Massless Dirac fermions, gauge fields, and underdoped cuprates

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We study 2+1 dimensional massless Dirac fermions and bosons coupled to a U(1) gauge field as a model for underdoped cuprates. We find that the uniform susceptibility and the specific heat coefficient are logarithmically enhanced (compared to linear-in-\(T\) behavior) due to the fluctuation of transverse gauge field which is the only massless mode at finite boson density. We analyze existing data, and find good agreement in the spin gap phase. Within our picture, the drop of the susceptibility below the superconducting \(T_c\) arises from the suppression of gauge fluctuations.

Recent experiments have indicated the existence in the normal state underdoped cuprate superconductor of a gap with the same anisotropy as the \(d\)-wave superconducting gap. One proposed explanation involves spin-charge separation: an electron in these highly correlated materials is a composite object made of a spin \(\frac{1}{2}\) neutral fermion (spinon) and a spinless charged boson (holon). The suppression of normal state magnetic excitation seen in NMR and neutron scattering is thus viewed as a singlet pairing of neutral fermions in the absence of coherence among holons. As a possible realization of this idea, two of us have taken the \(t\)-\(J\) model (which is believed to capture essential physics of \(\text{CuO}_2\) planes) and developed a slave boson mean field theory \([1]\) that extends the local SU(2) symmetry at half-filling to the finite concentration of holes by introducing a SU(2) doublet of slave boson field. Among the mean field phases reported in Ref. \([6]\) the so-called staggered flux (sF) phase (which is connected to \(d\)-wave pairing phase by a local SU(2) transformation) was argued to describe the pseudogap in underdoped cuprates. The low energy physics of this phase can be described by massless Dirac fermions, non-relativistic bosons, and a massless U(1) gauge field which together with two massive gauge fields forms SU(2) gauge fields that represent the fluctuations around the mean field.

The purpose of this paper is to address the low energy effective theory of the sF phase as a U(1) gauge theory problem. Although Dirac fermions coupled to a gauge field had been considered in several contexts in the past \([2]\), we shall see that interesting new physics emerges when massless Dirac fermions are coupled to a gauge field that is also coupled to a compressible boson current. More specifically, the Lorentz symmetry breaking due to coupling to the bosons results in the renormalization of fermion velocity which have consequences on physical properties such as uniform susceptibility \(\chi_u\) and electronic specific heat \(c_v^d\). Experimentally, \(\chi_u\) of underdoped cuprates begins to decrease with lowering of temperature far above the superconducting \(T_c\) \([3, 4]\). Electronic specific heat experiments \([3, 4]\) show that \(\gamma(T)\) \((\equiv c_v^d(T)/T)\) behaves quite similar to \(\chi_u\). Although constant Wilson ratio \((\gamma/\chi_u)\) is a hallmark of Fermi liquid theory, the anomalous temperature dependence calls for a departure from the time-honored theory of most metals. We make a case that the puzzling normal state behavior of \(\chi_u\) and \(\gamma\) may be viewed as enhancement over linear-in-\(T\) \(\chi_u\) and \(\gamma\) of Dirac fermions due to logarithmic decrease of Dirac velocity caused by fermion-gauge field interaction.

We begin with the following continuum effective Lagrangian for our problem

\[
\mathcal{L} = \bar{\Psi}_\alpha \left( \partial \mu \gamma^\mu + ia_\mu \gamma^\mu \right) \Psi_\alpha + \frac{1}{2m_B} b^\dagger (\nabla + ia)^2 b. \tag{1}
\]

