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Infinite single-particle bandwidth of a Mott–Hubbard insulator

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The conventional viewpoint of the strongly correlated electron metal-insulator transition is that a single band splits into two upper and lower Hubbard bands at the transition. Much work has investigated whether this transition is continuous or discontinuous. Here we focus on another aspect and ask the question of whether there are additional upper and lower Hubbard bands, which stretch all the way out to infinity — leading to an infinite single-particle bandwidth (or spectral range) for the Mott insulator. While we are not able to provide a rigorous proof of this result, we use exact diagonalization studies on small clusters to motivate the existence of these additional bands, and we discuss some different methods that might be utilized to provide such a proof. Even though the extra upper and lower Hubbard bands have very low total spectral weight, those states are expected to have extremely long lifetimes, leading to a nontrivial contribution to the transport density of states for *dc* transport and modifying the high temperature limit for the electrical resistivity.

Keywords: Mott–Hubbard insulator; Hubbard model; density of states.

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1. Introduction

In conventional band theory, metals are classified as systems whose Fermi level lies within the band and thereby can conduct electricity. But if the repulsive interaction between electrons is sufficiently large, it can induce a metal-to-insulator transition called the Mott–Hubbard transition.[1,2] One of the hallmarks of this transition is the appearance of a spectral gap in the single-particle density of states, creating separate upper and lower Hubbard bands from the original single band (in the absence of the electron–electron interaction) and an insulating state. Many numerical calculations confirm this picture.[3] We present evidence which shows that there actually are *an infinite number of upper and lower Hubbard bands* in the single-particle density of states! While we are not yet able to provide a rigorous proof of this result, we present arguments that show a possible pathway for such a proof.

The Mott–Hubbard transition has long been viewed as one of the most important and difficult problems to solve in condensed matter physics. Numerically exact solutions for the spectral function come from dynamical mean-field theory,[4] exact diagonalization of small systems[5] and density matrix renormalization group calculations.[6] In all of these solutions, one sees the prominent features of just one upper and one lower Hubbard band in the insulating state. But systematic projection onto subspaces with a fixed number of doubly occupied lattice sites—as first performed by Harris and Lange[7] and later extended by Olés and co-workers[8] — showed that there must be at least one more upper and lower Hubbard band, but with a spectral weight so low, it cannot be easily seen in a linear plot of the density of states.

We present strong evidence that supports the conjecture that this last result is just the tip of the iceberg — there actually exists an infinite number of upper and lower Hubbard bands — but the spectral weight of each of these additional bands is so exceedingly small, that it is difficult to see them in conventional calculations. Instead, we show (through an analysis of exact diagonalization studies and general arguments relating to the structure of the eigenfunctions) compelling evidence for the existence of these extra upper and lower bands. We hope that these results will ultimately lead to a proof of the counterintuitive result that the Mott–Hubbard insulator actually has an infinite single-particle bandwidth.

2. Formalism

We will be examining the Hubbard model, which is defined by the following Hamiltonian on a graph Λ with vertices $x \in \Lambda$ (which we refer to as sites on the graph)

$$\mathcal{H} = -\sum_{x,y\in\Lambda,\sigma} t_{xy} c^\dagger_{x\sigma} c_{y\sigma} - \mu \sum_{x\in\Lambda,\sigma} c^\dagger_{x\sigma} c_{x\sigma} + U \sum_{x\in\Lambda} c^\dagger_{x\uparrow} c_{x\uparrow} c^\dagger_{x\downarrow} c_{x\downarrow}\,. \tag{1}$$

Here the creation (annihilation) operator for a fermion of spin σ at site x is $c^\dagger_{x\sigma}$ ($c_{x\sigma}$) and they satisfy the canonical anticommutation relation $\{c^\dagger_{x\sigma}, c_{y\sigma'}\}_+ = \delta_{xy}\delta_{\sigma\sigma'}$ (with all creation operators anticommuting amongst themselves, and similarly for the annihilation operators). The matrix $-t_{xy}$ is the hopping matrix, which is

required to be Hermitian and to have a vanishing diagonal ($t_{xx} = 0$), μ is the chemical potential, and U is the on-site Hubbard interaction.

