Origin of the Mott Gap

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We show exactly that the only charged excitations that exist in the strong-coupling limit of the half-filled Hubbard model are gapped composite excitations generated by the dynamics of the charge $2e$ boson that appears upon explicit integration of the high-energy scale. At every momentum, such excitations have non-zero spectral weight at two distinct energy scales separated by the on-site repulsion $U$. The result is a gap in the spectrum for the composite excitations accompanied by a discontinuous vanishing of the density of states at the chemical potential when $U > 8t$ exceeds the bandwidth. Consequently, we resolve the long-standing problem of the cause of the charge gap in a half-filled band in the absence of symmetry breaking.

I. INTRODUCTION

In 1949, Sir Neville Mott\textsuperscript{1} proposed that transition metal oxides with half-filled bands possess a gap in the single-particle spectrum that is due entirely to the energy cost for placing two electrons on the same site. This explanation is clearly incomplete because even in the simplest model of a Mott insulator, the Hubbard model, none of the eigenstates have definite local occupation. Consequently, the charge gap in transition metal oxides does not have the simple interpretation as the energy gap between bands that represent electron motion among singly and doubly-occupied sites. What then are the degrees of freedom that account for the Mott gap in the half-filling, the charge gap in transition metal oxides does not have the simple interpretation as the energy gap between bands that represent electron motion among singly and doubly-occupied sites. What then are the degrees of freedom that lead to a turn-on of any kind. Second, we identify two dispersing degrees of freedom or composite excitations which lead to a turn-on of any kind. Second, we identify two dispersing degrees of freedom that are being gapped? Because mobile doubly occupied sites. What then are the degrees of freedom that are being gapped? Because mobile doubly occupied sites would be inconsistent with an insulating state, some\textsuperscript{2,3} have argued that in a Mott insulator, double occupancy is localized whereas in the metal doubly occupied sites form an itinerant fluid. Such localization requires a dynamical degree of freedom which has not been enunciated despite numerous simulations which display a Mott gap.\textsuperscript{5} In fact, the origin of the dynamical degree of freedom that generates the elementary excitations responsible for the Mott gap is the essential problem of Mottness. Knowledge of this degree of freedom and the excitations it mediates are crucial to the physics of high-temperature copper-oxide superconductors as they are doped Mott insulators. Indeed, the extreme difficulty in unearthing the mechanism for the localization of double occupancy led Laughlin\textsuperscript{6} to suggest that charge gaps in homogeneous time-reversal systems are impossible.

In this paper, we construct explicitly the dynamical degrees of freedom that account for the Mott gap in the absence of any symmetry breaking. There are two key elements to our proof. First, we show that the exact low-energy theory for a half-filled band described by the Hubbard model has no bare propagating degrees of freedom of any kind. Second, we identify two dispersing degrees of freedom or composite excitations which lead to a turn-on of the spectral weight centered at $\pm U/2$. If $U > 8t$, the composite excitations are orthogonal to one another in that the spectral weight they produce never exists in the same energy range. The result is a gap in the spectrum. In terms of the UV variables, the composite excitations represent bound states involving double occupancy or double holes and are the fundamental excitations that define the lower and upper Hubbard bands.

II. LOW-ENERGY ACTION

As pointed out by Laughlin\textsuperscript{6}, no one has identified the band structure of the elementary particles whose spectrum becomes gapped at half-filling. In this paper, we show that this can be done by utilizing the method we have recently developed to explicitly integrate out the degrees of freedom far from the chemical potential in the Hubbard model. We consider the Hubbard model on a square lattice in the limit in which the bands are well separated, that is, the on-site interaction $U$ exceeds the bandwidth, $W = 8t$, the hopping matrix element. At half-filling, the chemical potential lies in the Mott gap. As a consequence, both the degrees of freedom above and below the chemical potential must be integrated out if one wishes to construct a low-energy theory of the Mott insulator. This can be done by introducing two new fermionic fields which when constrained appropriately will correspond to the creation of double occupancy, $D_1$, and double holes, $\bar{D}_i$. In Lorentzian signature, the Lagrangian which makes this integration possible,

$$L_{UV}^\text{eff} = \int d^2 \theta \left[ i D^\dagger D - i \bar{D}^\dagger \bar{D} - \frac{U}{2} (D^\dagger D - \bar{D}^\dagger \bar{D}) + \frac{t}{2} D^\dagger \theta b + \frac{t}{2} \bar{D} \theta b + h.c. + s \theta \varphi^\dagger (D - \theta c_\uparrow c_\downarrow) + \bar{s} \bar{\theta} \bar{\varphi}^\dagger (\bar{D} - \theta \bar{c}_\uparrow \bar{c}_\downarrow) + h.c. \right],$$

