Resilient Fermi Liquid and Strength of Correlations near an Antiferromagnetic Quantum Critical Point

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Near the antiferromagnetic quantum critical point (QCP) of electron-doped cuprate superconductors, angle-resolved photoemission experiments detect hot spots where the Fermi surface disappears. Here, we demonstrate, using the two-particle self-consistent theory, that in the antinodal region the Fermi liquid remains stable for a broad range of angles on the Fermi surface and for all dopings near the QCP. We show how the quasiparticle weight Z and effective mass m^* change and then abruptly become meaningless as the hot spots are approached. We propose a dimensionless number, easily accessible in ARPES experiments, that can be used to gauge the strength of correlations.

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Introduction.—Fermi-liquid theory is the basis on which rests the description of electron behavior in metals. Although Landau Fermi-liquid theory was formulated for translationally invariant systems, the presence of a lattice leads to relatively small modifications of the original idea. Fermi-liquid quantities, such as the effective mass and the quasiparticle weight, acquire angular dependence along the Fermi surface, a relatively trivial modification. However, the concept of Fermi liquids has been challenged in strongly correlated materials, such as the high-temperature superconductors, where the notions of non-Fermi liquids [1,2] and marginal Fermi liquids [3] have emerged. The presence of magnetic zero-temperature quantum critical points (QCP) is often invoked as an explanation of non-Fermi-liquid behavior [2].

Detailed analysis of the Fermi surface quasiparticles through the extraction of the self-energy from ARPES measurements have been performed on multiple materials, such as Sr_2RuO_4 [4], organic metals [5], the hole-doped cuprates $Bi_2Sr_2CaCu_2O_8$ and $La_{2-x}Sr_xCuO_4$ [6,7], and the electron-doped cuprate $Pr_{1.3-x}La_{0.7}Ce_xCuO_4$ (PLCCO) [8]. In all these cases, Fermi-liquid quasiparticles have been shown to persist in some segments of the Fermi surface, especially away from putative QCPs in *overdoped* samples.

Here, we show, for the specific case of electron-doped cuprates, where ample experimental data are available [9–11], that the proximity to an antiferromagnetic QCP leaves the Fermi liquid unscathed for large portions of the Fermi surface and for all dopings in the vicinity of the QCP. While many theoretical studies have focused on "hot spots" where non-Fermi-liquid behavior is observed [12,13], we focus on the resilient Fermi-liquid segments that have interesting properties and that can dominate transport [14–16]. In particular, we show that the properties of the resilient portions of the Fermi liquid lead to a new way to quantify the strength of correlations that goes beyond earlier proposals based, for example, on sum rules [17].

In the electron-doped cuprates, an antiferromagnetic phase extends to high dopings, for example $x \sim 0.13$ in $Nd_{2-x}Ce_xCuO_4$ (NCCO) [10]. Antiferromagnetic fluctuations play an important role since a loss of spectral weight at the hot spots, connected by the antiferromagnetic (AFM) wave vector, has been observed through ARPES measurements [9,18–20]. Theoretical and experimental proposals have attributed these observations to antiferromagnetic fluctuations [10,21–23]. Moreover, in the electron-doped cuprate PLCCO, it was shown that the suppression of the AFM pseudogap through "protect annealing" could be due to the suppression of the AFM fluctuations [24].

Model and method.—We study the two-dimensional Hubbard model on a square lattice,

$$H = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}, \tag{1}$$

where $c^{(\dagger)}_{\mathbf{k}\sigma}$ annihilates (creates) an electron of spin σ and crystal momentum $\mathbf{k}$. Allowing first, second, and third nearest-neighbor hoppings, with respective hopping parameters $t = 1$, $t' = -0.175$, and $t'' = 0.05$ that model the electron-doped cuprate NCCO [21], the dispersion relation is $\epsilon_{\mathbf{k}} = -2t[\cos(k_x) + \cos(k_y)] - 4t' \cos(k_x)\cos(k_y) - 2t''[\cos(2k_x) + \cos(2k_y)]$. The strength of interactions is U and $n_{i\uparrow}, n_{i\downarrow}$ are number operators for, respectively, spin-up and spin-down electrons on site i. Planck's constant $\hbar$ is unity.

