Mott-Hubbard insulators for systems with orbital degeneracy

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We study how the electron hopping reduces the Mott-Hubbard band gap in the limit of a large Coulomb interaction \(U\) and as a function of the orbital degeneracy \(N\). The results support the conclusion that the hopping contribution grows as roughly \(\sqrt{NW}\), where \(W\) is the one-particle band width, but in certain models a crossover to a \(\sim NW\) behavior is found for sufficiently large \(N\).

I. INTRODUCTION

The Mott-Hubbard metal-insulator transition has attracted much interest since it was proposed by Mott,\(^{1,2}\) being an example of how strong correlation drastically changes the properties of the system. For simplicity, the Mott-Hubbard transition is usually studied for models without orbital degeneracy,\(^{3,4}\) e.g., the Hubbard model.\(^{5,6}\) For most real systems, however, the orbitals primarily involved in the transition are degenerate. We recently argued that in a Hubbard model with an orbital degeneracy \(N\), the ratio of \(U/W\) where the Mott-Hubbard transition takes place is increased by roughly a factor \(\sqrt{N}\) where \(U\) is the on-site Coulomb interaction and \(W\) is the one-electron band width.

This conclusion was based on a simple and suggestive but nonrigorous argument in the large \(U\)-limit, which said that the band gap \(E_g\) behaves as

\[
E_g \sim U - \sqrt{NW}.
\]

This argument was supported by exact diagonalization calculations for small clusters with \(N = 1, 2\) and 3. The argument was then extrapolated to intermediate values of \(U\), and the extrapolation was supported by quantum lattice Monte Carlo calculations for a model of \(A_2C_{60}\) (A=K, Rb) with the \(N = 3\). Similar results have recently also been obtained in Monte Carlo calculations by Han and Cox\(^{7}\) while L\(^{6}\) found a \((N+1)W\) behavior using the Gutzwiller Ansatz and Gutzwiller approximation.

Here we want to investigate the behavior in the large \(U\) limit further. We have in particular studied a model with hopping only between orbitals with the same orbital quantum number, referred to as an intraband hopping model. This model shows an interesting cross-over as the degeneracy \(N\) becomes larger than the number of nearest neighbor \(K\). Thus the hopping contribution tends to be \(\sim \sqrt{NW}\) for \(N \ll K\) but \(\sim NW\) for \(N \gg K\). When hopping between orbitals with different quantum numbers is included, interband hopping models, the results become more model dependent. The results obtained here support a behavior \(\sim \sqrt{NW}\) or a somewhat more rapid growth with \(N\).

In Sec. II we present some general arguments. In Sec. III we use exact diagonalization to study small clusters with intraband hopping and in Sec. IV this is extended to include interband hopping. The results are discussed in Sec. V.

II. GENERAL CONSIDERATIONS

We consider a system with \(M\) sites and the orbital degeneracy \(N\) at half-filling, i.e., with \(NM\) electrons. The band gap is then given by

\[
E_g = E(NM+1) + E(NM-1) - 2E(NM),
\]

where \(E(L)\) is the ground-state energy for \(L\) electrons. In the large \(U\)-limit, the \(NL\)-electron ground-state has exactly \(N\) electrons per site. The hopping of an electron to a neighboring site would cost the Coulomb energy \(U\) and is strongly suppressed in this limit. Therefore

\[
E(NM) = \frac{1}{2} N(N-1)MU + \mathcal{O}\left(\frac{t^2}{U}\right),
\]

where \(t\) is a hopping integral. For the states with an extra electron or hole the situation is more complicated, since the extra electron or hole can hop without any extra cost in Coulomb energy. We therefore focus on these states. We first form an antiferromagnetic state \(|\text{anti}\rangle\) with \(N\) electrons of a given spin on each site and with each site having as many neighboring sites of the opposite spin as possible. To be specific, the central site 1 has spin up. We then form a state with \(NM+1\) electrons

\[
|v_1\rangle = \psi_{11\uparrow}^\dagger|\text{anti}\rangle,
\]

