Exact Ground State Energy of Hubbard Rings in the Atomic Limit

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Using a straightforward extension of the analysis of Lieb and Wu, we derive a simple analytic form for the ground state energy of a one-dimensional Hubbard ring in the atomic limit. This result is valid for an arbitrary number of lattice sites \( L \) and electrons \( N \leq L \). Furthermore, our analysis, including an application of the theory of stochastic matrices, provides insight into the degeneracy and spin properties of the ground states in the atomic limit. We give numerical results which illustrate how the atomic limit is approached.

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I. INTRODUCTION

For nearly fifty years, the Hubbard model has been used to describe many-body effects in solids, capturing the dominant competition between the delocalizing effects of the kinetic energy (with strength described by a hopping energy \( t \)) and the localizing effects of the electron-electron repulsion (with strength described by an on-site Coulomb energy \( U \)). Despite its simple form, the Hubbard model has provided significant insight into many-body properties of solids such as metal-insulator transitions, high-temperature superconductivity, and magnetic states largely because of the accessibility of its analytic and numerical solutions.

The analytic understanding of the Hubbard model stems primarily from the seminal work of Lieb and Wu, who derived a “Bethe ansatz” method for determining eigenvalues and eigenfunctions of the single band, one-dimensional Hubbard model with \( L \) lattice sites and \( N \) electrons. They obtained an explicit expression for the ground state energy for a half-filled system in the thermodynamic limit (\( N = L \rightarrow \infty \)). In the intervening years, many authors have extended the Lieb-Wu analysis. For example, Essler, Korepin, and Schoutens have shown that for even \( L \) and periodic boundary conditions, it is possible to find operators to extend the Bethe ansatz solutions and to find a complete set of eigenstates for the model. Lieb and Wu and Goldbaum have presented some existence proofs for Bethe ansatz solutions for ground states. In addition, many authors have applied the Lieb-Wu equations to particular systems.

In the present paper, we reanalyze the Lieb-Wu solutions to the single band, one-dimensional Hubbard model for the case that there are \( L \) lattice sites (\( L \leq \infty \)) with periodic boundary conditions and \( N \) electrons (\( N \leq L \)) in the limit \( U/t \equiv u \rightarrow \infty \). This represents the strongly correlated regime of the system for which we find that the exact ground state energy can be expressed by the simple analytic form

\[
E_g = -2t \frac{\sin \left( \frac{\pi N}{L} \right)}{\sin \left( \frac{\pi}{L} \right)}.
\]  

II. DERIVATION OF GROUND STATE ENERGY

The Hamiltonian of the Hubbard model is

\[
H = H_{\text{hop}}(t) + H_{\text{int}}(U) = -t \sum_{\langle q,r \rangle} c_{q,\sigma}^\dagger c_{r,\sigma} + U \sum_q n_{q,\uparrow} n_{q,\downarrow},
\]

where \( c_{q,\sigma}^\dagger \) (\( c_{q,\sigma} \)) creates (annihilates) an electron with spin \( \sigma \) in the Wannier state localized at lattice site \( q \), and \( \langle q,r \rangle \) denotes that a sum is over nearest neighbor sites only. For the case of a one-dimensional system with periodic boundary conditions, the site index \( q \) (or \( r \)) takes values \( 1 \leq q \leq L \) and indices \( q \) and \( q + L \) are equivalent.

Lieb and Wu considered solutions to the one-dimensional Hubbard model for a specified electron spin distribution with \( N_{\uparrow} \) and \( N_{\downarrow} \) indicating the total number of up and down \( z \)-component spin orientations, respectively, where \( N = N_{\uparrow} + N_{\downarrow} \). Applying the Bethe ansatz,
the total energy eigenvalues are written in a form identical to that for independent electrons:

\[ E(N_1, N_\uparrow) = -2t \sum_{j=1}^{N} \cos k_j. \quad (3) \]

The so-called charge momenta \( k_j \), however, are not the wavevectors one finds in the absence of electron-electron interactions. To find the charge momenta requires solving the set of coupled nonlinear equations (the Lieb-Wu equations)

\[ Lk_j(N_1, N_\uparrow) = 2\pi I_j + 2 \sum_{\beta=1}^{N_1} \tan^{-1} \left( \frac{4}{u} (\lambda_\alpha - \sin k_j) - \lambda_\beta \right), \quad (4) \]

and

\[ 2 \sum_{j=1}^{N} \tan^{-1} \left( \frac{4}{u} (\lambda_\alpha - \sin k_j) \right) = 2\pi J_\alpha \]

\[ + 2 \sum_{\beta=1}^{N_1} \tan^{-1} \left( \frac{2}{u} (\lambda_\alpha - \lambda_\beta) \right). \quad (5) \]

In this formulation, Lieb and Wu assume \( N \leq L \) and \( N_1 \leq N_\uparrow \). The parameter \( I_j = I_j(N_1) \) is an integer (half-odd-integer) if \( N_\uparrow \) is even (odd), where \( 1 \leq j \leq N \). The parameter \( J_{\alpha} = J_{\alpha}(N_1) \) is an integer (half-odd-integer) if \( N_1 = N - N_\uparrow \) is odd (even), where \( 1 \leq \alpha \leq N_1 \). The \( \lambda_\alpha \)'s are a set of ordered, unequal real numbers \( \lambda_1 < \lambda_2 < ... < \lambda_{N_1} \). Details of the derivation of these equations are given in Yang’s examination of a one-dimensional system with delta function interaction\(^{19}\) as well as a more recent review of the Hubbard model by Lieb and Wu\(^{20}\).

