Evidence of Electron Fractionalization from Photoemission Spectra in the High Temperature Superconductors

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(Received 30 May 2000)

In the normal state of the high temperature superconductors $Bi_2Sr_2CaCu_2O_{8+\delta}$ and $La_{2-x}Sr_xCuO_4$, and in the related "stripe ordered" material, $La_{1.25}Nd_{0.6}Sr_{0.15}CuO_4$, there is sharp structure in the measured single hole spectral function, $A^<(\vec{k},\omega)$, considered as a function of $\vec{k}$ at fixed small binding energy ω. At the same time, as a function of ω at fixed $\vec{k}$ on much of the putative Fermi surface, any structure in $A^<(\vec{k},\omega)$, other than the Fermi cutoff, is very broad. This is characteristic of the situation in which there are no stable excitations with the quantum numbers of the electron, as is the case in the one-dimensional electron gas.

DOI: 10.1103/PhysRevLett.86.4362 PACS numbers: 74.25.Jb, 71.10.Pm, 71.20.–b, 79.60.–i

In a Fermi liquid, the elementary excitations have the quantum numbers of an electron, so the one particle spectral function, $A(\vec{k},\omega)$, is peaked at $\omega = \epsilon(\vec{k}) = \vec{v}_F(\vec{k}_F)\cdot(\vec{k} - \vec{k}_F)$, where $\epsilon(\vec{k})$ is the quasiparticle dispersion relation. The single hole piece, $A^<(\vec{k},\omega)$, can be measured using angle-resolved photoemission spectroscopy (ARPES). The lifetime of the quasiparticle, $\tau(\vec{k})$, can be determined from the width of the peak in the "energy distribution curve" (EDC) defined by considering $A^<(\vec{k},\omega)$ at fixed $\vec{k}$ as a function of ω:

$$1/\tau = \Delta\omega\,. \tag{1}$$

A check on the consistency of this picture can be obtained by studying the "momentum distribution curve" (MDC), i.e., by studying the width Δk of the peak in $A^<(\vec{k},\omega)$ at fixed binding energy, ω. As long as the quasiparticle excitation is well defined, (i.e., the decay rate is small compared to the binding energy), these two widths are related by

$$\Delta\omega = v_F\Delta k\,, \tag{2}$$

where v_F is the renormalized Fermi velocity which is directly measured. This well-established Fermi-liquid theoretic picture as applied to normal metals was recently observed in ARPES measurements of surface states on molybdenum by Valla *et al.* [1].

The ways in which strong correlation effects can lead to the breakdown of Fermi-liquid theory in more than one dimension are not well understood. However, non-Fermi-liquid behavior is generic in the theory of the one-dimensional electron gas (1DEG), where there are no elementary excitations with the quantum numbers of the hole [2]. Because of the celebrated separation of charge and spin, a hole (or an electron) is always unstable to decay into two or more elementary excitations, of which one or more carries its spin and one or more carries its charge. Consequently, $A^<(k,\omega)$ does not have a pole contribution, but rather consists of a multiparticle continuum. If both the spin and charge excitations are gapless, elementary kinematics implies that, at $T = 0$, $A^<(k,\omega)$ is nonzero only for negative frequencies such that

$$|\omega| \geq \min(v_c, v_s)\,|k|\,, \tag{3}$$

as shown in Fig. 1. [We define $A^<(k,\omega)$ as the Fourier transform of the hole piece of the single particle Green function with respect to $kx - \omega t$ and measure the wave vector and frequency relative to k_F and E_F, respectively, so $-\omega$ is the electron binding energy.]

Clearly, at $T = 0$ and constant energy ω there will be nonzero spectral weight in a region of k of width $\Delta k = 2|\omega|/\min(v_c, v_s)$, and a peak in the MDC with a full width at half maximum equal to some fraction of this. At finite temperature, one effectively averages over ω in a

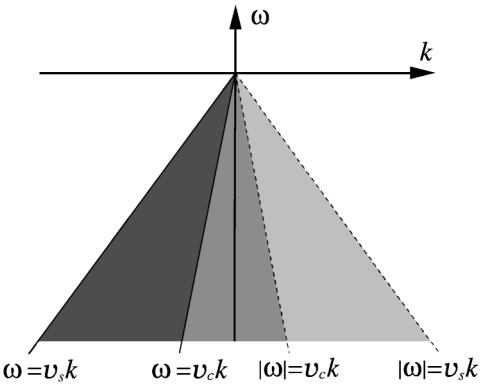

FIG. 1. Kinematic constraints: $A^<(k,\omega)$ for the 1DEG is nonzero at $T = 0$ only in the shaded region of the (k,ω) plane. In the spin rotationally invariant case, $K_s = 1$, $A^<(k,\omega) = 0$ in the lightly shaded region as well. If, in addition, $K_c = 1$, $A^<(k,\omega) = 0$ outside the darkest region. Here $v_c > v_s$.