The Fermi field \(\Psi_\alpha\) is a 2 \(\times\) 1 spinor: \(\Psi_\alpha = (\Psi_1^s, \Psi_2^s)\), \(\Psi_1^s = (f_{1s}^\dagger, f_{1so}^\dagger)\), \(\Psi_2^s = (f_{2so}^\dagger, f_{2se}^\dagger)\), where \(\alpha = 1, 2\) labels the two Fermi points, \(s = 1, ..., N\) labels fermion species \((N = 2\) for physical case \(s = \uparrow, \downarrow\)), and \(e, o\) stands for even and odd sites, respectively. The \(\gamma^\mu\) matrices are Pauli matrices \((\gamma^0, \gamma^1, \gamma^2) = (\sigma^3, \sigma^1, \sigma^2)\) and satisfy \([\gamma^\mu, \gamma^\nu] = 2\delta^{\mu\nu}\) \((\mu, \nu = 0, 1, 2)\). \(\Psi_\alpha \equiv \Psi_\alpha \gamma^0\). In the sF phase of Ref. \([6]\), the fermion dispersion near the fermi points is anisotropic, but we rescale it to an isotropic spectrum \(E(k) = v_D |k|\) where \(v_D = \sqrt{v_F v_E}\), the geometric mean of the two velocities \((v_E\) is proportional to the energy gap). We set \(v_D = 1\), unless otherwise specified. The gauge field \(a_\mu\) \((= (a_0, \mathbf{a})\) corresponds to the \(a_\mu^b\) part of the SU(2) gauge fields of Ref. \([6]\). The terms in Eq. \((1)\) involving the Bose field \(b\) (representing charge degree of freedom) are believed to play several important roles, including the suppression of chiral symmetry breaking (Neel ordering \([3]\) and instanton effects \([3]\). Most importantly, the compressible boson current screens the \(a_0\) field, making it massive. Unfortunately we do not have a detailed understanding of our boson subsystem. Therefore we shall draw upon only a few of qualitative features of the Bose sector while focusing mainly on the Fermi sector of the theory.

Eq. \((1)\) carries certain similarity to the uniform resonating valence bond (uR\(V\)B) gauge theory \([7, 10]\).
proposed to describe optimally and slightly overdoped cuprates, and some of the theoretical framework can be carried over to our problem. As in the uRVB case, the internal gauge field $a_µ$ does not have dynamics of its own, but it acquires dynamics from the polarization of fermions and bosons. Integrating out the matter fields generates the self energy term for the gauge field $E_a = \frac{1}{2} a_µ (\Pi_{µν}^{a} + \Pi_{νµ}^{a}) a_ν$, up to quadratic order. The fermion polarization $\Pi_{µν}^{a}$ from the two Dirac points is given by

$$\Pi_{µν}^{a}(q) = \frac{2N}{β} \sum_{k_0} \int \frac{d^d k}{(2π)^d} \text{tr} [G_F(k) γ^µ G_F(k + q) γ^ν],$$

where $G_F(k) = -(i k_ν γ^ν)^{-1}$ is the fermion Green’s function and $k$, $q$ denote 3-momentum; for example, $k = (k_0 = (2n + 1)πT, k)$. In the Coulomb gauge, the spatial part and the time part of the gauge field are decoupled, the propagators being $D^{00}(q) = (\Pi_{µν}^{00}(q) + Π_{νµ}^{10}(q))^{-1}$ and $D^0(q) = (δ_įj - q_i q_j/q^2) D^+(q)$, with $D^+(q) = (Π_{µν}^{1}p(q) + Π_{νµ}^{1}p(q))^{-1}$. As mentioned earlier, the bosons should have a finite compressibility ($Π_{µν}^{00}(q → 0) ≠ 0$) so the time component of the gauge field becomes massive (at finite temperature $Π_{µν}^{00}(q → 0)$ is also nonzero and contributes to the screening of $a_0$ field), but the spatial part of the gauge field, which is purely transverse, remains massless even at finite boson density and temperature, as long as the bosons are uncondensed (as in the spin gap phase). In the remainder of this paper, we will focus on the effect of this massless mode, ignoring the $a_0$ field.

