On the relationship between charge ordering and the Fermi arcs observed in underdoped high $T_c$ superconductors

N Harrison$^1$ and S E Sebastian$^2$

$^1$Mail Stop E536, Los Alamos National Labs, Los Alamos, NM 87545, USA
$^2$Cavendish Laboratory, Cambridge University, JJ Thomson Avenue, Cambridge CB3 OHE, UK
E-mail: nharrison@lanl.gov

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Abstract

We address the origin of the recently discovered close correspondence between the charge ordering wave vectors and the momentum-space separation between the tips of the Fermi arcs seen in angle-resolved photoemission measurements in underdoped high-temperature superconducting cuprates. This observation has been interpreted as a signature of charge order forming as an instability of pre-existing Fermi arcs of a different origin. We calculate the Fermi surface spectral weight for a charge density-wave model, considering a Fermi surface, charge ordering wave vectors and short correlation lengths similar to those found experimentally. We show that the observation of wave vectors spanning the tips of remnant Fermi surface sections is a natural consequence of a Fermi surface having been reconstructed by charge order. The presence of short-range charge order therefore cannot be ruled out as a potential origin of the observed Fermi arcs.

Keywords: superconductivity, charge density waves, Fermi surface
Introduction

The discovery of charge ordering in a growing number of underdoped high-temperature superconducting cuprates raises the possibility of this type of order being universal to the normal state [1–8]. Evidence for charge order is found in x-ray scattering [7, 8] and Raman spectroscopy [6] experiments at temperatures as high as the pseudogap onset $T^*$. Comparisons of the charge ordering wave vectors found in x-ray scattering and scanning tunneling microscopy (STM) measurements with the Fermi surface spectral weight found in angle-resolved photoemission spectroscopy (ARPES) have revealed an emerging pattern. The charge ordering wave vectors are found to span the tips of the residual nodal segments of spectral weight at the Fermi energy within the pseudogap regime termed ‘Fermi arcs’ [7–9]. It has been postulated [7, 8] that these observations point to a scenario in which the arcs themselves result from a primary antinodal Fermi surface instability that is distinct from charge ordering (see figure 1(b)) [10, 11].

In this paper, we show that charge ordering wave vectors spanning the tips of the Fermi arcs are a natural consequence of Fermi surface reconstruction by charge density-wave order [2, 3, 12–18] (see figure 1(a)). On calculating the ARPES spectral weight, considering a scenario in which a Fermi surface instability is caused by charge ordering, we find a correspondence between charge ordering wave vectors and the Fermi arc tips to be a robust feature of the reconstructed Fermi surface. Such a behavior mirrors that seen in several conventional charge density-wave materials [19–22]. Our calculations therefore indicate that charge ordering cannot be ruled out as a potential origin of Fermi arcs observed in cuprate superconductors [7–9].

Fermi surface model

For the purposes of the present calculations, the specific mechanism for the charge ordering is immaterial, with two scenarios involving an antinodal Fermi surface instability [12–14] and Fermi surface ‘hot spots’ [17, 18] having been proposed. In the absence of an accepted formalism for Fermi surface reconstruction in the cuprates that includes the effects of strong correlations, we adopt the former approach within a single particle scheme [16, 23, 24]. We consider a Fermi surface that is conducive to charge ordering instabilities of characteristic wave vector $Q_x$ and $Q_y$ in the antinodal regions of momentum-space, as depicted in figure 1(a). A Fermi surface of this geometry is produced by the tight binding dispersion

$$\varepsilon_{\pm} = -2t\left[\cos(k_x) + \cos(k_y)\right] + 2t'\left[\cos(ak_x) + \cos(ak_y - 2ak_x) + 2ak_x\right] - 2t''\left[\cos(2ak_x) - \mu\right]$$

(1)

on setting $t'/t = 0.5$ and $t''/t = 0.1$, in which we neglect small differences in the lattice dimensions in the $k_x$ and $k_y$ directions. Here, $t$, $t'$ and $t''$ are the nearest, next nearest and next next nearest hopping parameters, respectively, while $\mu$ is the chemical potential. These parameters have been chosen to yield a Fermi surface shape qualitatively similar to that measured [7, 25–27].
To model the Fermi surface spectral weight resulting from long-range charge order caused by an antinodal instability, we consider a biaxial density-wave picture, as shown schematically in Figure 1(a). We consider $\epsilon_k$ states with relative translations of the ordering wave vectors $Q_x = (2\pi \delta_x, 0)$ and $Q_y = (0, 2\pi \delta_y)$ \cite{15, 16, 23, 28} to be respectively coupled by $V_{k,x}$ and $V_{k,y}$, where $\delta_x$ and $\delta_y$ refer to the approximate dimensions of the wave vectors ($0.2 \lesssim \delta_{x,y} \lesssim 0.3$) found in x-ray scattering and STM experiments \cite{2–4, 7, 8, 12–14}. A reconstructed Fermi surface consisting of antinodal gaps at both $ak = (\pm \pi, 0)$ and $ak = (0, \pm \pi)$ \cite{15, 16, 28} and a nodal electron pocket consistent with quantum oscillation \cite{9, 29} and negative Hall effect \cite{30} measurements is produced by a Hamiltonian of the form