We solve the model with the two-particle self-consistent approach (TPSC). This method is nonperturbative and respects conservation laws, the Mermin-Wagner theorem, the Pauli exclusion principle, and consistency between single- and two-particle quantities [25,26]. This method is

valid for U ranging from zero to about 0.75 times the bandwidth. While it cannot reproduce the Mott transition, it enables the study of long-wavelength antiferromagnetic fluctuations and their interactions with electrons. It was the first method to accurately predict the condition under which an AFM pseudogap opens at the hot spots where the AFM Brillouin zone crosses the Fermi surface in the 2D Hubbard model without long-range order. Regions where the Fermi liquid disappears, so-called hot spots, occur when the Vilk criterion is satisfied, namely when the AFM correlation length becomes larger than the thermal de Broglie wavelength [10,22,25]. A similar phenomenon is seen with the TPSC approach for the attractive Hubbard model, with the prediction of the opening of a pairing pseudogap when the pairing correlation length becomes larger than the de Broglie wavelength [25,27]. In that case, the whole Fermi surface becomes "hot." The TPSC approach was previously used to study the electron-doped cuprate NCCO with the band parameters listed above [21], reproducing accurately the evolution of the Fermi surface as a function of doping, as observed in ARPES experiments. Unless stated otherwise, we use $U = 5.75t$ that was used to reproduce the NCCO ARPES spectra at $x = 0.15$.

The resilient Fermi liquid.—To study the effect of AFM fluctuations on Fermi-liquid quasiparticles, we study three different dopings: $x = 0.15$ in the underdoped regime (below the AFM QCP), $x = 0.20$ near the AFM QCP [28], and $x = 0.25$ in the overdoped regime (above the AFM QCP). As shown in Fig. 1, in the low but nonzero temperature regime, the AFM pseudogap at the hot spots is only present at $x = 0.15$, while the Fermi surface, at least when contemplated as a color plot, is well defined at $x = 0.20$ and $x = 0.25$.

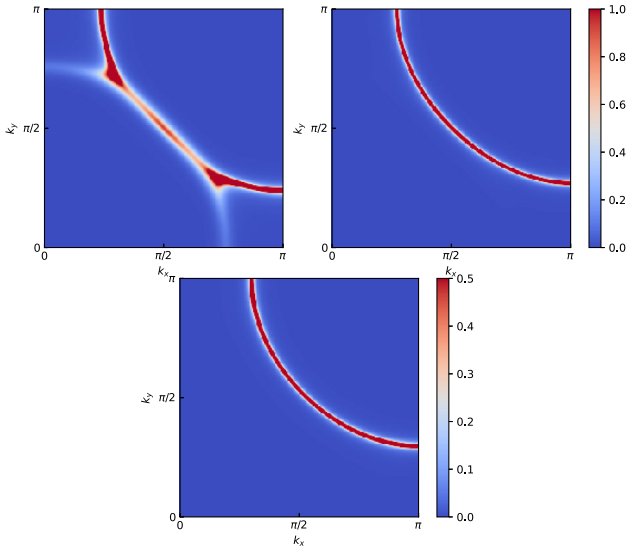

FIG. 1. Momentum distribution curves computed at $T = 0.04t$ for $x = 0.15$ (top panel, left), $x = 0.20$ (top panel, right) and $x = 0.25$ (bottom panel).

We first investigate the behavior of the quasiparticles as a function of the Fermi-surface angle θ, which is defined in Fig. 2. In a Fermi liquid, the expected form of the self-energy at low frequency is

$$\Sigma''(\omega, T) = a_0(T) - a_2\omega^2, \qquad \omega < \omega_c, \tag{2}$$

where T is temperature, ω is frequency, and ω_c is a cutoff frequency. The parameters a_2, a_0, and ω_c can be extracted from ARPES measurements [7,8]. In general, the self-energy is momentum dependent, even though we do not write it explicitly.