In the absence of detailed understanding of the Bose sector, we assume that the transverse gauge propagator is dominated by the fermion part. In other words, $D^+(q) ≈ D_F^+(q) = 1/Π_F^+(q)$. This approximation, which is often used in the uRVB gauge theory, may not be fully justified in our case, but it allows us to organize the infrared behavior of our theory within 1/N expansion. The full expression for analytically continued transverse polarization function $Π_F^+(ω, q)$ at finite temperature is rather complicated and therefore we shall not write it here, although it is used later in the evaluation of gauge fluctuation contribution to $χ_ν$ and $c_{ν}^el$. In the limiting case of $T > |q| > |ω|$, we have

$$Π_F^+(ω, q) ≈ -iC_1 \frac{ωT}{|q|} + C_2 \frac{q^2}{T},$$

while in the zero temperature limit,

$$\text{Im} Π_F^+(ω, q) = -N \text{sign}(ω)(|ω| - |q|) \sqrt{ω^2 - q^2}/8$$

$$\text{Re} Π_F^+(ω, q) = Nθ(|q| - |ω|) \sqrt{q^2 - ω^2}/8.$$ (4)

To the leading order in 1/N, fermion self energy due to transverse gauge fluctuations is

$$Σ(k) = \frac{1}{β} \sum_{q_0} \int \frac{d^d q}{(2π)^d} G_F(k + q) γ^2 D_F^+(q),$$

where $D_F^+(q) = (δ_įj - q_i q_j/q^2)/Π_F^+. At zero temperature, the self energy is [11]

$$N/8 \sum_{k_0} \int \frac{d^d q}{(2π)^d} \frac{−iγ^0}{(k_0 + q_0)} + iγ^2 \int \frac{d^d q}{(2π)^d} \frac{(k_x + q_x)(q_y - q^2 - 2q_i q_j(k_y + q_y))}{q^2(k + q)^2√q^2}.$$ (6)

We find, for $|k| > |k_0|,$

$$Σ(k) = -c i k_0 γ^0 A_0(k) + 2c i k · γ A_1(κ)$$ (7)

with $c = 4/(3Nπ²)$ and $A_0(k) ≈ A_1(κ) ≈ ln(Λ/|k|),$ where Λ is a UV cutoff. Now the pole of the renormalized Green’s function $G_F^+(k) = (G_F(k)^{-1} - Σ(k)^{-1})$ occurs at

$$E(k) = |k|(1 - 4/(Nπ²) ln(Λ/|k|)).$$ (8)

Note the presence of compressible bosons and the resulting breaking of Lorentz symmetry is crucial to have logarithmic velocity renormalization. Indeed, in the absence of bosons, the gauge propagator (gauge independent part) is given by $D^{µν}(q) = 8N(δ^{µν} - q_i q_j/q^2)/√q^2$ and the zero temperature fermion self energy takes the form $Σ = ik_µ γ^µ f(k^2);$ therefore the velocity is not renormalized.

Treating the quasiparticles described by Eq. (8) as “free”, we calculate $c_ν$ and $χ_ν$ up to $O(1/N^0)$:

$$c_{ν}^{el} = (9/π)ζ(3) N T^2(1 + (8/Nπ²) ln(Λ/T) + ..)$$

$$χ_ν = (2/π) N T(1 + (8/Nπ²) ln(Λ/T) + ..),$$ (9)

(ζ(3) = 1.202). These results are believed to be valid for two reasons: 1) $\text{Im} A_{0,1}(ν+i0^+,k) = 0$ for $|ν| < |k|$, so the quasiparticles are well-defined. 2) Unlike the usual Fermi liquid theory, the free particle response function vanishes as $T → 0$. To the extent the Landau parameters in Fermi liquid theory enter as in mean field theory, this means that Landau parameter correction vanish in $T → 0$. Indeed, it will be shown shortly that the calculation of $χ_ν$ and $c_{ν}^{el}$ from the free energy shift due to gauge fluctuation yields the same results.

The enhancement of $c_{ν}^{el}$ seen here finds its counterpart in the more familiar problems such as electron-phonon interaction in metals [14], uRVB gauge theory [10], and half-filled Landau level [15], where interactions induce mass enhancement which manifests itself in the specific heat. In the nonrelativistic analogues, however, mass renormalization does not necessarily result in the enhancement of compressibility and uniform susceptibility [14,16,17], because the corrections are tied to the Fermi
surface [14]. The crucial difference in our case is that there are only Fermi “points” instead of Fermi “surface”. Thus in contrast to the nonrelativistic case, we find that the susceptibility is also renormalized such that the Wilson ratio $\gamma(T)/\chi_{\omega}(T)$ is constant. In fact, the Wilson ratio is the same as that of free Dirac fermions because quasiparticles are well-defined and Fermi-liquid type corrections are absent, as discussed earlier.