$$H_{\text{bi}} = \begin{pmatrix} \epsilon_k & V_{k,x} & 0 & V_{k,y} & 0 & \cdots \\ V_{k,x} & \epsilon_{k+Q_x} & V_{k,x} & 0 & 0 & \cdots \\ 0 & V_{k,y} & \epsilon_{k+Q_y} & V_{k,x} & 0 & \cdots \\ V_{k,x} & 0 & V_{k,y} & \epsilon_{k+2Q_x} & 0 & \cdots \\ V_{k,y} & 0 & 0 & V_{k,x} & \epsilon_{k+Q_x+Q_y} & \cdots \\ 0 & V_{k,y} & 0 & 0 & V_{k,x} & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix},$$  \hspace{1cm} \text{(2)}$$

on adopting suitable forms for $V_{k,x}$ and $V_{k,y}$ \cite{15–17}. The diagonal elements $\epsilon_k, \epsilon_{k+Q_x}, \epsilon_{k+2Q_x} \ldots$ of equation (2) list the original dispersion in equation (1) translated by all possible multiples and combinations of $Q_x$ and $Q_y$. By approximating $\delta_{x,y}$ with a rational fraction $\delta_x = \delta_y = \frac{m}{n}$, a full Hamiltonian consisting of a $n \times n$ matrix can be constructed, from which $n \times n$ reconstructed electronic bands are obtained upon diagonalization \cite{16}. Here we neglect bilayer coupling, which, while important for understanding the detailed waveform of quantum oscillations \cite{31} and obtaining values of $\delta_x$ and $\delta_y$ closer to those in experiment \cite{24} in the bilayer cuprates, is less important for calculating the spectral weight.
The Fermi surface spectral weight is obtained by setting $\omega = 0$ for the excitation energy in the spectral function [32]

$$A_{bi}(k, \omega) = \frac{1}{\pi} \text{Im} \left( G_{bi} \right), \quad (3)$$

where

$$G_{bi}(k, \omega) = \left( (\omega + i\Gamma) I - H_{bi} \right)_1^{-1}, \quad (4)$$

is the corresponding Green’s function for the Hamiltonian given by equation (2). The subscript ‘11’ refers to the first diagonal element of the inverted matrix, where $I$ is the identity matrix and $\Gamma$ represents a simple elastic energy level broadening [28].

**Short-range charge order**

To simulate the effect of a finite charge order correlation length, as seen in x-ray scattering and STM experiments, we introduce a Gaussian statistical broadening of $\delta$ [7] (using $\delta = \delta_x = \delta_y$) in which $\sigma = \frac{a}{2\xi}$ is the standard deviation and $\xi$ is the correlation length. It is convenient, in this case, to consider a simplified Hamiltonian of the form [28]

$$H'_{bi} = \begin{pmatrix}
            \epsilon_k & V_{k,x} & V_{k,y} & V_{k,y} \\
            V_{k,x} & \epsilon_{k+Q_x} & 0 & 0 \\
            V_{k,y} & 0 & \epsilon_{k-Q_y} & 0 \\
            V_{k,y} & 0 & 0 & \epsilon_{k-Q_y}
          \end{pmatrix}, \quad (5)$$

noting that for period $n$ order the wave vectors $(n - 1)Q_x$ and $(n - 1)Q_y$ are equivalent to $-Q_x$ and $-Q_y$, respectively. The statistically broadened spectral weight is then obtained by setting $\omega = 0$ in

$$A'_{bi}(k, \omega, \sigma) = \int_{-\infty}^{\infty} \frac{1}{\pi} \text{Im} \left( G'_{bi} \right) \frac{1}{\sigma \sqrt{2\pi}} e^{-\frac{(\delta-\delta')^2}{2\sigma^2}} d\delta', \quad (6)$$

where

$$G'_{bi}(k, \omega) = \left( (\omega + i\Gamma) I - H'_{bi} \right)_1^{-1}. \quad (7)$$

Below we show that the spectral weight given by equation (6) produces very similar results to that given by equation (3) on taking the limit $\sigma \to 0$ (i.e., figures 2(c) and 4(a)), which corresponds to long-range order ($\xi \to \infty$), justifying the use of equation (5) in calculating the spectral weight.

