Universality of the single-particle spectra of cuprate superconductors

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All the available data for the dispersion and linewidth of the single-particle spectra above the superconducting gap and the pseudogap in metallic cuprates for any doping has universal features. The linewidth is linear in energy below a scale \( \omega_c \) and constant above. The cut-off in the linewidth at \( \omega_c \) mandates, due to causality, a “waterfall”, i.e., a vertical feature in the dispersion. These features are predicted by a recent microscopic theory. We find that all data can be quantitatively fitted by the theory with a coupling constant \( \lambda_0 \) and an upper cutoff at \( \omega_c \) which vary by less than 50\% among the different cuprates and for varying dopings. The microscopic theory also gives these values to within factors of \( O(2) \).

PACS numbers: 74.20.Mn, 74.25.Jb, 74.72.-h

Introduction. With increased refinement of technique and imaginative use, angle-resolved photoemission spectroscopy (ARPES) on the high temperature superconductors has revealed that novel physical principles determine the single-particle spectra in such compounds [1, 2]. Recently, the single-particle spectra over an energy range from the chemical potential to about 1 eV have been deduced for various metallic dopings in different cuprates [3, 4, 5, 6, 7, 8, 9, 10]. Also, recently a microscopic theory [11] has been formulated which derives the fluctuations leading to the phenomenological marginal Fermi liquid (MFL) [12] and their coupling to fermions. MFL had previously been tested only for low marginal Fermi liquid (MFL) [12] and their coupling to fermions. MFL had previously been tested only for low energies and near optimal doping in Bi2212 [13, 14, 15] with adjustable couplings. Here we test crucial new features of the microscopic theory including its universality, its cut-off and coupling functions, by comparing with recent ARPES data in 4 different cuprate families and at different dopings.

The most important results of these recent ARPES experiments may be summarized as follows:

(i) The spectra for energies \( \omega \) in the range of interest (above the superconducting gap and the pseudogap energy scales) are universal; they have the same functional form for all cuprates and for all metallic dopings. Moreover, even the parameters in the functional form vary less than by a factor of 2 over the entire range of cuprates for which data is available, irrespective of whether they are underdoped (UD), optimally doped (OP) or overdoped (OD).

(ii) The momentum distribution curves (MDC) at constant energy \( \omega \) is a Lorentzian with width \( \omega_k(\omega) \). In the energy range of interest \( \omega_k \) varies linearly with \( \omega \) up to a cutoff above which it is approximately a constant. This is modified if the bare velocity \( v(k) \) varies with \( \omega \), which happens as the bottom of the band is approached. See Fig. [3] below for representative experimental data.

(iii) The peak of the MDC as a function of \( \omega \) moves with \( k \) defining the renormalized dispersion \( \varepsilon(k) \). The observed dispersion \( \varepsilon(k) \) follows the band structure \( \epsilon_k \) with a smooth renormalization factor up to \( \omega \approx E_1 \). Above \( E_1 \), the “velocity” \( d\varepsilon(k)/dk \) sharply increases up to another cutoff \( E_2 \) where \( \varepsilon(k) \) resumes the normal dispersion. The nearly vertical dispersion has been picturesquely termed a “waterfall” [3]. In the energy range, \( E_1 \approx \omega \approx E_2 \), there is also an indication of multiple \( \varepsilon(k) \) for fixed \( \omega \) [6, 8]. \( E_1 \) varies systematically being largest in the \((\pi, \pi)\) direction and smallest in the \((0, 0)\) direction [8]. Similarly, the position of the “waterfall” in \( k \)-space varies systematically.

All these features follow quantitatively from the quantum-critical fluctuations derived recently [11]. We find that, given the bare band structure \( \epsilon_k \), all available data can be fitted with the two parameters of this theory, a sharp cutoff \( \omega_c \) and a coupling constant \( \lambda_0 \) calculable to factors of \( O(2) \).

