Mottness in high-temperature copper-oxide superconductors

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Abstract
The standard theory of metals, Fermi liquid theory, hinges on the key assumption that although the electrons interact, the low-energy excitation spectrum stands in a one-to-one correspondence with that of a non-interacting system. In the normal state of the copper-oxide high-temperature superconductors, drastic deviations from the Fermi liquid picture are obtained, highlighted by a pseudogap, broad spectral features and $T$-linear resistivity. A successful theory in this context must confront the highly constraining scaling argument which establishes that all 4-Fermi interactions are irrelevant (except for pairing) at a Fermi surface. This argument lays plain that new low-energy degrees of freedom are necessary. This paper focuses on the series of experiments on copper-oxide superconductors which reveal that the number of low-energy addition states per electron per spin exceeds unity, in direct violation of the key Fermi liquid tenet. These experiments point to new degrees of freedom, not made out of the elemental excitations, as the key mechanism by which Fermi liquid theory breaks down in the cuprates. A recent theoretical advance which permits an explicit integration of the high-energy scale in the standard model for the cuprates reveals the source of the new dynamical degrees of freedom at low energies, a charge 2$e$ bosonic field which has nothing to do with pairing but rather represents the mixing with the high-energy scales. We demonstrate explicitly that at half-filling, this new degree of freedom provides a dynamical mechanism for the generation of the charge gap and antiferromagnetism in the insulating phase. At finite doping, many of the anomalies of the normal state of the cuprates including the pseudogap, $T$-linear resistivity and the mid-infrared band are reproduced. A possible route to superconductivity is explored.

(Some figures in this article are in colour only in the electronic version)

This article was invited by Professor L Greene.

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1. Introduction

Superconductivity in copper-oxide ceramics stands as a grand challenge problem as its solution is fundamentally rooted in the physics of strong coupling. In such problems, traditional calculational schemes based on the properties of single free particles fail. Rather the physics of strong coupling resides in collective behaviour, signified typically by the emergence of new degrees of freedom at low energy. For example, in quantum-chromodynamics (QCD) the propagating degrees of freedom in the infrared (IR) are bound states not related straightforwardly to the ultra-violet (UV) scale physics. The key perspective presented here is that similar physics stems from the strong electron interactions in the copper-oxide superconductors. We will delineate precisely how the emergence of collective behaviour at low energy accounts for many of the anomalous properties of the normal state of the cuprates.

That the cuprates embody strong-coupling physics stems from the Mott insulating [1] nature of the parent state. Such materials possess a half-filled band but insulate, nonetheless. Their insulating behaviour derives from the large on-site interaction that two opposite-spin electrons encounter whenever they doubly occupy the same lattice site. For the cuprates [2], the on-site electron repulsion is typically \( U \simeq 4 \text{ eV} \) whereas the nearest-neighbour hopping matrix element is only \( t \simeq 0.4 \text{ eV} \). Although double occupancy is costly, there is no symmetry principle that forbids it even at half-filling. In the original proposal by Mott [1] to explain why NiO insulated, he assumed, as illustrated in figure 1, that each Ni atom remained neutral because

\[
U = E^{N+1} + E^{N-1} - 2E^N
\]

dominates all other energy scales. Here \( E^N \) is the ground state energy of an atom with \( N \) valence electrons. For each Ni atom, \( N = 2 \). Hence, the zero-temperature state envisioned by Mott is one in which no atom is excited with an occupation of \( N \pm 1 \) electrons. For NiO, this translates to no Ni\(^{+++}\) or Ni\(^{+}\) ions existing, as explicitly stated by Mott [1]. However, it is well known [3–5] that the ground state of a Mott insulator possesses doubly occupied sites at half-filling. As a result, the simple cartoon [1] that the Mott gap originates because double occupancy is forbidden is incomplete. Some have advocated [6] that in the Mott insulator, doubly occupied sites are immobile whereas in the metal they form a fluid. This account requires an explicit dynamical mechanism for the generation of the Mott gap. However, the dynamical degrees of freedom leading to the localization of double occupancy have not been unearthed. We offer here an explicit resolution of this problem.

A few of the properties of doped Mott insulators are sketched in the phase diagram in figure 2. Aside from \( d^{1-2}_{x^2-y^2} \) superconductivity, the pseudogap, the phase diagram, in which the single-particle density of states is suppressed [7, 8, 13], and the strange metal, characterized by the ubiquitous \( T \)-linear resistivity [14, 15], stand out. As the phase diagram suggests, the pseudogap and strange metal phases are intimately related. That is, a correct theory of the pseudogap state of matter should at higher temperatures yield a metallic phase in which the resistivity scales as a linear function of temperature. Nonetheless, numerous proposals [16–22] for the pseudogap abound that offer no resolution of \( T \)-linear resistivity. A part of the problem is that a series of associated phenomena, for example, incipient diamagnetism [23] indicative of incoherent pairing [20–22, 24], electronic inhomogeneity [16, 25–29], time-reversal symmetry breaking [30–33] and quantum oscillations [34] in the Hall conductivity, possibly associated with the emergence of closed electron (not hole) pockets in the first Brillouin zone (FBZ), obscure the efficient cause of the
pseudogap and its continuity with the strange metal. Despite this range of phenomena, a key experimental measure \[15, 35\] of the pseudogap onset is the temperature, \(T^*\), at which the first deviation from \(T\)-linear resistivity occurs. As a consequence, the physics underlying the strange metal must also yield a pseudogap at lower temperatures. Furthermore, it must do so in a natural way. In our work, we take the relationship between the strange metal and the pseudogap seriously and develop a theory \[9–11\] that explains both simultaneously. In addition, we show that the same theory is capable of explaining other anomalies of the normal state such as (1) absence of quasiparticles \[12\] in the normal state, (2) the mid-infrared band (MIB) in the optical conductivity \[36–41\], (3) spectral weight transfer across the Mott gap and (4) the high- and low-energy kinks in the electron removal spectrum.

While it has been acknowledged for some time \[42\] that the normal state of the cuprates is incompatible with Fermi liquid theory, precisely what replaces it has not been settled. In a Fermi liquid, the low-energy excitation spectrum stands in a one-to-one correspondence with that of a non-interacting system. This correspondence must clearly break down in the normal state of the cuprates. The arguments of Polchinski \[42\] and others \[43–45\] make it clear that breaking Fermi liquid theory in \(d = 2\) requires new degrees of freedom at low energy, not simply 4-fermion interactions as they are all (except for pairing) irrelevant at the Fermi liquid fixed point. One possible origin of the new degrees of freedom \[46\] is if spectral weight transfer between high and low energies mediates new electronic states at a low energy. As a result, new states will emerge at low energy that have no counterpart in the non-interacting system. We show quite generally that this state of affairs obtains in the minimal model for a doped Mott insulator, namely, the Hubbard model. Refinements of this model to include more details of the copper-oxide plane also retain this feature. We establish this result first through a simple physical argument which makes it plain that in a doped Mott insulator, the phase space available for adding a particle exceeds the number of ways that electrons can be added at a low energy. Consequently, some new degrees of freedom not made out of the elemental excitations must reside in the low-energy spectrum. By explicitly integrating out the degrees of freedom far away from the chemical potential, the Wilsonian program for constructing a proper low-energy theory, we show that this new excitation is a charge 2\(e\) bosonic field that in no way has anything to do with pairing. It is from this new degree of freedom that the pseudogap and \(T\)-linear resistivity follow immediately. Since this physics arises without any appeal to some further fact but relies only on the strong correlations of the doped Mott state, we have successfully isolated the efficient cause of the pseudogap. The associated phenomena mentioned above are supervenient on rather than central to the physics of the normal state. This review is organized as follows. In the next section, we discuss the experimental evidence for spectral weight transfer and show that it requires new degrees of freedom at low energy not made out of the elemental excitations. In section 3, we derive the exact low-energy theory by formally integrating out the degrees of freedom far away from the chemical potential. In section 4, we compare the predictions of the theory with experiment. We close with a perspective on the remaining problem of superconductivity.

2. Mottness

The origin of the Mott insulating state is subtle for two related reasons. First, the Mott gap cannot be easily deduced from the bare degrees of freedom in a model Hamiltonian. As remarked in the introduction, even in the Hubbard model, the ground state contains admixtures with the degrees of freedom, namely, double occupancy, that lie above the gap. That is, if one were to write the bare electron operator \[3\]

\[
c_i = (1 - n_{i\sigma})c_{i\sigma} + n_{i\sigma}c_{i\sigma}
\]

as a sum of two operators, one of which vanishes on doubly occupied sites, \(\eta_{i\sigma} = (1 - n_{i\sigma})c_{i\sigma}\), and its complement which is only non-zero when a site is doubly occupied, \(\eta_{i\sigma} = n_{i\sigma}c_{i\sigma}\), one would see immediately that such a separation is not canonical. As a result, \(\eta_{i\sigma}\) and \(\eta_{i\sigma}\) have a non-zero overlap and hence they do not propagate independently as would be required for them to be gapped. In fact, it is unclear precisely how to write down a set of canonically defined fermionic operators that do become gapped as a result of the energy cost for double occupancy. This is the Mott problem. Its persistence has led Laughlin \[47\] to assert that the Mott problem is fictitious and in reality does not exist. As mentioned in the preceding section, the real problem is that the Mott gap is fundamentally dynamical in nature. That it is difficult to write down the precise degrees of freedom that are becoming gapped is just a symptom of this fact. As will become clear from this review, the dynamical degrees of freedom that ultimately produce the Mott gap only appear when the high-energy scale is integrated out exactly.

Second, all known Mott insulators order antiferromagnetically at a sufficiently low temperature. To illustrate, two electrons on neighbouring sites with opposite spins can exchange their spins. This process proceeds through an intermediate state in which one of the sites is doubly occupied and hence the corresponding matrix element scales as \(t^2/U\). Antiferromagnetism in the cuprates arises from this mechanism. This mechanism is distinct from the weak-coupling Slater \[48\] process in which a half-filled band orders as a result of nesting at \(Q = (\pi, \pi)\). While antiferromagnetism is certainly a part of the Mott insulating story, it leaves much unexplained. It is that explanatory residue, namely, the properties of Mott insulators which do not necessitate ordering, which we refer to as Mottness. A simple property unexplained by ordering is the Mott gap itself. Above any temperature associated with ordering, an optical gap is obtained \[36, 37, 49\]. Another such property is spectral weight transfer.