The retarded Green's function is defined via the following trace over all fermionic states

$$G^R_{xy\sigma}(t) = -\frac{i}{\mathcal{Z}}\theta(t)\mathrm{Tr}[e^{-\beta\mathcal{H}}\{c_{x\sigma}(t), c^\dagger_{y\sigma}(0)\}_+]\,, \tag{2}$$

where $\mathcal{Z} = \mathrm{Tr}\exp[-\beta\mathcal{H}]$ is the partition function, $\theta(t)$ is the unit step function, $\beta = 1/T$ is the inverse temperature, and the fermionic operators are in the Heisenberg picture, where

$$c_{x\sigma}(t) = e^{i\mathcal{H}t}c_{x\sigma}e^{-i\mathcal{H}t}\,. \tag{3}$$

The Green's function is commonly expressed in frequency space after a Fourier transformation

$$G^R_{xy\sigma}(\omega) = \int_0^\infty dt e^{i\omega t}G^R_{xy\sigma}(t)\,, \tag{4}$$

and the local spectral function (or density of states) is then defined to be

$$A_{x\sigma}(\omega) = -\frac{1}{\pi}\mathrm{Im}G^R_{xx\sigma}(\omega)\,. \tag{5}$$

We will focus on the local density of states in this work. Note that if the graph corresponds to a translationally invariant lattice and the system is paramagnetic, then there is no spontaneous breaking of translational symmetry or of spin rotational symmetry due to ordered phases. In this case, the local density of states is independent of x and σ.

We let $|n\rangle$ denote an eigenstate of $\mathcal{H}$ with eigenvalue E_n, such that $\mathcal{H}|n\rangle = E_n|n\rangle$. Then, introducing the complete set of eigenstates to perform the trace, and introducing a second complete set of eigenstates inside the anticommutator, allows us to re-express the retarded Green's function in the Lehmann representation, as follows:

$$G^R_{xy\sigma}(\omega) = \frac{1}{\mathcal{Z}}\sum_{mn}\frac{e^{-\beta E_m} + e^{-\beta E_n}}{\omega + E_m - E_n + i0^+}\langle m|c_{x\sigma}|n\rangle\langle n|c^\dagger_{y\sigma}|m\rangle\,. \tag{6}$$

The local density of states then satisfies

$$\begin{aligned} A_{x\sigma}(\omega) = \frac{1}{\mathcal{Z}}\sum_{mn} e^{-\beta E_m}[&|\langle n|c^\dagger_{x\sigma}|m\rangle|^2\delta(\omega + E_m - E_n) \\ &+ |\langle n|c_{x\sigma}|m\rangle|^2\delta(\omega - E_m + E_n)]\,. \end{aligned} \tag{7}$$

We consider the case of half-filling, where there is one particle for every vertex on the graph. Let $|\Lambda|$ denote the number of vertices on the graph, then half-filling corresponds to the condition that the number of electrons N_e satisfies

$$N_e = \frac{1}{\mathcal{Z}}\mathrm{Tr} - \beta\mathcal{H}\sum_{x\sigma}c^\dagger_{x\sigma}c_{x\sigma} = |\Lambda|\,, \tag{8}$$

which is equivalent to the condition $\mu = U/2$ (in the grand canonical ensemble) when the hopping matrix is *bipartite*. A bipartite hopping matrix occurs when the graph can be separated into two disjoint graphs Λ_A and Λ_B such that the hopping matrix is nonzero only when x and y belong to different subgraphs. At half-filling, the largest contributions to Eq. (7) come from states where $|m\rangle$ is one of the half-filled states, with $N_e = |\Lambda|$, and the state $|n\rangle$ is one of the states with N_e+1 particles for the leftmost term and $N_e - 1$ particles for the rightmost term. At $T = 0$, $|m\rangle$ can only be the ground-state for half-filling, which we denote by $|\text{gs}\rangle$ (although all states with one additional or one fewer particle enter so the sum over n remains). For any finite T, all states must be summed over, so the character of the density of states can change for $T = 0$ versus $T \neq 0$, but all nonzero temperatures will have similar behavior, at least with respect to the question of whether the density of states is nonzero at any specific frequency. The question of whether there are states in the gap, and whether there are extra upper and lower Hubbard bands can be answered by examining just the "canonical" set of states where all states $|m\rangle$ are at half-filling (if the answers are affirmative). We focus on these states for the remainder of the paper.