We work in Matsubara frequencies where expansion of the Fermi-liquid self-energy at low frequency gives

$$\Sigma(\omega_n, T) = ia_0(T) + b_0(T) + ia_1\omega_n + ia_2\omega_n^2 + \mathcal{O}(\omega_n^3), \tag{3}$$

where $\omega_n = (2n+1)\pi T$ are fermionic Matsubara frequencies and a_0, b_0, a_1, and a_2 are real. One can obtain the imaginary part, Eq. (2), as well as the real part of the self-energy on the real axis,

$$\Sigma'(\omega, T) = b_0(T) + a_1\omega, \tag{4}$$

from the Matsubara expression Eq. (3) using the analytic continuation $\omega_n \to -i(\omega + i0^+)$.

From the real part of the self-energy, Eq. (4), we can extract the quasiparticle weight Z

$$Z = \left(1 - \frac{\partial\Sigma'(\omega)}{\partial\omega}\right)^{-1}\Bigg|_{\omega=0}, \\ = \frac{1}{1-a_1}. \tag{5}$$

The fitting procedure is described in Supplemental Material [29] Eqs. (S1)–(S3).

Figure 2 show the quasiparticle weight Z and the coefficient a_2 of the Fermi-liquid ω^2 dependence as a function of the Fermi-surface angle θ for $x = 0.15$, $x = 0.20$, and $x = 0.25$. At the largest doping studied, far from the AFM QCP, both Z and a_2 show little dependence on θ. However, we observe a qualitatively different behavior at $x = 0.20$. Even though the Fermi surface is still well defined at this doping and in the temperature range we study, the effect of antiferromagnetic fluctuations can be seen in the angle dependence of Z and a_2. Both parameters have a relatively small dependence in θ for angles close to the antinode (0°). However, as θ increases toward the hot spots and the node, we observe a sharp increase in a_2 that is not present in the large doping, $x = 0.25$, case. Finally, at $x = 0.15$, both Z and a_2 are ill defined for angles near the hot spot. The Fermi-liquid form for the self-energy does not hold near the hot spots and the node when the AFM pseudogap is opened [25]. Indeed, in this region, the a_1

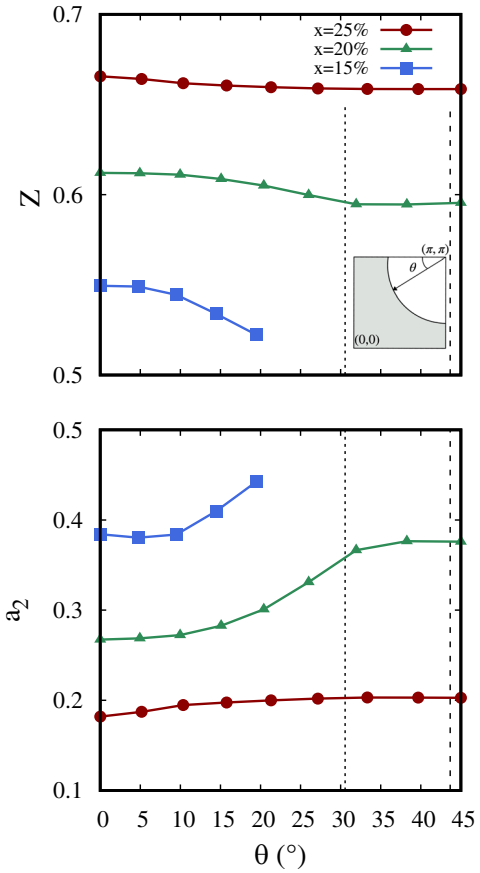

FIG. 2. Fermi-liquid parameters as a function of the angle on the Fermi surface θ for $x = 0.15$ (blue), $x = 0.20$ (green), and $x = 0.25$ (red). Top panel shows the quasiparticle weight Z. Bottom panel shows the ω^2 coefficient a_2 of the self-energy in units of $1/t$. The dotted and dashed lines show the hot-spot angle at $x = 0.15$ and at $x = 0.20$, respectively. The Fermi-surface angle θ is defined as shown in the inset in the top panel, with $\theta = 0°$ at the antinode and $\theta = 45°$ at the node. The calculations were performed in the temperature range $T = 0.02t$ to $T = 0.04t$ for $x = 0.20$ and $x = 0.25$. For $x = 0.15$, we did the calculations from $T = 0.04t$ to $T = 0.05t$ because the TPSC approach is not valid at low temperatures in the renormalized classical regime when the AFM pseudogap becomes too large [25].