 0031-9007/01/86(19)/4362(4)$15.00

range T, giving rise to a Δk proportional to the greater of T and $|\omega|$. By contrast, at $k = 0$, the shape of the EDC is not given by the kinematics at all, but is rather determined by the details of the matrix elements linking the one hole state to the various multiparticle hole states which form the continuum. In this case, the spectrum has a nonuniversal power-law behavior with exponents determined by the interactions in the 1DEG.

Figures 2 and 3 show finite temperature spectral functions of the 1DEG for various interaction strengths (i.e., for various values of the charge Luttinger exponent K_c). *It is a direct, general, and dramatic consequence of electron fractionalization that the MDC is much more highly constrained by kinematics than the EDC, which can often be very broad compared to the MDC.* When such a dichotomy can be established experimentally, we believe it represents strong evidence of electron fractionalization. This dichotomy has been observed in the measured spectral functions of $La_{1.25}Nd_{0.6}Sr_{0.15}CuO_4$ (LNSCO) [3,4] shown in Fig. 3, $La_{2-x}Sr_xCuO_4$ (LSCO) [4–6], and slightly underdoped and even optimally doped $Bi_2Sr_2CaCu_2O_{8+\delta}$ (BSCCO) [7,8] in the normal state (at $T > T_c$). (For instance, see Fig. 2 of Ref. [7].)

We would like to emphasize that spin-charge separation is sufficient but not necessary for fractionalization. The spinless 1DEG is an example where the electron decays into a multitude of left and right moving density waves. Here, too, the EDCs lack quasiparticle peaks and exhibit power-law tails. Similar signatures are found when quasiparticles are strongly scattered by (2 + 1)- or (3 + 1)-dimensional quantum critical fluctuations [9] and in a "marginal Fermi liquid" [10]. However, in these last two cases the spectral weight is highly peaked at $\omega = v_F k$ and Eq. (2) holds to good approximation; to logarithmic accuracy for the marginal Fermi liquid.

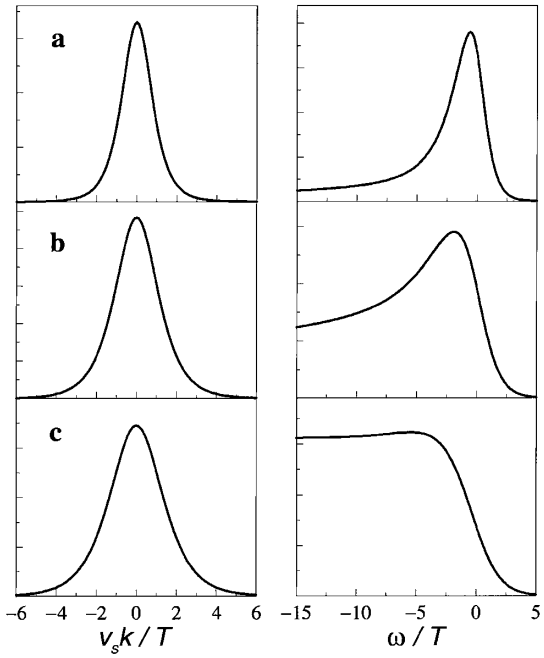

FIG. 2. MDCs for $\omega = 0$ (left) and EDCs for $k = 0$ (right) for the spin rotationally invariant 1DEG with $v_c/v_s = 3$, and (a) $\gamma_c = 0.1$, (b) $\gamma_c = 0.3$, and (c) $\gamma_c = 0.5$.

