Failure of Scattering Interference in the Pseudogap State of Cuprate Superconductors

S. Misra, M. Vershinin, P. Phillips, and A. Yazdani
Department of Physics and Fredrick Seitz Materials Research Laboratory, University of Illinois at Urbana-Champaign, Urbana, Illinois 61801
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We calculate scattering interference patterns for various electronic states proposed for the pseudogap regime of the cuprate superconductors. The scattering interference models all produce patterns whose wavelength changes as a function of energy, in contradiction to the energy-independent wavelength seen by scanning tunneling microscopy (STM) experiments in the pseudogap state. This suggests that the patterns seen in STM local density of states measurements are not due to scattering interference, but are rather the result of some form of ordering.

The origin of pseudogap phenomena is one of the key questions in the cuprate superconductors, as it profoundly affects their properties above the superconducting transition, and potentially influences the cuprate phase diagram. In a recent paper, we have used a scanning tunneling microscope to show that the electronic states in the pseudogap state of $Bi_2Sr_2CaCu_2O_{8+\delta}$ are spatially modulated. These electronic modulations in the local density of states, which are seen only for energies less than the pseudogap energy scale, are oriented along the copper-oxide bond direction and have an energy-independent, incommensurate wavelength. One interpretation of these experiments is that these modulations are caused by electronic ordering, a variety of which have been proposed for the cuprates in the pseudogap regime. Another possibility is that such modulations are the consequence of scattering interference from one of the electronic states proposed for the pseudogap. The interest in scattering interference as a possible explanation is motivated by the success of this idea in understanding similar modulations in the superconducting state, although even below $T_c$ there are a number of deviations from the scattering interference picture. In this paper, we elaborate on calculations reported in Ref. 2 to demonstrate the failure of the scattering interference scenario in describing the modulations observed in the pseudogap state. We show that this failure is a generic feature of scattering interference itself, regardless of the model chosen for the pseudogap electronic state. This shortcoming suggests that the modulations observed in the pseudogap regime are the signature of some form of ordering.

The scattering interference picture ascribes spatial modulations in the local density of states to interference between elastically scattered quasiparticles. A well-studied example of this phenomenon is the standing wave patterns seen on certain metal surfaces, in which electrons scattering from step edges and point impurities interfere coherently to form modulations in the density of states. The period of these modulations at a given energy $\omega$ is determined by the wavevector $\vec{q}$ that joins the two points on curves of constant electron energy in $\vec{k}$ space with the greatest weight, as determined by the electronic structure of the system. For a superconductor, the scattering interference contribution to the local density of states can be treated within the Born approximation, which introduces a correction.

$$\delta n(\vec{r}, \omega) = -\frac{1}{\pi} Im \{ \int d^2 \vec{r} 1 G_0(\vec{r} - \vec{r}, \omega) V(\vec{r}, \omega) G_0(\vec{r} - \vec{r}, \omega) - F_0(\vec{r} - \vec{r}, \omega) V(\vec{r}, \omega) F_0(\vec{r} - \vec{r}, \omega) \} \tag{1}$$

where $G_0$ and $F_0$ are the single particle and anomalous Green functions, respectively, and $V$ is a weak, finite-range scattering potential. For pure potential scattering, the Fourier transform of the Born correction $\delta n(\vec{q}, \omega) = -\frac{1}{\pi} Im \{ V(\vec{q}, \omega) \Lambda(\vec{q}, \omega) \}$ separates into a part

$$\Lambda(\vec{q}, \omega) = \int \{ d^2 \vec{k} G_0(\vec{k}, \omega) G_0(\vec{k} + \vec{q}, \omega) - F_0(\vec{k}, \omega) F_0(\vec{k} + \vec{q}, \omega) \} \tag{2}$$

which contains all the wave interference information, and a part

$$V(\vec{q}, \omega) = \int d^2 \vec{x} e^{-i \vec{q} \cdot \vec{x}} V(\vec{x}, \omega) \tag{3}$$

which acts like a static structure factor. For now, we will assume that the structure factor does not filter any wave interference information.

In order to develop a context in which to understand quantum interference in the pseudogap state, we will first review the quantum interference picture for the two cases already discussed in the literature- the superconducting state and the Fermi liquid normal state.
ing these previous works, scattering interference in the superconducting state can be modeled using the Green functions,

\[
G_0(\vec{k}, \omega) = \frac{\omega + i\delta + \epsilon^*_F}{(\omega + i\delta - \epsilon^*_F)(\omega + i\delta + \epsilon^*_F) - \Delta_F^2 - i\delta} - \frac{\Delta_F}{\omega + i\delta - \epsilon^*_F - \Delta_F^2 - i\delta}
\]

\[
F_0(\vec{k}, \omega) = \frac{\Delta_F}{(\omega + i\delta - \epsilon^*_F)(\omega + i\delta + \epsilon^*_F) - \Delta_F^2 - i\delta}
\]