3. Exact Diagonalization Studies

The Hubbard model has particle-hole symmetry when it is on a bipartite lattice which implies that the particle removal spectrum and the particle addition spectrum are related by the substitution $\omega \to -\omega$. Since the existence of the infinite bandwidth does not depend on the presence of particle-hole symmetry, but our exposition is greatly simplified when we take particle-hole symmetry into account, we will do so for convenience here. We will also assume a translationally invariant system. This allows us to focus solely on the local particle removal spectra given by

$$A_{\text{rem}}(\omega) = \frac{1}{\mathcal{Z}} \sum_{mn} e^{-\beta E_m} |\langle n|c_{x\sigma}|m\rangle|^2 \delta(\omega - E_m + E_n) \tag{9}$$

for any lattice site x (since it is the same for all lattice sites). At $T = 0$, the spectra only has weight at negative frequencies (usually called the lower Hubbard band) because $E_{m=\text{gs}} < E_n$ for all states n with $N_e = |\Lambda| - 1$ electrons. Surprisingly, the removal spectrum has contributions from the upper Hubbard band with $\omega > 0$ when we consider the nonzero temperature case (this is easiest to see for the repulsive Hubbard model by considering any half-filled state with $D = N_e/2 = |\Lambda|/2$ double occupancies, which, upon removal of a particle, overlaps with states that have $D' = N_e/2 - 1 = |\Lambda|/2 - 1$ double occupancies; these states have an energy that is on the order of $U/2$ lower — corresponding to a positive energy contribution in the upper Hubbard band).

In Fig. 1, we plot the electron removal spectra for the ground state (corresponding to $T = 0$) and for all half-filled states (corresponding to a "canonical" subset of the states at $T = \infty$). In addition, the extra upper and lower Hubbard bands

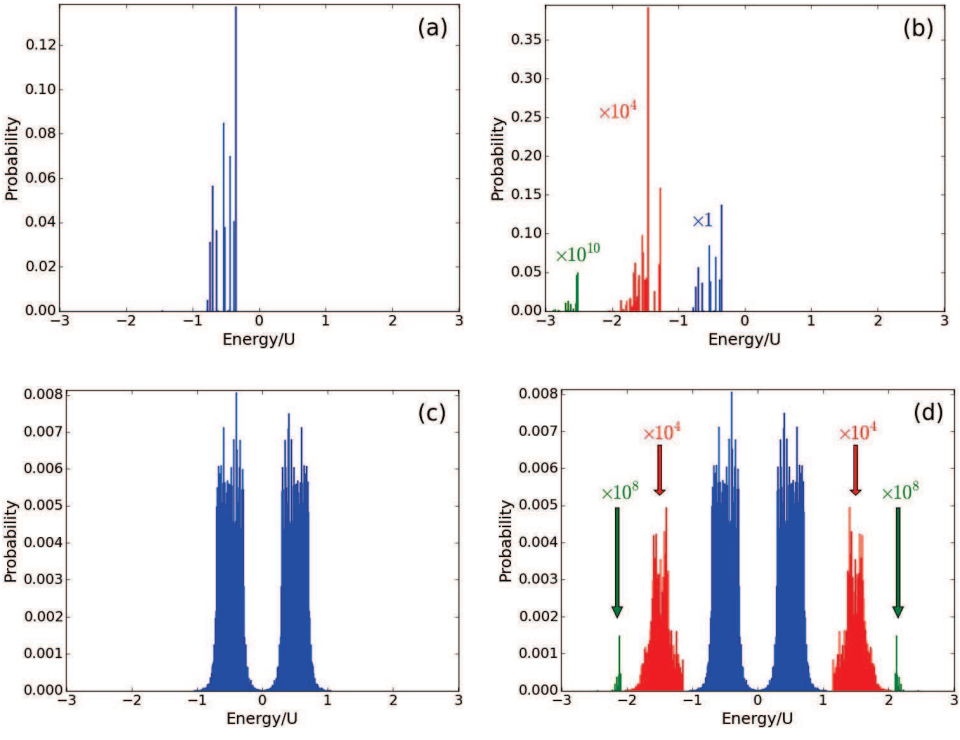

Fig. 1. (Color online) Binned weights of the electron removal spectral function for a $|\Lambda| = 6$ one-dimensional chain, with a bin width of $0.01U$. (a) $T = 0$ density of states. (b) $T = 0$ density of states with the extra bands magnified by the factors shown in the figure. (c) $T = \infty$ density of states in the "canonical approximation" which considers just the two electron numbers $N_e = 5, 6$ and (d) $T = \infty$ density of states with the extra bands color coded and magnified by the factors shown in the figure. Note that these results are not particle-hole symmetric, since the electron addition spectra needs to be added to create the electron-hole symmetric spectra (although the $T = \infty$ results are nearly so).