(1)

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. Mathematically, they are analogous to $\sigma$ in the non-linear sigma model. All operators in Eq. (1) have the same site index which is summed over. The Lagrangian also contains the integration, $d^2 \theta$, over the complex Grassman, $\theta$, and $b_i = \sum_j g_{ij} c_i \sigma V_{\sigma} c_{j,-\sigma}$ is a bond-singlet operator where $c_i^\dagger$ creates a fermion on site $i$ with spin $\sigma$, $g_{ij} = 1$ iff $i$...
and \( j \) are nearest neighbours, \( V_1 = -V_1 = 1 \) and \( s \) and \( s \) are constants appearing in the constraint which have units of energy. The theory (1) is completely equivalent to the Hubbard model. That this is so can be seen by integrating out \( \varphi_i \) and \( \varphi_i \) followed immediately by an integration over \( D_i \) and \( \bar{D}_i \) in the partition function,

\[
Z = \int [Dc \ Dc^\dagger \ DD \ DD^\dagger \ D\varphi \ D\varphi^\dagger] \exp - \int_0^t L_{\text{UV}}^{\text{ald}} dt . \tag{2}
\]

The \( \varphi \) and \( \bar{\varphi} \) integrations (over the real and imaginary parts) are precisely a representation of (a series of) \( \delta \)-functions of the form,

\[
\delta \left( \int d\theta D_i - \int d\theta \bar{c}_{i,\sigma} c_{i,\sigma} \right) , \tag{3}
\]

and

\[
\delta \left( \int d\theta \bar{D}_i - \int d\theta \bar{c}_{i,\sigma}^\dagger c_{i,\sigma}^\dagger \right) . \tag{4}
\]

We must now integrate over the \( D_i \) and and \( \bar{D}_i \). The dynamical terms yield,

\[
\int d^2 \theta \bar{\theta} \left[ c_{i,\sigma}^\dagger \partial_\theta \left( c_{i,\sigma} c_{i+1,\sigma} \right) - \partial_\theta \left( c_{i,\sigma} c_{i,\sigma} + c_{i+1,\sigma} c_{i+1,\sigma} \right) \right] \\
= \int d^2 \theta \bar{\theta} \sum_\sigma \partial_\theta c_{i,\sigma}^\dagger \partial_\theta c_{i,\sigma}^\dagger . \tag{5}
\]

The terms proportional to \( U \) lead to

\[
\frac{U}{2} \int d^2 \theta \left[ \bar{\theta} \eta_{i,\sigma} c_{i,\sigma}^\dagger c_{i,\sigma} - \bar{\theta} \eta_{i,\sigma} c_{i,\sigma}^\dagger c_{i,\sigma} + c_{i,\sigma} \right] \\
= \frac{U}{2} \int d^2 \theta \bar{\theta} \eta_{i,\sigma} n_{i,\sigma} c_{i,\sigma} + c_{i,\sigma} + h.c. . \tag{6}
\]

The standard interaction term in the Hubbard model in the Lorentzian signature. Finally, the terms proportional to \( V_\sigma \) yield

\[
\int d^2 \theta \bar{\theta} \sum_\sigma g_{ij} \left[ c_{i,\sigma} \bar{c}_{j,\sigma} c_{j+1,\sigma} c_{j+1,\sigma} - c_{i,\sigma} c_{j,\sigma} c_{j,\sigma} \right] + h.c. \\
= \int d^2 \theta \bar{\theta} \sum_\sigma g_{ij} n_{j,\sigma} c_{i,\sigma} + c_{i,\sigma} + h.c. . \tag{7}
\]

after the \( \varphi \) and \( D_i \) integrations, whereas the \( \bar{\varphi} \) and \( \bar{D}_i \) integrations yield the same final result except \( n_{j,\sigma} \) is replaced by \((1 - n_{j,\sigma})\). Hence, these terms add together to generate the kinetic term in the Hubbard model. Adding all these results together leads to \( \int d^2 \theta \bar{\theta} L_{\text{HUBB}} = L_{\text{HUBB}} \) for the Hubbard model. Hence, Eq. (1) is an equivalent way of writing the Hubbard model in which two canonical fermions describe the physics on the \( U \)-scale.

