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Strong-coupling theory of the universal linear temperature dependence of the nodal Fermi velocity in layered cuprates

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We explain the recently observed linear temperature dependence of the nodal Fermi velocity $v_F(T)$ in nearly optimally doped cuprates. We argue that it originates from electron-electron interaction and it is a fundamental property of an arbitrary two-dimensional (2D) Fermi liquid. We consider a spin-fermion model with input parameters extracted from the data, and we show that the T term is about 30% at 300 K, in agreement with the data. We show that the sub-leading term in $v_F(T)$ is a regular (and small) T^2 correction. We also show that at a $2k_F$ quantum-critical point, temperature corrections to the dispersion are singular.

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The origin of strong deviations from the Fermi-liquid behavior in the normal state of the hole-doped cuprates, the mechanism of d-wave superconductivity, and the nature of the pseudogap phase remain the subjects of active debate in the condensed-matter community. Deep inside the pseudogap phase, the cuprates are Mott-Hubbard insulators. Outside the pseudogap phase, angle-resolved photoemission spectroscopy (ARPES) and other measurements show a large Luttinger Fermi surface and an ω^2 behavior of the fermionic damping at the lowest energies,[1,2] consistent with the idea that in this range the system is a Fermi liquid with strong correlations.

We take the point of view that the crossover from a metal to a Mott insulator occurs inside the pseudogap phase, while to the right of the T^* line, the number of carriers is $1-x$, where x is doping. In the $1-x$ regime, the fermionic self-energy can be described in conventional terms, as originating from the interaction with some bosonic degrees of freedom. A boson can be a phonon, or it can be a collective electronic excitation in spin or charge channels. The same interaction is also thought to be primarily responsible for the pairing instability, which eventually leads to superconductivity.

The nature of the pairing boson in the cuprates is the subject of ongoing debate. In recent years several proposals to distinguish experimentally between phononic and electronic mechanisms have been discussed.[3–8] One of the proposals is to look at the temperature dependence of the Fermi velocity, $v_F(T)=v_F(T=0)[1+\delta(T)]$, taken along the diagonal of the Brillouin zone (BZ), where the $d_{x^2-y^2}$-wave superconducting gap has nodes (the “nodal” velocity). It was measured recently by Plumb *et al.*[9] in optimally doped $Bi_2Sr_2CaCu_2O_{8+\delta}$ by means of laser-based angle-resolved photoemission spectroscopy. They found that $\delta(T)$ is approximately linear in T up to at least 300 K. The linear behavior holds down to T_c, and the slope is quite large: $\delta(T)$ is about 0.35 between T_c and $T=250$ K. The linear T dependence of $\delta(T)$ is a challenge to theorists, as on general grounds one would expect an analytic T^2 dependence at the lowest T. The magnitude of $\delta(T)$ is another challenge, as the coupling to the boson is set by fits to other experimental data, including the value of T_c.

The linear in T dependences of various observables in the normal (nonpseudogap) state have been reported before and phenomenologically described in terms of marginal Fermi-liquid (MFL) behavior.[10,11] The linear in T behavior of the velocity is different for two reasons. First, the self-energy, which yields $\delta(T)\propto T$, scales as $\mathrm{Re}\,\Sigma \propto \omega T$, while MFL behavior originates from $\mathrm{Re}\,\Sigma \propto \omega \log \max(\omega,T)$ [and $\mathrm{Im}\,\Sigma \propto \max(\omega,T)$]. Second, the linear behavior of $\delta(T)$ has been measured down to energies ($\pi T \to \omega$) where $\mathrm{Im}\,\Sigma$ already has a Fermi liquid, in ω^2 form.[9] From this perspective, the linear in T dependence of the velocity appears to be a truly low-temperature asymptotic behavior, as opposed to MFL behavior, which likely holds only above the upper boundary of the Fermi liquid.[7,12]

The quasilinear T dependence of the Fermi velocity can be obtained due to electron-phonon interaction but only as approximate behavior in a limited T range above the Debye frequency ω_D,[13] where the temperature-dependent velocity slowly approaches its bare value after passing through a minimum at $T\sim\omega_D$. On the other hand, electron-electron interaction in two dimensions gives rise to a linear in T dependence of $\delta(T)$ down to the lowest temperatures, at which the system is still in the normal state.[14,15] The linear in T correction to the velocity comes from the ωT term in the real part of self-energy, which in turn originates from the nonanalytic $\mathrm{Im}\,\Sigma(\omega)\sim\omega^2 \log \omega$, coming from backscattering.[14,16]

Although the original analysis in Refs. 14 and 15 was a weak-coupling perturbation theory, one can show that $\delta(T)$ is linear in T in an arbitrary Fermi liquid. The reasoning parallels the one in Ref. 17 for the specific-heat coefficient, which is also linear in T in a two-dimensional (2D) Fermi liquid.

