Temperature dependence of the nodal Fermi velocity in layered cuprates

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We explain recently observed linear temperature dependence of the nodal Fermi velocity $v_F(T)$ in near-optimally doped cuprates. We argue that it originates from electron-electron interaction, and is a fundamental property of an arbitrary 2D Fermi liquid. We consider a spin-fermion model with the same parameters as in earlier studies, and show that the $T$ term is about 30\% at 300K, 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 $\omega^2$ behavior of the fermionic damping at the lowest energies\textsuperscript{[1,2]}, consistent with the idea that in this range the system is a Fermi liquid with strong correlations.

We take a 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 a superconductivity.

The nature of the pairing boson in the cuprates is the subject of outstanding debate, and in recent years several proposals to distinguish experimentally between phononic and electronic mechanisms have been discussed\textsuperscript{[3,4,5,6,7,8]}. One of the proposals is to look at the temperature dependence of the the Fermi velocity $v_F(T) = v_F(T = 0)(1 + \delta(T))$, taken along the diagonal of the Brillouine Zone (BZ) where the $d_{x^2-y^2}$-wave superconducting gap has nodes (the “nodal” velocity) It has been measured recently by Plumb et al.\textsuperscript{[9]} in optimally-doped Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ by means of laser-based angle-resolved photoemission spectroscopy. They found that $\delta(T)$ is approximately linear in $T$ up to at least 300K. The linear behavior holds down to $T_c$, and the slope is quite large: $\delta(T)$ is about 0.35 between $T_c$ and $T = 250K$. 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 $T$ dependence of various observables in the normal (non-pseudogap) state have been reported before and phenomenologically described in terms of marginal Fermi liquid (MFL) behavior\textsuperscript{[10,11]}. The linear in $T$ behavior of the velocity is different by two reasons. First, the self-energy which yields $\delta(T) \propto T$ scales as $Re \Sigma \propto \omega T$, while MFL behavior originates from $Re \Sigma \propto \omega \log \max(\omega, T)$ (and $Im \Sigma \propto \max(\omega, T)$). Second, the linear behavior of $\delta(T)$ has been measured down to energies ($\pi T \rightarrow \omega$) where $Im \Sigma$ already has a Fermi liquid, $\omega^2$ form\textsuperscript{[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\textsuperscript{[7,12]}. The quasi-linear $T$ dependence of the Fermi velocity can be obtained due to electron-phonon iteration, but only as approximate behavior in a limited $T$ range above the Debye frequency $\omega_D$\textsuperscript{[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 2D 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\textsuperscript{[15,16]}. The linear in $T$ correction to the velocity comes from $\omega T$ term in the real part of self-energy, which in turn originates from the non-analytic $Im \Sigma(\omega) \sim \omega^2 \log \omega$, coming from backscattering\textsuperscript{[14,15]}. Although the original analysis in\textsuperscript{[15,16]} 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.\textsuperscript{[17]} for the specific heat coeffi-
cient, which is also linear in $T$ in a 2D Fermi liquid.

The magnitude of $\delta T$ is a different issue. To second order in the interaction $U(q)$, the velocity renormalization is given by

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

where $A = p_F \log 2/(4\pi^2 v_F^2)$. The two terms in Eq. (1) account for the contributions from charge and spin channels. Approximating the measured FS of Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ (Bi2212) by a circle with $p_F \sim \sqrt{2} \times 0.6\pi = 2.7$ (Ref. 18), we set interatomic distance to one, $U(q)$ by $U \sim 2eV$, and using experimental $v_F \sim 1eV$ (Ref. 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 $T \sim 300K$, two orders of magnitude smaller than the experimental value.

The second-order estimate, however, is only valid in the weak coupling regime, when the system is far from a Pomeranchuk-type instability. There is a consensus among researchers that near optimal hole doping, the interaction between fermions and their collective bosonic excitations in the spin channel. Several groups have noted that $\delta(T)$ affects the functional form of $\delta(T)$. The purpose of this paper is to analyze the interplay between these two effects.

An analytic estimate is $\delta(T)$ given by

$$\delta(T) = \frac{3g}{4\pi^2} T \sum_{q_m} \int d^2 q \chi(q - 2k_F, i\Omega_m) \times \frac{1}{i(\omega_m + \Omega_m) - \varepsilon_{-k_F + k + q + Q}}$$

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

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

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

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

Further, $\chi(q, \Omega_m)$, 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 and bare static spin susceptibilities at momentum $2k_F$. We assume, based on neutron scattering data, that the momentum dependence of the static susceptibility is weak near $q = 0$, and approximate the full dynamic spin susceptibility at small $q$

$$\chi(q - 2k_F, i\Omega_m) = 1/(1 + \bar{g} \Pi(q - 2k_F, i\Omega_m))$$

where $\Pi(q - 2k_F, i\Omega_m)$ is the polarization bubble with momenta near $2k_F$ (the spin factor of 2 is included into $\Pi$).