Since the physics on the \( U \)-scale has been cleanly identified, the exact low-energy theory,

\[
L_{\text{IR}}^{4f} = - \left( s \varphi^\dagger + \frac{1}{2} t b^\dagger \right) L_{\text{UV}}^{4f} \left( s \varphi + \frac{1}{2} t b \right) \\
+ \left( s^\dagger \bar{\varphi} + \frac{1}{2} t \bar{b}^\dagger \right) L_{\text{UV}}^{4f} \left( s^\dagger \bar{\varphi} + \frac{1}{2} t \bar{b} \right) \\
- \left( s \varphi^\dagger - s^\dagger \bar{\varphi} \right) c_j c_{j+1} + h.c. , \tag{8}
\]

can be constructed by explicitly integrating out the massive fields \( D_i \) and \( \bar{D}_i \). Here, \( L_{\text{UV}}^{4f} = \frac{1}{2} \bar{b}^\dagger \bar{b} \left( \partial_\varphi - \frac{1}{2} \varphi \right) \). This integration is straightforward as it is strictly Gaussian. It is important to appreciate that the resulting theory is exact, and completely equivalent to the Hubbard model.

We would like to understand the physics of this model. It is clear from this presentation that the bosonic and fermionic fields do not represent weakly coupled degrees of freedom, as there are no quadratic terms in \( c_{i,\sigma} \) and the would-be boson propagators have no poles. Presumably, one would like to find an appropriate continuum limit, but the identification of the correct continuum limit is difficult. What we will find here is that Eq. (8) is a much better theory to work with than the Hubbard model, as it contains the seeds of the degrees of freedom that emerge at low energies. The Hubbard model contains only strongly interacting electrons, and any continuum limit that might be considered would presumably miss any collective degrees of freedom.

To proceed, we begin by recalling what happens in the free fermion Landau theory. There, the continuum limit is trivial to take, as we just scale towards the free fermion UV fixed point. The appropriate renormalization group flow is obtained\(^{15}\) by scaling momenta towards the Fermi surface, \( k = k_F + 1, 1 \rightarrow 0 \). The fundamental reason that the latter is done is that that is \( \text{where the spectral density lies}. \)

The correct degrees of freedom in the IR give rise to this spectral density. At the level of the Lagrangian, the spectral density is determined by the vanishing of the coefficient of the quadratic terms. The spectral density is highly peaked and the effects of renormalization are only to give weakly interacting (dressed) fermions.

We emulate this approach by determining where Eq. (8) predicts the spectral density to lie. Fortunately, we will find that this is highly peaked (at what we will call the upper and lower Hubbard bands), and so one might hope that the scaling towards that locus is well-defined. We will not go so far in this paper as to claim that a continuum limit exists, but we will use this insight to establish that a dynamical Mott gap emerges. The root cause of this effect is that hidden in Eq. (8) is the dynamical degree of freedom that mediates the Mott gap: both the electrons and bosons are locked into bound states and hence cannot propagate independently. As a result the most relevant term in the Lagrangian arises from the boson-fermion interaction. This is a purely strongly coupled effect which makes Mottness analogous to other problems of strong interactions, for example QCD. An important difference with QCD which Eq. (8) lays plain is that for Mottness, the exact low-energy Lagrangian may be derived. This should enable an identification of the proper collective degrees of freedom.