coefficient in Σ' cannot be calculated from Eqs. (3) or (S2) in Supplemental Material [29] since it changes sign near the hot spots, denoting the destruction of the quasiparticles [32]. However, even with the presence of the AFM pseudogap at $x = 0.15$, both Z and a_2 remain well defined near the antinode. The imaginary part of the self-energy at the antinode retains a Fermi-liquid form for this doping, which is situated below the AFM QCP.

This study of Z and a_2 as a function of the Fermi-surface angle points toward an anisotropic destruction of the Fermi-liquid quasiparticles on the Fermi surface, as shown by the survival of well-defined quasiparticles at the antinode below the AFM QCP. Moreover, this destruction seems to be gradual as a function of doping. Before the appearance of the AFM pseudogap, the AFM fluctuations at the QCP already influence the quasiparticles, as illustrated by the increase of a_2 near the hot spots at $x = 0.20$.

TABLE I. Corrections to the effective mass from the momentum dependence of the self-energy in percentages calculated using Eq. (7). Calculations were done at $T = 0.02$ for $x = 0.20$ and $x = 0.25$, and at $T = 0.04$ for $x = 0.15$. The values of Δk are 0.12 for the antinodal direction and 0.17 for the nodal direction.

	$x = 0.15$	$x = 0.20$	$x = 0.25$
AN, $-\Delta k$	2.6	5.2	5.7
AN, $+\Delta k$	2.8	5.3	5.7
N, $-\Delta k$	28	15	7.8
N, $+\Delta k$	77	14	7.8

An additional way to determine whether quasiparticles are well defined or not is to compute the effective mass m^*, which can be written as a function of the quasiparticle weight Z and of the momentum dependence of the self-energy perpendicular to the Fermi surface

$$\frac{m}{m^*} = Z\left(1 + \frac{\partial\Sigma'(\mathbf{k}, \omega = 0)}{\partial\xi_{\mathbf{k}}}\right), \tag{6}$$

$$\frac{\partial\Sigma'(\mathbf{k}, \omega = 0)}{\partial\xi_{\mathbf{k}}} = \frac{\hat{e}_{\mathbf{k}} \cdot \nabla_{\mathbf{k}}\Sigma'(\mathbf{k}, \omega = 0)}{\hat{e}_{\mathbf{k}} \cdot \nabla_{\mathbf{k}}\xi_{\mathbf{k}}}. \tag{7}$$

We calculate the gradients with small momentum differences Δk: $\nabla_{\mathbf{k}}\Sigma'(\mathbf{k}) \simeq [\Sigma'(\mathbf{k} \pm \Delta k) - \Sigma'(\mathbf{k})]/\Delta k$. We assess the ill- or well-defined character of the effective mass by comparing the derivatives calculated with positive and negative Δk. The results from Eq. (7) for $x = 0.15$, $x = 0.20$, and $x = 0.25$ are shown in Table I. We observe that the momentum-dependent correction to the effective mass is well defined at the antinode for all three dopings, since the left and right derivatives are equal and that these corrections are quite small, of the order of 5%. This is also true at the node at $x = 0.25$. At the node at $x = 0.20$, however, the correction is larger by an order of magnitude. This indicates a strong momentum dependence for this doping at the node, even without an AFM pseudogap. At the node at $x = 0.15$, the correction is large and the left and right derivatives disagree. These findings are consistent with our previous discussion of Z and a_2, and reinforce our conclusion that Fermi-liquid quasiparticles remain well defined at the antinode at $x = 0.15$.