The $2k_F$ particle-hole bubble has been calculated before$^{22, 23}$. It contains a regular part, which plays no role in our analysis and which we neglect, and a non-analytic part (a dynamic Kohn anomaly), which at finite $T$ is given by

$$\Pi_{NA}(q - 2k_F, i\Omega_m) = \frac{1}{4\pi v_F \beta} \int_{-\infty}^{+\infty} du \frac{\sqrt{u^2 + \Omega_m^2} + u}{4T \cosh^2 \frac{u - E_q}{4T}}$$

At $T = 0$, this reduces to

$$\Pi_{NA}^{T=0}(q - 2k_F, i\Omega_m) = \frac{1}{2\pi v_F \beta} \left[ E_q + \sqrt{\Omega_m^2 + E_q^2} \right]$$

where $E_q = -v_F q_x + \beta^2 q_y^2/2$ $^{24}$. The static $\Pi_{NA}^{T=0}(q - 2k_F, 0)$ is nonzero at the smallest $q$ only for $q_x < 0$ (a static Kohn anomaly). The non-analyticity that gives rise to our effect originates from the form of $\Pi_{NA}^{T=0}$ at $E_q < 0$, and $\Omega^2 \ll E_q^2$. In this limit $\Pi_{NA}^{T=0} \propto |\Omega_m|/|E_q|$, which for $q_x \sim q_y^2$ is of order $|\Omega_m|/|q_y|$. The existence of non-analytic $|q_y|$ in the denominator implies that $\Pi_{NA}^{T=0}$ gives rise to dynamic long-range interaction between fermions.

For the velocity renormalization, we need the real part of the self-energy $Re\Sigma(k, \omega)$ on the mass shell, to first order in fermionic frequency $\omega$. $Re\Sigma(\varepsilon_k, \omega) = \omega \lambda(T)$. The temperature variation of the velocity is related to
\[ \lambda(T) = \frac{v_F(T) - v_F(T = 0)}{v_F(T = 0)} = -\frac{\lambda(T) - \lambda(0)}{1 + \lambda(0)}, \]  

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

We first obtain \(\text{Im}\Sigma(k, \omega)\) using spectral representation, and then obtain \(\text{Re}\Sigma\) by Kramers-Kronig transformation. Substituting Eqs. \[9\]-\[13\] into Eq. \[2\], using spectral representation, evaluating the frequency sums, and re-scaling, we get

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

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

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

If the integral over \(y\) was convergent, the result of \(y\)-integration would be \(O(t)\). \(\text{Im}\Sigma\) would then be determined by \(t = O(1)\) and have a Fermi liquid form, \(\omega^2 + (\pi T)^2\). \(\text{Re}\Sigma\) would then only contain a regular \(\omega T^2\) 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 \(t/y \propto |\Omega_{\text{mag}}|/|q_y|\), this logarithmic singularity indeed originates from long-range dynamical interaction given by \(\Pi_{N.A}\).

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, \(\text{Im}\Sigma(k, \bar{\omega})\) is independent on \(k\), even in frequency, and the frequency dependence comes only via the Fermi function in \[7\]. Evaluating the integral over \(y\) in \[7\] with logarithmic accuracy and subtracting regular \(\omega^2 + (\pi T)^2\) terms, we obtain for the non-analytic part of \(\text{Im}\Sigma\)

\[
\text{Im}\Sigma(\bar{\omega})_{\text{N.A}} = \frac{3T^2}{\pi T_1} \int_0^{L^2/T} dt \times[t \log t^2 \left( n_F(t + \bar{\omega}) + n_F(t - \bar{\omega}) - 2n_F(t) \right)]
\]

Substituting \[10\] into Kramers-Kronig (KK) relation \(\text{Re}\Sigma(\bar{\omega}) = (2\bar{\omega}/\pi) \int_0^\infty \text{Im}\Sigma(s)/(s^2 - \bar{\omega}^2)\) and integrating over \(s\), we obtain after straightforward calculations that

at small \(\omega/T\)

\[
\text{Re}\Sigma(\omega) = \frac{6\omega T}{T_1} \int_0^{L^2/T} \tanh t dt = \left( \frac{6L^2}{T_1} \right) \omega - \left( \frac{6 \log 2}{T_1} \right) \omega T
\]

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 \(\omega T\) term which gives rise to a linear in \(T\) correction to the velocity:

\[
\delta(T) = \frac{6 \log 2}{1 + \lambda(0)} \frac{T}{T_1}
\]