To check this conclusion, we calculate $\chi_{\omega}$ and $e_{\nu}^{cl}$ in a gauge invariant way, using the correction to the free energy due to gauge fluctuations. We consider only the leading correction in $1/N$, which is $O(1/N^0)$:

$$\Delta F = \frac{1}{(2\pi)^3} \int d^2 q \int_{-\infty}^{\infty} d\omega n(\omega) \tan^{-1} \left( \frac{\text{Im}\Pi_F^{\perp}(\omega, q)}{\text{Re}\Pi_F^{\perp}(\omega, q)} \right).$$

The entropy shift $\Delta S = -\partial \Delta F/\partial T$ due to gauge fluctuation has two contributions: $\Delta S_1$ from the temperature dependence of the Bose function $n(\omega) = 1/\exp(\omega/T) - 1$ and $\Delta S_2$ from the temperature dependence of fermion polarization. Numerically we find that the former gives a $\sim T^2$ contribution to entropy, while the latter which can be written as

$$\Delta S_2 = -\frac{1}{(2\pi)^3} \int |q| < T_{UV} d^2 q \int_{-\infty}^{\infty} d\omega n(\omega) \text{Im}(D_F^{\perp} \frac{\partial}{\partial T} \Pi_F^{\perp}),$$

($T_{UV}$=high energy cutoff) gives a singular contribution $\propto -T^2 \ln T$. The gauge fluctuation contribution to $\chi_{\omega}$ ($\Delta\chi_{\omega}$) is obtained by taking $-\partial^2/\partial H^2$ at $H = 0$ of $\Delta F(H)$. This approach corresponds to summing the bubble diagrams for the vertex correction and the self energy correction. It takes the form

$$\Delta\chi_{\omega} = -\frac{1}{(2\pi)^3} \int |q| < T_{UV} d^2 q \int_{-\infty}^{\infty} d\omega n(\omega) \text{Im}(D_F^{\perp} \frac{\partial^2}{\partial \mu_F^2} \Pi_F^{\perp}),$$

where $\partial^2 \Pi^{\perp}/\partial \mu_F^2$ is a short-hand notation for $\partial^2 \Pi^{\perp}(\omega, q; \mu_F)/\partial \mu_F^2|_{\mu_F=0}$ in which $\Pi^{\perp}(\omega, q; \mu_F)$ is the transverse polarization function of Dirac fermions with finite chemical potential $\mu_F$. This expression, which closely resembles that of $\Delta S_2$, gives a singular contribution $\propto -T \ln T$. Note that the expressions for $\Delta S_2$ and $\Delta\chi_{\omega}$ are also applicable to (nonrelativistic) uRVB gauge theory [11,13], but they are usually ignored in that case because they give only subleading corrections while $\Delta S_1$ generates a singular correction $\propto T^{2/3}$ [13], unlike our case in which $\Delta S_2$ dominate at low temperatures.

Summarizing our numerical evaluation, we have

$$\Delta\chi_{\omega} = 0.358 \frac{v_D}{v_F^D} T \ln \frac{T_{UV}}{2.4T}, \quad \Delta e_{\nu}^{cl} = \frac{2.79}{v_F^D} T^2 \ln \frac{T_{UV}}{2.6T},$$

at low temperatures ($T < T_{UV}/5$) in agreement with Eqs. [13].