The magnitude of δT is a different issue. To second order in the interaction $U(q)$, the velocity renormalization is given by[14]

$$\delta(T) = AT\left\{\left[U(0)-\frac{1}{2}U(2k_F)\right]^2 + 3\left[\frac{U(2k_F)}{2}\right]^2\right\}, \quad (1)$$

where $A=p_F \log 2/(4\pi^2 v_F^3)$. The two terms in Eq. (1) account for the contributions from charge and spin channels. Approximating the measured Fermi surface (FS) of

$Bi_2Sr_2CaCu_2O_{8+\delta}$ (Bi2212) by a circle with $p_F \sim \sqrt{2}\times 0.6\pi = 2.7$ (we set the interatomic distance to 1) and $U(q)$ by $U \sim 2$ eV and using $v_F \sim 1$ eV (Refs. 18 and 19), we find $\delta(T) \sim 1.610^{-5}T$, where T is measured in kelvins. This yields $\delta(T) \sim 5\times 10^{-3}$ for $T \sim 300$ K, 2 orders of magnitude smaller than the experimental value.

The second-order estimate, however, is valid only in the weak-coupling regime, where the system is far from a Pomeranchuk-type instability. There is a consensus among researchers that near optimal hole doping, the coupling is actually strong. Strong interaction brings about two effects. On one hand, larger coupling leads to a larger $\delta(T)$. On the other hand, the effective screened interaction between quasiparticles deviates from the second-order $U^2\Pi$ form, where Π is the dynamic polarization bubble, and one has to consider the full effect of the screening. Since Π is temperature dependent, this generally affects the functional form of $\delta(T)$. The purpose of this Rapid Communication is to analyze the interplay between these two effects.

As a model for the dynamic screening, we consider the interaction between fermions and their collective bosonic excitations in the spin channel. Several groups argued[12,20,21] that this interaction is responsible for the normal-state self-energy and the pairing. We show that the velocity renormalization is *not* affected by the full dynamic screening of the effective interaction. The extra terms in $\delta(T)$, due to the difference between the full interaction and $U^2\Pi$, scale as T^2 and are small for all experimentally studied T. For the linear in T term, we find, using the same parameters as in earlier studies, $\delta(T) \approx 0.37$ at 250 K, in good agreement with the data.

The singular interaction in the spin channel is a $2k_F$ process, which for holelike cuprates' Fermi surface is an umklapp scattering between nodal fermions at $\mathbf{k}_F = (k_F, k_F)$ and $\mathbf{Q} - \mathbf{k}_F$. The normal-state fermionic self-energy due to nodal-nodal interaction was previously considered in the context of quantum-critical (QC) phenomena.[22] Here we consider the system behavior away from the QC point, when the bosonic propagator has a finite mass. In the notation $G^{-1}(\mathbf{k}, i\omega_m) = i\omega_m - \epsilon_{\mathbf{k}+\mathbf{k_F}} + \Sigma(\mathbf{k}, \omega_m)$, the self-energy due to coupling to spin fluctuations is given by

$$\Sigma(\mathbf{k}, i\omega_m) = -\frac{3\bar{g}}{4\pi^2} T \sum_{\Omega_m} \int d^2q \chi(\mathbf{q} - 2\mathbf{k}_F, i\Omega_m) \times \frac{1}{i(\omega_m + \Omega_m) - \epsilon_{-\mathbf{k}_F+\mathbf{k}+\mathbf{q}+\mathbf{Q}}}, \quad (2)$$

where $\mathbf{k_F}$ is the Fermi momentum along zone diagonal, counted from the (π,π) point $[(0.8\pi, 0.8\pi)$ for optimally doped Bi2212]. Near the Fermi surface

$$\varepsilon_{\mathbf{k}+k_F} = v_F k_x + \beta^2 k_y^2,$$

$$\varepsilon_{-\mathbf{k_F}+\mathbf{k}+\mathbf{q}+\mathbf{Q}} = -v_F(k_x + q_x) + \beta^2 (k_y + q_y)^2, \quad (3)$$

where x is set along the zone diagonal, toward $(-\pi, -\pi)$, and β parametrizes the curvature of the Fermi line, $\beta^2 = 1/(2m)$ for a circular FS.