To proceed, we switch to frequency and momentum space and specialize to a square lattice as our focus is the copper-oxide plane of the cuprates. Defining \( \varphi(t) = \int d\omega \ e^{-i\omega t} \varphi(\omega) \), the energy dispersion, \( \epsilon_p^{(k)} = 4 \sum_n \cos(k_n a/2) \cos(p_n a) \), where \( k \) and \( p \) are the center of mass and relative momenta of the fermion pair, and
the Fourier transform of $b_i$,
\[ b_k = \sum_p \varepsilon_p^{(k)} c_{k/2+p, \uparrow} c_{k/2-p, \downarrow} \]  
we arrive at the exact working expression,
\[ L_{\text{IR}}^{\text{hf}} = -\frac{|s|^2}{(w - U/2)} \varphi_{\omega, k}^\dagger \varphi_{\omega, k} + \frac{1}{(w + U/2)} \tilde{\varphi}_{-\omega, k} \tilde{\varphi}_{-\omega, k} \]
\[ + \frac{U t^2}{U^2 - 4 \omega^2} b_{\omega, k}^\dagger b_{\omega, k} \]
\[ + \left( s_0 \varepsilon_p^{(k)}(\omega) \varphi_{\omega, k}^\dagger + s \tilde{\alpha}_p^{(k)}(\omega) \tilde{\varphi}_{-\omega, k} \right) \]
\[ \times \left( c_{k/2+p, \uparrow} c_{k/2-p, \downarrow} \right) \omega + h.c. \]  
for the low-energy Lagrangian where we have suppressed the implied integration over frequency and introduced the coupling constants,
\[ \alpha_p^{(k)}(\omega) = \frac{U + t \varepsilon_p^{(k)} + 2 \omega}{U - 2 \omega} \]
\[ \tilde{\alpha}_p^{(k)}(\omega) = \frac{U + t \varepsilon_p^{(k)} + 2 \omega}{U + 2 \omega} \]  
which play a central role in this theory. They, in fact, will determine the spectral weight in the lower Hubbard (LHB) and upper Hubbard (UHB) bands, respectively. Note that in all of these expressions, $\omega$ is the frequency of the boson field $\varphi$ or $\tilde{\varphi}$. As we have retained the full frequency dependence, we will be able to determine the complete dynamics.

If the bosons were weakly coupled propagating degrees of freedom, setting the coefficient of the quadratic terms (in the Lagrangian) to zero would determine their dispersion. However, the coefficients of the naively quadratic terms never vanish for any momentum and frequency. Hence, on the surface of it, neither the bosons nor the electrons propagate and the spectral weight vanishes at all energies. The correct theory of the Mott gap should yield, however, a non-zero spectral weight in the UHB and LHB. Identifying this physics requires that we re-examine what should properly be considered to be a kinetic term. The structure of the frequency and momentum dependence of Eq. (10) suggests that the operators $\varphi^{cc}$ and $\tilde{\varphi}^{cc}$ play a central role and they determine where the spectral weight resides. These operators might then be thought of as the kinetic terms for composite excitations mediated by the charge $\pm 2e$ bosonic fields (loosely speaking, we might think of this as occurring because of the formation of bound states). Such an interpretation is warranted because the spin-spin interaction and all higher-order operators contained in the $|b_j|^2$ term are at least proportional to $|a|^4$ and hence are all sub-dominant to the composite interaction terms. Consequently, at the level of the Lagrangian, the turn-on of the spectral weight is governed by the vanishing of the coefficients of the coupled boson-fermion terms. That novel dynamics emerges from Eq. (10) can be seen by inspection of the coefficients (11). We note that the frequency poles appearing in the various terms of the Lagrangian are an artifact of our normalization, and could be absorbed into a redefinition of fields: $\varphi_\omega \to \sqrt{1 - 2\omega/U} \varphi_\omega$, $\tilde{\varphi}_\omega \to \sqrt{1 + 2\omega/U} \tilde{\varphi}_\omega$, and $(cc)_\omega \to \sqrt{1 - 4\omega^2/U^2} (cc)_\omega$. These scalings recast the Lagrangian as
\[ L_{\text{IR}}^{\text{hf}} \to \frac{2 |s|^2}{U} |\varphi_{\omega}|^2 + \frac{1}{U} |\tilde{\varphi}_{-\omega}|^2 + \frac{t^2}{U} |b|_\omega|^2 \]
\[ + s \varphi_p^{(k)}(\omega) \varphi_{\omega, k}^\dagger c_{k/2 + p, \uparrow} c_{k/2 - p, \downarrow} \]
\[ + s \tilde{\varphi}_p^{(k)}(\omega) \tilde{\varphi}_{-\omega, k}^\dagger c_{k/2 + p, \downarrow} c_{k/2 - p, \uparrow} + h.c. \]  
Effectively, we have rescaled the coefficients $\alpha, \tilde{\alpha}$ to
\[ \gamma_p^{(k)}(\omega) = \frac{U + t \varepsilon_p^{(k)} + 2 \omega}{U} \sqrt{1 + 2\omega/U} \]
\[ \tilde{\gamma}_p^{(k)}(\omega) = \frac{U + t \varepsilon_p^{(k)} + 2 \omega}{U} \sqrt{1 - 2\omega/U}, \]  
while the coefficients of other terms in the Lagrangian are just constants. The first thing to notice about these expressions is that the boson frequency appears in the combinations $U \mp 2\omega$. What this will ultimately mean is that the analytic structure is concentrated around $\omega = \pm U/2$.