2.1. Spectral weight transfer

While what constitutes the minimal model for the cuprates can certainly be debated, it is clear \[50–52\] that regardless of the model, the largest energy scale arises from doubly occupying the copper \(d_{x^2−y^2}\) orbital. This orbital can hybridize with
the in-plane $p_x$ and $p_y$ orbitals and hence a two-band model is natural. Since our emphasis is on the interplay between the high- and low-energy scales, we simplify to a one-band Hubbard [3] model:

$$H_{\text{Hubb}} = -t \sum_{i,j,\sigma} g_{ij} c_{i,\sigma}^\dagger c_{j,\sigma} + U \sum_{i,\sigma} c_{i,\uparrow}^\dagger c_{i,\downarrow} c_{i,\downarrow}^\dagger c_{i,\uparrow},$$

(3)

where $i, j$ label lattice sites, $g_{ij}$ is equal to one iff $i, j$ are nearest neighbours, $c_{i,\sigma}$ annihilates an electron with spin $\sigma$ on lattice site $i$, $t$ is the nearest-neighbour hopping matrix element and $U$ the energy cost when two electrons doubly occupy the same site. Our conclusions carry over naturally to any n-band model of the cuprates as long as the largest energy scale is the on-site energy, $U$, in equation (3). That the dynamics of the charge carriers in the cuprates are captured by this model was confirmed by oxygen 1s x-ray absorption [53] on La$_{2-x}$Sr$_x$CuO$_4$. In such experiments, an electron is promoted from the core 1s to an unoccupied level. The experimental observable is the fluorescence yield as a function of energy as electrons relax back to the valence states. The experiments, figure 3, show that at $x = 0$, all the available states lie at 530 eV. As a function of doping, the intensity in the high-energy peak decreases and is transferred to states at 528 eV. In fact, the lower peak grows faster than $2x$ while the upper peak decreases faster than $1-x$. The separation between these two peaks is the optical gap in the parent insulating material. Though this observation of transfer of spectral weight from high to low energy is not expected in a semiconductor or a Fermi liquid, it is certainly not an anomaly in strongly correlated systems. In fact, it is the fingerprint of Mottness as it has been observed in the classic Mott system NiO upon Li doping [49] and in all optical conductivity measurements on the cuprates [36, 37, 39–41] above any temperature having to do with ordering.

This generic behaviour of spectral weight transfer is captured by the Hubbard model. To illustrate, consider the half-filled Hubbard model. A charge gap splits the spectrum into two parts, lower and upper Hubbard bands. Roughly, the lower Hubbard band (LHB) describes particle motion on empty sites while particle motion on already singly occupied sites is captured by the upper Hubbard band (UHB). This relationship is only approximate because the UHB and LHB are mixed so that there are states in the LHB that have some doubly occupied character. To understand spectral weight transfer, we start in the atomic limit in which there is a clean gap of order $U$ between the UHB and LHB. For a system containing $N$ electrons on $N$ sites, the weight of the LHB is $N$ corresponding to $N$ ways to remove an electron. The corresponding weight in the UHB is $N$ as well as there are $N$ ways to add an electron to the system. These bands are shown in figure 4. Consequently, adding a hole in the atomic limit decreases the electron removal spectrum in the LHB by one state. The weight in the UHB is also affected as there are now $N-1$ ways to create a doubly occupied site. This leaves two states unaccounted for. The two extra states are part of the addition spectrum at low energies and correspond to the two ways of occupying the empty site by either a spin-up or a spin-down electron. In the atomic limit, the number of addition states scales as $2x$ [54, 55] when $x$ holes are created. In a semiconductor or a Fermi liquid, the number of addition states would be strictly $x$. Experimentally [36, 37, 39, 40, 41, 49, 53], however, the low-energy spectral weight (LESW) grows faster than $2x$. The excess of $2x$ can be understood simply by turning on the hopping [4]. When the hopping is non-zero, empty sites are created as a result of the creation of double occupancy. Such events increase the number of available states for particle addition and as a consequence the LESW increases faster than $2x$. It is important to recall that the argument leading to the LESW exceeding $2x$ relies on the strong-coupling limit. If this limit is not relevant to the ground state at a particular filling, the previous argument fails.
Polchinski [42] and others [43–45] considered Fermi liquid natural if there are no relevant perturbations. Several years ago, theory. A low-energy theory is properly considered to be if spectral weight transfer plays any role in a low-energy important? A way of gauging importance is to determine A natural question arises. Is spectral weight transfer electrons, there are no relevant interactions (except for pairing) [42–45] that as long as one posits that the charge carriers are theory from the standpoint of renormalization. They found [43–45] considered Fermi liquid theory from the standpoint of renormalization. They found [42–45] that as long as one posits that the charge carriers are electrons, there are no relevant interactions (except for pairing) that destroy the Fermi liquid state. The setup [42] as follows. Decompose the momenta into the Fermi momentum and a component orthogonal to the Fermi surface:

\[ p = k + \ell. \]  

(4)

Here \( \ell \) is the component orthogonal to the Fermi surface. Then consider scaling of energy and momentum towards the Fermi surface, in other words

\[ E \rightarrow uE, \quad k \rightarrow k, \quad \ell \rightarrow u\ell, \]  

(5)

where \( u \) is the scaling parameter. To quadratic order, the action is

\[ S = \int \! dt \, d^3 p \left[ i \bar{\psi}(p) \partial_t \psi(p) - (E(p) - E_F(p)) \bar{\psi}^*(p) \psi(p) \right]. \]

Hence, close to the Fermi surface

\[ E(p) - E_F(p) \sim \ell v_f, \quad v_F = \partial_p E, \]  

(6)

so that after scaling towards the Fermi surface (note that also \( t \rightarrow u^{-1} t \)) one finds that

\[ \psi \rightarrow u^{-1/2} \psi. \]  

(7)

Consider now the four-fermion interaction. The argument showing that such interactions are irrelevant is particularly simple. In terms of powers of the scaling parameter, \( u \), the measure over time contributes one negative power, the measure over the momenta orthogonal to the Fermi surface 4 powers and the 4-Fermi interaction \( \frac{1}{2} \) negative powers. The delta function over the 4-momenta generically does not scale. Hence, the overall scaling of the 4-Fermi interaction is governed by \( u^{-1+4-4/2} = u^1 \) and hence is irrelevant as the power of \( u \) is positive. The only exception to this argument if inversion symmetry is present is the Cooper pairing interaction. Consequently, as long as the charge carriers carry unit charge, there are no relevant interactions that destroy Fermi liquid theory. In the context of the cuprates, this argument is particularly powerful as it implies that in order to explain \( T^2 \)-linear resistivity, some new emergent degrees of freedom that have nothing to do with the electrons must be present. There have been attempts to circumvent this argument in the literature that amount to essentially free field theory. In light of the above argument, such attempts must reduce to Fermi liquid theory and hence must yield \( T^2 \) resistivity. Others \([56, 57]\) have directly confronted the Polchinski \([42]\) argument and added extra derivative couplings to the Fermi liquid action. However, the relationship of such continuum models \([56, 57]\) to any concrete realization of Mott physics is not clear.

It is straightforward to show that dynamical spectral weight transfer in a doped Mott insulator leads to a breakdown of the Fermi liquid picture and the emergence of new low-energy degrees of freedom. The interactions of the electrons with the new degrees of freedom can be formulated as a natural theory in which the electron spin–spin interaction is subdominant. As will be seen, the interactions with the new degrees of freedom govern all of the physics that is independent of ordering. In this sense, we arrive at a natural separation between spin-ordering and Mott physics. To proceed, we define the number of single-particle addition states per site at a low energy,

\[ L = \int_{\mu}^{E_F} N(\omega) \, d\omega, \]  

(8)

as the integral of the single-particle density of states \((N(\omega))\) from the chemical potential, \( \mu \), to a cutoff energy scale, \( A \), demarcating the IR and UV scales. As long as \( A \) is chosen to exclude the high-energy scale, \( L \) is a well-defined quantity which simply counts the number of states in the unoccupied part of the spectrum at a low energy. We compare this quantity with the number of ways an electron can be added to the holes created by the dopants. We call this quantity \( n_h \). Our usage of ‘ways’ here refers to the spin degree of freedom of the electron only and not to combinatorics. From the perspective of single-particle physics, the intensity of a band is always equal to the number of electrons the band can hold. Hence, strict adherence to the single-particle picture requires that \( L = n_h \), implying that the number of low-energy addition states per electron per Figure 4. Evolution of the single-particle density of states from half-filling to the one-hole limit in a doped Mott insulator described by the Hubbard model. Removal of an electron results in two empty states at a low energy as opposed to one in the band-insulator limit. The key difference from the Fermi liquid is that the total weight spectral weight carried by the LHB (analogue of the valence band in a Fermi liquid) is not a constant but a function of the filling.

2.2. Breakdown of fermi liquid theory: more than just electrons

A natural question arises. Is spectral weight transfer important? A way of gauging importance is to determine if spectral weight transfer plays any role in a low-energy theory. A low-energy theory is properly considered to be natural if there are no relevant perturbations. Several years ago, Polchinski \([42]\) and others \([43–45]\) found renormalization. They found \([42–45]\) that as long as one posits that the charge carriers are electrons, there are no relevant interactions (except for pairing) that destroy the Fermi liquid state. The setup \([42]\) is as follows. Decompose the momenta into the Fermi momentum and a component orthogonal to the Fermi surface:

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That mixing between the high- and low-energy scales is obtained only if double occupancy neighbours a hole. In the exact low-energy equation (16), the low-energy theory in terms of the bare fermions does not preserve double occupancy. The process shown here illustrates expansion of the projected transformed operators in terms of the bare electron operators (see equation (16)). As a result of the strictly above the $U_L=\infty$ charge

$$0 \leq \frac{t}{U_L} \ll 1$$

in perturbation theory contributes to as shown first by Harris and Lange [4]. In fact, every order $L/t/U$ double occupancy and as a result empty sites with weight $x$ remains fixed at $2x$ in a real doped Mott insulator, $L/n_h > 1$. Hence, real Mott systems are not in the atomic limit. In strong coupling, finite hopping with matrix element $t$ creates double occupancy and as a result empty sites with weight $t/U$. Such empty sites with fractional weight contribute to $L$ as shown first by Harris and Lange [4]. In fact, every order in perturbation theory contributes to $L$. Consequently, when $0 < \frac{t}{U} \ll 1$, $L$ is strictly larger than $2x$. Such hopping processes or quantum fluctuations do not affect the number of electrons that can be added to the system, however. Since $n_h$ remains fixed at $2x$, in a real doped Mott system, $L/n_h > 1$. Consequently, in contrast to a Fermi liquid, simply counting the number of electrons that can be added does not exhaust the available phase space to add a particle at a low energy. That is, additional states that do not have the quantum numbers of an electron must exist as illustrated in figure 6. Since the number of ways of adding a particle exceeds the number of electrons that can be added, the additional states must be gapped to the addition of an electron. This gap can manifest itself straightforwardly as a depression in the density of states at the chemical potential or more subtly as a reconstruction [58] of the non-interacting Fermi surface, for example, one that has electron (or hole) pockets that shrink in size as the doping decreases. Numerical simulations show [59] that such reconstructions do not necessitate broken symmetry but result entirely from the strong correlations in a doped Mott insulator. In either case, the one-to-one correspondence between the excitation spectrum in the free and interacting systems breaks down. In doped Mott systems, this breakdown arises entirely from the strong correlations in a doped Mott insulator. Thus, additional degrees of freedom at a low energy, not discussed in section 4.1) has not been deduced previously. Hence, the physics governed by the new degrees of freedom breaks down in a doped Mott insulator.
2.3. Perturbative approaches

It is possible to account for the dynamical contribution to the LESW using degenerate perturbation theory. While this method does not shed any light on the missing degree of freedom at low energy, it does serve to illustrate that the limits of the LESW using degenerate perturbation theory. While this must emerge from the new collective charge $2e$. The new theory we construct, in which we integrate out exactly the high-energy scale, has such a degree of freedom which does in fact mediate the dynamical part of $L$. In light of Polchinski’s argument [42], any non-Fermi liquid behaviour must emerge from the new collective charge $2e$ excitation. We show that this is in fact the case.