Because the gapless Tomonaga-Luttinger liquid is a quantum critical system, its response functions have a scaling form. Recently we obtained [11] explicit analytic expressions for these scaling functions under various conditions. In the spin rotationally invariant case, the result for $A^<(\tilde{k}, \tilde{\omega})$ at finite temperature in terms of the scaled variables $\tilde{\omega} = \omega/2\pi T$ and $\tilde{k} = v_s k/2\pi T$ is

$$A^<(\tilde{k}, \tilde{\omega}) \propto \int_{-\infty}^{\infty} dq h_{\gamma_c+1/2}[\tilde{\omega} - \tilde{k} + (1 + r)q] \times h_{\gamma_c}[\tilde{\omega} - \tilde{k} - (1 - r)q] h_{1/2}(2\tilde{k} - 2rq), \tag{4}$$

where $r = v_s/v_c$ is the ratio of the spin and charge velocities and h is related to the beta function, $B(x, y)$,

$$h_\gamma(k) = \mathrm{Re}\left[(2i)^\gamma B\left(\frac{\gamma - ik}{2}, 1 - \gamma\right)\right]. \tag{5}$$

Here, we have introduced the critical exponents

$$\gamma_\alpha = \tfrac{1}{8}(K_\alpha + K_\alpha^{-1} - 2), \tag{6}$$

which are expressed in terms of the Luttinger parameters K_α with $\alpha = c, s$ for charge and spin, respectively. For a spin rotationally invariant system, K_s approaches 1 at the fixed point. Therefore we have set $K_s = 1$.

The kinematics discussed following Eq. (3) becomes evident once the $T \to 0$ limit of Eq. (4) is considered, by using the asymptotic behavior $h_\gamma(|k| \to \infty) \propto (-k)^{\gamma-1}\Theta(-k)$. An interesting subtlety occurs in the spin rotationally invariant case, which results in a more stringent constraint on the extent of the multiparticle continuum than is implied by pure kinematics. In this case, at the fixed point, the spin correlators do not mix left and right moving pieces. As a consequence, $A^<(T = 0)$ vanishes if $v_s < v_c$ and $k > 0$ when ω is in the range $v_s k \le |\omega| \le v_c k$, even if the kinematic constraints in Eq. (3) are satisfied (see Fig. 1).

If $v_s < v_c$ and both $K_s = 1$ and $K_c = 1$, so that the charge piece also does not mix left and right movers, $A^<(T = 0)$ vanishes unless $k < 0$ and $v_s|k| \le |\omega| \le v_c|k|$, as shown in Fig. 1. There is, of course, no special reason why K_c should be precisely equal to 1, but if the interactions are only moderately strong (i.e., $\gamma_c \lesssim 0.2$), most of the spectral weight is still concentrated in this region. In such a circumstance, even though the electron fractionalizes, as long as v_c/v_s is not too large, $\Delta\omega \sim (v_c - v_s)|k|$ and $\Delta k \sim [(v_c - v_s)/v_c v_s]|\omega|$ at $T = 0$ and similar expressions with T substituting for k/v_F and ω, respectively, at elevated temperatures. Thus, the spectral function resembles that of a marginal Fermi liquid.

In Fig. 2 we plot EDCs (for $k = 0$) and MDCs (for $\omega = 0$) generated by using Eq. (4) for $v_s/v_c \equiv r = 1/3$

and various values of γ_c. The results depend only weakly on r. However, as a function of γ_c, the EDCs change much more dramatically than do the MDCs. In particular it is possible to eliminate any peak structure in the EDCs without broadening the MDCs substantially.

It is also possible to obtain expressions for the spectral function of the spin gapped Luther-Emery liquid with $K_s = 1/2$ [11]. While different in detail, the results in this case are grossly similar to those in the gapless case, aside from the fact that the Fermi edge is pushed back from the Fermi energy by the magnitude of the spin gap.

The spectra in Fig. 2 are very reminiscent of the ARPES spectra seen in the cuprates. While the details vary from material to material, the MDCs are always fairly sharp, while the EDCs broaden dramatically with underdoping, especially in the $(\pi, 0)$ region of the Brillouin zone (BZ). *We take this as evidence of electron fractionalization in the normal state of these materials.*