Single-particle spectral function. The single-particle spectral function deduced by ARPES is given

\[
A(k, \omega) = \frac{-\text{Im}\Sigma(\omega, k)/\pi}{[\omega - \text{Re}\Sigma(\omega, k) - \epsilon_k]^2 + [\text{Im}\Sigma(\omega, k)]^2},
\]

where \( \Sigma(\omega, k) \) is the self-energy function. The band structure \( \epsilon_k \) is in general fitted by the tight-binding dispersion [10].

Microscopic Theory. A microscopic theory for the cuprates [11, 17, 18] is based on the realization, that the central organizing feature in the physics of the metallic phase of the cuprates are quantum critical fluctuations of loop currents. In this theory the ordering of these loop currents below \( T_g \) (PG in inset of Fig. [1]) leads to a phase which breaks time-reversal symmetry but preserves translational symmetry. Direct evidences for such an ordered state have been obtained by polarized neutron scattering in \( \text{YBa}_2\text{Cu}_3\text{O}_{6+x} \) [19] and by dichroic ARPES experiments in \( \text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+x} \) [20], for various \( x \) in the pseudo-gap phase. The properties in the entire funnel shaped region (I) in inset of Fig. [1] are determined by the quantum critical fluctuations of the loop currents. Therefore universal properties are predicted for \( \omega \) larger than the superconducting gap or the pseudogap for all \( x \) in the metallic phases on either side of \( x_c \).
The microscopic theory of the quantum-critical fluctuations [11] gives their absorptive part to be

$$\text{Im}\chi(q, \nu) = -\chi_0 \tanh \frac{\nu}{2\pi T}, \quad |\nu| < \omega_c;$$
$$\text{Im}\chi(q, \nu) = 0, \quad |\nu| > \omega_c. \quad (2)$$

$\omega_c$ is a cutoff and $\chi_0$ gives the integrated weight of the fluctuations. In the microscopic theory [11], $\omega_c^2 \approx 2EV/R$, where $E$ is the local repulsion or charging energy parameter, $V$ the nearest neighbor Cu-O interaction, and $R$ is the dimensionless loop-current order parameter. $\chi_0 \approx R/\omega_c$. For $E \approx 5eV$, $V \approx 1 - 2eV$ and $R \approx 0.1$ which is consistent with the neutron measurements, we expect $\omega_c \approx 0.3 - 0.5eV$.

**Calculation of the Self-energy.** The loop current fluctuations scatter fermions from $k$ to $k'$ with the amplitude $\gamma(k, k')$. From the microscopic model, we find [21]

$$\gamma(k, k') = \pm \frac{V}{2} (s_{\alpha} (k + k') s_{\alpha} (k - k') - x \leftrightarrow y) S_{\alpha \beta}(k, k'),$$

where $s_{\alpha \beta}(k) \equiv \sin(k_{\alpha} a / 2)$, $s_{\alpha \beta}(k) \equiv \sqrt{s_{\alpha}^2 (k) + s_{\alpha}^2 (k')}$, $S_{\alpha \beta}(k, k') \equiv (s_{\alpha}^{-1} (k) + s_{\alpha}^{-1} (k'))$. The leading self-energy contribution is

$$\Sigma(i\omega_n, k) = T \sum_{q, i\nu_n} |\gamma(k, k + q)|^2 G(i\omega_n + i\nu_n, k + q) \chi(q, i\nu_n),$$

where $\omega_n$, $\nu_n$ are Matsubara frequencies of the quasi-particle and the fluctuating mode, respectively. Given a $q$-independent $\chi$ and $\gamma(k, k')$ of the form of Eq. (3), the self-energy variation with $k$ on a Fermi surface comes only from the separable $s$-wave part of $|\gamma(k, k')|^2$ which is $\propto (1 - \cos k_{\alpha} a \cos k_{\beta} a) (k \rightarrow k')$. This gives $\lambda_0 \propto (1 - \cos k_{\alpha} a \cos k_{\beta} a)$ which varies by about a factor of 2 from the $(\pi, \pi)$ to the $(\pi, 0)$ directions for the Fermi surface of Bi2212 near optimal doping.