The goal of perturbative approaches [63–68] in this context is to bring the Hubbard model into diagonal form with respect to double occupancy. As with any matrix diagonalization problem, the new basis which makes double occupancy a good quantum number involves some linear combination of the old states. The subtlety that this introduces is that the no double-occupancy condition applies only to the transformed fermions, not to the original bare electrons. This is an oft-overlooked fact that has led to much confusion over what precisely the accepted low-energy reduction of the Hubbard model, namely, the $t$–$J$ model [69], entails. We review the derivation with an eye on isolating the processes which lead to dynamical spectral weight transfer. Let $f_{i\sigma}$ be the dressed operators which make the Hubbard model block diagonal with respect to ‘double occupancy.’ Following Eskes et al [63], for any operator $O$, we define $\hat{O}$ such that $O \equiv \mathbf{O}(c)$ and $\hat{O} \equiv \mathbf{O}(f)$, simply by replacing the Fermi operators $c_{i\sigma}$ with the transformed fermions $f_{i\sigma}$. To block diagonalize the Hubbard model,

$$H[f] \equiv e^{\frac{1}{U}(\tilde{T}_{i+} - \tilde{T}_{i-})},$$

one constructs a similarity transformation $S[f] = e^{\frac{1}{U}(\tilde{T}_{i+} - \tilde{T}_{i-})}$, which connects sectors that differ by at most one ’fictive’ doubly occupied site, that is, a doubly occupied site in the transformed basis. To lowest order,

$$S^{(1)} = \frac{1}{U}(\tilde{T}_{i+} - \tilde{T}_{i-}),$$

where

$$\tilde{T}_{i+} = -t \sum_{j,\sigma} g_{ij} c_{i\sigma} f_{j\sigma} (1 - n_{j\sigma}),$$

which increases the quantum number $\tilde{V} = \sum_{i} n_{i\uparrow} n_{i\downarrow}$ by one. Likewise, $\tilde{T}_{i-} = (T_{i\uparrow})^\dagger$ decreases $\tilde{V}$ by one. In the new basis, $[H, \tilde{V}] = 0$, implying that double occupation of the transformed fermions is a good quantum number, and all of the eigenstates can be indexed as such. This does not mean that $[H, V] = 0$. If it were, there would have been no reason to do the similarity transformation in the first place. $\tilde{V}$, and not $V$, is conserved. Assuming that $V$ is the conserved quantity results in a spurious local $SU(2)$ [70, 71] symmetry in the strong-coupling limit at half-filling.

To expose the dynamical contribution to spectral weight transfer, we focus on the relationship between the physical and transformed fermions. As expected in any degenerate perturbation scheme, the bare fermions,

$$c_{i\sigma} = e^S f_{i\sigma} e^{-S} \approx f_{i\sigma} - \frac{t}{U} \sum_{j,\sigma} \langle \bar{n}_{j\sigma} - \bar{n}_{j\bar{\sigma}} \rangle f_{j\sigma}$$

$$- \frac{f_{i\sigma}^\dagger f_{i\sigma} + f_{i\sigma} f_{i\sigma}^\dagger f_{j\bar{\sigma}} \rangle},$$

are linear combinations of the multiparticle states in the transformed basis. We invert this relationship to find that

$$f_{i\sigma} \approx c_{i\sigma} + \frac{t}{U} \sum_{j} g_{ij} X_{ij\sigma},$$

where

$$X_{ij\sigma} \equiv \langle (n_{j\sigma} - n_{i\sigma}) c_{j\sigma} - c_{j\sigma} c_{i\sigma} c_{i\sigma} + c_{j\sigma} c_{i\sigma} c_{j\bar{\sigma}} \rangle.$$  

Since the low-energy theory is captured by the sector in the transformed basis which has no double occupancy, it is most relevant to focus on the form of the projected transformed fermions. Using the relations above, we find that, as expected, the projected transformed fermions

$$(1 - \bar{n}_{i\bar{\sigma}}) f_{i\sigma} \approx (1 - n_{i\sigma}) c_{i\sigma} + \frac{t}{U} V_{i\sigma} c_{i\sigma} b_i$$

$$+ \frac{t}{U} \sum_{j} g_{ij} [n_{j\sigma} c_{j\sigma} + n_{\bar{\sigma}} (1 - n_{j\bar{\sigma}}) c_{j\bar{\sigma}}]$$

$$(1 - n_{j\bar{\sigma}})(c_{j\sigma} c_{i\sigma} - c_{j\sigma} c_{i\sigma} c_{i\bar{\sigma}})$$

involve double occupancy in the bare fermion basis. Here $V_{\sigma} = -V_{\sigma} = 1$ and $b_i = \sum_j V_{ij} c_{i\sigma} c_{j\sigma}$, where $j$ is summed over the nearest neighbours of $i$. The projected bare fermion, $(1 - n_{i\bar{\sigma}})c_{i\sigma}$, yields the 2x sum rule, whereas it is the admixture with the doubly occupied sector that mediates the $t/U$ corrections. A process mediated by these terms is shown in figure 5. This can be seen more clearly by computing $L$ directly using equation (13). The standard treatment [60–62, 69] of the $t$–$J$ model ignores the dynamical corrections as a hard projection scheme is implemented in which the no double-occupancy condition applies not only to the transformed but also to the bare fermions. As we have pointed out in the introduction, the physics left out by projecting out double occupancy is important because it tells us immediately that $L/n_{ib} > 1$ as can be seen from the expression
Simulations on finite-size systems reveal that however, in the Hubbard model, the situation is not as clear. It is in these corrections that the explicit non-Fermi liquid projected part, their contribution cannot be ignored because $Z_L$.

As is evident, $2\langle (1 - n_{i\sigma})(1 - n_{j\sigma}) \rangle = 2x$ in the projected Hilbert space of the dressed fermions which corresponds to the $2x$ sum rule of the static part in the LESW. The dynamical part of $L$ arises from the $t/U$ corrections. It is these corrections that prevent the operator in equation (16) from being regarded as a free excitation. Rather it describes a non-Fermi liquid $(L/n_h > 1)$.

However, it is particularly cumbersome to extract physical insight from the canonical transformation method. The primary reason is that any information regarding the bare fermions requires that the similarity transformation be undone when any experimentally relevant quantity is calculated. Consider, for example, the electron spectral function. In the hard-projected version of the $t$–$J$ model [60–62, 69], the electron spectral function is assumed to be given by simply the time-ordered anticommutator of the transformed fermions. However, equation (13) illustrates that this is not so. In actuality, the single-particle Green function,

$$G(k,\omega) = -\text{iFT}(T c_{i\sigma} c_{j\sigma}^\dagger) = -\text{iFT}(T f_{i\sigma} f_{j\sigma}^\dagger)$$

has $t/U$ corrections in the transformed basis. Although these corrections are naively down by a factor of $t/U$ relative to the projected part, their contribution cannot be ignored because it is in these corrections that the explicit non-Fermi liquid behaviour is hidden. To illustrate, all calculations on the $t$–$J$ model of the single hole problem [72–75] in a quantum antiferromagnet yield a finite value of $Z$ proportional to $J/t$. However, in the Hubbard model, the situation is not as clear. Simulations on finite-size systems reveal that $Z \propto L^{-\alpha_c}$, where $\alpha > 0$ and hence tends to zero as the system size increases. While this calculation is not conclusive, it is consistent with the fact that similar dynamical mean-field treatments of the $t$–$J$ and Hubbard models at finite doping yield a finite conductivity as $T \to 0$ in the $t$–$J$ model [76, 77] but a vanishing value in the Hubbard model as $T \to 0 |8 – 78]$. These differences are summarized in table 1. The most striking results in table 1 are those for the exponents governing the asymptotic fall-off of the density correlations, $\alpha_c$, and momentum distribution functions ($\theta$) in the $t$–$J$ (with $t = J$, the supersymmetric point) and Hubbard models in $d = 1$. Here these quantities can be obtained exactly [79–81] for both models using Bethe ansatz.

Table 1. Comparison between Hubbard and $t$–$J$ models. The exponents $\alpha_c$ and $\theta$ were computed using Bethe ansatz for the supersymmetric ($t = J$) $t$–$J$ and Hubbard models in $d = 1$. Respectively, these exponents govern the asymptotic form of the density correlations and the momentum distribution functions. $Z_{Lh}$ denotes the quasiparticle weight for a single hole in Mott insulator described by either the Hubbard or $t$–$J$ model, $\sigma(T = 0, n > 0.9)$ the conductivity for fillings exceeding $n = 0.9$ and mid-IR denotes the MIB in the optical conductivity.

| Model        | $\alpha_c(n = 0)$ | $\theta$ | $Z_{Lh}$ | Mid-IR | Luttinger surface |
|--------------|-------------------|----------|----------|--------|------------------|
| $t$–$J$      | 4 [79]            | $2[80]$  | Finite   | None   | None             |
| Hubbard      | $\alpha_c – 4\sigma^2/16\alpha_c$ [79] | $1/8$    | $L^\infty$ [75] | Yes    | Yes              |
| at $n = 1$   |                   |          |          |        |                  |

3. New theory: hidden charge 2e boson

The Wilsonian program for constructing a low-energy theory is to explicitly integrate over the fields at high energy. The theory that results from this procedure should contain all of the physics at low energy. In the context of the Hubbard model, it should explicitly tell us that $L/n_h > 1$, a key defining feature of a gapped phase without symmetry breaking. We now show how this comes about.

For the Hubbard model, one has to cleanly associate the physics on the energy scale $U$ with an elemental field that can be integrated out by using either fermionic or bosonic path-integral methods. The Hubbard model in its traditional form does not admit such a treatment. However, one can bring the
Hubbard model into the appropriate form by introducing an elemental field that describes the excitations far away from the chemical potential. For hole doping, this constitutes the excitations in the UHB. In our construction, we will extend the Hilbert space of the Hubbard model to include an extra degree of freedom which will represent the UHB. By a constraint, the new field will represent the creation of double occupancy. This field will enter the Lagrangian with a mass of $U$. When the constraint is solved, we recover the Hubbard model. However, since the new field has a mass of $U$, the exact low-energy theory is obtained by integrating over this field rather than by solving the constraint. Consequently, the new low-energy theory will contain an extra degree of freedom having to do with the coupling with the high-energy scale. Since the constraint field has to do with double occupancy, it must have charge $2e$.

3.1. Bohm/Pines redux

There is a great similarity between our treatment of the new collective mode in the Hubbard model and the Bohm–Pines derivation of plasmons. Here we briefly introduce the approach used by Bohm and Pines [90] to describe the collective excitation of the interacting electron gas. Shankar [91] also used a similar approach in their dipole analysis of the $v = 1/2$ quantum Hall state. The basic idea is to re-express the Hamiltonian in such a way that the long-range part of the Coulomb interactions between the electron is described in terms of collective fields (plasma mode) by enlarging the original Hilbert space. After we remove the unphysical states by a constraint, the resultant Hamiltonian will transform to an interacting electron gas with only short-range Coulomb interactions coupled to a plasma oscillating mode.

The starting point is the general interacting electron Hamiltonian,

$$
H = \sum_i \frac{p_i^2}{2m} + 2\pi e^2 \sum_{k_i} \frac{e^{ik(x_i-x_k)}}{k^2} - 2\pi ne^2 \sum_k \frac{1}{k^2},
$$

where $n$ is the total electron density, the first term corresponds to the kinetic energy of the electrons, the second term is their Coulomb interaction and the third term is the self-energy which represents a uniform positive charge background.