We now discuss our results in light of the experiments. In Fig. 1a we plot $\chi_{\omega}$ of YBa$_2$Cu$_3$O$_{6.63}$, a prototypical underdoped (bilayer) cuprate, from the Knight shift data of Takigawa et al. [18] We took the liberty of moving the zero of $\chi_{\omega}$ by 0.27 states/eV Cu(2), which is within the error bars corresponding to uncertainty in the orbital contributions $K^{\text{orb}}$ ($\chi_{\omega} \propto K - K^{\text{orb}}$). This change avoids the unphysical situation of Ref. [13] in which $63 K^{\text{iso}}, 17 K^{\text{spin}}, 17 K^{\text{spin}} < 0$ at $T = 0$. Further support for the adjustment of 0 comes from precision measurements of the Knight shifts in YBa$_2$Cu$_3$O$_{6}$ by Brinkmann and collaborators [19] who made substantial upward shift of $K^{\text{spin}}$ from their previous values [13]. We find that the normal state data of Ref. [19] are well-fitted (solid line) by $\chi_{\omega}(T; v_D, T_{UV}) = \Delta\chi_{\omega} + \chi_{\omega}^0$. Here $\Delta\chi_{\omega}$ is the numerical evaluation of Eq. (12) whose low $T$ behavior is given by Eq. (13), and $\chi_{\omega}^0$ is the uniform susceptibility of bare Dirac fermions with the same upper cutoff $T_{UV}$: $\chi_{\omega}^0 = -4v_F^2 T F(T_{UV}/2T)F(x) = J y/cosh^2 y dy$. The two parameters in the fit are chosen to be $v_D = 0.76 J$ and $T_{UV} = 0.63 J$, where we set the antiferromagnetic exchange energy $J = 1500$ K. We expect the gauge fluctuations to be suppressed in the superconducting state (due to Higgs mechanism) so that $\chi_{\omega}$ should cross-over to $\chi_{\omega}^0$ (dashed line) at low temperatures. This is in qualitative agreement with the data below $T_c$. The inset of Fig 1a shows a similar fit for the spin Knight shifts of YBa$_2$Cu$_4$Os [18], which is again very good. Thus our theory can account for the susceptibility in both the normal and superconducting states, without the need to adjust the energy scale of the gap parameter. Using the same parameters $v_D$ and $T_{UV}$ as in the fitting of YBa$_2$Cu$_3$O$_{6.63}$ Knight shift data, we plot $\gamma = \Delta e_{\nu}^{cl}/T + \gamma^0$ (where
\[ \gamma^0 = \frac{16\pi^2}{v_D} G(2T_{UV}/T), G(x) = \int_0^x dy^2/\cosh^2 y \] in Fig 1b. Also shown is the experimental data for \( \gamma(T) \) of YBa\(_2\)Cu\(_3\)O\(_{6.67}\) [8]. Rough agreement of scales between the curves is quite encouraging.

In monolayer La\(_{2-x}\)Sr\(_x\)CuO\(_4\), the uniform susceptibility is usually deduced from bulk susceptibility by subtracting the core diamagnetism \( \chi_c \) and Van Vleck paramagnetism \( \chi_{vv} \). Fig. 1c shows \( \chi_u \) of La\(_{2-x}\)Sr\(_x\)CuO\(_4\) obtained by subtracting the powder average value \( \chi_{vv} + \chi_c = -0.5 \) states/eV [3] (there’s some uncertainty in the value of \( \chi_{vv} \)) from the bulk susceptibility \( \chi \) [14]. The data can be characterized by \( \chi_u = \Delta \chi_u + \chi_u^0 + \chi_\text{const} \) with \( (v_D = 0.99 J, T_{UV} = 1.17 J) \) for \( x = 0.10 \) and \( (v_D = 0.79 J, T_{UV} = 0.65 J) \) for \( x = 0.14 \). Unlike the YBCO compounds, temperature independent part \( \chi_\text{const} > 0 \) is needed for a reasonable fit. Regarding the specific heat data of LSCO, cutoffs significantly smaller than the ones used for \( \chi_u \) are needed to fit \( \gamma \) of the same compound in terms of \( \gamma = \Delta \gamma^0 + \gamma_\text{const} \) in Fig. 1d we have kept the same \( v_D \) as in Fig. 1c, but used smaller cutoffs \( (T_{UV} = 0.8 J \text{ for } x = 0.1, T_{UV} = 0.49 J \text{ for } x = 0.135) \) to fit the \( \gamma \)-data [4]. This discrepancy and the origin of nonzero \( \gamma_\text{const} \) and \( \chi_\text{const} \) are not well understood. The \( \gamma_\text{const} \) \( > 0 \) feature in LSCO has been emphasized by some [4] to be an important evidence that the bilayer structure is important for spin gap behavior. Recent experiments on trilayer HgBa\(_2\)Cu\(_2\)O\(_{8+\delta}\) [57] and monolayer HgBa\(_2\)Cu\(_4\)O\(_{4+\delta}\) [58], however, find similar spin gap behaviors as in YBCO, suggesting that LSCO is a rather special case.

