Hall and optical conductivity experiments on the cuprates indicate that the low-energy fermionic degrees of freedom in a doped Mott insulator possess a component that is dynamically generated and hence determined by the temperature. We show explicitly how the spectrum in the lower Hubbard band should be partitioned to describe such dynamically generated charge degrees of freedom and corroborate this picture with the results from the exact low-energy theory of the Hubbard model. A consequence of such dynamics is that the Landau one-to-one correspondence between bare electrons and the effective fermionic degrees of freedom at low energies breaks down explicitly. This state of affairs obtains because the total hole number is not conserved as it contains a dynamical contribution. We propose that any experimental probe that couples to the low-energy dynamics of a doped Mott insulator, quantum oscillation experiments included, should be interpreted in terms of the total dynamically generated hole number rather than the bare value.

In 1993, Meinders, Eskes, and Sawatzky\textsuperscript{1} concluded based on an exact diagonalization study that because the effective number of low-energy degrees of freedom in a doped Mott insulator is a function of the hybridization and therefore the volume and temperature, “...it is not possible to define a Hamiltonian that describes the low-energy-scale physics unless one accepts an effective non-particle conservation.” Particle non-conservation as used here refers to the fact that the number of low-energy degrees of freedom is not strictly determined by the electron filling or equivalently the doping level but rather by dynamical degrees of freedom generated from the hybridization and hence the temperature. If this statement is correct, then it must be the case that the chemical potential for the static fermionic low-energy degrees of freedom in any realistic model for a doped Mott insulator is not equivalent to that of the conserved charge, namely the bare electrons. Thus far, an explicit construction demonstrating this has not been advanced. Given the obvious importance of this result, it is surprising how little attention it has attracted. In this paper, we directly address the question of how particle conservation breaks down in a low-energy theory of a doped Mott insulator. We first show that experiments on the Hall and optical conductivities and general theoretical considerations support this claim. Finally, we propose a simple partitioning of the spectral weight in the lower Hubbard band (LHB) which isolates the explicit hybridization-dependent degrees of freedom that are responsible for the dynamical generation of charge degrees of freedom and hence effective particle non-conservation as defined above. We show that these degrees of freedom can be understood within the recently derived exact low-energy theory of the Hubbard model.

I. EXPERIMENTAL MOTIVATION

Is there any experimental indication in doped Mott systems that the number of charge carriers is dynamically generated? It would suffice to show that either 1) the carrier density is temperature dependent or 2) the number of charge carriers exceeds the nominal doping level, hereafter referred to as $x$. Consider first the experiments on the Hall coefficient in La$_2$Sr$_{2-x}$CuO$_4$ (LSCO). In the underdoped regime, the inverse Hall number is strongly temperature dependent$^{2,3}$. Gor’kov and Teitel’baum$^{2,3}$ observed that a two-component empirical formula,

$$n_{\text{Hall}}(x, T) = n_0(x) + n_1(x) \exp(-\Delta(x)/T),$$

accurately describes the inverse Hall coefficient in LSCO in the underdoped regime. One of the components is independent of temperature, $n_0(x)$, given by the static 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 $n_{\text{Hall}}$ is carried entirely within $\Delta(x, T)$ which defines a characteristic activation energy scale for the system. Gor’kov and Teitel’baum$^{2,3}$ 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.

Additionally, optical conductivity experiments indicate that the effective number of charge carriers exceeds the nominal count provided by the doping. In the experiment, the integrated optical conductivity,

$$N_{\text{eff}}(\Omega) = \frac{2mV_{\text{cell}}}{\pi e^2} \int_0^\Omega \sigma(\omega) d\omega$$

is generally plotted in which the cutoff is set by the optical gap, which for LSCO is $\Omega \approx 1.2eV$. Here $\sigma(\omega)$ is the optical conductivity, $V_{\text{cell}}$ the unit-cell volume per formula unit, $m$ the free electron mass, and $e$ the electron charge. In a rigid-band semiconductor model in which spectral weight transfer is absent, $N_{\text{eff}} = x$. However, in all cuprates, regardless of whether they are electron$^{4,5}$ or hole-doped$^{4,5}$, $N_{\text{eff}}$ exceeds $x$ in the underdoped regime.