are highlighted by magnifying their signal by the factors shown in the figures. Note how the extra bands are robust, but have very small total weight. In Fig. 2, we plot the energy levels for the half-filled case, and for the cases with one more and one fewer electron. The ground state connects to eigenstates with all possible double occupancy values in the $N_e = |\Lambda| - 1$ sector.

In the large U limit, the zeroth-order energy is given by $DU - N_e\mu$ where D is the number of double occupancies and N_e is the number of electrons. These states are highly degenerate and require degenerate perturbation theory to determine both the energies and the eigenfunctions in an expansion in powers of t/U. The $\mathcal{O}(t)$ corrections to the energies arise from linear combinations of the zeroth-order eigenfunctions with a fixed number of double occupancies. Higher order corrections to the wavefunction involve $\mathcal{O}(t/U)$ combinations that have $D \pm 1$, and in general $\mathcal{O}([t/U]^\alpha)$ combinations with $D \pm \alpha$. In the perturbative expansion for many

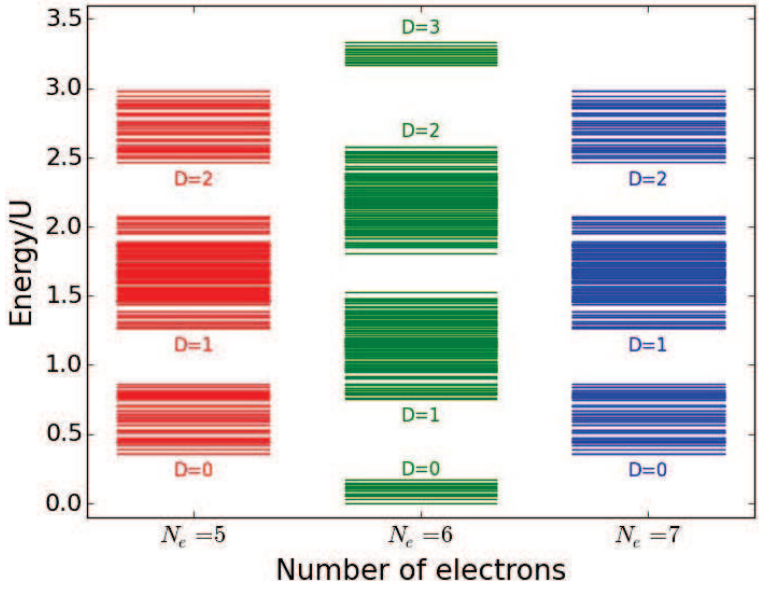

Fig. 2. (Color online) Energy spectra for the half-filled and half-filled plus or minus one particle cases of the $|\Lambda| = 6$ one-dimensional chain with $U/t = 10$. Note how the eigenstates with different double occupancies (as labeled in the figure) are grouped together for this typical large-U case.

eigenfunctions, the expansion terminates after a finite number of terms. What is important here is identifying the minimal power in t/U for a state with a given double occupancy to be present in the expansion for the eigenfunction, to estimate the t/U dependence of the matrix elements in the expansion for the spectral function.

However, this approach is not sufficient to get a correct estimate. For example, consider the ground state and the states it couples to with the removal of an electron. The ground state of the half-filled repulsive Hubbard model has $D = 0$ as $U \to \infty$, and the ground state for finite U includes an $\mathcal{O}(1)$ contribution with $D = 0$, an $\mathcal{O}(t/U)$ admixture with $D = 1$, an $\mathcal{O}([t/U]^2)$ admixture with $D = 2$ and so on. The eigenfunction when there are $N_e = |\Lambda| - 1$ electrons has similar behavior, with an $\mathcal{O}(1)$ contribution with $D = 0$, an $\mathcal{O}(t/U)$ admixture with $D = 1$, and so on. Hence, the overlap between the ground state at half-filling after an electron is removed, and a state with one fewer electron is $\mathcal{O}(1)$ for the $D = 0$ subspace with $|\Lambda| - 1$ electrons. The energy difference $E_{\rm gs} - E_n$ is approximately $-U/2$ plus corrections of $\mathcal{O}(t)$ (recall that $\mu = U/2$). These are states that contribute to the first lower Hubbard band. We expect the next lower Hubbard band to have energies centered near $-3U/2$. The overlap of the half-filled ground state and states with one fewer electron that have $D = 1$ in the large U limit, should have matrix elements that go like t/U and hence the weight of the band should be of order $(t/U)^2$, but it is of order $(t/U)^4$, as seen in the results above. Similar arguments for the next lower band $(-5U/2)$ would put that weight at order $(t/U)^4$, but we saw