Further, $\chi(\mathbf{q}, \Omega_m)$, normalized to $\chi(0,0) = 1$, is the dimensionless dynamical spin susceptibility and $\bar{g} = [U(2k_F)/2]K$ is the effective enhanced coupling in the spin channel. The factor K, which reduces to 1 at weak coupling, is the ratio of the actual to the bare static spin susceptibility at momentum $2k_F$. We assume, based on neutron-scattering data, that the momentum dependence of the static susceptibility is weak near $\mathbf{q} = 0$ and approximate the full dynamic spin susceptibility at small $\mathbf{q}$ as $\chi(\mathbf{q} - 2\mathbf{k}_F, i\Omega_m) = 1/[1 + \bar{g}\Pi(\mathbf{q} - 2\mathbf{k}_F, i\Omega_m)]$, where $\Pi(\mathbf{q} - 2\mathbf{k}_F, i\Omega_m)$ is the polarization bubble with momenta near $2\mathbf{k}_F$ (the spin factor of 2 is included in Π).

The $2k_F$ particle-hole bubble was calculated before.[22] It contains a regular part, which plays no role in our analysis and which we neglect, and a nonanalytic part (a dynamic Kohn anomaly), which at finite T is given by

$$\Pi_{\rm NA}(\mathbf{q} - 2\mathbf{k}_F, i\Omega_m) = \frac{1}{4\pi v_F \beta} \int_{-\infty}^{+\infty} du \frac{\sqrt{\sqrt{u^2 + \Omega_m^2} + u}}{4T \cosh^2 \frac{u - E_{\mathbf{q}}}{4T}}. \quad (4)$$

At $T = 0$, this reduces to

$$\Pi_{\rm NA}^{T=0}(\mathbf{q} - 2\mathbf{k}_F, i\Omega_m) = \frac{1}{2\pi v_F \beta} \sqrt{E_{\mathbf{q}} + \sqrt{\Omega_m^2 + E_{\mathbf{q}}^2}}, \quad (5)$$

where $E_{\mathbf{q}} = -v_F q_x + \beta^2 q_y^2/2$.[23] The static $\Pi_{\rm NA}^{T=0}(\mathbf{q} - 2\mathbf{k}_F, 0)$ is nonzero at the smallest q only for $q_x < 0$ (a static Kohn anomaly). The nonanalyticity that gives rise to our effect originates from $\Pi_{\rm NA}^{T=0}$ at $E_{\mathbf{q}} < 0$, and $\Omega^2 \ll E_{\mathbf{q}}^2$. In this limit $\Pi_{\rm NA}^{T=0} \propto |\Omega_m| / \sqrt{|E_{\mathbf{q}}|}$, which for $q_x \sim q_y^2$ is on the order of $|\Omega_m|/|q_y|$. The existence of nonanalytic $|q_y|$ in the denominator implies that $\Pi_{\rm NA}^{T=0}$ gives rise to *dynamic* long-range interaction between fermions.

For velocity renormalization, we need the real part of the self-energy $\mathrm{Re}\,\Sigma(\mathbf{k}, \omega)$ on the mass shell to first order in fermionic frequency ω: $\mathrm{Re}\,\Sigma(\varepsilon_k = \omega, \omega) = \omega\lambda(T)$. The temperature variation of v_F is related to $\lambda(T)$ as

$$\delta(T) = \frac{v_F(T) - v_F(T=0)}{v_F(T=0)} = -\frac{\lambda(T) - \lambda(0)}{1 + \lambda(0)}, \quad (6)$$

where $v_F(T=0) = v_F/[1 + \lambda(0)]$. The zero-temperature $\lambda(0)$ is cutoff dependent.[22] The temperature dependence of λ on the other hand comes from processes near the Fermi surface and is not sensitive to a cutoff.

We first obtain $\mathrm{Im}\,\Sigma(\mathbf{k}, \omega)$ using spectral representation and then obtain $\mathrm{Re}\,\Sigma$ by Kramers-Kronig transformation. Substituting Eqs. (3) and (4) into Eq. (2), using spectral representation, evaluating the frequency sums, and rescaling, we get

$$\mathrm{Im}\,\Sigma(\mathbf{k}, \bar{\omega}) = -\frac{6}{\pi} \frac{T^2}{T_1} \int_{-\infty}^{+\infty} dt [n_B(t) + n_F(t + \bar{\omega})] \times \int_0^{L/\sqrt{T}} \frac{dy\, \mathrm{Im}\, Z}{\left[1 + \left(\frac{T}{T_1}\right)^{1/2} \mathrm{Re}\, Z\right]^2 + \left[\left(\frac{T}{T_1}\right)^{1/2} \mathrm{Im}\, Z\right]^2}, \quad (7)$$

