Two-fluid model of the pseudogap of high-temperature cuprate superconductors based on charge-2*e* bosons

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Starting from the effective low-energy theory of a doped Mott insulator, obtained by exactly integrating out the high-energy scale, we show that the effective carrier density in the underdoped regime agrees with a two-fluid description. Namely, it has distinct temperature-independent and thermally activated components. We identify the thermally activated component as the bound state of a hole and a charge-2*e* boson, which occurs naturally in the effective theory. The thermally activated unbinding of this state leads to the strange metal and subsequent *T*-linear resistivity. We find that the doping dependence of the binding energy is in excellent agreement with the experimentally determined pseudogap energy scale in cuprate superconductors.

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The normal state of the high-T_c copper oxide superconductors exhibits a variety of anomalous features in the underdoped regime which any successful theory of these materials must explain. Central to the exotica of the underdoped cuprates are the pseudogap[1,2] and strange metal phases. These phases are closely linked because once the suppression of the density of states at the chemical potential, a key experimental signature of the pseudogap, ceases at some critical temperature, T^*, a metallic state ensues. Such behavior is suggestive of a localized, or more properly, a "bound" electronic state, that is, liberated at T^*. While the upturn[3,4] of the resistivity at low temperatures is consistent with this bound-state scenario or charge localization[5–8] a more direct signature is the activated temperature dependence[10–12] of the Hall coefficient. In a Fermi liquid, the inverse of the Hall coefficient is a measure of the carrier density which of course is independent of temperature. However, in the underdoped cuprates, the inverse of the Hall coefficient is strongly temperature dependent.[10–12] Gor'kov and Teitel'baum[9] observed remarkably that the charge-carrier concentration, n_{Hall}, extracted from the inverse of the Hall coefficient in $La_{2-x}Sr_xCuO_4$ (LSCO) obeys an empirical formula,

$$n_{\mathrm{Hall}}(x,T) = n_0(x) + n_1(x)\exp[-\Delta(x)/T], \tag{1}$$

appropriate or a two-component or two-fluid system. One of the components is independent of temperature, $n_0(x)$ (x the doping level) while the other is strongly temperature dependent, $n_1(x)\exp[-\Delta(x)/T]$. The key observation here is that the temperature dependence in n_{Hall} is carried entirely within $\Delta(x,T)$ which defines a characteristic activation energy scale for the system. Gor'kov and Teitel'baum's[9] analysis suggests that the activation energy is set by the pseudogap energy scale. Consequently, the bound component should be liberated beyond the T^* scale for the onset of the pseudogap. Should n_{Hall} be an accurate representation of the effective charge-carrier concentration in the cuprates, the above observation indicates that the underdoped or pseudogap phase necessitates a two-fluid description, which has been championed[13] recently to explain NMR, inelastic neutron-scattering and thermodynamic measurements on these systems. Nonetheless, the microscopic origin of the two fluids has not been advanced. That is, there is no microscopic prescription for the precise nature of the propagating degrees of freedom that underlie the temperature dependence of n_{Hall}. For example, Gor'kov and Teitel'baum[9] attributed the unbinding of the localized charges above T^* to excitations from van Hove singularities at the bottom of the band up to the chemical potential.

By contrast, our explanation of the two fluids relies entirely on the strong correlations of a doped Mott insulator, that is, Mottness. Here we show that the exact low-energy theory of a doped Mott insulator[14–16] described by the Hubbard model naturally resolves the two-component conundrum in the cuprates. The propagating degrees of freedom that constitute the two fluids are the standard projected electron in the lower Hubbard band and a bound composite excitation composed of a charge-2*e* boson and a hole. It is the unbinding of the latter that gives rise to the strange metal regime. The binding energy is found to be in excellent agreement with experimental values for the pseudogap energy scale.