**Results**

Figure 2(a) shows the unreconstructed Fermi surface according to equation (1) in which $\mu$ has been adjusted to produce a Fermi surface corresponding to a hole filling of $p = 0.08$ (relative to the half-filled band). Figure 2(b) shows the reconstructed Fermi surface calculated for the same
hole doping using $\delta = \frac{1}{4}$ (which lies within the range of values found in x-ray scattering and STM experiments [2–4, 7, 8, 12–14]). We use a form $V_{k\chi} = \frac{V}{2} \left( 1 - \cos ak^i_\chi \right)$ and $V_{k\gamma} = \frac{V}{2} \left( 1 - \cos ak^i_\gamma \right)$ (which has the property of being large in the antinodal regions of the Brillouin zone where a gap is created at the Fermi surface [16]) and $V_0/t = 0.3$. These parameters are the same as those used in [16]. On calculating $A_{\alpha\beta}(k, \omega)$ in figure 2(c) for the full $n \times n = 16 \times 16$ Hamiltonian given by equation (2), the Fermi arcs obtained display similarities to those found by Li et al [15] and Norman [28]. Here they correspond to one side of the reconstructed electron pocket in figure 2(b) (where they are plotted in red). A salient feature of the Fermi surface spectral weight calculated using our charge ordering model in figure 2(c) is that the Fermi arc tips are separated in momentum-space by $Q_x$ and $Q_y$. This arises from the correspondence of the ‘Fermi arc’ to one side of the reconstructed electron pocket (plotted in red in figure 2(b)) in this charge ordering model. The spacing between reconstructed electron pockets in the repeated Brillouin zone (shown in figure 2(b)) is consequently given by $2\pi\delta_x = Q_x$, and $2\pi\delta_y = Q_y$, yielding a separation between Fermi arc tips also of $Q_x$ and $Q_y$. A similar connection between the ends of the arcs in the spectral weight and $Q$ vector is found in well-known model charge density-wave systems [19–22], as shown for the case of SmTe$_3$ in figure 3.

3 After [16], where $k'_i = k_i + n'_i Q_x$ and $k'_\gamma = k_\gamma + n'_\gamma Q_x$, where $n'_i Q_x + n'_\gamma Q_x$ is the vector by which $\epsilon_k$ is translated. The chosen forms of $V_{k\chi}$ and $V_{k\gamma}$ have the useful property of being invariant under transformation by $Q_x$ and $Q_y$.

4 For this reason, the charge ordering wave vectors $Q_x$ and $Q_y$ continue to span the tips of the Fermi arcs even when these vectors no longer connect the antinodal regions of the Fermi surface (see appendix).
In figure 4 we show that the charge ordering wave vectors span the tips of the Fermi arcs irrespective of the correlation length $\xi$. For $\xi \to \infty$ in figures 2(c) and 4(a), our calculations find band backfolding features at the ends of the Fermi arcs that are associated with the reconstructed electron pocket in figure 2(b). These features become significantly smeared on including a correlation length $\xi = 100$ Å in figure 4(b), and more so on simulating the effect of a finite ARPES experimental resolution in figure 4(c), potentially explaining their absence in ARPES measured in materials with shorter correlation lengths [7, 8, 12, 14, 27]. Our model also
produces a weak spectral weight within the gap in the antinodal regions of the Brillouin zone that is congruent with the unreconstructed Fermi surface. A residual antinodal spectral weight appears to be observed in Bi$_2$Sr$_2$-$x$La$_x$CuO$_6$+$\delta$ ARPES data [25].

Conclusion

The recent discoveries of short-range or long-range charge order extending to high temperatures within the pseudogap regime have led to renewed debate as to the contribution of charge ordering to the formation of the pseudogap and its relevance to superconductivity [1–6, 11, 17, 18]. A notable experimental feature is the close correspondence between the measured ordering wave vectors and the momentum-space separation of the Fermi arcs seen by ARPES [7–9]. While arguments have been made for this correspondence signalling charge order being an instability of the Fermi arcs, our model shows that such a correspondence is in fact a natural consequence of a Fermi surface reconstructed by charge order, as seen in archetypal charge density-wave materials [19–22].

Were strong electronic correlations to be included, their effect might be to renormalize the effective hopping parameters so as to result in smaller values of the ratios $t'/t$ and $t''/t$ [10]. Even though the charge ordering wave vector no longer connects the antinodal regions of the Fermi surface in such a case, it still continues to connect the tips of the arcs in the calculated Fermi surface spectral weight (see appendix). In this event, a different mechanism would need to be invoked to reduce the spectral weight intensity in the antinodal region to levels comparable with ARPES experiments.

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Appendix

In figure 5 we consider a scenario whereby reduced values of $t'/t$ and $t''/t$ cause the shape of the Fermi surface to be modified from that shown in figures 1 and 2. Consequently the values of $Q_x$ and $Q_y$ are not matched to the antinodal separation of the Fermi surface, in the manner proposed in [7]. In such a case, $Q_x$ and $Q_y$ continue to span the separation between Fermi arcs while leaving behind residual sections of Fermi surface at the antinodes in our non-interacting model (see figure 5). The backfolding features at the ends of the arcs are the result of the effects of a finite correlation length or a finite experimental resolution having not been included. In this case, remnant antinodal Fermi surface sections result, requiring an additional mechanism to reduce the antinodal spectral weight to levels corresponding with ARPES experiments.

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