Consequently, experimental probes which couple to the current reveal that the number of charge carriers in the
cuprates is 1) temperature dependent and 2) exceeds the nominal doping level, consistent with Meinders, et al. An interesting question is how does one define the chemical potential for such dynamically generated charge degrees of freedom. Clearly it is not equal to that of the bare electrons as the the effective number of charge degrees of freedom exceeds the bare charge count. We argue below that the effective doping level that captures the dynamical generation of the charge degrees of freedom as in Eq. (1) is given by

$$x' = x + \alpha$$  \hspace{1cm} (3)

where $$\alpha$$ is a dynamical correction determined by the hybridization. This redefinition of the doping level naturally arises from the exact low-energy theory of the Hubbard model which has been shown to explain both Eq. (1) and Eq. (2).

II. REDEFINITION OF CHEMICAL POTENTIAL

The goal in this section is to redefine the chemical potential so that the effective number of fermionic charge carriers is consistent with dynamical generation of charge degrees of freedom discussed in the previous section. In the standard theory of metals, the intensity or spectral weight of a band is completely exhausted by counting the number of electrons it can hold. That is, it is a constant given by one per unit cell and per spin direction. Essential to this view is the robustness of electron quasiparticles even in the presence of interactions. Because of the one-to-one correspondence between electrons and quasiparticles, the chemical potential, $$\mu$$, can be defined either by counting electrons

$$n = \int_{-\infty}^{\mu} N(\omega) d\omega,$$  \hspace{1cm} (4)

or by integrating,

$$y = \int_{\mu}^{\infty} N(\omega) d\omega,$$  \hspace{1cm} (5)

the unoccupied part of the spectrum. Here $$N(\omega)$$ is the single-particle electron density of states and $$A_g$$ is a cut-off demarcating the low-energy physics. As a result of the electron-quasiparticle correspondence, $$y$$ is identical to the number of doped holes, $$x$$, and the electron filling is given by $$n = 2 - x$$ (for a single band).

In stark contrast, the empty part of the spectrum per spin at low energies, Eq. (5), exceeds the doping level in strongly correlated systems such as doped Mott insulators. The inherent problem with strongly correlated systems is that the energy bands are not the traditional static bands that typify band insulator systems. This can be illustrated simply by considering the Hubbard model

$$H_{\text{Hubb}} = -t \sum_{(i,j), \sigma} c_{i\sigma}^{\dagger} c_{j\sigma} + U \sum_i c_{i\uparrow}^{\dagger} c_{i\downarrow}^{\dagger} c_{i\downarrow} c_{i\uparrow},$$  \hspace{1cm} (6)

in which electrons hop among a set of lattice sites, but pay an energy cost $$U$$ whenever they doubly occupy the same site. Here $$i, j$$ label lattice sites, $$(i, j)$$ indicates nearest neighbors, $$c_{i\sigma}$$ annihilates an electron with spin $$\sigma$$ on site $$i$$ and $$t$$ is the nearest-neighbor hopping matrix element. When $$t = 0$$, the Hamiltonian is diagonal

$$H_U = U \sum_i n_{i\uparrow} n_{i\downarrow} = \frac{U}{2} \sum_{\sigma} \eta_{i\sigma} \bar{\eta}_{i\sigma},$$  \hspace{1cm} (7)

where $$\eta_{i\sigma} = c_{i\sigma} n_{i\bar{\sigma}}$$ creates the excitations above the gap in the upper Hubbard band (UHB) on sites occupied by a single electron. Its complement, $$\xi_{i\sigma} = c_{i\sigma} (1 - n_{i\bar{\sigma}})$$ creates excitations strictly on empty sites and hence describes particle motion below the gap. Here $$\bar{\sigma} = -\sigma$$. Consequently, the anticommutator

$$m_{\text{LHB}}^0 = \frac{1}{N} \sum_{i, \sigma} \langle \xi_{i\sigma}, \xi_{i\sigma}^{\dagger} \rangle = 2 - n,$$  \hspace{1cm} (8)

determines the spectral weight in the lower Hubbard band (LHB). Since each hole in a half-filled band decreases the single occupancy by one, the weight of the UHB is $$1 - x$$. Because the total weight of the UHB and LHB must be 2, we find that $$2 - n + 1 - x = 2$$ or $$n = 1 - x$$ and $$m_{\text{LHB}}^0 = 1 + x$$ in the atomic limit. The weights $$1 + x$$ and $$1 - x$$ also determine the total ways electrons can occupy each of the bands. Thus, in the atomic limit, electrons alone exhaust the total degrees of freedom of each band. Further, since each hole leaves behind an empty site that can be occupied by either a spin up or a spin down electron, the electron addition spectrum in the LHB has weight $$y = 2$$.