$$Z=\int_{-\infty}^{+\infty}\frac{dz}{\cosh^2 z}\sqrt{4z+t+\bar{\omega}+\bar{k}-y^2/2+\sqrt{(4z+t+\bar{\omega}+\bar{k}-y^2/2)^2-(t+i\delta)^2}}, \tag{8}$$

where $t=\Omega/T$ is the running dimensionless frequency variable, $y\propto q_y/\sqrt{T}$ is the dimensional momentum variable along the Fermi surface, and $n_{F,B}(t)=(e^t\pm 1)^{-1}$ are Bose and Fermi functions, respectively. L is the upper limit of the momentum integral along the Fermi surface, $T_1=(4\pi v_F\beta/\bar{g})^2$, and $\bar{\omega}=\omega/T$, $\bar{k}=v_F k/T$. The second-order perturbative result is obtained by neglecting Z in the denominator of Eq. (7).

If the integral over y was convergent, the result of y integration would be $O(t)$. Im Σ would then be determined by $t=O(1)$ and have a Fermi-liquid form, $\omega^2+(\pi T)^2$. Re Σ would then contain only a regular ωT^2 term, and the renormalization of the Fermi velocity would be T^2. On a more careful look, however, we find that at large y, Z scales as $-2it/y$ and the y integral is logarithmic. As $t/y\propto|\Omega|/|q_y|$, this logarithmic singularity indeed originates from long-range dynamical interaction given by Π_{NA}.

We assume and then verify that the logarithmic accuracy is sufficient for the T dependence of the velocity renormalization and that the logarithm is cut at the lower end by $|t|$. To this accuracy, Im $\Sigma(\mathbf{k},\bar{\omega})$ is independent of k, even in frequency, and the frequency dependence comes only via the Fermi function in Eq. (7). Evaluating the integral over y in Eq. (7) with logarithmic accuracy and subtracting regular $\omega^2+(\pi T)^2$ terms, we obtain the following for the nonanalytic part of Im Σ:

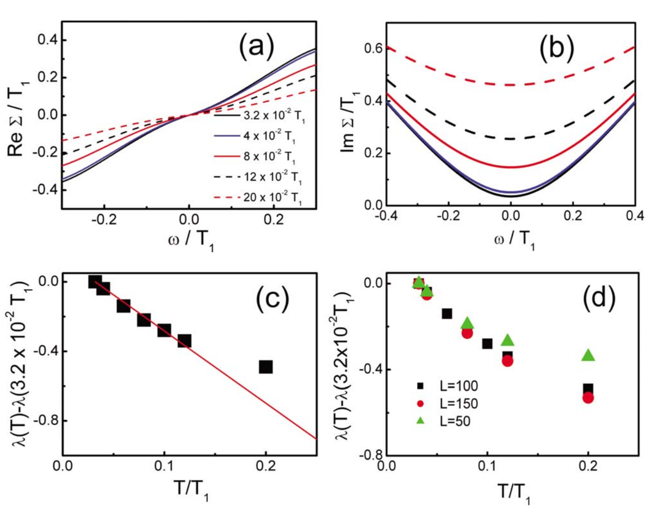

FIG. 1. (Color online) [(a) and (b)] The real and imaginary parts of the self-energy for various temperatures in the normal state [from the numerical solution of Eqs. (7) and (8) and Kramers-Kronig transform]. (c) The temperature dependence of the coupling constant, $\lambda(T)=d\,\mathrm{Re}\,\Sigma(\omega\to 0,T)/d\omega$. The straight line is the analytical result at low T, Eq. (11). (d) The coupling $\lambda(T)$ for three different upper cutoffs of the momentum integration L. The aim is to demonstrate that the T-dependent part of λ is independent of L.

$$\mathrm{Im}\,\Sigma(\bar{\omega})_{\mathrm{NA}}=-\frac{3T^2}{\pi T_1}\int_0^{L^2/T}dt\times t\log t^2[n_F(t+\bar{\omega})+n_F(t-\bar{\omega})-2n_F(t)]. \tag{9}$$

Substituting Eq. (9) into the Kramers-Kronig (KK) relation $\mathrm{Re}\,\Sigma(\bar{\omega})=(2\bar{\omega}/\pi)\int_0^{\infty}\mathrm{Im}\,\Sigma(s)/(s^2-\bar{\omega}^2)$ and integrating over s, we obtain after straightforward calculations that at small ω/T

$$\mathrm{Re}\,\Sigma(\omega)=\frac{6\omega T}{T_1}\int_0^{L^2/T}\tanh t\,dt=\left(\frac{6L^2}{T_1}\right)\omega-\left(\frac{6\log 2}{T_1}\right)\omega T. \tag{10}$$

The first term is a cutoff-dependent zero-temperature contribution $\lambda(0)\omega$. The second term, on the other hand, is a universal cutoff-independent ωT term which gives rise to a linear in T correction to the velocity:

$$\delta(T)=\frac{6\log 2}{1+\lambda(0)}\frac{T}{T_1}. \tag{11}$$

We emphasize that this universal term comes from the *upper* limit of the integration over the frequency variable t, justifying our assumption that the integral over y is cut by t rather than by the external parameters $\bar{\omega}$ and $v_F\bar{k}$.