where \(\psi_{im\sigma}^\dagger\) creates an electron on site \(i\) in the orbital \(m\) with spin \(\sigma\). Thus site 1 in the state \(|v_1\rangle\) has an additional electron. A spin up electron can hop from this site to a neighboring spin down site, forming a state

\[
|v_2\rangle = \frac{1}{\sqrt{NK}} \psi_{11\downarrow}^\dagger \sum_{im} \psi_{im\uparrow}^\dagger \psi_{im\downarrow}|\text{anti}\rangle,
\]

where the sum \(i\) is over the \(L (\leq K)\) neighboring sites with opposite spin to site 1. The spin down electron on
site 1 can also hop to neighboring sites with spin up, but we neglect this for the moment. The matrix element between the states in Eqs. (4) can then be calculated.

\[ \langle v_2 \vert H \vert v_1 \rangle = \sqrt{NL}t, \]  

where we have considered the case when there is a hopping matrix element only between orbitals of the same \( m \) quantum number on the neighboring sites. The argument can also be repeated for more general hopping. The important aspect of the result (4) is that it has a factor \( \sqrt{N} \) relative to the one-particle case. This is a consequence of the fact that any of the \( N \) spin up electrons can hop to the neighboring site, as illustrated in Fig. 1. For a bipartite system with \( N = 1 \), the ferromagnetic arrangement in Fig. 1a is favorable according to Nagaoka’s theorem. For \( N > 1 \) the situation in Fig. 1b is in general more favorable, since the hopping can then take place in \( N \) channels.

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{fig1}
\caption{Illustration how an extra electron can hop against a half-filled background. a) ferromagnetically aligned neighbor: There is only one hopping-channel. b) antiferromagnetically aligned neighbor: There are \( N \) different ways for hopping.}
\end{figure}

For one single electron in the system, the hopping energy is of the order of \( W/2 \), where \( W \) is the one-electron band width. The extra factor \( \sqrt{N} \) in Eq. (4) suggests that the hopping energy is correspondingly larger for the \( NM + 1 \) electron case and that the total energy is

\[ E(NM + 1) \approx E(NM) + NU + \sqrt{NW}/2. \]  

Analogous arguments then suggest a similar result for \( E(NM - 1) \) and we obtain

\[ E_g = U - \sqrt{NW}. \]  

As pointed out in Ref. [4], these arguments are not rigorous. As the extra occupancy moves through the system it reduces the spins along its path. There is therefore no one to one correspondence to the one-particle case. We therefore need to consider the arguments in more detail. To be specific, we consider a degenerate multiband Hubbard model

\[ H = \sum_{\langle i,j \rangle \sigma} t_{im,jm'} \psi^\dagger_{im\sigma} \psi_{jm'\sigma} + U \sum_i \left( n_{i\uparrow} n_{i\downarrow} - \frac{1}{2} \right), \]  

with hopping only between orbitals on nearest neighbor sites. In part of the discussion we furthermore consider the intraband hopping model, where \( t_{im,jm'} = \delta_{mm'} \), i.e., only hopping between orbitals with the same quantum number \( m \).

To calculate the energies of the states with an extra hole or electron, we use the Lanczos method. In this method a set of basis states \( \vert v_n \rangle \) are generated according to the prescription

\[ b_{n+1} \vert v_{n+1} \rangle = H \vert v_n \rangle - a_n \vert v_n \rangle - b_n \vert v_{n-1} \rangle \]  

where \( b_{n+1} \) is determined by the requirement that \( \vert v_{n+1} \rangle \) is normalized. In this way the Hamiltonian is transformed into a tridiagonal form, where the diagonal elements are given by \( a_n \) and the nondiagonal elements by \( b_n \). The starting state \( \vert v_1 \rangle \) is defined in Eq. (4) and \( \vert v_0 \rangle = 0 \).