The collective mode can be described by first enlarging the Hilbert space of the original electron gas to include a new set of canonical variables $(\pi_k, \theta_k)$ such that $[\theta_k, \pi_k] = i\hbar \delta_{k,k'}$. The original Hamiltonian becomes

$$
H = \sum_i \frac{p_i^2}{2m} - 2\pi ne^2 \sum_k \left( \frac{1}{k^2} \right)
+ \frac{\sqrt{4\pi} e}{m} \sum_{ik} \epsilon_k \cdot (p_i - \hbar k/2) \theta_k e^{ikx_k} - \sum_k \frac{1}{2} \pi_{-k} \pi_{-k}
+ \frac{2\pi e^2}{m} \sum_{ik}\epsilon_k \epsilon_{ik} \theta_k \theta_{ik} e^{ikx_k}.
$$

Here, $\epsilon_k$ is the unit vector along the $k$ direction. The relevant equation can be derived by rewriting the Hamiltonian as a non-interacting electron system coupled to an external electric field, $E(x)$,

$$
H = \sum_i \frac{p_i^2}{2m} \left( 1 - e^{iA(x)} \right)^2 + \frac{1}{8\pi} E(x)^2,
$$

such that

$$
E(x) = \sqrt{4\pi} \sum_k \pi_{-k} \epsilon_k e^{ikx}.
$$

The corresponding longitudinal vector potential $A(x)$ is

$$
A(x) = \sqrt{4\pi} e^2 \sum_k \theta_k \epsilon_k e^{ikx}.
$$

Here, both $A(x)$ and $E(x)$ are real and the unphysical states can be removed by the constraint

$$
\Omega_k = \pi_k - i \left( \frac{4\pi e^2}{k^2} \right)^{1/2} \sum_i e^{-ikx} = 0 \quad \forall k,
$$

which was obtained by equating the electric field energy $E(x)^2/8\pi$ with the electron–electron interaction energy. For the last term in equation (20), the dominant part comes from $k = -l$. By defining the plasma frequency

$$
\omega_p^2 = \frac{4\pi ne^2}{m},
$$

we are able to simplify the Hamiltonian

$$
H = \sum_i \frac{p_i^2}{2m} - 2\pi ne^2 \sum_k \left( \frac{1}{k^2} \right)
+ \frac{\sqrt{4\pi} e}{m} \sum_{ik} \epsilon_k \cdot (p_i - \hbar k/2) \theta_k e^{ikx_k}
- \frac{1}{2} \sum_k (\pi_k \pi_{-k} + \omega_p^2 \theta_k \theta_{-k}),
$$

which describes the non-interacting electron gas coupled with the plasma mode of frequency $\omega_p$. Here, we have simplified the derivation by assuming that the collective modes can oscillate with any frequency. In a realistic system, a maximum cutoff frequency, $k_c$, determined by the electron density, arises so that only the long-range electron–electron interaction can be transformed into the plasma mode, and the electron gas retains a short-range Coulomb interaction. The magnitude of $k_c$ can be determined self-consistently by minimizing the total energy. To summarize, we have mapped the original electron–electron interacting Hamiltonian to a non-interacting electron gas coupled to the plasma mode. The key trick that made this happen was enlarging the original Hilbert space.

3.2. Charge $2e$ boson

The essence of the Bohm–Pines [90] derivation is that plasmons, as an independent degree of freedom, are only apparent when the constraint is relaxed in the extended Hilbert space. As we will see, the same is true for a doped Mott insulator. To this end [9, 10], we extend the Hilbert space $\otimes (F^+ \otimes F^+ \otimes F^D)$, where $F$ denotes a fermionic Fock space.
In the left frame of figure 7, we indicate the states of the extended Hilbert space for a single site. The new extended states are shown in red. Such states will be removed by a suitably chosen constraint which will associate $D_i$ with the creation of double occupancy. In order to limit the Hilbert space to single occupation in the $D$ sector, we will take $D$ to be fermionic. The field $D$ will enter the theory as an elemental field with a large (order $U$) quadratic term and precise interactions with electronic degrees of freedom; the low-energy (IR) theory is obtained by integrating out $D$. Because $D$ is fermionic, a trick is required to associate it with the creation of double occupancy which clearly transforms as a boson. Essentially, we will have to fermionize double occupancy. This can be done by imposing a constraint on the $D_i$ field such that

$$D_i \approx \theta c_{i,\uparrow}^\dagger c_{i,\downarrow}^\dagger,$$  
(27)

where $\theta$ is a Grassmann field which is normalized as

$$\int d^2 \theta \bar{\theta} \theta = 1.$$  
(28)

The constraint will be imposed through the use of a $\delta$-function and hence will enter the action upon subsequent exponentiation as in the implementation of the constraint in the non-linear $\sigma$-model. While there is some similarity between $\theta$ and a super-coordinate, this association is strictly formal in our case as any dependence on the Grassmann parameter $\theta$ disappears.

For hole doping, it is the UHB that must be integrated out. The appropriate hopping processes that must be included in the Lagrangian are given in the right-hand panel of figure 7. The Euclidean Lagrangian in the extended Hilbert space which describes the hopping processes detailed above can be written as

$$\mathcal{L} = \int d^2 \bar{\theta} \theta \left[ \bar{\theta} \sum_{i,\sigma} (1 - n_{i,\sigma}) c_{i,\sigma}^\dagger \dot{c}_{i,\sigma} + \sum_i D_i^\dagger D_i ight. + U \sum_j \sum_i D_i j - t \sum_{i,j,\sigma} g_{ij} [c_{i,\sigma}^\dagger c_{j,\sigma}^\dagger c_{j,\sigma} c_{i,\sigma} + D_i^\dagger c_{i,\sigma}^\dagger c_{i,\sigma} D_j^\dagger c_{j,\sigma} + (D_i^\dagger \theta c_{i,\sigma} V_\sigma c_{j,\sigma} - h.c.)] + H_{\text{con}} \right].$$  
(29)

Here, $g_{ij}$ selects nearest neighbours (note that if we wanted to include next-to-nearest neighbour interactions, we need just modify the matrix $g_{ij}$ accordingly), the parameter $V_\sigma$ has values $V_{\uparrow} = 1$, $V_{\downarrow} = -1$ and simply ensures that $D$ couples to the spin singlet and the operator $C_{i,\sigma}$ is of the form $C_{i,\sigma} \equiv \theta \bar{\theta} \alpha_{i,\sigma} \equiv \bar{\theta} \theta (1 - n_{i,\sigma})(1 - n_{j,\sigma})$ with number operators $n_{i,\sigma} \equiv c_{i,\sigma}^\dagger c_{i,\sigma}$. Note that the dynamical terms that appear in the Lagrangian exclude, as they must, those sites already singly occupied, as they describe the dynamics in the LHB. The constraint Hamiltonian $H_{\text{con}}$ is taken to be

$$H_{\text{con}} = s \bar{\theta} \sum_j [\theta \dot{\phi}_j - \theta j \theta \phi_j + \text{h.c.}],$$  
(30)

where $\phi$ is a complex charge $2e$ bosonic field which enters the theory as a Lagrange multiplier. The constant $s$ has been inserted to carry the units of energy. It could be absorbed into the definition of the constraint field $\phi$. There is a natural connection between $\phi_i$ in our theory and $\sigma$ in the non-linear $\sigma$-model. Both start their lives as Lagrange multipliers but both end up affecting the low-energy physics. At this point, there is some ambiguity in the normalization of $\phi$, but we expect that this will be set dynamically. We will find that if a true IR limit exists, then $s$ must be of the order of the hopping matrix element $t$.

Now, as noted previously, we have chosen Lagrangian (29) so that this theory is equivalent to the Hubbard model. To demonstrate this, we first show that once the constraint is solved, we obtain the Hubbard model. Hence, the Lagrangian we have formulated is the Hubbard model written in a non-traditional form—in a sense, we have inserted unity into the Hubbard model path integral in a rather complicated fashion. To this end, we compute the partition function

$$Z = \int [Dc \theta c_{\uparrow} \theta c_{\downarrow}] \exp \left[ \int t \mathcal{L} \right],$$  
(31)

with $\mathcal{L}$ given by (29). We note that $\phi$ is a Lagrange multiplier. As shown previously [10], in the Euclidean signature, the fluctuations of the real and imaginary parts of $\phi_i$ must be integrated along the imaginary axis for $\phi_i$ to be regarded as a Lagrangian multiplier. The $\phi$ integrations (over the real and imaginary parts) are precisely a representation of (a series of) $\delta$-functions of the form

$$\delta \left( \int \bar{\theta} \theta D_i - \int \bar{\theta} \theta c_{i,\uparrow}^\dagger c_{i,\downarrow}^\dagger \right).$$  
(32)

If we wish to recover the Hubbard model, we need only integrate over $D_i$, which is straightforward because of the $\delta$-functions. The dynamical terms yield

$$\int d^2 \theta \bar{\theta} \left[ \sum_{i,\sigma} (1 - n_{i,\sigma}) c_{i,\sigma}^\dagger \dot{c}_{i,\sigma} + c_{i,\sigma}^\dagger \dot{c}_{i,\sigma}^\dagger + \sum_i c_{i,\uparrow}^\dagger c_{i,\downarrow}^\dagger \dot{c}_{i,\downarrow}^\dagger c_{i,\uparrow}^\dagger - h.c. \right] = \int d^2 \theta \bar{\theta} \theta \left[ \sum_{i,\sigma} (1 - n_{i,\sigma}) c_{i,\sigma}^\dagger \dot{c}_{i,\sigma} + n_{i,\sigma} c_{i,\sigma}^\dagger \dot{c}_{i,\sigma}^\dagger \right] = \int d^2 \theta \bar{\theta} \theta \left[ \sum_{i,\sigma} c_{i,\sigma} \dot{c}_{i,\sigma} \right].$$  
(33)
Likewise the term proportional to $V_\sigma$ yields
\[
\int d^2\theta \, \theta \sum_{i,j} g_{ij} [c_{i,j,\sigma}^\dagger c_{j,i,\sigma}^\dagger (c_{i,j,\sigma} c_{j,i,\sigma} - c_{i,i,\sigma}^\dagger c_{j,j,\sigma}^\dagger)] + \text{h.c.}
\]
\[
= \int d^2\theta \, \theta \sum_{i,j,\sigma} g_{ij} n_{j,-\sigma} c_{i,\sigma}^\dagger c_{i,\sigma} + \text{h.c.}
\] (34)

Finally, the two $D$ field terms give rise to
\[
\int d^2\theta \, \theta \sum_{i,j} g_{ij} [c_{i,j,\sigma}^\dagger c_{j,i,\sigma}^\dagger (c_{i,j,\sigma} c_{j,i,\sigma} + c_{i,i,\sigma}^\dagger c_{j,j,\sigma}^\dagger)]
\]
\[
= - \int d^2\theta \, \theta \sum_{i,j} g_{ij} n_{j,-\sigma} n_{i,-\sigma} c_{i,\sigma}^\dagger c_{j,\sigma}. \tag{35}
\]

Equations (34) and (35) add to the constrained hopping term in the Lagrangian (the term proportional to $C_{ij,\sigma}$) to yield the standard kinetic energy term in the Hubbard model. Finally, the $D^2$ term generates the on-site repulsion of the Hubbard model. Consequently, by integrating over $\varphi_i$ followed by an integration over $D_i$, we recover the Lagrangian
\[
\int d^2\theta \, \theta \sum_{i,\sigma} \bar{c}_{i,\sigma} \dot{\bar{c}}_{i,\sigma} + H_{\text{Hab}}. \tag{36}
\]
of the Hubbard model. This constitutes the UV limit of our theory. In this limit, it is clear that the Grassmann variables amount to an insertion of unity and hence play no role. Further, in this limit the extended Hilbert space contracts, unphysical states such as $|1,0,1\rangle$, $|0,1,1\rangle$, $|1,1,1\rangle$ are set to zero and we identify $|1,1,0\rangle$ with $|0,0,1\rangle$. Note there is no contradiction between treating $D$ as fermionic and the constraint in equation (30). The constraint never governs the commutation relation for $D$. The value of $D$ is determined by equation (30) only when $\varphi$ is integrated over. This is followed immediately by an integration over $D$ at which point $D$ is eliminated from the theory.