At $T = 0$ the self-energy is easily evaluated to be

$$\text{Im}\Sigma(\omega, k) = -\lambda(k) \frac{\pi}{2} \left[ |\omega|, \quad |\omega| < \omega_c \right.$$
$$\text{Re}\Sigma(\omega, k) = -\frac{\lambda(k)}{2} \left[ \omega \ln \frac{\omega + \omega_c}{\omega_c} + (\omega - \omega_c) \ln \frac{\omega - \omega_c}{\omega_c} \right.$$ \quad (5)

$$\left. - (\omega \rightarrow -\omega) \right],$$

where $\lambda(k) = \chi_0 \langle \gamma^2(k') \rangle$, $\lambda_0 = N(0)(V^2/4)\chi_0$, and $\langle \gamma^2 \rangle$ is the average of $|\gamma(k, k')|^2$ over $k'$ on the Fermi surface. For the density of states per one spin species $N(0) \approx 1.1V^{-1}$ and other parameters used above, we expect $\lambda_0 \approx 1$.

Given such a weakly momentum dependent self-energy, the vertex corrections [22] to the self-energy are only of $O(\lambda_0/w)$, where $W$ is the bare bandwidth of the conduction band. Using the $\omega_c$ and $\lambda$ fitted to the experiments, this ratio is of $O(0.1)$. The remaining processes, repeated scattering (self-consistent Born approximation) produce no singular corrections. At low energies compared to $\omega_c$, Eq. (5) reduces to the MFL form deduced earlier [12], except for the weak momentum dependence.

**The Waterfall.** The dispersion of the quasi-particles, $\varepsilon(k)$, given by

$$\varepsilon(k) - \text{Re}\Sigma(\varepsilon(k)) - \epsilon_k = 0. \quad (6)$$

As shown in Fig. 1, $\omega - \text{Re}\Sigma(\omega)$ has a wide reentrant region from $\omega_1 \leq \omega \leq \omega_2$. The solution of Eq. (6) therefore produces a “waterfall” in the dispersion $\varepsilon(k)$ because it varies over the large energy range $\omega_1$ to $\omega_2$ for a very small variation in $k$. The multiple solutions obtained in this region are within $\text{Im}\Sigma(\omega)$ for $\lambda$ of $O(1)$.

**Comparison with Experiments:** The calculated self-energy at $\lambda_0 = 1$ (suitable to fit the experimental data [8] for La$_{1.83}$Sr$_{0.17}$CuO$_{4}$) is shown in Fig. 1. The experimental MDC width for this compound and the calculated widths for three different cuts are compared with experiment in Fig. 3. In Fig. 1 (a)-(c), we compare the experiments [3] for the dispersion of three Bi2212 samples at different dopings with calculations with $\omega_c = 0.5$, $\lambda_0 \sim 1$. In Fig. 3 (d), we compare the measured linewidth for an UD-LSCO sample, an OP-Bi2201 sample and an OP-Bi2212 sample with calculations with parameters given
In the figure caption.

**Universalities of the Data:** The data and the comparison with experiments in Fig. 3 and Fig. 4 (a)-(d) attest to the universality of the single-particle spectra of the cuprates and of the quantitative success of the theory. Now we consider in detail each of the points (i) to (iii) of the experimental data and explain them successively.

(i) The physical properties in any quantum critical regime are universal, controlled by the scale-invariant critical fluctuations. Specifically, for \( \omega \) larger than the superconducting gap or the pseudogap the self-energy is of MFL form and given in terms of only the two parameters \( \omega_c, \lambda_0 \) for each compound for all \( x \). Weak dependencies in these parameters from variation in microscopic parameters due to varying \( x \) or \( T \) may occur of course. We find however that for a given compound, a single value of these parameters is adequate to fit all the available data for different \( x \) and for all momentum directions.

It is worth noting that the spectra of energies below the pseudogap energy and \( T \lesssim T_g \) is also scale-invariant with a new scale \( \propto T_g(x) \).