it was either order $(t/U)^8$ or $(t/U)^{10}$. So there is a conundrum about the weight of the extra bands, in that they are not consistent with a simple power-counting argument based on perturbation theory. It requires a more sophisticated analysis. This is discussed in more detail in the next section.

Another question is whether these extra bands, which are present for finite systems, remain in the thermodynamic limit. The canonical projection method, described briefly in the next section, shows that the next upper and lower Hubbard bands do survive into the thermodynamic limit. Yet another question to ask is, do they survive in the infinite-dimensional limit of dynamical mean-field theory, where the hopping is scaled to zero as the inverse square root of the dimension. Here, the question is easily posed for the Bethe lattice (with its finite bandwidth for the noninteracting case). For the hypercubic lattice, which has a Gaussian density of states for the noninteracting problem, one has to search for the enhancement of the extra bands (which are power law) versus the Gaussian decaying tails coming from the noninteracting band to see the extra bands, which is much harder to do. Unfortunately, there are no known calculational methods that are accurate enough to determine whether these extra upper and lower Hubbard bands exist for the Hubbard model. But for the spinless Falicov–Kimball model, it is known that they do not exist for the Bethe lattice, since there is an exact cubic equation for the density of states that has only a single upper and lower Hubbard band in the insulating phase. They also do not look like they are present on the hypercubic lattice.

4. Canonical Projection Methods

The canonical projection method was introduced by Harris and Lange[7] shortly after the Hubbard model was created. They described the first extra upper and lower Hubbard bands. Olés and co-workers[8] confirmed this result along with the fact that the weight of these bands is of order $(t/U)^4$. This clearly demonstrates the existence of extra upper and lower Hubbard bands that survive the thermodynamic limit.

The approach of Harris and Lange involves using canonical transformations to project the Hubbard model onto different sectors with fixed double occupancies. The lowest-energy sector for the repulsive model is the $D = 0$ sector. The projection approach is to determine the canonical representation of the creation and annihilation operators projected onto the different constant double occupancy sectors. Using these results, one can show the different weights of the spectral function in the different sectors. The approach is tedious and becomes increasingly difficult for higher orders. To date, it has only been carried out far enough to show the weight of the next upper and lower Hubbard bands being $(t/U)^4$. It explains the lower order of the weight than the naive prediction made in the previous section arises from a sum rule which is related to a commutator, which vanishes to lowest order. Since we expect there to be a similar effect occurring for the next extra upper and lower Hubbard bands, due to their very low weight, this indicates that there

may be an interesting algebra associated with the weights of these bands. A full extension of the Harris–Lange procedure to higher order could lead both to a proof of the existence of the extra upper and lower Hubbard bands and to a determination of the weight of those extra bands as well. It is not clear whether this can be done analytically for the general case.

5. Towards a Full Proof

There is another strategy that can be used to determine the energy differences of the coupled states. It starts by using one of two identities to determine the energy difference

$$(E_{\rm gs}-E_n)\langle n|c_{x\sigma}|{\rm gs}\rangle = -\langle n|[\mathcal{H},c_{x\sigma}]_-|{\rm gs}\rangle \tag{10}$$

and

$$(E_{\rm gs}-E_n)\langle n|c_{x\sigma}c^\dagger_{x-\sigma}c_{x-\sigma}|{\rm gs}\rangle = -\langle n|[\mathcal{H},c_{x\sigma}c^\dagger_{x-\sigma}c_{x-\sigma}]_-|{\rm gs}\rangle\,. \tag{11}$$