This approach gives the energy of the lowest eigenstate which is nonorthogonal to the state \( \vert v_1 \rangle \). If our choice of \( \vert v_1 \rangle \) is orthogonal to the ground-state of the \( (NM + 1) \)-system, the energies of these ground-states are overestimated. We then obtain an upper limit to \( E_g \), since we know the energy of the half-filled state in the large \( U \)-limit. This remains true if the iterative steps implied by Eq. (10) are interrupted before convergence, since the lowest eigenvalue obtained from the tridiagonal matrix is decreased as more (nonzero) elements are added to the matrix. We furthermore observe that if \( \vert v_1 \rangle \) is chosen poorly in the sense that it is very different from the ground-state, the ground-state energy is still obtained after sufficiently many steps, as long as \( \vert v_1 \rangle \) is not orthogonal to the ground-state.

In the following we often use a classical Néel state to construct the states \( \langle \text{anti} \rangle \) and \( \langle 1 \rangle \). These states are convenient to handle, but not necessarily the best starting point, due to the tendency of the system to form a singlet (or a doublet with an extra electron or hole for \( N > 1 \)). Due to the arguments above this will at worst mean that we underestimate the hopping reduction of the gap.

In the case of a half-filled system with an additional hole or electron, the Coulomb energy is minimized if there are exactly \( N \) electrons per site, except for one site with the extra electron or hole. Since we consider the large-\( U \) limit we allow only such states in the following. The Coulomb energy is then a constant which we choose as energy-zero. We thus arrive at a \( t-J \) model with \( J = 0 \). Let \( T_{\text{lo}}(NM \pm 1) \) and \( T_{\text{hi}}(NM \pm 1) \) denote the lowest and highest eigenenergy of the Hamiltonian. In the large \( U \)-limit
\[ T_{\text{lo}}(NM \pm 1) = -T_{\text{hi}}(NM \mp 1). \quad (11) \]

It is therefore sufficient to study, e.g., the \((NM + 1)\)-electron case, which gives
\[ E_g = U + T_{\text{lo}}(NM + 1) - T_{\text{hi}}(NM + 1). \quad (12) \]

### III. INTRABAND HOPPING

We have studied a few small clusters of atoms, where the system is small enough to allow an exact diagonalization. We first consider intraband hopping models. In these models the one-particle band width of each channel \(m\) is the same and independent of \(N\).

#### A. Diatomic molecule

We first study the case of just two sites, orbital degeneracy \(N\) and \(2N + 1\) electrons. We form one state \(|a\rangle\), with \(N + 1\) electrons on site 1. This state is a linear combination of states, where the first state has \(N\) spin up electrons and one spin down electron with, say, \(m = 1\) on site 1 and \(N\) spin down electrons on site 2. To generate further states in \(|a\rangle\), we let one of the spin up electrons hop to site 2 and one spin down electron to site 2 hop to site 1. This gives \(N(N - 1)\) states which are added to state \(|a\rangle\). In this way we form all possible states with \(N + 1\) electrons on site 1 and include them in \(|a\rangle\). In this process we also generate all possible states with \(N + 1\) electrons on site 2, which are included in a state \(|b\rangle\). For symmetry reasons, state \(|a\rangle\) and \(|b\rangle\) include equally many terms \(L\) and therefore have the same normalization factor \(1/\sqrt{N}\).

In calculating the matrix element \(<b|H|a\rangle\), we notice that in each \((m, \sigma)\) channel except \((m = 1, \downarrow)\), there is only one electron. Each one of the \(L\) states in \(|a\rangle\) then connects to exactly \(N\) states in \(|b\rangle\), since \(N\) of the electrons (spin up or down) on site 1 can hop to site 2, and only the electron in the orbital \((m = 1, \downarrow)\) cannot hop. There are then \(NL\) contributions \(t\) to the matrix element. After taking the normalization factor into account, we then find that the matrix element is \(Nt\). The corresponding result for the gap in the large \(U\) limit is then
\[ E_g = U - 2Nt = U - NW. \quad (13) \]

The reduction of the band gap due to hopping is thus proportional to \(N\) and not \(\sqrt{N}\) as the arguments in the previous section suggested. If we start the Lanczos procedure from the antiferromagnetic state discussed before (Eq. (4)), \(b_2 = \sqrt{Nt}\). For \(n \sim N\), however, \(b_n \sim Nt\). The ground-state of the \((2N + 1)\)-electron system is a doublet. It is then not surprising that a large number of Lanczos steps is needed to generate this state from antiferromagnetic state \(|v_1\rangle\) in Eq. (4).