A. Propagating Degrees of Freedom at Half-filling: Mott Gap

To determine where the spectral weight resides, we calculate where the coefficients $\gamma_p^k$ and $\tilde{\gamma}_p^k$ vanish. Consider initially $k = 0$ so that the dispersion simplifies to $\varepsilon_\rho^{(0)} = 4 \sum_{\mu} \cos \alpha p_{\mu}$. When $\omega = \pm U/2$, $\gamma_p^0$ ($\tilde{\gamma}_p^0$) vanish along the
momentum corresponds to the diamond \( a_p = \left( a_{p_x} \pm \pi - a_{p_z} \right) \) depicted in Fig. (1). These features define the center of the LHB \((-U/2)\) and UHB \((U/2)\) for the composite excitations. For all momenta outside the diamond, \(|p| > \pi\), \( \gamma_p \) vanishes for \( U/2 < \omega \leq U/2 + 4t \) while \( \tilde{\gamma}_p = 0 \) for \(-U/2 < \omega < -U/2 + 4t\). Within the diamond, \(|p| < \pi\), \( \gamma_p = 0 \) in the energy range \( U/2 - 4t \leq \omega < U/2 \) while in the interval \([-U/2 - 4t, -U/2]\) the coefficient \( \tilde{\gamma}_p \) vanishes. Consequently, for each momentum, spectral weight turns on at two distinct energies, one in the LHB \((\gamma_p = 0)\) and the other in the UHB \((\gamma_p = 0)\) with a separation of \( U \). Note that \( \gamma_p \) and \( \tilde{\gamma}_p \) never vanish at the same energy provided that \( U > 8t \). Consequently, for \( U > W \), a hard gap opens (the Mott gap) in the spectrum and the excitations defined by the vanishing of \( \gamma \) and \( \tilde{\gamma} \) propagate independently above and below the gap, respectively. In terms of the composite excitations, the Mott gap opens continuously but the spectral weight at the chemical potential rises discontinuously as is seen in numerical calculations on finite-dimensional lattices\cite{11,12,13} but in contrast to the \( d = \infty \) solution. The composite excitations which lead to the turn-on of the spectral weight correspond to the bound states of \( \varphi^\dagger cc \) (UHB) and \( \varphi^\dagger cc \) (LHB): they represent the collective modes or in essence the propagating charge degrees of freedom of the half-filled Hubbard model. This is our principal conclusion. As our analysis thus far is exact, we conclude that in the absence of any symmetry breaking, the coefficients \( \gamma_p \) and \( \tilde{\gamma}_p \) determine the dispersion for the excitations that comprise the here-to-fore undefined UHB and LHB. The center-of-mass momentum \( k \) simply shifts the momentum at which \( \tilde{\gamma}^p \) changes sign, thereby keeping the Mott gap intact.

Ultimately, it is the overlap between the composite excitations and the bare electrons that determines the turn-on of the electron spectral density. Consequently, the gap in the electron spectrum is at least that of the composite excitations. To determine the overlap, it is tempting to complete the square on the \( \varphi^\dagger cc \) term bringing it into a quadratic form, \( \Psi^\dagger \Psi \) with \( \Psi = A \varphi + B ccc \). This would lead to composite excitations having charge \( 2e \), a vanishing of the overlap and hence no electron spectral density of any kind. However, the actual excitations that underlie the operator \( \varphi^\dagger cc \) correspond to a linear combination of charge objects, \( c^\dagger \) and \( \varphi^\dagger c \). In terms of the UV variables, the latter can be thought of as a doubly occupied site bound to a hole. To support this claim, we construct the exact representation of the electron creation operator in the IR at half-filling

\[
\begin{align*}
\hat{c}_i^\dagger \rightarrow \tilde{\hat{c}}_i & = -\frac{V_c}{U} \left( \hat{c}_{i,-\sigma} \hat{b}_i^\dagger + \hat{b}_i \hat{c}_{i,-\sigma} \right) + \frac{V_c^2}{U} \left( \hat{s} \hat{\varphi}_i^\dagger + \Delta \hat{\varphi}_i^\dagger \right) c_{i,-\sigma}
\end{align*}
\]