Evaluating each commutator and dividing by the matrix element (in cases when the matrix element is nonzero) yields

$$E_{\rm gs}-E_n = -\sum_{x\in\Lambda} t_{xy}\frac{\langle n|c_{y\sigma}|{\rm gs}\rangle}{\langle n|c_{x\sigma}|{\rm gs}\rangle} + U\frac{\langle n|c_{x\sigma}c^\dagger_{x-\sigma}c_{x-\sigma}|{\rm gs}\rangle}{\langle n|c_{x\sigma}|{\rm gs}\rangle} \tag{12}$$

and

$$\begin{aligned}E_{\rm gs}-E_n = &-\sum_{x\in\Lambda} t_{xy}\frac{\langle n|c_{y\sigma}c^\dagger_{x-\sigma}c_{x-\sigma}|{\rm gs}\rangle}{\langle n|c_{x\sigma}c^\dagger_{x-\sigma}c_{x-\sigma}|{\rm gs}\rangle} - \sum_{x\in\Lambda} t_{xy}\frac{\langle n|c_{x\sigma}c^\dagger_{x-\sigma}c_{y-\sigma}|{\rm gs}\rangle}{\langle n|c_{x\sigma}c^\dagger_{x-\sigma}c_{x-\sigma}|{\rm gs}\rangle}\\ &+\sum_{x\in\Lambda} t_{xy}\frac{\langle n|c_{x\sigma}c^\dagger_{y-\sigma}c_{x-\sigma}|{\rm gs}\rangle}{\langle n|c_{x\sigma}c^\dagger_{x-\sigma}c_{x-\sigma}|{\rm gs}\rangle} + U\,.\end{aligned} \tag{13}$$

We can also evaluate similar commutators using creation and annihilation operators for one-electron states that are eigenstates of the hopping term in the Hamiltonian by starting with the hopping matrix eigenvectors

$$-\sum_{y\in\Lambda} t_{xy}f^\lambda_y = \epsilon_\lambda f^\lambda_x \tag{14}$$

and forming the additional matrix element identities (by dividing by the matrix element when it is nonzero) to give the following:

$$E_{\rm gs}-E_n = \epsilon_\lambda + U\frac{\langle n|\sum_{x\in\Lambda} f^{\lambda*}_x c_{x\sigma}c^\dagger_{x-\sigma}c_{x-\sigma}|{\rm gs}\rangle}{\langle n|\sum_{x\in\Lambda} f^{\lambda*}_x c_{x\sigma}|{\rm gs}\rangle} \tag{15}$$

and

$$E_{\rm gs}-E_n = -\frac{\langle n|\sum_{x\in\Lambda} t_{xy}f^{\lambda*}_x c_{y\sigma}c^\dagger_{x-\sigma}c_{x-\sigma}|{\rm gs}\rangle}{\langle n|\sum_{x\in\Lambda} f^{\lambda*}_x c_{x\sigma}c^\dagger_{x-\sigma}c_{x-\sigma}|{\rm gs}\rangle} - \frac{\langle n|\sum_{x\in\Lambda} t_{xy}f^{\lambda*}_x c_{x\sigma}c^\dagger_{x-\sigma}c_{y-\sigma}|{\rm gs}\rangle}{\langle n|\sum_{x\in\Lambda} f^{\lambda*}_x c_{x\sigma}c^\dagger_{x-\sigma}c_{x-\sigma}|{\rm gs}\rangle}$$

$$+\frac{\langle n|\sum_{x\in\Lambda} t_{xy} f_x^{\lambda *} c_{x\sigma} c_{y-\sigma}^{\dagger} c_{x-\sigma}|\mathrm{gs}\rangle}{\langle n|\sum_{x\in\Lambda} f_x^{\lambda *} c_{x\sigma} c_{x-\sigma}^{\dagger} c_{x-\sigma}|\mathrm{gs}\rangle} + U\,. \tag{16}$$

Since these identities hold in all cases when the denominators on the right-hand side are nonzero, they must hold in the cases of the extra upper and lower Hubbard bands. But the details for exactly how that happens are not yet clear. This does seem like a good starting place, though, to try to complete a rigorous proof of the existence of the extra upper and lower Hubbard bands. If one could show that the second term on the right-hand side of Eq. (15) is close to a positive integer, then we would prove the existence of the extra lower Hubbard bands.