To estimate the slope, we recall that $\bar{g}=[U(2k_F)/2]K$, where K is the ratio of the actual and to the bare static spin susceptibility at momentum $2k_F$. The bare susceptibility $\chi_0=p_F/\pi v_F\sim 0.9$ states/eV. The measured χ has a flat top between (π,π) and $2k_F$, at about 13 states/eV.[24] Using the ratio as the estimate for K and $U(2k_F)\sim 2$ eV, $p_F\sim\sqrt{2}\times 0.6\pi/a=2.7$, and $v_F\sim 1$ eV ($E_F\sim 1.35$ eV), we obtain $T_1\sim 2.5\times 10^3$ K (Ref. 25). Using next $\lambda(0)=0.7$ extracted from ARPES fits,[26] we find $\delta T\approx 0.15\times 10^{-2}$ T. For $T=250$ K, this gives $\delta(T)\approx 0.37$, in good agreement with the data.

We next consider the subleading terms. By power counting, the subleading terms, obtained by expanding in Z from the denominator in Eq. (7), should scale as $\sqrt{T/T_1}$. As $T_1\sim 2500$ K and the measurements are performed up to $T\sim 300$ K, such corrections would be substantial. We argue, however, that the corrections to Eq. (11) are in fact regular T^2 terms. To see this, we observe that both Re Z and Im Z in Eq. (7) vanish at large y, such that expanding the denominator in Eq. (7) in powers of Z and integrating over y, we lose the log t^2 term, which was the source of nonanalyticity. Integrating further over t, we find that the expansion of Im $\Sigma(\omega)$ is regular and holds in even powers of ω^2 and T^2, in which case the renormalization of the Fermi velocity holds in powers of T^2. Alternatively speaking, the T term in $v_F(T)$

comes from Im Z term in Eq. (7), while Z-dependent terms in the denominator in Eq. (7) give rise only to regular T^2 corrections to the Fermi velocity.

To estimate these regular corrections, we computed the velocity renormalization numerically. We used Eq. (7) as a point of departure, evaluated Im $\Sigma(\bar{k},\bar{\omega})$ by explicit three-dimensional (3D) integration, and subtracted antisymmetric contributions to Im Σ which do not affect linear in ω term in Re Σ (such contributions are generally present because the dispersion is not particle-hole symmetric). In Figs. 1(a) and 1(b) we present the results for the real and imaginary parts of the self-energy for various temperatures, measured in units of T_1. We see that the slope of the real part of the self-energy decreases with increasing temperature and is negative. In Fig. 1(c) we plot the T-dependent part of $\lambda(T)$ vs Eq. (11). We see that the agreement is perfect up to approximately $0.1T_1$. At larger T, the actual $\lambda(T)$ flattens. In Fig. 1(d), we show that the T-dependent part of λ [but not $\lambda(0)$] is insensitive to the upper cutoff of the momentum integration, in agreement with Eq. (11).

For completeness, we computed velocity renormalization in the QC regime and found $\omega=\tilde{\epsilon}_k[1-0.82(\tilde{\epsilon}_k/T)^{1/4}]$, where $\tilde{\epsilon}_k \propto (k-k_F)^{4/3}$. Observe that a given k, ω still increases with increasing T.

To conclude, in this Rapid Communication we considered the temperature dependence of the nodal Fermi velocity in 2D systems, $v_F(T)=v_F(0)[1+\delta(T)]$. We have found that $\delta(T)$ is positive and linear in T in any Fermi liquid. The linear in T term comes from the screening of the interaction by just one particle-hole bubble. The corrections due to extra dynamical screening give rise only to regular T^2 terms. The slope of the linear term is quite large in the cuprates and agrees with the measurements on optimally doped Bi2212.

The experiments by Plumb *et al.*[9] were performed only at optimal doping. In our theory, the prefactor of the T term increases with decreasing doping; i.e., it should get larger in the underdoped regime. The measurements of the doping dependence of the slope are clearly called for.

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