Temperature dependence of the scattering rate.—Further signatures of the anisotropy between the node and the antinode at the QCP, $x = 0.20$, can be found through the temperature scaling of the self-energy. Following Appendix B of Ref. [22], we assume ω/T scaling for the imaginary part of the self-energy in real frequencies

$$\Sigma''(\omega) = a(\pi T)^{\nu}\phi\left(\frac{\omega}{\pi T}\right), \tag{8}$$

where a is a constant. This allows us to find the exponent ν at $\omega = 0$ with the procedure described in Supplemental Material [29], Eqs. (S6)–(S11). The exponent $\nu = 2$ corresponds to Fermi-liquid behavior, while $\nu < 2$ corresponds to non-Fermi-liquid behavior.

We calculate the exponent ν at the node and at the antinode for $x = 0.20$ and $x = 0.25$. At the antinode, we recover $\nu \simeq 2$ for both dopings. While $\nu \simeq 2$ is also true at the node for $x = 0.25$, it is not the case at $x = 0.20$, where $\nu \simeq 1.4$. Similarly to our calculation of a_2 as a function of the Fermi-surface angle, this scaling analysis shows that the Fermi liquid is resilient only near the antinode at the AFM QCP ($x = 0.20$).

Fermi liquid and strength of interactions.—The properties of the antinodal Fermi liquid can be used to quantify the strength of interactions. It has been proposed that the Fermi-liquid cutoff frequency ω_c, namely the frequency at which ω^2 behavior disappears, can indicate the strength of the interactions in a correlated material [8]. We focus on the antinodal direction for $x = 0.15$, $x = 0.20$, and $x = 0.25$, and on the nodal direction for $x = 0.25$, where the Fermi liquid is stable. We vary U from $1t$ to $5t$. Evidently, the determination of the cutoff frequency ω_c has some arbitrariness, but as long as one adheres to a definition, the results are consistent. Here, we calculate the deviation between the imaginary part of the linearly interpolated Matsubara self-energy we obtain from our calculation and the fit using Eq. (3). We take ω_c as the frequency at which this deviation reaches a threshold of 10%, 15%, or 20% for a fixed temperature $T = 0.02$.

As shown in Fig. S4 of Supplemental Material [29], ω_c decreases with U and increases with the quasiparticle weight Z, so that ω_c can indeed measure the strength of interactions. Moreover, for a fixed value of U, ω_c increases with doping, which means that ω_c is a measure of electronic correlations in a broader sense. Given the angular dependence of Z illustrated in Fig. 2, it is clear that this measure of interaction is not uniquely defined for a given compound.

Horio *et al.* [8] also suggested a spectroscopic analog of the Kadowaki-Woods ratio that would relate a_2 and Z, two quantities we obtained in our calculations for multiple values of U. This is discussed in Fig. S5 in Supplemental Material [29]. We propose instead that the dimensionless number $a_2 \times \omega_c$ is a more robust estimate that scales as $(Z^{-1} - 1)$. It is shown in Fig. 3 (left panel) with ω_c calculated using a threshold of 15%. This scaling is a general result that follows from the Kramers-Kronig relation. More precisely, we find

$$Z_{\mathbf{k}}^{-1} - 1 = \frac{4\xi_{\mathbf{k}}}{\pi}\omega_{c,\mathbf{k}}a_{2,\mathbf{k}}, \tag{9}$$

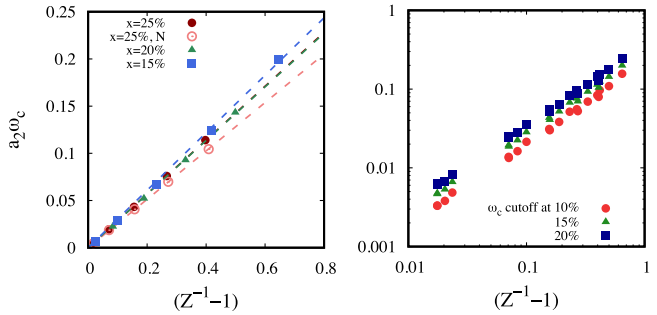

FIG. 3. The product of a_2, the coefficient of ω^2 in Σ'', and of ω_c, the Fermi-liquid cutoff frequency, is related to the quasiparticle weight Z through a Kramers-Kronig relation. Here, all the dots are computed for different values of U (shown in Supplemental Material, Fig. S4 [29]). Left panel shows data at the antinode, for dopings $x = 0.25$ (red), $x = 0.20$ (green), and $x = 0.15$ (blue), and at the node for $x = 0.25$ (pink), with ω_c calculated with a relative deviation threshold from ω_n^2 of 15%. The right panel shows a log-log plot of the data for the dopings listed above, with ω_c calculated with three different thresholds, 10% (orange), 15% (green), and 20% (blue). Note that for a given threshold, all dopings of the left panel here fall on the same straight line, with only small variations.