is indeed a sum of two composite excitations, the first having to do with spin fluctuations \( (\hat{b}^\dagger c) \) and the other with high-energy physics, \( \hat{\varphi}^\dagger c \) and \( \hat{\varphi} c \), that is, excitations in the UHB and LHB, respectively. It is important to note that Eq. (15) is the exact expression for the low-energy electron at half-filling. Consequently, we formulate the overlap

\[
O = |\langle \hat{c}^\dagger | \hat{c}^\dagger \rangle |^2 P}\Psi
\]

for the the physical process of passing an electron through a Mott insulator in terms of the overlap between the bare electron with the low-energy excitations of Eq. (15), \( \langle \hat{c}^\dagger | \hat{c}^\dagger \rangle \), and the overlap with the propagating degrees of freedom, \( \langle \hat{c}^\dagger | \Psi \rangle \) with \( P\Psi \), the propagator for the composite excitations. As a result of the dependence on the bosonic fields in Eq. (15), \( O \) contains destructive interference between states above and below the chemical potential. Such destructive interference between excitations across the chemical potential leads to a vanishing of the spectral weight at low energies\cite{11,13,14}. Consequently, the turn-on of the electron spectral weight cannot be viewed simply as a sum of the spectral weight for the composite excitations. As a result of the destructive interference, the gap in the electron spectrum will always exceed that for the composite excitations. Hence, establishing (Fig. 11) that the composite excitations display a gap is a sufficient condition for the existence of a charge gap in the electron spectrum, a key conclusion of this work.

### B. Electron Spectral Function

We confirm the argument in the previous section on the origin of the gap in the electron basis by an explicit calculation of the electron spectral function. Because the action lacks any derivative terms with respect to \( \varphi_i \), we can treat \( \varphi \) as a spatially homogeneous field. While \( A \) priori, such gradient terms with respect to \( \varphi_i \) are possible, their presence at half-filling would indicate that freely propagating bosonic degree of freedom exist at half-filling. The absence of such terms at half-filling makes it possible to identify that the only propagating degrees of freedom at half-filling are gapped composite excitations.

We proceed by rewriting the coefficient of the boson-fermi terms as

\[
\Delta(k, \omega, \varphi, \tilde{\varphi}) = -s(\hat{\varphi}^\dagger - \varphi) + \frac{st}{U - 2\omega - i\delta}(\hat{\varphi}^\dagger + \hat{\varphi})(\hat{\varphi}^\dagger + \hat{\varphi})(\hat{\varphi}^\dagger + \hat{\varphi})\alpha(k)
\]

and

\[
\alpha(k) = 2t(\cos(k_x) + \cos(k_y))
\]

(17)
Any non-trivial dynamics underlying the Mott gap will arise only from the second term in \( \Delta(k, \omega, \varphi, \bar{\varphi}) \). Upon Wick rotation, \( \varphi \rightarrow i\varphi \) and \( \varphi^* \rightarrow i\varphi^* \), we rewrite the single-particle electron Green function as

\[
G(k, \omega) = \int d\varphi \int d\bar{\varphi} G(k, \omega, \varphi, \bar{\varphi}) \exp^{-\int d\omega L_{\text{Mott}}} \tag{18}
\]

where \( L_{\text{Mott}} \) is the IR Lagrangian with the \(|b|^2\) term dropped and

\[
G(k, \omega, \varphi, \bar{\varphi}) = \frac{i\delta}{|\Delta(k, \omega, \varphi, \bar{\varphi})|^2 + i\delta}. \tag{19}
\]

As our analysis thus far demonstrates that the \(|b|^2\) term has no bearing on the Mott gap justifies our use of the truncated Lagrangian, \( L_{\text{Mott}} \) which has only the charge degrees of freedom. Because of the \( i\delta \) in the gap function, \( \Delta(k, \omega, \varphi, \bar{\varphi}) \), the imaginary part of the Green function

\[
\Im G(k, \omega, \varphi, \bar{\varphi}) = \lim_{\delta \to 0} \left[ \frac{(U - 2\omega)^2 + \delta^2}{\left[(U + 2\omega)^2 + \delta^2\right]} - \frac{\delta}{A^2 + (2A\varphi + \bar{\varphi} + B)^2}\delta^2 + O(\delta^4) \right]
\]

\[
\times \frac{A^2 + (2A\varphi + \bar{\varphi} + B)^2\delta^2 + O(\delta^4)}{(U - 2\omega)^2(U + 2\omega)^2\delta(A)} \tag{20}
\]

is explicitly non-zero. We have defined

\[
A = \left[U^2 - 4\omega^2 - 2\alpha_k(U + 2\omega)\right] \varphi
\]

\[
+ \left[U^2 - 4\omega^2 - 2\alpha_k(U - 2\omega)\right] \bar{\varphi}
\]

\[
B = 2\varphi(2\omega + \alpha_k) + 2\bar{\varphi}(2\omega + \alpha_k). \tag{21}
\]