We review some of the key features of the our effective low-energy theory of Mottness, the complete details of which have been worked out elsewhere.[14–17] Our starting point is the usual Hubbard model

$$H_{\mathrm{Hubb}} = -t\sum_{i,j,\sigma} g_{ij}c^{\dagger}_{i,\sigma}c_{j,\sigma} + U\sum_{i,\sigma} c^{\dagger}_{i,\uparrow}c^{\dagger}_{i,\downarrow}c_{i,\downarrow}c_{i,\uparrow}, \tag{2}$$

where i,j are label lattice sites, g_{ij} is equal to one if i,j are nearest neighbors, $c_{i\sigma}$ annihilates an electron with spin σ on lattice site i, t is the nearest-neighbor hopping matrix element, and U the energy cost when two electrons doubly occupy the same site. The cuprates live in the strongly coupled regime in which the interactions dominate as $t \approx 0.5$ eV and $U=4$ eV. A low-energy effective action is then obtained by integrating out the physics on the U scale. Because double occupancy occurs in the ground state, integrating out the U-scale physics is not equivalent to integrating out double occupancy. We solved this problem by extending the Hilbert space to include a new fermionic oscillator which represents the creation or annihilation of double occupancy only when a constraint is solved. The new fermionic oscillator enters the

action with a mass of U and hence represents the high-energy scale, which must be integrated out to generate the low-energy action. The corresponding low-energy theory contains new degrees of freedom, namely, a charge-$2e$ boson, denoted by φ_i, that are absent in the original model and are not made out of the elemental excitations. φ_i enters the theory initially as the Lagrange multiplier to maintain the constraint that in the extended Hilbert space the heavy fermionic field represents the creation of double occupancy. To leading order in t/U, the effective Hamiltonian

$$H_{\text{eff}} = -t\sum_{i,j,\sigma} g_{ij}\alpha_{ij\sigma}c^{\dagger}_{i\sigma}c_{j\sigma} - \frac{t^2}{U}\sum_{j} b^{\dagger}_{j}b_{j} - \frac{t^2}{U}\sum_{j}\varphi^{\dagger}_{j}\varphi_{j} - t\sum_{j}\varphi^{\dagger}_{j}c_{j\uparrow}c_{j\downarrow} - \frac{t^2}{U}\sum_{i}\varphi^{\dagger}_{i}b_{i} + \text{H.c.} \tag{3}$$

contains the t-J model (the first two terms) and new interactions with the charge-$2e$ boson, φ_i which represent mixing with the sectors with varying numbers of doubly occupied sites. Here $b_i=\Sigma_j b_{ij}=\Sigma_{j\sigma} g_{ij}c_{j,\sigma}V_\sigma c_{i,-\sigma}$ with $V_\uparrow=-V_\downarrow=1$. The $|b_i|^2$ term contains the spin-spin interaction as well as the three-site hopping term. A gradient expansion of this term shows that the spin-spin term scales as a^4, a the lattice constant, whereas the terms linear in b are proportional to a^2. Hence, relative to the terms linear in b, the $|b|^2$ term is irrelevant. Our key contention which has been worked out extensively for the cuprates[14–17] is that as far as the charge degrees of freedom are concerned, it is the interactions with the φ_i sector that determine the propagating degrees of freedom, not the dynamics arising from the spin-spin term. In particular, we show that it is the φ terms that give rise to a gap in the single-particle electron spectrum. As this gap is on the order of t, any contribution from the spin-spin term will be subdominant.

It is important to realize that once the heavy field is integrated out, the Hilbert space reverts back that of the Hubbard model. Further, as φ_i has no bare dynamics and φ has no Fock space of its own, its only contribution will be to create bound states within the Hilbert space of the Hubbard model. This can be seen initially by considering how the electron operator transforms[14–17]

$$c^{\dagger}_{i,\sigma} \rightarrow (1-n_{i,-\sigma})c^{\dagger}_{i,\sigma} + V_\sigma\frac{t}{U}b_i c_{i,-\sigma} + V_\sigma\frac{t}{U}\varphi^{\dagger}_{i}c_{i,-\sigma} \tag{4}$$