Because the operators $$\xi$$ and $$\eta$$ do not diagonalize the hopping term, the total intensity of the LHB

$$m_{\text{LHB}} = 1 + x + \frac{2t}{U} \sum_{i,j,\sigma} g_{ij} \langle \tilde{c}_{i\sigma} \tilde{c}_{j\sigma}^{\dagger} \rangle + \cdots = 1 + x + \alpha,$$  \hspace{1cm} (9)

has $$t/U$$ corrections as shown by Harris and Langro15. Here $$\tilde{c}_{i\sigma}$$ are related to the original bare fermion operators via a canonical transformation that brings the Hubbard model into block diagonal form in which the energy of each block is $$nU$$. In fact, all orders of perturbation theory increase the intensity of the LHB beyond its atomic limit of $$1 + x$$. It is these dynamical corrections that $$\alpha$$ denotes. While the intensity of the LHB increases away from the atomic limit, the total number of ways of assigning electrons to the LHB still remains fixed at $$1 + x$$. Consequently, the total weight of the LHB exceeds the fermionic phase space and additional degrees of freedom are needed.

Nonetheless, the sum of the spectral weights in the LHB and UHB must be 2 by charge conservation. Consequently, the weight in the UHB, $$m_{\text{UHB}} = 1 - x - \alpha$$, decreases faster than $$1 - x$$. How should the spectrum in
FIG. 1. Redistribution of spectral weight in the Hubbard model upon doping the insulating state with \( x \) holes. \( \alpha \) is the dynamical correction mediated by the doubly occupied sector. To order \( t/U \), this correction worked out by Harris and Lange\(^\text{14}\) in which the occupied part of the lower band is fixed to the electron filling \( 1-x \). a) The traditional approach\(^\text{11–17}\) in which the occupied part of the lower band is fixed to the electron filling \( 1-x \). b) New assignment of the spectral weight in terms of dynamically generated charge carriers. In this picture, the weight of the empty part of the LHB per spin is the effective doping level, \( x'=x+\alpha \).

Doped Mott Insulator
\[
\begin{array}{c}
\begin{array}{c}
\xrightarrow{1-x} \\
\xrightarrow{1-x-\alpha} \\
\xrightarrow{2x+\alpha} \\
\xrightarrow{E_F} \\
\xrightarrow{1+x+\alpha} \\
\xrightarrow{2x+2\alpha} \\
\xrightarrow{1-x-\alpha} \\
\xrightarrow{E_F} \\
\xrightarrow{U} \\
\end{array}
\end{array}
\]

We now show how the spectrum can be partitioned so that the chemical potential accounts for a charge number consistent with Eq. (1). Note we have some degree of freedom in describing the physics in the LHB since it is not a rigid band. If the dynamical contribution can be removed through a re-definition of the chemical potential, then the empty part of the spectrum per spin will be the effective hole number. The justification for this picture is as follows. In a hole-doped system, turning on a finite \( t/U \) creates pairs of double occupancies and empty sites (doublon-holon pairs). The weight in the UHB corresponds to adding one electron in the high energy sector, in other words creating double occupancy. Doublon-holon pairs clearly deplete this intensity leading to a loss of spectral in the UHB faster than the atomic limit value of \( 1-x \). The occupied weight in the LHB corresponds to removing an electron in the low-energy sector. In other words, the occupied part of the spectrum corresponds to removing an electron such that the number of double occupancies remains conserved. Hence the occupied part of the LHB is a measure of single-occupancy whose weight as well must decrease on creation of doublon-holon pairs. In other words, the weights in the occupied part of the LHB and the UHB must be the same, since both provide a measure of the same phase space. Therefore, we propose that the consistent definition of the chemical potential for the low-energy fermionic degrees of freedom can be obtained by demanding that the two weights be equal. Note this says nothing about the nature of the excitations which live in the high-energy scale. Consequently, we arrive at the assignments of the spectral weights in Fig. (1b). The occupied part of the LHB has weight \((1-x-\alpha)\) and the unoccupied part \((2(x+\alpha))\). The fermionic degrees of freedom that are associated with this assignment of the chemical potential reflect the dynamical generation of the charge degrees of freedom. As a result of the dynamics, \( x'=x+\alpha \) now denotes the effective number of hole degrees of freedom per spin at low energy. Consequently, we propose that it is with respect to \( x' \) that a Luttinger theorem exists not \( x \), the bare hole number.