Note the arguments of the \( \delta \) functions are closely related to the coefficients \( \gamma \) and \( \xi \) that led to the turn-on of the spectral weight. However, in the electron basis, the spectral weight is not a simple sum of the spectral weight at \( \pm U/2 \). As a result of the integration over \( \varphi_i \) and \( \bar{\varphi}_i \), the spectral function for the electrons arises from a complicated intereference between excitations in the LHB and UHB. Consequently, to complete the calculation, we performed the \( \varphi_i \) and \( \bar{\varphi}_i \) integrations numerically. The resultant electron spectral function for \( U = 8t \) shown in Fig. 2 demonstrates clearly that a Mott gap exists and the spectral weight is momentum dependent. This calculation supports the physical argument made in the previous section that the Mott gap in the electron basis arises from a non-trivial interference between the excitations at \( \pm U/2 \). At \((\pi, \pi)\), the spectral weight lies predominantly in the UHB whereas at \((0, 0)\) it lies in the LHB. Consequently, the real part of the Green function must change sign along some momentum surface that lies between these two extreme momenta. The location of the zero surface or Luttinger surface is the Fermi surface of the non-interacting system as it must be\(^{16,17}\) for the half-filled system with particle-hole symmetry. We find then that the Mott gap arises from the dynamics of the two charge \(2|e| \) bosonic fields. This is the first time the Mott gap has been derived dynamically, in particular by a collective degree of freedom of the lower and upper Hubbard bands. Relative to the gap in the spectrum for the composite excitations that diagonalize the fermion-boson terms in Eq. \((13)\), 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. While our treatment of the charge \( \pm 2|e| \) boson is approximate, it does suffice to capture the essence of of the collective mode, namely it mixes all sectors with varying numbers of doubly occupied sites. In addition, we anticipate that the electron spectral function should evolve as the Mott transition is approached in a similar fashion to that in terms of the composite particle basis. That is, the gap should close continuously without a coherence peak at zero energy. Consequently, the spectral weight at the chemical potential should jump discontinuously from zero to the value in the free system at the Mott transition as is seen in simulations of the Mott transition in finite-dimensional systems. In addition, the momentum dependence of the spectral function is identical to that obtained by dynamical mean-field calculations\(^{18,19}\) thereby lending credence to such cluster calculations\(^{14}\) near the Mott transition.

**III. Final Remarks**

What this analysis demonstrates is that the spin-spin interaction, contained in the \(|b|^2\) term, plays a spectator role in the generation of the Mott gap. Nonetheless, there is a natural candidate for the antiferromagnetic order, namely \( B_{ij} = \langle g_{ij}\varphi^i_1\bar{c}^i_1c^j_1 \rangle \). 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 \( \gamma_i \). Such an antiferromagnet, which has no continuity with weak-coupling theory, is composed of composite excitations which can form excitonic bound states in the two-particle spectrum and hence is not inconsistent with the excitonic modes found in the mid-
infrared absorption of numerous parent cuprates. In essence, the composite excitations described by the coefficients $\gamma^k$ and $\tilde{\gamma^k}$ represent the orthogonal (they never lead to a turn-on of the spectral weight in the same energy range) low-energy degrees modes that render the original UV problem weakly coupled. That such new degrees of freedom emerge as the dispersing modes is a typical feature of strong coupling. In fact, an analogy can be made here between our demonstration that the propagating modes at strong coupling in the Hubbard model are composite excitations (not electrons) mediated by an auxiliary field that has no bare dynamics with 't Hooft's demonstration that meson states, not free quarks, also mediated by a non-propagating auxiliary field, are the dispersing modes in QCD in $1+1$ dimensions. Our analysis suggests that a fixed point underlies the formation of such composite excitations. Whether the $\beta$ function can be calculated within this formalism remains the outstanding question.

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