From the results above it is immediately clear that for sufficiently large values of \(N\), the reduction of the band gap due to hopping must at least be of the order \(Nt\) even for a larger system. This can be seen by simply, arbitrarily, picking two neighboring atoms in the system of interest and then constructing a state like above. This already gives a reduction of the band gap \(\sim Nt \sim NW\), and any improvement of this simple construction can only make the reduction larger.

#### B. “Bethe” lattice

To obtain a system where an atom has several neighbors, we have studied a simple version of a finite Bethe lattice, where atom 1 connects to \(K\) neighboring atoms, while these atoms only connect back to the first atom and has no other neighbors. We have solved this problem using exact diagonalization for a number of values of \(N\) and \(K\) and find that the results are described by
\[ E_g = \begin{cases} U - \sqrt{N + (N^2 - 1)/KW} & \text{if } K > 1; \\ U - NW & \text{if } K = 1. \end{cases} \quad (14) \]

This result shows an interesting cross over behavior. For \(N << K\), the reduction of the band gap is proportional to \(\sqrt{NW}\), as suggested by the argument in Sec. II. On the other hand, for \(N >> K\), the reduction is proportional to \(NW\), as suggested by the previous section (IIIA). The limit \(N < K\) should apply to most cases of practical interest, but the result for \(N >> K\) is also interesting.

\[
\begin{array}{ccc}
\text{a)} & \text{b)} & \text{c)} \\
\includegraphics[width=0.3\textwidth]{a.png} & \includegraphics[width=0.3\textwidth]{b.png} & \includegraphics[width=0.3\textwidth]{c.png}
\end{array}
\]

\[
\begin{array}{ccc}
\text{d)} & \text{e)} \\
\includegraphics[width=0.3\textwidth]{d.png} & \includegraphics[width=0.3\textwidth]{e.png}
\end{array}
\]

FIG. 2. Schematic picture of small clusters studied by exact diagonalization. Each circle indicates a site and the lines show the hopping between these sites.
C. Other small clusters

The results for the Bethe cluster are instructive, but because of the simplicity of the model it is not clear to what extent they apply to more realistic models. We have therefore studied a few models which are small enough to allow exact diagonalization. In Fig. 2 we show these models schematically. We define a quantity

\[ C(N) = \lim_{U \to \infty} \frac{U - E_g(N)}{U - E_g(N = 1)} \sqrt{N}. \]

where \( E_g(N) \) is the band gap for the orbital degeneracy \( N \). \( C(N) \equiv 1 \) implies that hopping reduction of the band gap is proportional to \( \sqrt{N} \). The results are shown in Fig. 3. The figure supports the results found in Sec. III for the “Bethe” lattice, in the sense that \( C(N) \) is closer to a constant the larger \( K \) is, but that \( C(N) \) grows when \( N \sim K \).

![Figure 3](image)

**FIG. 3.** The ratio \( C(N) \) between \( U - E_g \) for a given value of the orbital degeneracy \( N \) and the same quantity for \( N = 1 \) divided by \( \sqrt{N} \). Thus if the reduction of the band gap were proportional to \( \sqrt{N} \), \( C(N) \) would be identically unity. The figure illustrates how this tends to be true when the number \( K \) of nearest neighbors is much larger than \( N \). The labels refer to Fig. 2. We have also included the results for a diatomic molecule \((K = 1)\).

D. Tetrahedron

In this section we study the tetrahedron \((c)\) in Fig. 2, in somewhat more detail. This system has four sites with equal hopping matrix elements \( t < 0 \) between all the sites. In the one-particle case, there is one nondegenerate eigenvalue \( 3t \) and a three-fold degenerate eigenvalue \(-t\). The band width is then

\[ W = 4t. \]

We notice that the band width is reduced by the frustration, since it is not possible to find a fully anti-bonding state.