The advantage of our starting Lagrangian over the traditional writing of the Hubbard model is that we are able to coarse grain the system cleanly for $U \gg t$. The energy scale associated with $D$ is the large on-site energy $U$. Hence, it makes sense, instead of solving the constraint, to integrate out $D$. The resultant theory will contain explicitly the bosonic field, $\varphi$. As a result of this field, double occupancy will remain, though the energy cost will be shifted from the UV to the IR. Because the theory is Gaussian, the integration over $D_i$ can be done exactly. This is the ultimate utility of the expansion of the Hilbert space—we have isolated the high-energy physics into this Gaussian field. As a result of the dynamical term in the action, integration over $D$ will yield a theory that is frequency dependent. The frequency will enter in the combination $\omega + U$ which will appear in the denominators. Since $U$ is the largest energy scale, we expand in powers of $\omega/U$; the leading term yields the proper $\omega = 0$ low-energy theory. Since the theory is Gaussian, it suffices to complete the square in the $D$-field. To accomplish this, we define the matrix
\[
\mathcal{M}_{ij} = \delta_{ij} - \frac{t}{(\omega + U)} g_{ij} \sum_\sigma c_{i,\sigma}^\dagger c_{i,\sigma}. \tag{37}
\]

and $b_i = \sum_j b_{ij} = \sum_{j,\sigma} g_{ij} c_{j,\sigma} V_\sigma c_{i,-\sigma}$. At zero frequency the Hamiltonian is
\[
H_h^{\text{IR}} = -t \sum_{i,j,\sigma} g_{ij} a_{i,j,\sigma} c_{i,\sigma}^\dagger c_{j,\sigma} + H_{\text{int}} - \frac{1}{\beta} \text{Tr} \ln \mathcal{M},
\]
where
\[
H_{\text{int}} = - \frac{s^2}{U} \sum_{i,j} b_{ij} (M^{-1})_{ij} b_{ij} - \frac{s}{U} \sum_{i,j} \varphi_i (M^{-1})_{ij} \varphi_j - \frac{s t}{U} \sum_{i,j} \varphi_i (M^{-1})_{ij} b_{ij} + \text{h.c.}. \tag{38}
\]
which constitutes the true (IR) limit as long as the energy scale $s$ is not of order $U$. As we have retained all powers of $t/U$, equation (38) is exact. If $s \sim O(U)$ then we should also integrate out $\varphi_i$—this integration is again Gaussian and can be done exactly; one can easily check that this leads precisely back to the UV theory, the Hubbard model. Hence, the only way in which a low-energy theory of the Hubbard model exists is if the energy scale for the dynamics that $\varphi$ mediates is $O(t)$. This observation is significant because it lays plain the principal condition for the existence of an IR limit of the Hubbard model. Since the order of integrations we have performed here does not matter, integration over $\varphi_i$ in the path integral for the action corresponding to equation (38) also yields the Hubbard model. As we have shown elsewhere [10], the Wick rotation must be taken into consideration to complete the Gaussian integration over $\varphi_i$. Finally, as we have shown previously [10], the theory derived here could easily have been constructed in terms of the Hubbard operators, $\xi$ and $\eta$. This offers no further complication. In doing so, the spin–spin interaction which arises from the first term in equation (38) would have been projected onto a subspace which prohibits double occupancy. That is, it would be equivalent to the spin–spin interaction in the standard $t–J$ model. Since double occupancy still survives at low energies and is mediated by the $\varphi_i$ terms, such a rewriting of the low-energy Hamiltonian is strictly optional.

To fix the constant $s$, we determine how the electron operator transforms in the exact theory. As is standard, we add a source term to the starting Lagrangian which generates the canonical electron operator when the constraint is solved. For hole doping, the appropriate transformation that yields the canonical electron operator when the constraint is solved. However, in the IR in which we only integrate over the heavy degree of freedom, $D_i$, the electron creation operator becomes
\[
c_{i,\sigma}^\dagger \rightarrow (1 - n_{i,-\sigma}) c_{i,\sigma}^\dagger + V_\sigma \frac{t}{U} b_{i} c_{i,-\sigma} + V_\sigma \frac{s t}{U} \varphi_i c_{i,-\sigma} \tag{39}
\]
to linear order in $t/U$. This equation resembles the transformed electron operator in equation (16). In fact, the first two terms are identical. The last term in equation (16) is associated with double occupation. In equation (39), this role is played by $\varphi_i$. The demand that equations (16) and
agree requires that \( s = t \), thereby eliminating any ambiguity associated with the constraint field. Consequently, the complicated interactions appearing in equation (16) as a result of the inequivalence between \( c_{\sigma a} \) and \( f_{\sigma a} \) are replaced by a single change 2e bosonic field \( \varphi \), which generates dynamical spectral weight transfer across the Mott gap. The interaction in figure 5, corresponding to the second-order process in the term \( \psi_i^\dagger h_i \), is the key physical process that enters the dynamics at low energy. That the dynamical spectral weight transfer can be captured by a charge 2e bosonic degree of freedom is the key outcome of the exact integration of the high-energy scale. This bosonic field represents a collective excitation of the UHB and LHB. Hence, we have successfully unearthed the extra degree of freedom associated with the \( L/n_b > 1 \) physics in a doped Mott insulator.

3.3. Half-filling: Mott gap and antiferromagnetism

There is an important simplification that is obtained at half-filling that points to one of the potential uses of this theory: the dynamical mode that generates the Mott gap. Recall that our ultimate task was to integrate out the degrees of freedom far away from the chemical potential. At half-filling, both the LHB and UHB are at high energy. Hence, both must be integrated out to obtain the true low-energy theory. However, at present, we have only integrated out the UHB. Because the integration of the UHB is not equivalent to simply integrating out double occupancy, a trivial particle–hole transformation does not help us to determine how the low-energy theory should be formulated in this case.

Ultimately we have to introduce two new fermionic fields \( D \) and \( \bar{D} \) associated with the double occupancy and double holes, respectively. To proceed, we consider the Lagrangian,

\[
\mathcal{L}_{\text{UV}}^b = \int d^2 \theta \left[ iD_i^\dagger \dot{D}_i + i\bar{D}_i \dot{\bar{D}}_i^\dagger - \frac{U}{2} (D_i^\dagger D_i - \bar{D}_i \bar{D}_i) \right] + \frac{1}{2} D_i^\dagger b \bar{b} + \frac{1}{2} \bar{b} \bar{b} + h.c. + s\varphi_i^\dagger (D - \bar{D} c_i c_i^\dagger) + \bar{s}\varphi_i (\bar{D} - \bar{D} c_i c_i^\dagger) + h.c.,
\]

(40)

contains the two constraint charge \( \pm 2e \) bosonic fields, \( \varphi_i^\dagger \) (charge 2e) and \( \bar{\varphi}_i^\dagger \) (charge \(-2e\)) which enter the theory as Lagrange multipliers for the creation of double occupancy and double holes, respectively. Similar to the previous result, if we first integrate out both the bosonic fields \( \varphi_i \) and then \( D_i \), \( \bar{D}_i \), the Hubbard model is obtained and the generalized theory (equation (40)) yields the correct UV limit. However, a different IR limit is obtained if we first integrate out \( D_i \) and \( \bar{D}_i \),

\[
\mathcal{L}_{\text{IR}}^b = - (s\varphi_i + \frac{i}{t}b \bar{b}) L_i^{-1} (s\varphi_i + \frac{i}{t}b \bar{b}) + (\bar{s}\varphi_i + \frac{i}{t}b \bar{b}) L_i^{-1} (\bar{s}\varphi_i + \frac{i}{t}b \bar{b}) - (s\varphi_i - \bar{s}\varphi_i) c_i c_i^\dagger + h.c.,
\]

(41)

where \( L \pm = \frac{1}{2} \pm \frac{t}{2} \). This theory is exact and hence should contain the source of the Mott gap. This Lagrangian is invariant under the transformation \( c_{i,\sigma} \rightarrow \exp(iQ \cdot R) c_{i,\sigma}^\dagger, \varphi_i \leftrightarrow \bar{\varphi}_i \) and \( s \leftrightarrow \bar{s} \). This invariance reflects the symmetry between the double occupancy and the double hole in the system at half-filling. In contrast to the doped case as in equation (38), no \( M \) matrices appear in the IR theory at half-filling. Consequently, we arrive at a closed form for the low-energy theory at half-filling in which no bare field has dynamics. The \( b^\dagger b + \bar{b}^\dagger \bar{b} \) terms include a spin–spin interaction as well as a three-site hopping term. However, at half-filling, the three-site hopping term vanishes.

It is interesting to note that equation (41), as an exact low-energy theory of the Hubbard model, is not equivalent to the Heisenberg model. Only the \( b^\dagger b \) terms yield the Heisenberg model. Hence, we consider the separation

\[
\mathcal{L}_{\text{Mott}} = \mathcal{L}_{\text{IR}}^b + \frac{1}{4} t^2 b_i^\dagger L_i^{-1} b_i + \frac{1}{4} t^2 b_i^\dagger b_i^\dagger L_i^{-1} b_i,
\]

(42)

which explicitly removes the spin–spin term from the low-energy Lagrangian. As will be seen, the dynamics leading to the Mott gap can be constructed entirely from \( \mathcal{L}_{\text{Mott}} \). That \( \mathcal{L}_{\text{IR}}^b \) is not equivalent to the Heisenberg model is not surprising for three related reasons. First, explicit evaluation of the path integral over the new degrees of freedom must regenerate the original Hubbard model. Hence, there must be something left over once we subtract the Heisenberg terms from the low-energy theory of the Hubbard model. Second, as pointed out previously [70, 71], the Heisenberg model has a local SU(2) symmetry, not the global SU(2) symmetry of the Hubbard model. Hence, the true low-energy theory of the Hubbard model at half-filling must have other terms that break the local SU(2) and restate the global SU(2) symmetry. As we have shown previously [10], all of the terms involving the \( \varphi_i \) and \( \bar{\varphi}_i \) degrees of freedom restore the global SU(2) symmetry. Consequently, the emergence of the new local SU(2) symmetry is a function entirely of projection onto the singly occupied electron subspace. Third, at half-filling, the Hubbard model possesses a surface of zeros \([86, 87]\) of the single-particle Green function along a connected surface in momentum space, whereas the Heisenberg model does not. The absence of such a surface of zeros, the Luttinger surface, is also a function of projection. In fact, all of these three failures of the Heisenberg model arise from hard projection, which equation (16) shows is not correct even at half-filling. The non-trivial implication of the zero surface is that the real part of the Green function

\[
R_\sigma(k, 0) = - \int_{-\infty}^{\Delta_c} \frac{d\epsilon}{\epsilon} \frac{A_\sigma(k, \epsilon)}{\epsilon} = \int_{-\Delta_c}^{\Delta_c} \frac{d\epsilon}{\epsilon} \frac{A_\sigma(k, \epsilon)}{\epsilon},
\]

(43)

vanishes. Here \( A_\sigma(k, \epsilon) \) is the single-particle spectral function which we assume to have a gap of width 2\( \Delta \) symmetrically located about the chemical potential at \( \epsilon = 0 \). Because \( A(k, \epsilon) > 0 \) away from the gap, and \( \epsilon \) changes sign above and below the gap, equation (43) can pass through zero. For this state of affairs to occur, the pieces of the integral below and above the gap must be retained. Projected models which throw away the UHB fail to recover the zero surface.
3.3.1. Origin of the Mott gap. What equation (41) makes clear is that all of the information regarding the surface of zeros is now encoded into the bosonic fields $\phi_i$ and $\tilde{\phi}_i$. While numerical methods [92, 93] exist which lead to a Mott gap, there has been no explicit demonstration of the dynamical degrees of freedom that ultimately generate this gap. The bosonic degrees of freedom in equation (41) solve this problem.