where \( \epsilon^*_F = 120.5 - 595.1 \times (\cos k_x + \cos k_y)/2 + 163.6 \times \cos k_x \cos k_y - 51.9 \times (\cos 2k_x + \cos 2k_y)/2 - 111.7 \times (\cos 2k_x \cos k_y + \cos k_x \cos 2k_y)/2 + 51.0 \times (\cos 2k_x \cos 2k_y) \) is the \( Bi_2Sr_2CuCu_2O_{8+\delta} \) band structure from ARPES for slightly underdoped (\( \delta = .12 \)) samples. \( \Delta_F = 45.0 \times (\cos k_x + \cos k_y)/2 \) is the superconducting gap function, and \( \delta \) is a broadening term. As shown in Figures 1a and b, this yields pictures with sharp peaks in q-space which disperse. To understand the origin of the dispersion qualitatively, it helps to consider a simplified version of scattering interference, the so-called octet model, introduced by Hoffman et al. and McElroy et al. Quasiparticles can elastically scatter between points on contours of constant electron energy in k-space (Fig. 1). The shape of these contours changes continuously as the energy increases. Consequently, the length of the characteristic scattering interference wavevector (q-space) changes, leading to dispersion. This picture changes dramatically if, instead of a superconducting Green function, we use a Fermi liquid normal state Green function by setting \( \Delta_F = 0 \) in Equation 4. The sharp peaks in q-space for the superconducting state have been replaced with dispersing caustics (Figs. 1a and d). The equivalence of all points in k-space leads directly to an absence of sharp peaks in q-space. The dispersion is now a direct consequence of the band structure itself. Although the Fermi liquid scattering interference picture is useful in determining the effect of the band structure on scattering interference, it is not applicable to the pseudogap, as it omits two key features of this state: the pseudogap in the density of states, and the ill-defined nature of quasiparticles.

To extend the scattering interference model into the pseudogap regime, we must first choose an appropriate Green function with which to model the pseudogap state. Although its origin is still not understood, the pseudogap has been thoroughly characterized by ARPES in the underdoped cuprate superconductors. At all energies, peaks in the ARPES spectral function are so broad that it is unclear whether quasiparticles are still well-defined. Meanwhile, at the Fermi energy, the spectral function shows extended arcs centered at the nodal points (Fig. 2a) in k-space. As energy increases towards the pseudogap energy scale, these arcs extend towards the Brillouin zone boundary. Theoretical attempts at understanding the measured behaviour have either followed a phenomenological approach, or have proposed exotic electronic states for the pseudogap. We will first focus on the phenomenological attempts. Norman et al. have modeled the ARPES data in the pseudogap regime using the Green function

\[
G_0(\vec{k}, \omega) = (\omega - \epsilon^*_F - \Sigma^*(\vec{k}))^{-1}
\]
and $F_0 = 0$, where the self energy,

$$\Sigma(\mathbf{k}, \omega) = -i\Gamma_1 + \Delta_\mathbf{k}^2/(\omega + \epsilon_\mathbf{k} + i\Gamma_0),$$

(6)

$\Gamma_1$ is a single particle scattering rate, $\Gamma_0$ is a measure of decoherence, and $\Delta_\mathbf{k}$ is a gap function with a $\mathbf{k}$ dependence which matches the Fermi arcs. The calculated scattering interference patterns (Fig. 2b) have two notable shortcomings in comparison with the measured data shown in Figure 3a. First, the calculated patterns contain caustics, while the measured patterns contain discrete points along the $(0, \pi)$ directions. This shortcoming can be overcome by assuming, for example, that the STM tunneling matrix element has a $d$-wave symmetry and selectively filters the density of states along the $(0, \pi)$ direction. Second, the scattering interference patterns calculated from this phenomenological description still show features along the $(0, \pi)$ directions that disperse (Fig. 2d). This dispersion curve resembles that in the superconducting state, as the characteristic wavevector for scattering interference is of a similar length at the gap energy, but is shallower because this wavevector is much shorter than the Fermi energy in the pseudogap regime (Figs. 1d and 2a). Even this shallower dispersion results in a change of wavelength between $7a_0$ and $35a_0$ for the Fermi energy and the pseudogap energy, whereas STM experiments show a fixed wavelength of $4.7 \pm 0.2a_0$ over this energy range.