(ii) Suppose at certain energy \( \omega \), Eq. (3) is satisfied for \( k = k_0 \). Since the self-energy does not depend significantly on \( k \), we can expand the spectral function in \( (k - k_0) \). The MDC is then a Lorentzian with width \( w_k \) given by \( \text{Im} \Sigma(\omega)/\nu(k_0) \) where \( \nu(k_0) = \nu_y(k_0) + \nu_x(k_0)(k_x - k_{x0})/(k_y - k_{y0}) \), is the bare velocity in the momentum-cut direction. This expansion also requires that within \( (k - k_0) \approx w_k \), the velocity \( v_k \) is nearly a constant.

As discussed above \( \text{Im} \Sigma(\omega) \) increases linearly in \( \omega \) for \( \omega \lesssim \omega_c \) and is constant beyond. Therefore if \( \nu_0(k) \) varies slowly with \( k \) as in cut 2 in Fig. 2, MDC linewidths also
vary linearly in $\omega$, i.e., $w_k \propto \omega$. Away from the nodal momentum directions, $v_0(k)$ varies considerably as in cut 4 and higher of Fig. 2. As a result, MDCs’ linewidth deviates from the linear-$\omega$ dependence. This accounts for the MDC width of cut 5 shown as an example in Fig. 3 and the higher cuts. If the MDC linewidth is obtained both in theory and the experiments.

(iii) Comparing Figs. 2(d-f), we can see that there are two distinct reasons for the “waterfalls”. If $c_k$ reaches $\omega_k - \text{Re} \Sigma(\omega_k)$ at $k \approx k_0$ as $k$ is varied along the momentum cut, e.g., cut 2 in Fig. 2, $\varepsilon(k)$ follows the “waterfall” between $\omega_1$ and $\omega_2$, which correspond to $E_1$ and $E_2$ defined in experiments.

If the momentum cuts are sufficiently away from the nodal cut such that the bottom of the band is very shallow, $c_k$ never reaches $\omega_k - \text{Re} \Sigma(\omega_k)$; e.g., cuts 5-8 in Fig. 2. The observed dispersion $\varepsilon(k)$ then follows Eq. (6) to its maximum value at the bottom of the band $k_m$. For higher energies, there are no solutions to Eq. (6). In this case the MDC curves stay centered at $k_m$ which leads to another type of “waterfall”. $E_1$ in this case is nearly the energy of the bottom of the renormalized band, and gets continuously smaller as the bottom of the band (where the velocity is zero) becomes continuously more shallow from the $(\pi, \pi)$ to the $(\pi, 0)$ direction. The variation of the position of the “waterfall”’s, Fig. 3 of Ref. [8] and Fig. 3 of Ref. [6] is thereby explained. In addition, the linewidth is no longer given by $\text{Im} \Sigma(\omega_k)$, leading to an additional cusp in linewidth at $E_1$ (e.g., cut 5 in Fig. 3).

However, if radial cuts are taken to avoid the shallow band, the position of the “waterfall” in momentum space is always the locus of $k$ where $\varepsilon(k) \approx \omega_1$. This locus is shown in Fig. 2(a) for radial cuts and is to be compared with data in Fig. 4 of Ref. [8] and Fig. 4 of Ref. [6].

Concluding remarks. The experimental results discussed place strong constraints on a theory applicable to the cuprates. Specifically, the experiments give a scattering rate linear in $\omega$ up to a sharp cut-off at $\omega_c$ and constant above with a coefficient which is a weak function of $k$. This behavior is found in the entire ‘strange metal’ region of the phase diagram. We do not know any ideas proposed for cuprates besides those discussed here which give these properties.

In this paper, we have pointed out the universal aspects of the measured single-particle self-energy in cuprates and shown that its functional form and even its magnitude is consistent with the recent microscopic theory of quantum critical fluctuations [11]. These fluctuations are predicated on the existence of an unusual symmetry breaking in underdoped cuprates for which considerable experimental evidence has also been adduced.

Acknowledgments. CMV is especially grateful to J. Mesot for interesting him in the problem and to him, J. Chang, S. Pailliès and C. Mudry for a detailed discussion of the data. Thanks are also due to J. Graf and A. Lanzara for communications regarding their data.

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