upon the integration of the high-energy scale. The first two terms represent the standard electron operator in the lower Hubbard band dressed with spin fluctuations. However, the last term represents the correction due to dynamical spectral weight transfer,[18] that is the mixing with doubly occupied sites. All such processes are mediated by φ_i which represents a collective charge-$2e$ mode arising from the dynamics of double occupancy. The quantity $\varphi^{\dagger}_{i}c_{i,-\sigma}$ represents a bound complex with a nonpropagating local degree of freedom. It is from this term that the bound-state dynamics emerges. Roughly, the two-fluid emerge from the fact that an electron at low energies is a linear superposition of an essentially free part, the first two terms in Eq. (4) and the last term in Eq. (4) from which the bound-state[16,17] dynamics (that is, pseudogap physics) emerges. As a result of φ_i, the conserved charge is no longer just the total number of electrons but

$$Q = \sum_{i\sigma} c^{\dagger}_{i\sigma}c_{i\sigma} + 2\sum_{i}\varphi^{\dagger}_{i}\varphi_{i}. \tag{5}$$

In order to obtain the electron Green function for the effective Hamiltonian, we treat φ_i as spatially independent, owing to a lack of gradient terms in that field in the Hamiltonian. To keep track of the dependence on φ_i it is helpful to introduce the rescaling $\varphi_i \rightarrow s\varphi_i$. The electron Green function is then written as a path integral over the φ fields as

$$G(\mathbf{k},\omega) = \frac{1}{Z}\int [D\varphi^*][D\varphi]FT\left\{\int [dc^*_i][dc_i]c_i(t)c^*_i(0) \times \exp\left[-\int L(c,\varphi)dt\right]\right\}, \tag{6}$$

where the effective Lagrangian L is expressed in a diagonalized form

$$L = \sum_{k\sigma}\gamma^*_{k\sigma}\dot{\gamma}_{k\sigma} + \sum_{k}(E_0+E_k-\lambda_k) + \sum_{k\sigma}\lambda_k\gamma^*_k\gamma_k, \tag{7}$$

where the $\gamma_{k\sigma}$ are the Boguliubov quasiparticles and are given by

$$\gamma^*_{k\uparrow} = \cos\,\theta_k c^*_{k\uparrow} + \sin\,\theta_k c_{-k\downarrow}, \tag{8}$$

$$\gamma_{k\downarrow} = -\sin\,\theta_k c^*_{k\uparrow} + \cos\,\theta_k c_{-k\downarrow}, \tag{9}$$

where $\cos^2\,\theta_k=\frac{1}{2}(1+\frac{E_k}{\lambda_k})$, $\alpha_k=2(\cos\,k_x+\cos\,k_y)$, $E_0=(-2\mu+\frac{s^2}{U})\varphi^*\varphi$, $E_k=-g_t t\alpha_k-\mu$, $\lambda_k=\sqrt{E_k^2+\Delta_k^2}$, the gap is proportional to s, $\Delta_k=s\varphi^*(1-\frac{2t}{U}\alpha_k)$, and hence vanishes when φ is absent and $g_t=\frac{2\delta}{1+\delta}$, $\delta=1-n$. The g_t term originates from the correlated hopping term, $(1-n_{i\bar{\sigma}})c^{\dagger}_{i\sigma}c_{j\sigma}(1-n_{j\bar{\sigma}})$. The $\gamma_{k\sigma}$'s play the role of the fundamental low-energy degrees of freedom in a doped Mott insulator. That is, they are the natural propagating charge degrees of freedom. Note they depend in a complicated way on the φ_i field and consequently are heavily mixed with the doubly occupied sector. Starting from Eq. (7), we integrate over the fermions in Eq. (6) to obtain,

$$G(k,\omega) = \frac{1}{Z}\int [D\varphi^*][D\varphi]G(k,\omega,\varphi) \times \exp^{-\Sigma_k[E_0+E_k-\lambda_k-2/\beta\,\ln(1+e^{-\beta\lambda_k})]}, \tag{10}$$

where

$$G(k,\omega,\varphi) = \frac{\sin^2\,\theta_k[\varphi]}{\omega+\lambda_k[\varphi]} + \frac{\cos^2\,\theta_k[\varphi]}{\omega-\lambda_k[\varphi]} \tag{11}$$

is the exact Green function corresponding to the Lagrangian, Eq. (7), which has a two-branch structure, corresponding to the bare electrons and the coupled holon-doublon state, respectively. The role of the φ field, which determines the weight of the second branch, is vital to our understanding of the properties of Mott systems, as was demonstrated previously.[16,17] It is trivial to see that in the limit of vanishing s (no φ field), the $\gamma_{k\sigma}$'s reduce to the bare electron operators c_k and the first term in Eq. (11) vanishes. The two-fluid na-