We next consider the scattering interference scenario for various exotic electronic states proposed for the pseudogap regime. We will discuss how four of these exotic Green functions (two based on preformed pairs, and two based on ordering) produce dispersions which should be resolved in the data. Chen et al. have proposed the Green function in Equation 5 with the self energy in Equation 6 to describe preformed pairs. However, unlike the Fermi arc model, they use a $d$-wave gap function. For small values of $\Gamma_0$, the scattering pictures resemble those calculated for the superconducting state, and for larger values, they resemble broader versions of those calculated for the Fermi liquid (not shown). Both these dispersions, similar to the ones shown in Figure 1a, should be resolved by the experiment. Another example of a preformed pairs calculation appears in Perep-Beane and Franz, where the authors take a $QED_3$ Green function $G_0(\mathbf{k}, \omega) = (\omega + \epsilon_\mathbf{k})/(\omega^2 + \epsilon_\mathbf{k}^2 + \Delta_\mathbf{k}^2)^{1-n/2}$, with $n$ being an anomalous dimension exponent which increases the amount of decoherence of the patterns for larger values. As noted by the authors, the scattering interference patterns show a dispersion identical to the superconducting state for $\eta < 0.5$, which is shown here explicitly in Figures 3a and b. We have also calculated the dispersion for a simplified $d$-density wave (DDW) ordering Green function $G_0(\mathbf{k}, \omega) = (\omega + \Delta_\mu - \epsilon_\mathbf{k} + \mathbf{Q})/(\omega - \Delta_\mu + \Delta_\mathbf{k} - \epsilon_\mathbf{k} + \mathbf{Q} - D_{\mathbf{k}}^2)$, where $D_{\mathbf{k}} = D_0(\cos k_x - \cos k_y)/2$ is the DDW gap, $\Delta_\mu$ is a chemical potential shift, and $\mathbf{Q} = (\pi, \pi)$. As can be seen in Figures 3a and c, the simplified DDW Green function produces scattering interference patterns which disperse through a range of wavelengths ($\Delta \lambda = 0.8a_0$ between -15mV and 35mV) which should be easily resolved by the STM experiment (maximum $\Delta \lambda = 0.4a_0$ over the same range of energies). Using a more complete DDW treatment results in an identical dispersion, and very similar scattering pictures (not shown). Finally, in Figures 3a and d, we show the quantum interference pat-
chemical potential shift of +40 meV. Features in q-space. (C) The power spectrum of \(\delta n\) become more diffuse until, by energies \(\omega < \omega_c\), the patterns in q-space become more diffuse until, by \(\eta \approx 1\), there are no discernable features in q-space. (C) The power spectrum of \(\delta n(q, \omega)\) for a QED Green function is shown here in the first Brillouin zone at \(\omega = 20mV\). The patterns were calculated using a value of \(\eta = 0.4\) and a broadening of 1mV. For increased \(\eta\), the patterns in q-space become more diffuse until, by \(\eta \approx 1\), there are no discernable features in q-space. (C) The power spectrum of \(\delta n(q, \omega)\) for a QED Green function is shown here in the first Brillouin zone at \(\omega = 20mV\). (D) The power spectrum of \(\delta n(q, \omega)\) for a circulating current Green function using a broadening of 1mV and a chemical potential shift of +40meV is shown here in the first Brillouin zone at \(\omega = 20mV\). Non-zero values of \(D_0\) result in the slowest dispersing mode along the \((0, \pi)\) direction (arrow) being replaced by a faster dispersing mode (circle) at energies \(\omega < 2|x_0|\). The dispersion shown in part (A) is for \(D_0 = 0\), corresponding to the slowest dispersing mode.

The Green Function for this phase, given by \(G_0(k, \omega) = (\omega - \epsilon_F + D(k) - \Sigma(k, \omega))^{-1}\) for \(k >> k_f\) with \(\Sigma(k, \omega) = \lambda \omega \log x/\omega_c + i \pi x/\cosh D(k)/x\), \(x = (\omega^2 + \pi^2 T^2)^{1/2}\) and \(D(k) = D_0 (\cos(k_2a) - \cos(k_ya))^2\), produces patterns which disperse in a fashion similar to the band structure. Thus, it also fails to match the dispersionless feature seen in STM in the pseudogap regime (Fig. 3). The failure of these approaches points to a fundamental problem: any Green function will result in a wave contribution to Born scattering which disperses. The Green function is being asked to accomplish two contradictory tasks: on one hand, the imaginary part of the Green function (the density of states) must disperse in order to match the ARPES band structure, and on the other hand, the imaginary part of the Green function convolved with itself cannot disperse if it is to match the STM data in the pseudogap state. In order for Born scattering to simultaneously match the ARPES and STM data, the structure factor, assumed to be an all-pass filter until now, could be chosen to pass only contributions near \(q = 2\pi/a_0(0, 1/4.7)\) inside the pseudogap. The real space scattering potential corresponding to such a structure factor is an incommensurate, bond-oriented square lattice of scattering centers. While this can be justified on various physical grounds, it amounts to an ad hoc assumption that ordering exists. Moreover, any choice of Green function would then adequately describe the data, thus demonstrating that scattering interference fails to describe the interesting physics revealed in the experiment.

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