In the case of electron doping, the chemical potential
(\mu) lies in the UHB where 2x electron removal states are created below \mu and the weight above \mu is given by 1 - x in the atomic limit. Turning on a finite t/U creates doublon-holon pairs. In this case, the holes belong to the LHB and represent the high-energy configurations of the system. The weight above \mu represents the amplitude for adding an electron to the UHB, or creating a double occupancy, which is depleted upon creation of doublon-holon pairs since neither holons nor doublons can contribute to the creation of double occupancies upon addition of a single electron. This weight is analogous to that of the occupied part of the LHB in the case of hole doping. For charge-transfer systems, such as the cuprates, the same argument applies because of the equivalences with the Hubbard model for realistic values of the hybridization between the bands.

To counter the argument that the dynamical corrections might not affect the physics on all energy scales, it suffices to compute the cross correlator between \xi_{i\sigma} = c_{i\sigma}(1 - n_{i\sigma}) and \eta_{i\sigma} = c_{i\sigma}n_{i\sigma}. The full electron spectral function, A(k, \omega) = -\text{Im} FT(\theta(t - t')(\{c_{i\sigma}(t)c_{j\sigma}^{\dagger}(t')\})/\pi = A_{\eta \eta} + A_{\xi \xi} + 2A_{\eta \xi}, contains two diagonal terms A_{\eta \eta} and A_{\xi \xi} and a cross term A_{\eta \xi} which represents the mixing with double occupancy and double holes respectively. For hole doping, the conserved charge \text{Q} is given by 1 - x = \sum_{i} c_{i\sigma}^{\dagger}c_{i\sigma} + 2x. Clearly shown is that the occupied part (red triangles) of the one-particle spectrum has a weight less than 1 - x (solid blue line).

FIG. 2. Integrated spectral weight in the occupied part of the lower Hubbard band, \Lambda_{\mu-}, from the charge 2e low-energy theory\textsuperscript{9–12} with U/t = 8. Here x is the doping level for the conserved charge, Q = \sum_{i} c_{i\sigma}^{\dagger}c_{i\sigma} + 2x. Clearly shown is that the occupied part (red triangles) of the one-particle spectrum has a weight less than 1 - x (solid blue line).

III. CONFIRMATION FROM EXACT LOW-ENERGY THEORY

Since the weight of the band in which the chemical potential resides in a doped Mott insulator exceeds the electron count, new degrees of freedom are required in any consistent low-energy theory. The extra degrees of freedom are generated from mixing with the doubly occupied sector and hence should emerge upon integration of the states far away from the chemical potential. We have carried\textsuperscript{18–20} out this Wilsonian program exactly for the Hubbard model and showed that a charge 2e bosonic field emerges. The boson which is non-propagating has charge 2e for hole doping and -2e for electron doping, represents the mixing with double occupancy and double holes respectively. For hole doping, the conserved charge Q, which equals the total electron filling n\textsuperscript{11–12}, is a sum of two components,

\[ Q = \sum_{i} a_{i\sigma}^{\dagger}a_{i\sigma} + 2x, \] (11)
immediately implying that the weight of the fermionic part must be less than the conserved charge. Here \( a_{i\sigma} \) is the annihilation operator for the fermionic degree of freedom that results when the high-energy scale is integrated out and \( \varphi \) is a charge 2e boson. That \( Q \) is the conserved charge can be verified by inspection as it trivially commutes with the low-energy effective Hamiltonian. In fact, Eq. (11) gives a prescription for \( \alpha \), namely the bosonic charge, if we interpret \( Q \) as \( 1 - x \) and the fermionic quasiparticle density as \( 1 - x' \). In this theory\(^{2,11}\), the quasiparticles are transformed at low energies to

\[
\tilde{c}_{i,\sigma} \rightarrow (1 - n_{i,\sigma}) c_{i,\sigma} + V_0 \sum_j b_{ij} \tilde{c}_{j,\sigma} + V_\sigma \sum_{\bar{\sigma}} \tilde{\varphi}_i^\dagger \tilde{c}_{i,\bar{\sigma}}, \tag{12}
\]