It is instructive to obtain this result from the Lanczos method. The nonzero coefficients \( a_n \) and \( b_n \) are shown in Table I. The process stops already after two step, since

\[ H|v_2\rangle - a_2|v_2\rangle - b_2|v_1\rangle = 0. \]

We note that in the present case an electron on a given site can hop to four other sites. The effect of one such hop is cancelled by the term \( b_n|v_{n-1}\rangle \). The remaining hops may contribute to \( b_{n+1} \) or to \( a_n \). In the present case the contribution goes to \( b_{n+1} \) in the first step but to \( a_n \) in the second step. For the many-body case the coefficients \( a_n \) are typically smaller and a larger part of the hopping contribution instead goes to \( b_{n+1} \).

For \( N = 1 \), 2 and 3 the lowest possible \((NM \pm 1)\)-energy is reached after just a few \((4-8)\) Lanczos steps, illustrating that the choice in Eq. (4) of \( |v_1\rangle \) leads to the ground-states. The situation is different for \( N = \infty \). We have calculated the first 40 coefficients \( b_{n+1} \), of which the first few are shown in Table I. At least up to \( n = 40 \) \( b_{n+1}/\sqrt{N} \) keeps increasing with \( n \), which suggests that the reduction of the band gap due to hopping grows faster that \( \sqrt{N} \), in agreement with the arguments in Sec. III.A-B that a contribution \( \sim N \) may be expected for \( N >> K \).

**TABLE I.** The coefficients \( a_n \) and \( b_n \) for a tetrahedron. Both the one-particle and \((NM \sim 1)\) many-particle problems are considered, where in the latter case the orbital degeneracies \( N = 1, 2, 3 \) and \( \infty \) are considered. The coefficients are given in units of \( \sqrt{N} \), where \( t \) is the hopping matrix element.

| \( n \) | One-particle | Many-particle |
|-------|------------|--------------|
|       | \( N = 1 \) | \( N = 2 \) | \( N = 3 \) | \( N = \infty \) |
| \( a_n \) | 1.00 | 1.73 | 0.00 | 1.73 | 0.00 | 1.58 | 0.00 | 1.53 | 0.00 | 1.41 |
| \( b_{n+1} \) | 2.00 | 0.00 | 0.67 | 1.25 | 0.57 | 1.30 | 0.49 | 1.32 | 0.00 | 1.41 |
| \( a_n \) | 3.00 | 0.19 | 1.51 | 0.44 | 1.48 | 0.45 | 1.39 | 0.00 | 1.49 | 0.00 | 1.58 |
| \( b_{n+1} \) | 4.00 | 0.25 | 1.07 | 0.31 | 1.21 | 0.24 | 1.34 | 0.00 | 1.76 |
| \( a_n \) | 5.00 | -0.11 | 0.00 | -0.17 | 0.98 | -0.00 | 1.37 | 0.00 | 1.94 |
| \( b_{n+1} \) | 6.00 | 1.15 | 0.97 | 0.55 | 1.21 | 0.00 | 1.96 |
| \( a_n \) | 7.00 | -0.17 | 0.00 | -0.20 | 0.92 | 0.00 | 2.24 |
| \( b_{n+1} \) | 8.00 | 0.94 | 0.91 | 0.00 | 2.17 |
| \( a_n \) | 9.00 | -0.16 | 0.00 | 0.00 | 2.46 |

To discuss the large \( N \)-limit, we first discuss the general situation when each site is surrounded by \( L(\leq K) \) other sites with the opposite spin. To leading order in \( N \) there are then \( L \) ways of hopping to a neighboring site increasing the number of flipped spins. In addition a spin flipped in a previous hop can be restored. This is immediately seen by applying the Hamiltonian to \( |v_2\rangle \) in Eq. (16) which can take us back to \( |v_1\rangle \). This latter contribution is cancelled by the term \(-b_n|v_{n-1}\rangle \) in Eq. (16) in the first few steps. Furthermore \( a_n/\sqrt{N} \equiv 0 \) in the \( N \to \infty \) limit, for any finite \( n \). We then find that \( b_{n+1} = \sqrt{LN}t \).
for the first few terms. This is illustrated in Table I, where $L = 2$.