Despite reasonable agreement, we feel that above comparisons do not provide a conclusive test, because the \( T_c \) is too high to probe the normal state infrared behavior for a wide range of temperature. In fact, most of the bending feature seen in the \( \gamma(T) \) data is presumably related to the high energy cutoff (the deviation from linear Dirac spectrum) which have been treated in a cavalier manner here by using a hard cutoff \( T_{UV} \). The low-\( T \) curvature in \( \chi_u \) data \( (d^2\chi_u/dT^2 < 0 ; \text{ faster decrease at lower temperature}) \) seems to support the gauge fluctuation picture, but it may not be simple to separate this effect from the curvature due to high energy cutoff. Nevertheless, we view that the theory advocated here presents a simple and appealing picture of the spin gap phase. In this theory, no new energy scale is introduced to distinguish the spin gap phase and the superconducting phase; the Dirac velocity in both phases is taken to be the same. Rather, it is the gauge fluctuation that distinguishes the phases by causing the enhancement of \( \chi_u \) and \( \gamma \) in the normal state.

Instead of conclusion, we recapitulate some issues that have been glossed over. We have ignored the \( a_0 \) field whose effect may not be totally innocuous [3]. In fact, we have checked that in the absence of bosons the contributions to \( \chi \) and \( \epsilon^d \) derived from the free energy shift due to the \( a_0 \) fluctuation cancel the singular contributions from transverse gauge fluctuation, in agreement with non-renormalization of Dirac velocity in a Lorentz invariant situation. Secondly, we have not treated contributions from the Bose sector, especially in regard to the entropy. Lastly, we mention the issue of whether the renormalization of fermion propagator feeds back to the gauge propagator. In the non-relativistic gauge theory [10-13], the density-density correlation function and the transverse gauge propagator receive only sub-leading corrections [17]. This might not hold any longer in our case. At present it is not clear to what extent the transverse propagator is modified by “feedback effect” and to what extent this affects the physical picture.

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[1] X.G. Wen and P.A. Lee, Phys. Rev. Lett. 76, 503 (1996). See also P.A. Lee et al., submitted to Phys. Rev. B.
[2] J.B. Marston, Phys. Rev. Lett. 64, 1166 (1990).
[3] T. Nakano et al., Phys. Rev. B 49, 16000 (1994).
[4] M. Takigawa et al., Phys. Rev. B 43, 247 (1991).
[5] M. Bankay et al., Phys. Rev. B 50, 6416 (1994).
[6] J.W. Loram et al., Proceedings of 10th Anniv. HTS Workshop, Houston, March 1996.
[7] W.Y. Liang et al., Physica C 263, 277 (1996).
[8] N. Nagaosa, Phys. Rev. Lett. 71, 4210 (1993).
[9] L.B. Ioffe and A.I. Larkin, Phys. Rev. B 39, 8988 (1988).
[10] P.A. Lee and N. Nagaosa, Phys. Rev. B 46, 5621 (1992).
[11] At finite temperature infrared divergence (analogous to those encountered in nonrelativistic gauge theory) occurs in \( \Sigma(k) \rightarrow \nu + i\epsilon^d \), for \( \nu \leq |k| \) due to the soft overdamped mode that exists for \( |q| < T \) (Eq. (3)).