to leading order in \( t/U \) upon the integration of the high energy scale. Here \( b_i = \sum_j b_{ij} = \sum_{j,\sigma} c_{j,\sigma} 3 V_0 c_{i,\bar{\sigma}} \) with \( V_1 = -V_\perp = 1 \) and \( j \) a nearest-neighbour of site \( i \). The first two terms represent the standard electron operator in the lower Hubbard band dressed with spin fluctuations which constitutes the quasiparticles or the effective fermionic degrees of freedom. However, the last term represents the correction due to dynamical spectral weight transfer. Eq. (12) lays plain that an electron at low energy contains a propagating part that arises from the charge 2e boson. To illustrate that more than just the fermions are needed to satisfy the \( 1 - x \) sum rule, we computed the pure fermionic part of the spectral function by evaluating the Green function:

\[
\int d\varphi^i d\varphi^j \langle \{ \mathcal{D}^i c_i(t) c_i^\dagger (0) \} \exp(-\sum_i L_{IR}(dt)) \rangle / Z.
\]

\( L_{IR} \) is the low-energy Lagrangian\(^{4,12}\) obtained by integrating out the UHB and \( Z \) the partition function. We computed this quantity assuming that the boson is spatially homogeneous, which is justified\(^{12,22}\) since there are no gradient terms of the boson in the low-energy action. The results in Fig. 2 demonstrate that the integrated weight in the occupied part of the spectrum is indeed less than \( 1 - x \). That this weight is less than \( 1 - x \) is independent of the approximations used to calculate the spectral function. This follows entirely from the fact that the conserved charge, \( Q \) is a sum of a fermionic and a bosonic part. The deficit from \( 1 - x \) is carried in the \( \varphi^i c_{i,\bar{\sigma}} \) term. The difference between the red triangles and the solid line approximates \( \alpha \).

**IV. CONCLUDING REMARKS**

Experimentally, any measurement which probes the fermionic low-energy degrees of freedom should be interpreted in terms of the total number of hole degrees of freedom, \( x + \alpha \) not \( x \). For example, the superfluid density should exceed \( x \) and scale as \( x + \alpha \), already confirmed in YBa\(_2\)Cu\(_3\)O\(_6+x\) (YBCO). Similarly, Fermi surface volumes, that is the total volume of the hole pockets minus that of the electron pockets, extracted from quantum oscillation experiments\(^{21}\), whose origin is still not understood, should be compared with \( x' \) not \( x \) as the experimental probe is the current. This is particularly germane because the Fermi surface volumes extracted experimentally\(^{21,22}\) for YBCO are not consistent with any integer multiple of the physically doped holes. Interestingly, the first experiments of this type observed oscillations in the Hall coefficient\(^{21}\). Hence, it is perfectly reasonable that the effective doping level should be consistent with the physics that leads to Eq. (1).

Finally, Fermi liquid theory is recovered when the charge 2e boson decouples from the electronic spectrum. By decoupling we mean that the UHB collapses and the LHB has a weight of 2. In this limit, there is no true high-energy scale and \( \varphi \) should be an irrelevant degree of freedom. To illustrate, using the appropriate\(^{23}\) scaling such that the kinetic energy remains constant in the limit \( d \rightarrow \infty \), that is, \( t \rightarrow 0(1/\sqrt{d}) \), and averages of the form \( \langle c_i^\dagger c_i \rangle \propto 1/\sqrt{d} \) (note as \( d \rightarrow \infty \) the scaling of \( c \) and \( \tilde{c} \) (Eq. (11)) are not trivially related), we find that the boson-dependent terms in the exact low energy theory, \( t \sum_i \varphi_i^\dagger c_i^\dagger c_i \propto O(1/\sqrt{d}) \), \( t^2/U \sum_i \varphi_i^\dagger \varphi_i \propto O(1/d) \), and \( t^2/U \sum_{(ij)} \varphi_i^\dagger b_{ij} \propto O(d \times (1/\sqrt{d})^3) \), vanish when \( d = \infty \). Consequently, no breakdown of Fermi liquid theory obtains as seen numerically\(^{21,22}\) for \( d = \infty \) and \( n \neq 1 \). In finite dimensions, the precise value of the coupling constant and doping level at which the bosonic degrees of freedom decouples remains the open problem in Mottness.

**ACKNOWLEDGMENTS**

This work was funded by the NSF DMR-0605769, NSF PHY05-51164 (KITP) and Samsung scholarship (S. Hong). We also thank F. Krüger, T. Stanescu, R. Leigh, and G. Sawatzky for critical remarks.

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