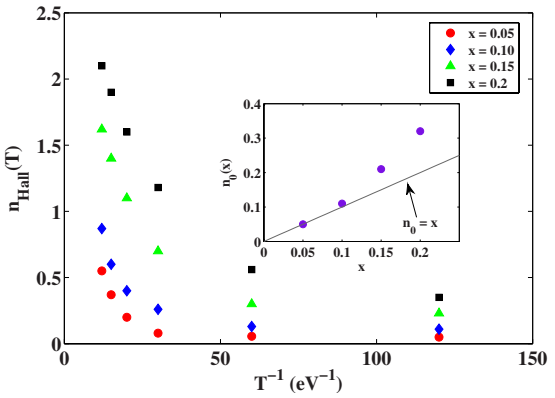

FIG. 1. (Color online) n_{Hall} plotted as a function of inverse temperature for four different values of hole doping x: (1) solid circles, $x=0.05$, (2) diamonds, $x=0.10$, (3) triangles, $x=0.15$, and (4) squares, $x=0.2$. The inset shows the temperature-independent part of the carrier density as a function of x. Note it exceeds the nominal doping level indicated by the straight line.

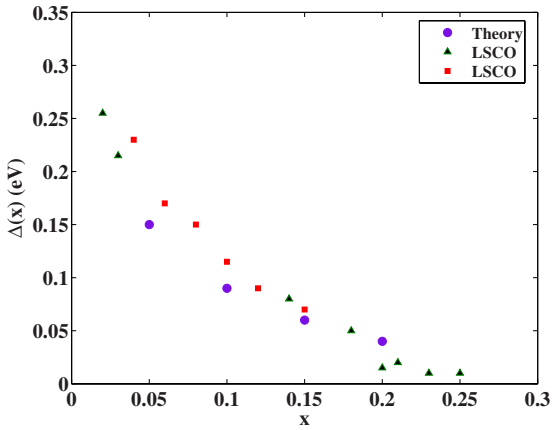

FIG. 2. (Color online) $\Delta(x)$ (solid circles) obtained from fitting the plots in Fig. 1 to Eq. (1) plotted as a function of hole doping x. The experimental values are also shown for LSCO: solid triangles (Refs. 11, 12, and 21) and squares (Ref. 10). The excellent agreement indicates that the bound component contributing to the charge density does in fact give rise to the pseudogap.

ture of the response stems from this fact of the theory. Namely, the first term contributes only when $\varphi \neq 0$ and the second when $\varphi=0$. These contributions correspond to the dynamical and static components of the spectral weight, respectively.

We obtained the Green function $G(\mathbf{k},\omega)$ by a numerical integration of Eq. (10) over the φ field. The Hall coefficient R_H was computed from the spectral function $A(\mathbf{k},\omega)$ using the Kubo formula[19]

$$R_H = \sigma_{xy}/\sigma_{xx}^2, \tag{12}$$

where

$$\sigma_{xy} = \frac{2\pi^2|e|^3aB}{3\hbar^2}\int d\omega\left[\frac{\partial f(\omega)}{\partial\omega}\right]\frac{1}{N}\sum_{\mathbf{k}}\left(\frac{\partial\epsilon_{\mathbf{k}}}{\partial k_x}\right)^2 \times \frac{\partial^2\epsilon_{\mathbf{k}}}{\partial k_y^2}A(\mathbf{k},\omega)^3 \tag{13}$$

and

$$\sigma_{xx} = \frac{\pi e^2}{2\hbar a}\int d\omega\left[-\frac{\partial f(\omega)}{\partial\omega}\right]\frac{1}{N}\sum_{\mathbf{k}}\left(\frac{\partial\epsilon_{\mathbf{k}}}{\partial k_x}\right)^2 A(\mathbf{k},\omega)^2 \tag{14}$$

with σ_{xx} and σ_{xy} the diagonal and off-diagonal components of the conductivity tensor, respectively, $f(\omega)$ is the Fermi distribution function and B is the normal component of the external magnetic field. The effective charge-carrier density n_{Hall} is then obtained using the relation $R_H=-1/(n_{\mathrm{Hall}}e)$.