where $\xi_{\mathbf{k}}$ is a constant that varies between 2 and 4 in our calculations. It can be both momentum dependent and material dependent, as seen from the different slopes in the left panel of Fig. 3. It also depends on the criterion that defines the cutoff frequency ω_c. This highlights the challenge in finding Z from spectroscopic data. Nevertheless, for general trends, it is quite useful as shown on the right panel of Fig. 3. There we show on a log-log plot the scaling $a_2 \times \omega_c$ vs $(Z^{-1} - 1)$ for the different dopings and angles as a function of the threshold for the cutoff frequency ω_c. On this scale, only the choice of threshold for the cutoff frequency, shown in different colors, has a visible effect on the result.

Discussion.—One could argue that the resilience of the antinodal Fermi liquid is not surprising given that the electron Fermi-surface pocket of the $T = 0$ antiferromagnet basically coincides for a large part with the antinodal section in the normal state. This is not so trivial, however, since a hole pocket also develops in the nodal direction in the AFM that eventually occurs at $T = 0$, while that part of the Fermi surface disappears completely in the pseudogap regime, at least for the temperatures we could consider.

An angle dependence of the a_2 coefficient analogous to what we observe here has been previously measured in the hole-doped cuprate LSCO in the overdoped regime, outside of the pseudogap phase [7]. In the case of LSCO, the a_2 coefficient was found to be stable around the node and to increase as the angle decreases toward the antinode, before vanishing at an angle of $\phi_0 \simeq 15°$. This behavior is analogous to the one described here, but the roles of the antinode and the node are exchanged. This is expected from

the fact that, in the hole-doped cuprates, the pseudogap opens in the antinodal region of the Fermi surface.

In contrast, recent ARPES experiments have shown that the a_2 coefficient in the electron-doped cuprate PLCCO is constant as a function of the Fermi-surface angle in the overdoped regime [8]. These measurements are reminiscent of our results at $x = 0.25$, far from the AFM QCP. The case of LSCO also illustrates that different portions of the Fermi surface can be affected very differently by interactions, analogous to what we have seen in our calculations (Fig. 2).

Our plot Fig. 3, based on the stable Fermi-liquid portions of the various compounds, quantifies the relative strength of interactions. The two quantities a_2, the coefficient of the ω^2 dependence, and ω_c the cutoff frequency for Fermi-liquid behavior, can be obtained experimentally from ARPES data. Given a future agreement between researchers on a reference case and on the way the cutoff frequency ω_c is determined, it becomes possible to compare the correlation strength in different materials using the proportionality between $a_2 \times \omega_c$ and $Z^{-1} - 1$. At this stage, we cannot compare quantitatively our results to experimental measurements because we obtained ω_c from the Matsubara self-energy. Nevertheless, using the data presented in Refs. [7,8], we obtain $a_2 \times \omega_c = 0.90 \pm 0.07$ for PLCCO while for LSCO, depending on the Fermi-surface angle, we obtain $a_2 \times \omega_c$ ranging from 1.0 ± 0.4 to 1.7 ± 0.2. This supports previous theoretical suggestions that hole-doped cuprates are more strongly correlated than electron-doped cuprates [33–35].

Conclusion.—The stability of the Fermi liquid on portions of the Fermi surface should be a general property of materials where electrons scatter off critical fluctuations with nonzero wave vector [15]. In such a case, the hot-spot phenomenon occurs and "cold regions" are bound to be stable Fermi liquids whose product $a_2 \times \omega_c$, accessible in ARPES experiments, can be used to provide a dimensionless scale that quantifies the strength of interactions.

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