To proceed, we transform to frequency and momentum space and focus on a square lattice as in the cuprates. Defining $\psi(t) = \int f \exp(\text{i}k\cdot r) \phi_i$, the energy dispersion, $\epsilon^{(k)}_0 = 4 \sum_\mu \cos(k_\mu a/2) \cos(p_\mu a)$, and the Fourier transform of $b_i$,

$$b_k = \sum_p \epsilon^{(k)}_p c_{k/2p,\uparrow}^\dagger c_{k/2-p,\downarrow},$$

we arrive at the exact working expression,

$$L^{\text{IR}}_{\text{IR}} = - \frac{|s|^2}{(\omega - U/2)} \psi_{\omega,k} \psi^\dagger_{\omega,k} + \frac{|s|^2}{(\omega + U/2)} \tilde{\psi}_{\omega,k} \tilde{\psi}^\dagger_{\omega,k}$$

$$+ \frac{U^2}{U^2 - 4\alpha s^2} b_{\omega,k} b^\dagger_{\omega,k} + (\alpha_{c_p}(\omega) \psi^\dagger_{\omega,k}$$

$$+ \sum_\omega \gamma(\omega) \psi^\dagger_{\omega-k} + (c_{k/2p,\uparrow}^\dagger c_{k/2-p,\downarrow}) + \text{h.c.},$$

(45)

for the low-energy Lagrangian where we have suppressed the implied integration over frequency and introduced the coupling constants,

$$\gamma_p^{(k)}(\omega) = \frac{U - t\epsilon^{(k)}_p - 2\omega}{U - 2\omega},$$

$$\gamma_\tilde{p}^{(k)}(\omega) = \frac{U + t\epsilon^{(k)}_p + 2\omega}{U + 2\omega},$$

(46)

which play a central role in this theory. They, in fact, will determine the spectral weight in the LHB and UHB, respectively.

Although equation (45) lacks any kinetic terms, an analysis similar to that used by Polchinski [42] in the context of Fermi liquids can be used. The key point in that argument is that all renormalizations are towards the surface in momentum space where the spectral weight resides. In a theory of weakly coupled constituents, setting the coefficient of the quadratic terms in a Lagrangian would determine their dispersion. As is evident from equation (45), the coupling constants for all the quadratic terms never vanish. All else being equal, this implies that there is no spectral weight anywhere. What we have shown [95] is that the terms in which the bosonic degrees of freedom and the fermions are coupled determine where spectral weight resides. In fact, it is these terms that should be properly regarded as quadratic. To this end, we make the transformation $\phi_{\omega} \rightarrow \sqrt{1 - 2\omega/U} \phi_{\omega}$, $\psi_{\omega} \rightarrow \sqrt{1 + 2\omega/U} \psi_{\omega}$ and $(cc)_{\omega} \rightarrow \sqrt{1 - 4\alpha^2/\omega^2} (cc)_{\omega}$ which recasts the Lagrangian as

$$L^{\text{IR}}_{\text{IR}} = \frac{\sqrt{2}|s|^2}{U} |\phi_{\omega}|^2 + \frac{2|s|^2}{U} |\tilde{\phi}_{\omega}|^2 + \frac{t^2}{U} |b_{\omega}|^2,$$

$$+ s \gamma_p^{(k)}(\omega) \psi^\dagger_{\omega,k} c_{k/2-p,\uparrow} + s \gamma_\tilde{p}^{(k)}(\omega) \tilde{\psi}_{\omega-k} c_{k/2-p,\downarrow},$$

(47)

$$+ \sum_\omega \gamma(\omega) \psi^\dagger_{\omega-k} + (c_{k/2p,\uparrow}^\dagger c_{k/2-p,\downarrow}) + \text{h.c.},$$

(48)

Figure 8. (a) Diamond-shaped surface in momentum space where the particle dispersion changes sign. (b) Turn-on of the spectral weight in the UHB and LHB as a function of energy and momentum. In the UHB, the spectral density is determined to be $\gamma_p$ while for the LHB it is governed by $\gamma_\tilde{p}$. The corresponding operators which describe the turn-on of the spectral weight are the composite excitations $\psi^{cc}$ (UHB) and $\tilde{\psi}^{cc}$ (LHB).

where

$$\gamma_p^{(k)}(\omega) = \frac{-U + t\epsilon^{(k)}_p + 2\omega}{U} \sqrt{1 + 2\omega/U},$$

$$\gamma_\tilde{p}^{(k)}(\omega) = \frac{-U + t\epsilon^{(k)}_p + 2\omega}{U} \sqrt{1 - 2\omega/U}. (50)$$

The vanishing of the coefficients $\gamma_p$ and $\gamma_\tilde{p}$ determines where the spectral weight lies. Consider initially $k = 0$ so that the dispersion simplifies to $4 \sum_\mu \cos p_\mu$. When $\omega = U/2$, $\omega = -U/2$, $\sum_\mu \cos p_\mu = 0$, defines the momentum surface along which $\gamma_p$ ($\gamma_\tilde{p}$) vanishes. This surface corresponds to the diamond $a = (ap, \pm \pi - ap)$ depicted in figure 8. These features define the centre of the LHB ($-U/2$) and UHB ($U/2$). At each momentum in the FBZ, spectral weight develops at two distinct energies. This state of affairs occurs because $\gamma_p = 0$ between $U/2 - 4\omega \leq \omega \leq U/2 + 4\omega$, whereas $(\pi, \pi)$ sits at the top of each band at $\omega = U/2 + 4\omega$ and $\omega = U/2 + 4\omega$. Consequently, at each momentum, the splitting between the turn-on of the spectral weight in the UHB and LHB is $U$. When $U > W$, each momentum state lacks spectral weight over a common range of energies. As a consequence, a hard gap opens in the spectrum. This is the Mott gap (for the composite excitations, not the electrons), and its origin is the emergence of composite excitations described by the operators $\psi^{ec}$ (UHB) and $\tilde{\psi}^{cc}$ (LHB), which we loosely interpret as bound states. As our analysis thus far is exact, we conclude that in the absence of any symmetry breaking, the coefficients $\gamma_p$ and $\gamma_\tilde{p}$ determine the dispersion for the excitations that comprise the heretofore undefined [47] UHB and LHB. Inclusion of the centre-of-mass momentum $k$ simply shifts the value of the momentum at which the dispersion changes sign, thereby keeping the Mott gap intact.

Thus far, we have established the Mott gap in terms of a set of composite excitations. Ultimately, we would like to know
Performing the Wick rotation, \(\phi\) implies that we can treat \(\varphi\) as a spatially homogeneous field. \textit{A priori}, gradient terms with respect to \(\varphi\) are possible. However, such terms are absent from the exact low-energy theory as such terms would indicate the presence of a freely propagating bosonic degree of freedom at half-filling. It is precisely because such terms are absent that we were able to identify that the only propagating degrees of freedom at half-filling are possible. However, such terms are absent from the exact spectral function in terms of the original electron degrees of freedom. At \(\beta = 0\), it lies in the UHB whereas at \((\pi, \pi)\) the gap arises from the dynamics of the two charge \(2e\) bosonic fields. This is the first time that the Mott gap has been derived dynamically, in particular by a collective degree of freedom of the LHB and UHB. Relative to the gap in the spectrum for the composite excitations that diagonalize the fermion-boson terms in equation (49), the gap in the electron spectrum is larger. This is not surprising as the bare electrons do not have unit overlap with the composite excitations. In addition, the momentum dependence of the spectral function is identical to that obtained by dynamical mean-field calculations [92], thereby lending credence to such a cluster [94].

An open question that this analysis provokes is whether or not the turn-on of the spectral weight in a Mott insulator is governed by a fixed point. If so, then in analogy of the Fermi liquid analysis [42], all the interactions except those that govern the turn-on of the spectral weight should be irrelevant. That is, the \(\psi_c\) and \(\bar{\psi}_c\) terms represent a natural theory. Indeed, the analysis presented above demonstrates that the spin–spin term has nothing to do with the turn-on of the spectral weight, as foreshadowed by Mott [1]. Namely, the gap in the spectrum at half-filling is independent of ordering. While a naive scaling analysis suggests that the spin–spin interaction is indeed subdominant, we have been unable to compute the \(\beta\)-function to show that a true fixed point underlies the physics at half-filling. Such a computation stands as a true challenge for Mottness.

Nonetheless, antiferromagnetism with an ordering wavevector of \((\pi, \pi)\) can also be understood within this formalism. Within this theory, there is a natural candidate for the antiferromagnetic order parameter, namely \(B_{ij} = \langle \hat{S}_{ij}\hat{\psi}^\dagger_c c_i \hat{\psi}_c \rangle\). The vacuum expectation value of this quantity is clearly non-zero as it is easily obtained from a functional derivative of the partition function with respect to \(\gamma_{\beta}\). That is, this is the relevant order parameter instead of the traditional one follows from the fact that the spin–spin interaction and all higher-order operators contained in \(\langle b^\dagger b \rangle\) are at least proportional to \(a^\dagger a\) (\(a\) the lattice constant) and hence are subdominant to the composite terms. Hence, a non-traditional order parameter must govern the turn-on of antiferromagnetism. We advocate that \(B_{ij}\) characterizes the antiferromagnet that describes the strong-coupling limit of the LHB and UHB.
the Hubbard model and as a consequence the insulating state of the cuprates. An antiferromagnet of this kind has no continuity with the antiferromagnet at weak coupling because it is mediated by the collective mode \( \varphi \) or \( \bar{\varphi} \). Hence, both the Mott gap and subsequent antiferromagnetic order emerge from composite excitations that have no counterpart in the original UV Lagrangian but only become apparent in a proper low-energy theory in which the high-energy degrees of freedom are explicitly integrated out. Away from half-filling, a similar state of affairs is obtained.

4. Hole doping: experimental consequences

The charge 2\( e \) boson has much to tell us about the normal state of a doped Mott insulator. Here we compute the electron spectral function, the specific heat, the thermal conductivity, the optical conductivity as well as the dielectric function. In each of these, the charge 2\( e \) boson produces a distinct signature that accounts for the anomalies of the doped state of a Mott insulator.