If all the elements $b_{n+1}$ would stay constant in the large $N$-limit, $b_{n+1} = \alpha \sqrt{Nt} \ (\alpha \geq 0)$, it is easy to show that the lowest state has the hopping energy $-2\alpha \sqrt{Nt}$ and the band gap is $E_g = U - 4\alpha \sqrt{Nt}$ for large $U$. In reality, however, after a few steps the situation becomes more complicated than discussed above.

After three steps, terms proportional to

$$\sum_{m m' m''} \psi_{1 m}^\dagger \psi_{1 m'}^\dagger \psi_{2 m}^\dagger \psi_{2 m'}^\dagger \psi_{1 m''}^\dagger \psi_{1 m''}^\dagger |\text{anti}\rangle,$$

(18)

enter the calculation. Since the states with $m < m''$ are equal to the states with $m > m''$, the norm of the state in Eq. (18) is $4N^2(N-1)/2 \approx 2N^3$. As a result $b_3$ in Table I is $\sqrt{2.5Nt}$ instead of $\sqrt{2Nt}$.

After four steps certain states can be reached in two different ways. This is illustrated schematically in Fig. 4. The amplitudes for these states then have to be added. The contribution of such a state to $b_{n+1}^2$ is then not $\sim (1^2 + 1^2)$ as assumed above but $\sim 2^2$. This increases the value of $b_{n+1}$. In addition, the restoration of a flipped spin can be done in different ways, leading to new states not contained in $b_n|v_{n-1}\rangle$ in Eq. (14). This is illustrated in Fig. 5 and it also increases $b_{n+1}^2$.

**FIG. 4.** The arrows illustrate how the double extra occupancy hops from site 1 to 2 and back, followed by a hop to 3 and back. In each hop a spin is reduced. The same final state can be obtained by hops $1 \to 3 \to 1 \to 2 \to 1$, and the corresponding amplitudes are added.

**FIG. 5.** a) Shows one contribution to $|v_n\rangle$. b) and c) show contributions to $H|v_n\rangle$. b) Shows how a contribution in $|v_{n-1}\rangle$ can be recovered by allowing the extra occupancy to hop back from site 2 to site 3 and thereby increasing the spins of sites 2 and 3. c) Shows how the extra occupancy instead can hop to site 1, increasing the spins of site 1 and 2 and creating a new state in $|v_{n+1}\rangle$.

### E. Bipartite and non-bipartite systems

A bipartite system is a system where it is possible to partition the system in two sublattices with hopping only between the sublattices. Nagaoka’s theorem states that for such a system with the orbital degeneracy $N = 1$ and $U = \infty$, the system is ferromagnetic when it has one electron or one hole relative to half-filling. The electron or the hole then have the same hopping possibilities as in the one-electron case and it follows that in the large $U$-limit $E_g = U - W$, with the prefactor exactly equal to one. For $N > 1$ or for many of the cases with $N = 1$ but a non-bipartite lattice, where the Nagaoka’s theorem has not been proven, the reduction of $E_g$ due to hopping is larger than $W$. This illustrates that Nagaoka’s theorem is not valid in these cases. Cases with $N = 1$ but a non-bipartite lattice are studied below.

For a bipartite lattice where all nonzero hopping integrals are equal, we can always construct states which are fully bonding or antibonding, by letting the coefficients of the orbitals on the two sublattices have the same or the opposite sign. This is in general not possible for a non-bipartite lattice. For instance, for the tetrahedron we found a bonding state with the energy $3t$ but the antibonding states have only the energy $-t$. In the Lanczos formalism, this result comes about because an electron can hop in a closed loop using an odd number of
hops. This leads to nonzero coefficients $a_n$, which makes the spectrum nonsymmetric around $\varepsilon = 0$. This also reduces the coefficients $b_{n+1}$ as discussed in Sec. III.D. In the many-body case, the hopping of an electron along a closed loop usually does not bring us back to the original state, since spins have been flipped along the path of the electron. This tends to reduce the values of $a_n$ and to increase $b_n$, as is illustrated in Table II. Even for $N=1$, hopping may therefore reduce the band gap more than one would expect from the one-particle band width. This is illustrated in Table II. In the cases we have studied the effect is of the order 15-30%.