Figure 1 shows a set of plots of n_{Hall} as a function of the inverse temperature, each corresponding to a different value of hole doping, x, in the underdoped regime (x ranging from 0.05 to 0.20). The plots fit remarkably well to an exponentially decaying form. In other words, the computed charge-carrier density within the charge-2e boson theory of a doped Mott insulator agrees well with the form given in Eq. (1) proposed by Gor'kov and Teitel'baum.[9] The inset shows the temperature-independent part of the charge density as a function of x. This quantity exceeds the nominal doping level. This deviation is expected as the Hall coefficient is expected to change sign around $x=0.3$ (Ref. 20) in hole-doped samples.

The "binding energy," $\Delta(x)$, was extracted for each doping and plotted in Fig. 2 using Eq. (1). Shown here also are the values for the experimentally determined pseudogap energy for LSCO.[11,12,21] The magnitude of $\Delta(x)$ falls with increasing hole doping as is seen experimentally and hence is consistent with its interpretation, even quantitatively, as a measure of the pseudogap temperature T^*. A rough estimate of T^*,

$$T^*(x) \approx -\Delta(x)/\ln(x), \tag{15}$$

may be obtained from $\Delta(x)$, by equating the number of doped carriers x with that of the activated ones $n_1(x)\exp[-\Delta(x,T)]$ as proposed by Gor'kov and Teitel'baum.[9] Figure 3 shows a plot of T^* as a function of x.

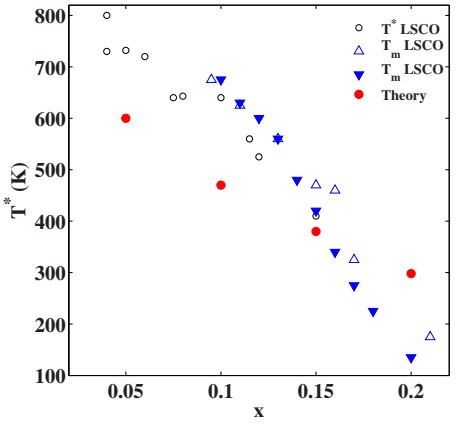

FIG. 3. (Color online) $T^*(x)$ (solid circles) obtained from Eq. (15) plotted as a function of hole doping x. The experimental data were gleaned from the following: open circles are from Ref. 1 T^*, open triangles (T_m) from Ref. 22, and closed triangles (T_m) from Ref. 23.

This is in qualitative agreement with the experimentally obtained estimates of T^*.[1,22,23]

Ultimately it is not surprising that the pseudogap[14,16] appears within the charge-2e boson theory. As mentioned previously, the charge-2e boson is a local collective nonpropagating mode that is restricted to mediate electronic states within the Hilbert space of the Hubbard model. The only option is that the boson binds to a hole to form a new charge-e state. As an electron at low energies [Eq. (4)] is a linear superposition of the standard state in the lower Hubbard band and the bound state mediated by the charge-2e boson, a two-fluid charge model is a natural consequence. This further supports the idea[16] that the pseudogap temperature T^* represents the boundary between bound and unbound charge-2e bosons where the binding energy to excite a boson vanishes and T-linear resistivity obtains.[16,17] The mechanism for T-linear resistivity is simple within this model. Once the binding energy of the boson vanishes, bosons are free to scatter off the electrons. The resistivity of electrons scattering off of bosons is well known to scale linearly with temperature above the energy to create a boson. Hence, this mechanism is robust and should persist to high temperatures. Consequently, the charge-2e boson theory offers a resolution of the pseudogap and the transition to the strange metal regime of the cuprates.

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