4.1. Spectral function: pseudogap

Since we have demonstrated that \( \mathcal{L}_{\text{Mott}} \) captures the strong-coupling physics of the Mott insulating state, we focus on the evolution of this theory with doping. The lack of any gradient terms in the action with respect to the bosonic fields and the absence of any bare dynamics associated with \( \varphi_i \) suggests that we can treat \( \varphi_i \) as a homogeneous field. Further, since we are not interested in the dynamics on the Mott scale, we treat \( \varphi \) as a static field. Its sole role is to mix the subsectors which differ in the number of doubly occupied sites. Consequently, our results are valid provided that \( \omega < U \) and \( U \gg t \). Under these assumptions, the single-particle electron Green function

\[
G(k, \omega) = \frac{-i\text{FT}[Tc_i(t)c_j^\dagger(0)]}{\omega - \epsilon_k}\,
\]

can be calculated rigorously in the path-integral formalism as

\[
G(k, \omega) = \frac{-i\text{FT} \int [D\varphi_i^\dagger][D\varphi_i] \int [Dc_i^\dagger][Dc_i]c_i(t)c_j^\dagger(0) \exp \left\{-\int \mathcal{L}[c, \varphi] \text{d}t \right\}}{\omega - \epsilon_k},
\]

where \( \text{FT} \) refers to the Fourier transform and \( T \) is the time-ordering operation. The explicit spin–spin term is not contained in \( \mathcal{L}_{\text{Mott}} \). This term will also be dropped in the doped case because even in this limit, the spin–spin term is subdominant (in a naive continuum limit sense) to the other interactions in \( \mathcal{L} \). This state of affairs arises because the spin–spin term in \( b^\dagger b \) contains four spatial derivatives, whereas the \( \varphi^\dagger b \) term contains only two. As a result, all of the physics we present below is associated with the charge rather than the spin degrees of freedom. The continuity of the analysis with that of the half-filled system raises the question that perhaps a fixed point at half-filling persists to finite doping as well in which only the fermion-boson terms are relevant. While our analysis is highly suggestive that such a state of affairs is obtained, the possible existence of such a fixed point remains a conjecture as of this writing.

To proceed, we will organize the calculation of \( G(k, \omega) \) by first integrating out the fermions (holding \( \varphi \) fixed)

\[
G(k, \omega) = \int [D\varphi^\dagger][D\varphi] \text{iFT} \left\{ \left( \int [Dc_i^\dagger][Dc_i]c_i(t)c_j^\dagger(0) \exp \left\{-\int \mathcal{L}[c, \varphi] \text{d}t \right\} \right) \right\},
\]

where now

\[
\mathcal{L} = \sum_{i\sigma} \left( 1 - n_{i\sigma} \right) c_{i\sigma}^\dagger c_{i\sigma} - \left( 2\mu + \frac{\omega^2}{U} \right) \varphi^\dagger \varphi - \sum_{k\sigma} (g_1 \dot{\alpha}_k + \mu) c_{k\sigma}^\dagger c_{k\sigma} + sq^\dagger \sum_{k} \left( 1 - \frac{2t}{U} \right) c_{-k\dagger} c_{k\dagger} + \text{c.c.}
\]

The effective Lagrangian can be diagonalized and written in terms of a collection of Bogoliubov quasiparticles [11]. The remaining \( \varphi \) integration can then be done numerically to obtain the spectral function.

The spectral functions in figures 10 and 11 exhibit four key features. First, there is a low-energy kink in the electron dispersion that is independent of doping. The low-energy kink occurs at roughly \( 0.2t \approx 100 \text{ meV} \). By treating the mass term for the boson as a variable parameter, we verified that the low-energy kink is determined by the bare mass. In the effective low-energy theory, the bare mass is \( r^2/U \). This mass is independent of doping. Experimentally, the low-energy kink [96] does not change with doping. Consequently, the charge 2\( e \) bosonic field provides a natural mechanism for the kink that is distinct from the phonon schemes that have been proposed [96].

Second, a high-energy kink appears at roughly \( 0.5t \approx 250 \text{ meV} \) which closely resembles the experimental kink at 300 meV [97]. Cluster [98] and exact diagonalization methods [99] also find a high-energy kink. At sufficiently high doping (see figures 11(a) and (b)), the high-energy kink disappears. Third, the electron dispersion bifurcates at the second kink. This is precisely the behaviour that is seen experimentally [97]. The energy difference between the two branches is maximum at \( \omega = 0 \) as is seen experimentally. A computation of the spectral function at \( U = 20t \) and \( n = 0.9 \) reveals that the dispersion as well as the bifurcation still persists. Further, the magnitude of the splitting does not change, indicating that the energy scale for the bifurcation and the maximum energy splitting are set by \( t \) and not \( U \). The origin of the two branches is captured in figure 10(c). The two branches below the chemical potential correspond to the standard band in the LHB (filled squares in figure 10(c)) on which \( \varphi \) vanishes and a branch on which \( \varphi \neq 0 \) (filled circles in figure 10(c)). Simulations on the Hubbard model clearly resolve either the low-energy feature [92–94] or the high-energy kink [98, 99]. In the studies showing the high-energy kink, the low-energy feature is not discernible [98, 99]. What is new here is that both features (but with drastically different intensities as is seen experimentally) are captured. The two branches indicate that there are two local maxima.
in the integrand in equation (58), a feature not captured by a saddle-point approximation. Above the chemical potential only one branch survives. The split electron dispersion below the chemical potential is consistent with the composite nature of the electron operator dictated by equation (39). At low energies, the electron is a linear superposition of two states, one the standard band in the LHB described by excitations of the form \( c_{i\sigma}^\dagger (1 - n_{i\bar{\sigma}}) \) and the other a composite excitation consisting of a bound hole and the charge \( 2e \) boson, \( c_{i\bar{\sigma}} \phi_i^\dagger \). The former contributes to the static part of the spectral weight transfer (2x) while the new charge \( e \) excitation gives rise to the dynamical contribution to the spectral weight transfer. Because the new charge \( e \) state is strongly dependent on the hopping, it should disperse as is evident from figure 11 and also confirmed experimentally [97].

The formation of the composite excitation, \( c_{i\bar{\sigma}} \phi_i^\dagger \), is the new dynamical degree of freedom in the doped theory. This dynamical degree of freedom has no counterpart in the UV scale. Such a binding of a hole and the charge \( 2e \) bosonic field leads to a pseudogap at the chemical potential, as evidenced by the absence of spectral weight at the chemical potential for both \( n = 0.9 \) and \( n = 0.8 \). A non-zero spectral weight resides at the chemical potential in the heavily overdoped regime, \( n = 0.4 \), consistent with the vanishing of the pseudogap beyond a critical doping away from half-filling. Because the density of states vanishes at the chemical potential, the electrical resistivity diverges as \( T \to 0 \). Such a divergence is shown in figure 12(a) and is consistent with our previous calculations of the dc resistivity using a local dynamical cluster method [78]. In the absence of the boson (figure 12(b)), localization ceases. Although this calculation does not constitute a proof, it is consistent with localization induced by the formation of the bound composite excitation, \( c_{i\bar{\sigma}} \phi_i^\dagger \). This state of affairs is obtained because the boson has no bare dynamics. It may acquire dynamics at \( O(t^3/U^2) \) as can be seen by expanding the \( M \) matrix in equation (38).

Such bound-state formation makes plain how the strong-coupling regime of a doped Mott insulator depends on the
the divergence of the resistivity as \( T \rightarrow 0 \). This suggests that it is the strong binding between the fermionic and bosonic degrees of freedom that ultimately leads to the insulating behaviour in the normal state of a doped Mott insulator.

As is clear from figure 15, Naively, doped Mott insulators are expected to either have a far-IR or an UV or UHB scale absorption. Hence, one of the true surprises in the optical response of the cuprates is the nature of the underlying fixed point remains an open problem.

4.2. Mid-infrared band

Naively, doped Mott insulators are expected to either have a far-IR or an UV or UHB scale absorption. Hence, one of the true surprises in the optical response of the cuprates is the MIB. While many mechanisms have been proposed [41], no explanation has risen to the fore. A hint as to the origin of this band is that the intensity in the MIB increases with doping at the expense of spectral weight at a high energy and the energy scale for the peak in the MIB is the hopping matrix element \( t \). Since the MIB arises from the high-energy scale, the current theory which accurately integrates out the high-energy degrees of freedom should capture this physics. We work in the non-crossing approximation,

\[
\sigma_{\text{xx}}(\omega) = 2\pi e^2 \int d^2k \int d\omega'(2\pi sin k_x)^2 \times \left(-\frac{f(\omega') - f(\omega' + \omega)}{\omega}\right) A(\omega + \omega', k)A(\omega', k),
\]

to the Kubo formula for the conductivity where \( f(\omega) \) is the Fermi distribution function and \( A(\omega, k) \) is the spectral function. In our treatment, the vertex corrections arise solely from the interactions with the bosonic degrees of freedom. Since the boson acquires dynamics only through electron motion and the leading such term is \( O(t^3/U^2) \), the treatment here should suffice to provide the leading behaviour of the optical conductivity. Shown in figure 14 is the optical conductivity which peaks at \( \omega_{\text{max}} \approx 0.5t \) forming the MIB. We have substracted the Drude weight at \( \omega = 0 \) to focus sharply on the MIB. As the inset indicates, \( \omega_{\text{max}} \) is an increasing function of the electron filling \( n \), whereas the integrated weight

\[
N_{\text{eff}} = \frac{2m^*}{\pi e^2} \int_0^{\Omega_c} \sigma(\omega)d\omega
\]

decreases. However, \( N_{\text{eff}} \) does not vanish at half-filling indicating that the mechanism that causes the mid-IR is evident even in the Mott state. We set the integration cutoff to \( \Omega_c = 2t = 1/m^* \). The magnitude and filling dependence of \( \Omega_{\text{max}} \) are all consistent with that of the MIB in the optical conductivity in the cuprates [36, 37, 39–41]. We determined what sets the scale for the MIB by studying its evolution as a function of \( U \). As is clear from figure 15, \( \omega_{\text{max}} \) is set essentially by the hopping matrix element \( t \) and depends only weakly on \( J \). The physical processes that determine this physics.
are determined by the coupled boson-Fermi terms in the low-energy theory. The $\psi_i \psi_i$ term has a constant of $t$ whereas the $\psi_i \bar{b}_i$ scales as $t^2/U$. Together both terms give rise to a MIB band that scales as $\omega_{max}/t \approx 0.8 - 2.21 t/U$ (see the inset of figure 15). Since $t/U \approx O(0.1)$ for the cuprates, the first term dominates and the MIB is determined predominantly by the hopping matrix element $t$. Within the interpretation that $\varphi$ represents a bound state between a doubly occupied site and a hole, second-order perturbation theory with the $\psi_i \bar{b}_i$ term mediates the process shown in figure 5. It is the resonance between these two states that results in the MIB. Interestingly, this resonance persists even at half-filling and hence the non-vanishing of $N_{eff}$ at half-filling is not evidence that the cuprates are not doped Mott insulators as has been recently claimed [84].

As the physics in figure 5 is not present in projective models which prohibit double occupancy in the Hubbard basis (not simply the transformed fermion basis of the $t-J$ model), it is instructive to see what calculations of the optical conductivity in the $t-J$ model reveal. All existing calculations [40, 77, 82, 83] on the $t-J$ model find that the MIB scales as $J$. In some of these calculations, superconductivity is needed to induce an MIB [82] also at an energy scale of $J$. In others, phonons are invoked to overcome the failure of the hard-projected $t-J$ model to yield a MIB. Experimentally [36, 37, 41], it is clear that the MIB is set by the $t$ scale rather than $J$. In fact, since the MIB grows at the expense of spectral weight in the UHB, it is not surprising that the $t-J$ model cannot describe this physics as first pointed out by Uchida et al [37]. The physical mechanism we have identified here, figure 5 clearly derives from the high-energy scale, has the correct energy dependence and hence satisfies the key experimental constraints on the origin of the MIB. Since the physics in figure 5 is crucial to the mid-IR, it is not surprising that single-site analysis [84] fails to obtain a non-zero intercept in the extreme Mott limit. The non-zero intercept of $N_{eff}$ is a consequence of Mottness and appears to be seen experimentally in a wide range of cuprates [36, 103, 104, 105].