There is experimental evidence that the physics of the 1DEG is also relevant to aspects of the electronic spectrum of the cuprates, especially at finite frequencies where local considerations are important. $La_{1.4-x}Nd_{0.6}Sr_xCuO_4$ ($x = 0.1, 0.12, 0.15$) is a "stripe ordered" nonsuperconducting relative of the high temperature superconductors [12]. The low energy ARPES spectral weight is largely confined within patches in the "antinodal" region of the BZ with $k_x \approx \pm\pi/4$ and k_y within 25% of π (and symmetry related regions of the BZ) [3], consistent with the idea that the spectrum is dominated by the 1DEG that lives along nearly quarter-filled stripes. *Static* stripe order has been detected in $La_{2-x}Sr_xCuO_4$ with $x < 0.13$, but not for $x > 0.13$, or in BSCCO or $YBa_2Cu_3O_{7-\delta}$ with $T_c \approx 90$ K. However, in both LSCO with $x > 0.13$ and underdoped $YBa_2Cu_3O_{7-\delta}$, evidence of slowly fluctuating spin order has been detected with inelastic neutron scattering [13,14]. Evidence for fluctuating charge stripe order has also been reported [14].

The idea that the ARPES spectrum in the antinodal regions of BSCCO is dominated by quasi-one–dimensional physics has been discussed in a previous paper [15]. Flat EDCs in the antinodal regions have been observed in stripe ordered LNSCO [3,4] and LSCO [5,6]. Similarly in BSCCO, a dichotomy between a sharp peak in the MDC and the absence of a peak in the corresponding EDC can be clearly seen in Fig. 3 of Ref. [7]. This dichotomy is most pronounced in the underdoped materials. The structures in the EDCs tend to sharpen with overdoping. Moreover, the spectral function shown in Fig. 1d of Ref. [7] is consistent with our Fig. 1.

Electron fractionalization in the normal state of BSCCO near $(\pi, 0)$ was inferred previously by us [15] based on an independent, although somewhat less direct, analysis. It was observed that a sharp quasi-particle-like feature emerges in the superconducting state with $\Delta\omega \sim \Delta k/v_F$, and a weight which is strongly temperature and doping dependent [16–18]. Empirically, it is observed that the weight is roughly proportional to the superfluid density [18]. We have shown [15] that this behavior can be understood as arising from a dimensional crossover from a one dimensional (spin-charge separated) spectrum above T_c to a two-dimensional spectrum, consistent with the existence of an electronlike quasiparticle, below T_c.

It was recently discovered [4] that there is a second component to the spectrum in LNSCO with small spectral weight in the "nodal" region, concentrated along straight Fermi segments perpendicular to the $(0, 0)$ to (π, π) ray, as indicated in Fig. 3. Thus, the distribution of low energy spectral weight in the BZ looks qualitatively similar to that found in LSCO and BSCCO although in the latter the nodal Fermi segments are considerably more curved. The origin of these nodal segments is not clear. Possible sources for them may include a fluctuating stripe array [19] and bond-centered stripes [20]. It is also presently unknown whether such models lead to a fractionalized spectrum in the nodal region, although for sufficiently flat Fermi segments and strong interactions this may be the case [21]. In the following we will take a heuristic approach and also compare the nodal data with the 1DEG predictions.