TABLE II. The reduction $U - E_g$ due to hopping for $N=1$ relative to the one-particle band width $W$ for some non-bipartite systems. The notations of the systems refer to Fig. 2 and “triang” refers to a system with three atoms coupling to each others.

| System | $[U - E_g(N=1)]/W$ |
|--------|---------------------|
| c      | 1.25                |
| d      | 1.15                |
| e      | 1.19                |
| triang | 1.33                |

IV. INTERBAND HOPPING

In the previous sections, we have for simplicity assumed that there is only hopping between orbitals on different sites with the same $m$ quantum number. Here we consider the more general case of hopping also between different $m$ quantum numbers. We first consider the step in the Lanczos procedure. In the one-particle case, this gives

\[ (b_2^{(m)})^2 = \sum_{imu'} |t_{1mu'}|^2, \tag{19} \]

where the electron is located in orbital $m$ on site 1 in the starting state. In the many-body case, we start from the state in Eq. (3) and obtain

\[ (b_2)^2 = \sum_{imu'} |t_{1mu'}|^2. \tag{20} \]

We compare this with the average of the coefficients $(b_2^{(m)})^2$ in the one-particle case

\[ \frac{1}{N} \sum_m (b_2^{(m)})^2 = \frac{1}{N} (b_2)^2, \tag{21} \]

i.e., $b_2$ is typically a factor $\sqrt{N}$ larger in the many-body case than in the one-particle case. This is the same factor as was found when the hopping between different $m$-quantum numbers was neglected. The inter-orbital hopping increases $b_2$ by a factor $\sqrt{N}$ in both the one-particle and many-body cases, but leaves their ratio ($= \sqrt{N}$) unchanged.

TABLE III. The band gap for a six-atom cluster (d) in Fig. 2. In all cases the absolute value of the hopping matrix elements is $t$. In the “sp”-model we have chosen the signs as if the two orbitals had $s$- ($N=1$) and $p$- character ($N=2$). In the “rand” model the signs were chosen randomly. For this model $K = 4$ and for the “sp”-model $K$ is effectively somewhat smaller.

| Syst | $d(N) = |U - E_g|/(W(N)\sqrt{N})$ | $d(2)/d(1)$ |
|------|---------------------------------|-------------|
| sp   | 1.15 1.31 1.14                  |             |
| “rand” | 1.23 1.10 0.89                |             |

In Eqs. (19,20) the sign of $t_{imu',jmu''}$ does not matter. When we continue to higher coefficients $b_n$ the sign becomes important and we have to specify the model in more detail. We can, for instance, specify the orbitals involved and the geometrical structure of the lattice. In Table III we show results for the lattice d) in Fig. 2, including a $s$-orbital and a $p$-orbital with the lobe along the direction of the three atoms. This defines the signs of the hopping integrals. The magnitudes are assumed to be identical. Alternatively, we can pick the sign randomly. The latter procedure is appropriate when we want to vary $N$, since it is not clear how to define an appropriate set of orbitals for an arbitrary value of $N$. Table III shows the ratio

\[ d(N) = \frac{U - E_g(N)}{W(N)\sqrt{N}}, \tag{22} \]

where $W(N)$ is the one-particle band width for the orbital degeneracy $N$. In contrast to the intraband model, the one-particle band $W(N)$ width now depends on $N$. We also show the ratio $d(2)/d(1)$, which would be unity if the reduction of band gap due to hopping were proportional to $\sqrt{NW(N)}$. This is roughly the case in Table III, but the results are too limited to allow more definite conclusions.