4.3. Dielectric function: experimental prediction

We have shown thus far that there are two branches in the electronic spectral function below the chemical potential. Such physics is explained by the dynamical formation of a new composite excitation, representing a bound state, consisting of a bound hole and a charge $2e$ boson, $\bar{\sigma} \sigma_i \bar{\sigma}$. We demonstrated that for the MIB in the optical conductivity such an excitation also appears. Such composite charge excitations should show up in response functions which are sensitive to all the charge degrees of freedom, for example, the energy loss function, $\Im(\epsilon(\omega, q))$, where $\epsilon(\omega, q)$ is the dielectric function. We show here that this is the case.

To this end, we calculate the inverse dielectric function, $\Im \frac{1}{\epsilon(\omega, q)} = \pi U \sum_p \int d\omega'(f(\omega') - f(\omega + \omega')) \times A(\omega + \omega', p + q) A(\omega', p)$, using the non-crossing approximation discussed earlier. Our results are shown in figure 16 for $n = 0.9$ and $n = 0.6$ for $q$ along the diagonal. Two features are distinct. First, there is a broad band (red arrow in figure 16) with the width of order $t$ that disperses with $q$, terminating when $q \approx (\pi, \pi)$. Physically, the sharp peak represents a quasiparticle excitation of the composite object, $\bar{\sigma} \sigma_i \bar{\sigma}$, the charge $2e$ boson and a hole. Therefore, we predict that if this new composite charge excitation, $\bar{\sigma} \sigma_i \bar{\sigma}$, is a real physical entity, as it seems to
be, it will give rise to a sharp peak in addition to the particle–hole continuum in the inverse dielectric function. Since this function has not been measured at present, our work here represents a prediction. Electron-energy loss spectroscopy can be used to measure the inverse dielectric function. Our key prediction is that momentum-dependent scattering should reveal a sharp peak that appears at low energy in a doped Mott insulator. We have checked numerically the weight under the peaks in the inverse dielectric function and the sharp peak is important. Hence, the new charge $e$ particle we have identified here should be experimentally observable. The two dispersing particle–hole features found here are distinct from a similar feature in stripe models [106]. In such models the second branch [106] has vanishing weight whereas in the current model we have identified LHB leaving the new state mediated by spin terms renormalize the standard fermionic branch in the Mott insulators is dominated by dynamical degrees of freedom. As we have focused entirely on the bosonic degree of freedom and not on the contribution from the spin–spin interaction terms, we have overestimated the kinetic energy. Such terms do not affect the pseudogap found here though they do change the doping dependence.

4.4. Heat conductivity and heat capacity

Loram and collaborators [107] have shown from their extensive measurements that the heat capacity in the cuprates in the normal state scales as $T^2$. It is a trivial exercise to show that such a temperature dependence requires a V-shaped gap density of states as a function of energy. The slope of the density of states in the vicinity of the chemical potential determines the coefficient of the $T^2$ term. Because the slope of the density of states decreases as the pseudogap closes, the magnitude of the $T^2$ term should diminish as the doping increases. As we showed in the previous section, the boson creates a pseudogap. The energy dependence of the gap is shown in the inset of figure 17. A linear dependence on energy is apparent. We calculated the heat capacity shown in figure 17(a) via the relationship $C_v = \frac{\partial^2 E}{\partial T^2}$, where the internal energy, $E$, is

$$E = \int d\omega D(\omega)\omega f(\omega)$$

and $D(\omega) = \sum_n A(\omega, n)$. As expected, the temperature dependence is quadratic in the doping regime where the pseudogap is present as is seen experimentally [107]. As it is the boson that underlies the pseudogap, it is the efficient cause of the $T^2$ dependence of the heat capacity. In our theory, the steeper slope occurs at smaller doping which gives rise to the largest heat capacity at half filling. This doping dependence of the heat capacity seems to contradict the experimental observations [107]. A key in determining the magnitude of the heat capacity is the spin degrees of freedom. As we have focused entirely on the bosonic degree of freedom and not on the contribution from the spin–spin interaction terms, we have overestimated the kinetic energy. Such terms do not affect the pseudogap found here though they do change the doping dependence [77]. From equation (39) it is clear that the spin–spin terms renormalize the standard fermionic branch in the LHB leaving the new state mediated by $\phi_i$ untouched.

Additionally, the thermal conductivity, $\tau(T)$, can be calculated using the Kubo formula in non-crossing approximation,

$$\tau(T) = \frac{e}{4k_B T} \sum_k \int \frac{d\omega}{2\pi} (\nu_k)^2 \omega^2 \left(-\frac{\partial f(\omega)}{\partial \omega}\right) A(k, \omega)^2.$$ 

The thermal conductivity shown in figure 17 scales as $T^2$ which is identical to that of the heat capacity. However, the system exhibits a larger thermal conductivity as the doping increases in contrast to the heat capacity which decreases as the doping increases. Physically, this signifies that the carriers are more mobile as the doping increases.

4.5. T-linear resistivity

A key theme of this review is that the normal state of doped Mott insulators is dominated by dynamical degrees of freedom that could not have been deduced from the UV physics. Further, as stated in the introduction, the correct theory of the pseudogap phase should also explain the $T$-linear resistivity. The standard explanation [108] attributes $T$-linear resistivity to quantum criticality. However, one of us has recently shown [108] that under three general assumptions, (1) one-parameter
in the critical region, the energy to create a boson vanishes as shown in figure 18 and hence the resistivity arising from electron–boson scattering should be linear in temperature. This mechanism is robust (assuming the unbound boson has classical dynamics) as it relies solely on the vanishing of the boson energy at criticality and not on the form of the coupling.

To the right of the quantum critical point, standard electron–electron interactions dominate and Fermi liquid behaviour is obtained. In this scenario, the quantum critical point coincides with the termination of the pseudogap phase, or equivalently with the unbinding of the bosonic degrees of freedom. Since it is the bound state of the boson that creates the new charge $e$ state giving rise to $L/n_b > 1$ and this state is generated as a result of dynamical spectral weight transfer, the $T^*$ line defines the temperature below which dynamical spectral weight transfer contributes to the LESW. Consequently, the mechanism proposed here is experimentally testable. Simply repeat the x-ray K-edge experiments presented in figure 3 below and above the $T^*$ line. Above $T^*$ the integrated weight should be $2x$ whereas below it should exceed $2x$.

### 4.6. Towards superconductivity

Our emphasis thus far has been on identifying a unifying principle for the normal state of the cuprates. As we have seen, strong correlations mediate new composite excitations made partly out of the emergent charge $2e$ boson that results by exactly integrating out the high-energy scale in the Hubbard model. An important question concerns the relevance of the physics we have identified here to the superconducting phase. Equivalently, what role, if any, does dynamical spectral weight transfer play in the superconducting state? We answer this question by focusing on a correlate of high-temperature superconductivity. As the phase diagram indicates, the superconducting region is roughly dome shaped. Why it is ‘dome’ shaped is not known. To offer some insight into this puzzle, we focus on an experimental quantity which exhibits an abrupt sign change near optimal doping. As shown in figure 19, at a doping level corresponding to the highest superconducting transition temperature, optimal doping, the thermopower vanishes [110] for a wide range of cuprates. Consequently, the sign change of $S$ occurs at the doping value defining the top of the ‘dome’. While this might be an accident, the fact that the thermopower vanishes at the same doping level for most cuprates indicates that the reason might have something to do with the superconducting mechanism.

The thermopower measures the thermoelectric voltage induced across a material in response to an applied temperature gradient. Microscopically, the thermopower is a measure of the entropy per charge carrier. Further, it reveals the nature of the dominant charge carriers, being positive for holes and negative for electrons. Should the entropy per carrier be identical for particles and holes, the thermopower vanishes. Consider hole doping a Mott insulator. Because transport occurs in the LHB, naively a vanishing of the thermopower [112] is expected whenever the number of states above and below the chemical potential is equal. In the atomic limit, this corresponds to the
condition $2x = 1 - x$, the solution of which is $x_{\text{crit}} = 1/3$. This result is corroborated by the large $U$ limit of the thermopower,

$$S = -\frac{k_B}{e} \ln \frac{2x}{1-x},$$  \hspace{1cm} (63)

computed by Beni [113] roughly 20 years before spectral weight transfer was discovered. Since $2x$ and $1 - x$ are the exact values for the electron addition and removal states, respectively, in the atomic limit, it is easy to see that the logarithm is precisely the entropy per carrier. The logarithm vanishes at $x_{\text{crit}} = 1/3$, which is the single particle–hole symmetric condition for the LHB in the atomic limit. Finite $t/U$ corrections will increase $L$ and as a result decrease $x_{\text{crit}}$. However, this is not all. The spectral function is strongly momentum dependent when $t/U \neq 0$. As a result, strict particle–hole symmetry is not needed to make the thermopower (or even the Hall coefficient) vanish as can be seen directly from the exact [114] expression. Both of these effects conspire to move the doping level at which the thermopower vanishes significantly below the atomic limit of $x = 1/3$. As this change is made entirely from the $t/U$ corrections to the thermopower, it is the dynamical spectral weight transfer that is ultimately responsible for the precise value of doping at which the thermopower vanishes in the cuprates. Consequently, the dynamical spectral weight transfer plays a role in maximizing $T_c$. As a result, superconductivity in the cuprates is determined fundamentally by the mixing between the high- and low-energy scales in a doped Mott insulator. The collective degree of freedom $\varphi$ which results from the spectral weight transfer is consequently central to the superconducting mechanism.

Optical conductivity experiments [115–117] certainly have shown plainly that the onset of superconductivity results in a decrease in the spectral weight in the UHB. It would seem then that the ultimate solution to superconductivity hinges on the precise dynamics of the collective charge $2e$ boson that we have shown to exist in the exact low-energy theory of a doped Mott insulator.

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Figure 19. (a) Universal behaviour of the thermoelectric power [110] (290 K) as a function of planar hole density ($P_{pl}$), for various families of hole-doped cuprates. All exhibit a sign change at $P_{pl} = 0.23$. Above the solid-bold horizontal line, the thermopower obeys the functional form, $S_{\text{emp}}(P_{pl}) = 392 \exp(-19.7P_{pl})$ for 0.01 $< P_{pl} < 0.21$. Below the solid-bold horizontal line, $S_{\text{emp}}(P_{pl}) = 40.47 - 163.4P_{pl}$ for 0.21 $< P_{pl} < 0.34$. These functional forms were used [110] to determine the hole doping levels for all the cuprates rather than the widely used empirical formula [111] $1 - T_c/T_{\text{max}} = 82.6(x - 0.16)^2$ which artificially fixes the optimal doping level of all cuprates to be 0.16. The thermopower scale is unbiased in this regard and has been shown [110] to corroborate independent measures of the doping level even in Y123 and Tl-2201 in which it is the oxygen content that determines the doping level. (b) Maximum transition temperature as a function of the planar hole density using the thermopower scale to determine the doping level. Except for three single-layer materials, the vanishing of the thermopower coincides with the doping level at which the transition temperature is maximized.
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