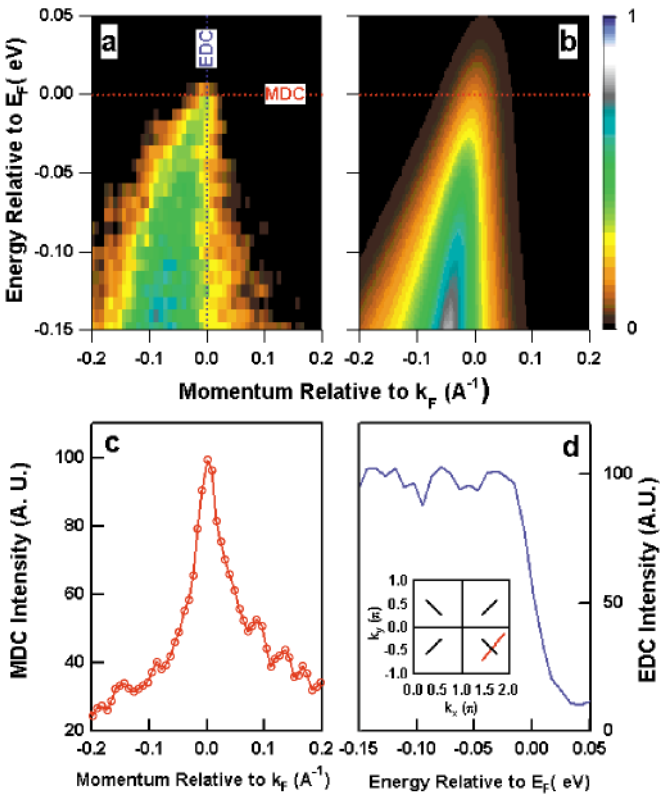

FIG. 3 (color). Spectral functions of $La_{1.25}Nd_{0.6}Sr_{0.15}CuO_4$ (experiment) and a spin rotationally invariant 1DEG (theory) with $\gamma_c = 0.5$, $v_s = 0.7$ eV Å and $v_c = 3.5$ eV Å. In both cases, $T = 15$ K: (a) Experimental contour plot of $A^<(\vec{k}, \omega)$. The data was collected along the line in the second BZ shown in red in the inset. The black diagonal lines indicate the position of the low energy Fermi segments; (b) contour plot for the 1DEG; (c) experimental MDC at $\omega = 0$; (d) experimental EDC at $\vec{k} = (1.6\pi, -0.4\pi)$.

In Fig. 3 we show the one particle spectral function obtained in recent experiments [4] on LNSCO along a ray perpendicular to the Fermi surface at the "nodal point" $\vec{k}_F = (1.6\pi, -0.4\pi)$ (a similar but weaker signal, due to matrix element effects, is observed along an equivalent cut in the first BZ). The measured spectra look similar to those of the spin rotationally invariant 1DEG with $\gamma_c = 0.5$ (Figs. 2c and 3d) and spin and charge velocities $v_s \approx 0.7$ eV Å and $v_c \approx 3.5$ eV Å. The value of $\gamma_c \sim 0.5$ corresponds to very strong interactions. (In comparing theory with experiment, we confine ourselves to the portion of the spectrum with binding energies less than the antiferromagnetic exchange energy, $J \sim 0.1$ eV.)

ARPES measurements along the nodal direction of underdoped, optimally doped, and overdoped LSCO [4–6] reveal behavior of $A^<(\vec{k}, \omega)$ similar to that displayed in Fig. 3. Normal state data from the nodal direction in BSCCO are shown in Refs. [7,22–24]. Here there is [23] a well-formed peak in the MDC, and a comparably sharp peak in the EDC with $\Delta k \approx \Delta\omega/v_F$. If we compare the spectral function with that of a 1DEG, we find that they look fairly similar provided we assume that $\gamma_c \approx 0.2$. Of course, in this case it is also possible to imagine more quasi-particle-like interpretations of the data.

One such interpretation [10] in terms of the marginal Fermi-liquid phenomenology is based on the recent observation [7] that, over most of the Fermi surface of BSCCO, the width of the MDC approximately satisfies the relation $\Delta k \approx (\Delta k)_0 + (\Delta k)_1 T$ for a range of temperatures above T_c, where $(\Delta k)_0$ depends on position along the Fermi surface but $(\Delta k)_1$ does not. However, in the same study it was found that, except for an interval of Fermi surface near the nodal direction (comprising, perhaps, 30% of it), the EDC has little or no peak. Thus, taken at face value, the measured widths of the EDCs outside this interval are *inconsistent* with a marginal Fermi-liquid form of the spectral function. We note that it has been stressed for many years by Anderson [25] and Laughlin [26] that the breadth of the measured EDCs provides strong evidence of electron fractionalization in the high temperature superconductors; the present analysis is similar in outline, although it differs in many particulars.

While some aspects of the data admit to mundane explanations, such as surface disorder, resolution effects where the dispersion is steep, and ambiguities due to any background signal, the data set as a whole is more constraining. For example, while disorder could explain the breadth of the EDC near $(\pi, 0)$, this explanation is in apparent conflict with the sharpness of the MDC and, at least in BSCCO, with the emergence of a sharp peak in the EDC below T_c. Moreover, the structure in the EDC gets sharper with overdoping, although the dispersion does not change substantially, and, at least in LSCO, the density of impurities increases.

We acknowledge stimulating discussions with P. Johnson, J. Tranquada, and T. Valla. We thank S. A. Kellar, P. V. Bogdanov, A. Lanzara, Z. Hussain, T. Yoshida, A. Fujimori, and S. Uchida for collaboration. S. A. K. and E. W. C. were supported in part by NSF Grant No. DMR 98-14289. V. J. E. was supported in part by DOE Grant No. DE-AC02-98CH10886. Data in Fig. 3 were collected at the Advanced Light Source. The SSRL work was supported by DOE Grant No. DE-AC03-76SF00098.

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