave vector $\mathbf{k}^*$, as defined in the text, plotted as a function of temperature. The open symbols are for without coherence factors and the solid symbols are for with coherence factors. The square symbols correspond to 2-meV broadening of the energy conserving δ function and the circles to 1-meV broadening. The electron-electron interaction parameter $\lambda=1.5$ eV.

$$M_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3,\mathbf{k}_4}=\lambda[-V_{\mathbf{k}_1}V_{\mathbf{k}_2}U_{\mathbf{k}_3}V_{\mathbf{k}_4}+V_{\mathbf{k}_1}U_{\mathbf{k}_2}V_{\mathbf{k}_3}V_{\mathbf{k}_4}-U_{\mathbf{k}_1}V_{\mathbf{k}_2}U_{\mathbf{k}_3}U_{\mathbf{k}_4}+U_{\mathbf{k}_1}V_{\mathbf{k}_2}V_{\mathbf{k}_3}U_{\mathbf{k}_4}] \quad (14)$$

and

$$N_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3,\mathbf{k}_4}=\lambda[-V_{\mathbf{k}_1}V_{\mathbf{k}_2}V_{\mathbf{k}_3}V_{\mathbf{k}_4}-U_{\mathbf{k}_1}U_{\mathbf{k}_2}U_{\mathbf{k}_3}U_{\mathbf{k}_4}-U_{\mathbf{k}_1}V_{\mathbf{k}_2}V_{\mathbf{k}_3}U_{\mathbf{k}_4}-V_{\mathbf{k}_1}U_{\mathbf{k}_2}U_{\mathbf{k}_3}V_{\mathbf{k}_4}+U_{\mathbf{k}_1}V_{\mathbf{k}_2}U_{\mathbf{k}_3}V_{\mathbf{k}_4}-V_{\mathbf{k}_1}U_{\mathbf{k}_2}U_{\mathbf{k}_3}V_{\mathbf{k}_4}-U_{\mathbf{k}_1}V_{\mathbf{k}_2}V_{\mathbf{k}_3}U_{\mathbf{k}_4}+V_{\mathbf{k}_1}U_{\mathbf{k}_2}V_{\mathbf{k}_3}U_{\mathbf{k}_4}], \quad (15)$$

where

$$\left.\begin{matrix}U^2_{\mathbf{k}}\\V^2_{\mathbf{k}}\end{matrix}\right\}=\frac{1}{2}\left(1\pm\frac{E_-(\mathbf{k})-\mu}{\mathcal{E}(\mathbf{k})}\right). \quad (16)$$

This form of the interaction allows us to capture the difference between the matrix elements in the pseudogap and superconducting states.

Our results are displayed in Fig. 3, where the decay rates are plotted against temperature. In these plots we have kept

the total gap $\mathcal{E}_{k*}$ fixed and equal to 0.06 eV, while assuming a mean-field temperature dependence for the superconducting gap:

$$\Delta_0(T)=\Delta_0(0)\left(1-\frac{T}{T_c}\right)^{1/2}, \tag{17}$$

with $\Delta_0(0)=0.03$ eV and $T_c=60$ K. This implicitly defines the temperature dependence of the DDW gap, which is weak close to T_c, as noted earlier.

It is apparent from this figure that the decay rate drops dramatically as a result of the development of superconducting order. From the calculation for model *A*, we see that there is a substantial drop resulting from the elimination of phase space. From model *B*, we see that the coherence factors reduce the decay rate further by a large amount.

The absence of an antinodal quasiparticle peak in the pseudogap state and its subsequent emergence in the superconducting state has been interpreted here as the increase of its width as T_c is approached. However, when the width becomes comparable to the quasiparticle energy, i.e., as the curve reaches the dashed line in Fig. 3, the quasiparticle concept breaks down. Once this occurs, our perturbative calculation can no longer be trusted, and it is not meaningful to assign a width or weight to the quasiparticle. What is significant is that it *is* possible to have a reasonably well-defined quasiparticle in the superconducting state as a result of phase-space restrictions and coherence factors, as we have found.

The broken-symmetry state may or may not have well-defined quasiparticles at the single-particle gap edge. It depends on many nonuniversal details: the locus in momentum space, the doping level, the interaction strength, etc. Thus, the absence of a well-defined antinodal quasiparticle does not preclude a broken-symmetry state. However, it may have important effects on nonuniversal aspects of the state, such as the temperature dependence of the order parameter which may, as a result, be strongly non-mean-field-like. Also, our calculation leaves out fluctuation effects, which must be considered in the future.

We end with three concluding remarks.

(1) Although hole pockets cannot be observed in ARPES, other experimental probes can be used to look for their signature, for example, infrared Hall angle measurement in the underdoped regime.[7]

(2) Because the interlayer tunneling matrix element is so strongly peaked at $(\pi,0)$,[8] we expect the *c*-axis optical conductivity to show a strong temperature dependence at T_c, given our lifetime calculation. Indeed, this is consistent with the known measurements.[9]

(3) We have not yet studied in detail the doping dependence. Nonetheless, it is possible to make a qualitative observation. There are two competing effects. As the system is moderately underdoped, the DDW order parameter must increase. Thus, the quasiparticle in the $(\pi,0)$ regime will have higher energy, increasing its scattering rate. On the other hand, the Fermi arcs will also shrink and the phase space for particle-hole scattering will decrease. We wish to return to these issues in the near future.

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