6. Transport

We next discuss dc transport for a translationally invariant lattice that has momentum as a good quantum number. If we neglect vertex corrections (which is usually a good first approximation), the dc conductivity is equal to

$$\sigma(t) = \sigma_0 \sum_{\mathbf{k}\sigma} \int d\omega |\mathbf{v}_{\mathbf{k}}|^2 \left(-\frac{df(\omega)}{d\omega}\right) A_\sigma^2(\mathbf{k},\omega)\,, \tag{17}$$

where $\mathbf{v}_{\mathbf{k}} = \nabla\epsilon_{\mathbf{k}}$ is the band velocity, $A_\sigma(\mathbf{k},\omega) = -\mathrm{Im}G_\sigma^R(\mathbf{k},\omega)/\pi$ is the spectral function, $f(\omega) = 1/[1+\exp(\beta\omega)]$ is the Fermi–Dirac distribution function and σ_0 is some dimensionful constant that gives the dimensions of conductivity to the final expression. The momentum-dependent retarded Green's function is defined precisely as before for the real-space Green's functions, except we use the creation and annihilation operators that have definite momentum, because they diagonalize the hopping matrix. Since the zeroth moment of the imaginary part of the self-energy satisfies a sum rule which holds to high accuracy when one uses just the integration over the first upper and lower Hubbard bands, the imaginary part of the self-energy in the extra bands must be small in magnitude.

If we make an approximation that there is no momentum dependence to the self-energy in these extra upper and lower bands, then we can perform the integrals by transforming the sum over momentum to an integral over the noninteracting transport density of states $\rho_{tr}(\epsilon)$ which is defined by

$$\rho_{\mathrm{tr}}(\epsilon) = \sum_{\mathbf{k}} |\mathbf{v}_{\mathbf{k}}|^2 \delta(\epsilon - \epsilon_{\mathbf{k}}) \tag{18}$$

and can be related to the noninteracting density of states via a differential equation[9] that usually takes the form

$$\frac{d}{d\epsilon}\rho_{\mathrm{tr}}(\epsilon) = -c\epsilon\rho(\epsilon) \tag{19}$$

for some constant c. We define a transport Green's function $G_{\mathrm{tr}}(\omega)$ via

$$G_{\mathrm{tr}}(\omega) = \int d\epsilon \rho_{\mathrm{tr}}(\epsilon) \frac{1}{\omega + \mu - \Sigma(\omega) - \epsilon} \tag{20}$$

[with $\Sigma(\omega)$ the self-energy] and then find the conductivity can be written as

$$\sigma(T) = \sigma_0 \int d\omega \left(-\frac{df(\omega)}{d\omega} \right) \tau(\omega) \,, \tag{21}$$

where the many-body transport relaxation time (neglecting vertex corrections) is

$$\tau(\omega) = \frac{1}{\pi^2} \left[\frac{\mathrm{Im} G_{\mathrm{tr}}(\omega)}{\mathrm{Im}\Sigma(\omega)} - \frac{dG_{\mathrm{tr}}(\omega)}{d\mu} \right] . \tag{22}$$

Hence, the transport relaxation time has a term proportional to the ratio of the imaginary part of the transport Green's function to the imaginary part of the self-energy. Both imaginary parts are small, but their ratio can be substantial and hence it can contribute to the high-temperature transport. This is one reason why the existence of these low spectral weight bands may, nevertheless, be important when studying properties of the insulating phase of the Hubbard model.

7. Conclusions

In this work, we provided evidence for the existence of additional upper and lower Hubbard bands going beyond the classic canonical transformation work of Harris and Lange[7] who established the existence of one additional lower and upper Hubbard band. The evidence comes from small cluster calculations which clearly show how these extra bands must extend out to an infinite number in the thermodynamic limit. Those results also showed that the weights get extremely small for these higher bands, which explains why they are not ordinarily seen in conventional calculations.

We described some methods that might be able to be used to rigorously show the existence of these extra bands, but we are not able to complete such a proof at this time. We also discussed why such small bands might, nevertheless, have an important contribution to high-temperature transport.

There is another question that is similar to what we discussed here but appears to require more work to establish, which is the question of whether the Mott gap fills in as a function of temperature for high T. There is numerical evidence to indicate this is true close to the metal-insulator transition,[10] but it appears that it should hold for all U. We do not have a proof for this either, but it is an interesting area for further study.

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