For the diatomic molecule, discussed in Sec. III.A, and the “Bethe” lattice, discussed in Sec. III.B, we can go to larger values of $N$. The results are shown in Fig. 3. These results support a reduction of the band gap due to hopping which is at least proportional to $\sqrt{NW(N)}$. Although the results are still too limited to draw definite conclusions, they do not support a behavior proportional to $NW(N)$. The $NW(N)$ behaviour found for the diatomic molecule with only intraband hopping, is therefore probably an artifact of the simple model used in that case.
V. DISCUSSION

Above we have studied two types of models, namely models with only intraband hopping (between orbitals with the same quantum number \( m \)) and models also with interband hopping. We have calculated the reduction of the band gap due to hopping in the large-\( U \)-limit for different orbital degeneracies \( N \) and for lattices with different number \( K \) of nearest neighbors. In the intraband models we find that the hopping contribution grows at least as \( \sqrt{NW} \), where \( W \) is the one-particle band width. For \( N > K \) there is an interesting crossover, and the hopping contribution grows as \( NW \). This limit should not, however, apply to most systems of interest. In the interband models the hopping contribution seems to be closer to a \( \sqrt{NW} \) behavior than a \( NW \) behavior even when \( K \) is small. Our present results therefore support a degeneracy dependence of roughly \( \sqrt{NW} \) or a somewhat stronger \( N \) dependence for most systems.

It has been suggested that in a strongly correlated system the hopping should be strongly suppressed and it should not reduce the band gap much. For instance, in models of the High-\( T_c \) compounds, e.g., the \( t-J \) model, it is found that the string of flipped spins in the trace of a moving particle tends to strongly reduce the dispersion of this particle and that in addition the weight of the quasi-particle is strongly reduced. This might suggest that hopping is very inefficient in this case. In the present problem we are, however, not interested in the quasi-particle dispersion but in total energies (Eq. (3)). The total energy can be obtained by integrating the Green’s function over frequencies and momenta. Since the weight of the quasi-particle is strongly reduced in correlated systems, this means that the spectral function must have substantial weight also for other frequencies. To argue in terms of the quasi-particle alone neglects important contributions to the total energy. It is then more convenient to follow the Lanczos approach used here, which gives an important hopping contribution to the band gap.

It is, nevertheless, true that hopping is suppressed in for large \( U \), as one would expect for strongly correlated systems. The band gap is, however, an energy difference between ground-state energies, where hopping has been suppressed differently. Thus hopping is suppressed very strongly in the \( NM \)-particle state and less strongly in the \( (NM \pm 1) \)-particle states, so that in the difference (Eq. (3)) it appears as if the hopping had been enhanced.

The reduced spins along the path of a moving extra occupancy plays two different roles. One role is that when the extra occupancy moves along different paths to a given site, the resulting states depend on this path. This is in contrast to the one-electron problem, and it has appreciable effects on the Lanczos matrix elements \( a_n \) and \( b_{n+1} \). This is seen in the greater tendency to put weights into the diagonal elements \( a_n \) in the one-particle case, and a reduction of the one-particle band width for non-bipartite lattices. For the non-bipartite clusters considered here, the hopping reduction of the band gap is therefore \textit{larger} than the single-particle band width, even for \( N = 1 \), contrary to the intuitive feeling that the flipped spins should reduce the hopping contribution (see Table II). The second effect is that the reduction of spins costs energy. This does not enter for \( U \rightarrow \infty \), since the energy cost (\( \sim t^2/U \)) for flipping the spin of one electron then goes to zero. Even for finite values of \( U \) this does not enter in the first element \( a_1 \), but gradually becomes more important for the higher coefficients. Normally, however, the spin flip energy is small compared with the band width \( W \). Since the nondiagonal elements \( b_{n+1} \) are of the order \( \sqrt{NW} \) or larger, these elements should tend to dominate the spin-flip energy, in particular in the large degeneracy limit.

\begin{figure}
\centering
\includegraphics[width=\textwidth]{figure6.png}
\caption{The ratio \( d(N) \) (Eq. (4)) between the reduction of the band gap due to hopping and \( \sqrt{NW} \). The figure shows results for the diatomic molecule \((K = 1)\) and the “Bethe” lattice with \( K = 2 \) and \( K = 3 \).}
\end{figure}

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