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

To estimate the slope, we recall that \(\bar{\gamma} = (U(2k_F)/2) * K\), where \(K\) is the ratio of the actual and bare static spin susceptibilities at momentum \(2k_F\). The bare susceptibility \(\chi_0 = p_F/\pi v_F \sim 0.9 \text{states/eV}\). The measured \(\chi\) has a flat top between \((\pi, \pi)\) and \(2k_F\), at about \(13 \text{states/eV} \[23\]. Using the ratio as the estimate for \(K\), and \(U(2k_F) = 2eV, p_F \sim \sqrt{2} * 0.6 \pi/a = 2.7, v_F \sim 1eV\) \(E_F \sim 1.35eV\), we obtain \(T_1 \sim 2.5 \times 10^3 K\) \(\text{Ref. 26}\). Using next \(\lambda(0) = 0.7\) extracted from ARPES fits \[27\], we find \(\delta T \approx 0.15 \times 10^{-2} T\). For \(T = 250 K\), this gives \(\delta(T) \approx 0.37\), in a 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. \[11\], 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 \(\text{Re}Z\) and \(\text{Im}Z\) in Eq. \[11\] vanish at large \(y\),
such that expanding the denominator in $\Sigma$ in powers of $Z$ and integrating over $y$, we loose the $\log t^2$ term, which was the source of non-analyticity. Integrating further over $t$ we find that the expansion of $\text{Im} \Sigma(\omega)$ is regular and holds in even powers of $\omega^2$ 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 $\text{Im} Z$ term in Eq. (7), while $Z$-dependent terms in the denominator in $\Sigma$ only give rise 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 $\text{Im} \Sigma(\vec{k}, \omega)$ by explicit 3D integration, and subtracted antisymmetric contributions to $\Sigma$ which do not affect linear in $\omega$ term in $\text{Re} \Sigma$ (such contributions are generally present because the dispersion is not particle-hole symmetric). In Fig. 1a we present the results for the real part of the self-energy for various temperatures, measured in units $T_\lambda$. We see that the slope of the real part of the self-energy decreases with increasing temperature and is negative. In Fig. 1b we plot the $T$-dependent part of $\lambda(T)$ vs Eq. (11). We see that the agreement is perfect up to approximately $0.1T_\lambda$. At larger $T$, the actual $\lambda(T)$ flattens. In the insert to this figure, we show that the $T$ dependent part of $\lambda$ (but not $\lambda(0)$) is insensitive to the upper cutoff of the momentum integration, in agreement with Eq. (11).

The linear in $T$ dependence of the Fermi velocity cannot be carried over to the $2k_F$ QC, non-Fermi liquid regime, because the pre-factor for the $T$ term contains the divergent static spin susceptibility at $2k_F$ (via $\frac{\delta}{\delta g}$. This quantum-critical regime is relevant for electron-doped cuprates, in which antiferromagnetism emerges near the electron density at which the Fermi surface passes through $(\pi/2, \pi/2)$, i.e., along zone diagonal $2k_F = (\pi, \pi)$ (Refs. [22, 23]). We computed the 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 $k$, $\omega$ still increases with increasing $T$.

To conclude, in this paper we considered 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 only give rise 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. In the quantum-critical regime, the correction to the zero-temperature dispersion is singular, and scales as $1/T^{0.15}$ at the lowest $T$, and as $1/T^{0.25}$ at intermediate temperatures.

The experiments by Plumb et al [8] have been performed only at optimal doping. In the theory, the prefactor of the $T$ term increases with decreasing doping, hence the prefactor should decrease in the overdoped regime, and increase in the underdoped regime. The measurements of the doping dependence of the slope are clearly called for.

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If the self-energy was analytic, $\text{Im}\Sigma(\omega)$ would be expandable in even powers of $\omega^2$, and $\text{Re}\Sigma$ in odd powers of $\omega^2$. The $T$ dependence of the velocity then would be $T^2$. Note also that in arbitrary $D < 3$, $\text{Im}\Sigma \propto \omega^2 + O(\omega^D)$, and the $T$ dependence of the velocity is $T^{D-1}$.

For $2k_F = Q = (\pi, \pi)$ considered in earlier work \[23\], $\Pi(\mathbf{q}, i\Omega_n)$ contains an additional contribution from umklapp processes. In our case, the umklapp term in $\Pi(\mathbf{q}, i\Omega_n)$ is linear in $\Omega$ and is smaller than the direct term which at $\mathbf{q} = 0$ scales as $\sqrt{|\Omega|}$.

In earlier works \[12, 25\], one of us used a smaller $U \sim 1\text{eV}$ to fit ARPES data near the hot spots. This was based on earlier estimate of $v_F$, which was roughly two times smaller than $1\text{eV}$. To get the same fits using $v_F = 1\text{eV}$, one needs $U = 2\text{eV}$.