In the present paper, we focus on the limit \( u \rightarrow \infty \), henceforth referred to as the atomic limit. This limit, which represents a highly correlated system, simplifies the mathematical properties of the Hubbard model considerably. In particular, since we are considering the case where \( N \leq L \), it is reasonable to assume that the charge momenta for the ground state are real so that terms of the form \( (\sin k_j) / u \) in Eqs. (4) and (5) vanish in the atomic limit. This assumption is not valid if \( N > L \) since the ground state energy is linear in \( u \), making the \( k_j \)'s necessarily complex\(^{10}\). As a result, Eq. (4) simplifies to

\[ 2N \tan^{-1} \left( \frac{4\lambda_\alpha}{u} \right) = 2\pi J_\alpha + 2 \sum_{\beta=1}^{N_1} \tan^{-1} \left( \frac{2}{u} (\lambda_\alpha - \lambda_\beta) \right). \quad (6) \]

By substituting this expression into Eq. (6), we obtain an equation for the charge momenta at \( u = \infty \):

\[ k_j(N_1, N_\uparrow) = \frac{2\pi}{L} \left[ I_j + \frac{1}{N} \sum_{\beta=1}^{N_1} J_\beta \right]. \quad (7) \]

In order to analyze the ground state, one possibility\(^3\) is to choose \( I_j \) and \( J_\alpha \) to be consecutive integers (or half-odd-integers) centered around the origin. We will consider other possibilities later. With this choice, if \( N \) is even,

\[ \sum_{\beta=1}^{N_1} J_\beta = 0; \quad (8) \]

otherwise, if \( N \) is odd,

\[ \sum_{\beta=1}^{N_1} J_\beta = \frac{N_1}{2}. \quad (9) \]

It thus follows that the charge momenta have the following relationships

\[ k_j(N_1, N_\uparrow) = \begin{cases} \frac{2\pi I_j}{L}, & N \text{ even} \\ \frac{2\pi}{L} \left( I_j + \frac{N_1}{2N} \right), & N \text{ odd}. \end{cases} \quad (10) \]

For a given system of \( L \) sites and \( N \leq L \) electrons, we now show that the lowest energy obtained by substituting the charge momenta given in Eq. (10) into the energy expression given in Eq. (3) is not necessarily the energy of the ground state. To do so, we present some examples where this is not the case.

First, we consider a configuration with all electrons having the same spin \( (N_1, N_\uparrow) = (0, N) \). The eigenstates of the Hubbard model in this configuration can be represented in terms of an antisymmetrized product of independent electron states in a Bloch basis, where the single particle energies are given by

\[ \epsilon_j = -2t \cos \left( \frac{2\pi j}{L} \right). \quad (11) \]

In this expression, the \( j \)'s are a set of any \( L \) consecutive integers. The minimum energy of this system is thus obtained by summing \( N \) terms of the Bloch contributions\(^{11}\), resulting in the analytic form for \( E_{\text{min}}(0, N) \):

\[ \begin{cases} -2t \sum_{j=-\frac{L}{2}+1}^{\frac{L}{2}} \cos \left( \frac{2\pi j}{L} \right) = E_g \cos \left( \frac{\pi}{L} \right), & N \text{ even} \\ -2t \sum_{j=-\frac{N-1}{2}}^{\frac{N-1}{2}} \cos \left( \frac{2\pi j}{L} \right) = E_g, & N \text{ odd}, \end{cases} \quad (12) \]

where \( E_g \) is the energy given in Eq. (11). The form of Eq. (12) shows an interesting simplification: if \( N = L - 1 \) is odd, then \( E_{\text{min}}(0, N) = -2t \). Interestingly, Trugman\(^{20}\) proved the general result that the lowest bound energy of the ground state of the one dimensional Hubbard model in the atomic limit is exactly \(-2t(L - N)\), where \( L - N \) is
we consider the relationships between systems and the number of holes. Therefore it follows that the ground state energy of a one-hole system with an odd number of electrons must be \( E_g = -2t \). Furthermore, there must exist precisely one state with that energy with maximal total spin.

We continue our examination of a one-hole system with the special case \( N = L - 1 = 4n + 1 \) and \( N_1 = 2n \), where \( n \) is an integer. In this case, Eq. (10) becomes

\[
k_{ij}(2n, 2n + 1) = \frac{2\pi}{4n + 2} \left[ j + \frac{n}{4n + 1} \right],
\]

where \( j \) is an integer. We find the possible energies of the system by summing over \( j \) in the formula given in Eq. (8); the lowest energy obtained is plotted in Fig. 1 as a function of \( n \). Inspection of this plot reveals that using the charge momenta given in Eq. (13) to evaluate Eq. (3) results in energies that are above the ground state energy of \(-2t\), except in the one-electron case \( (n = 0) \) and the thermodynamic limit \( (n = \infty) \). The failure of this example for systems of finite size, indicates that Eq. (10) should be reexamined.

To address this problem, we recall that the Hubbard Hamiltonian obeys the commutation relations

\[
[\mathcal{H}, \mathbf{S}^2] = [\mathcal{H}, S_z] = [\mathcal{H}, S_{\pm}] = 0,
\]

where \( \mathbf{S}^2 \) and \( S_z \) are the operators for total spin and \( z \)-component of spin, and \( S_{\pm} \) are the spin raising and lowering operators. Because of these relations, it is possible to find the energy eigenstates of the Hubbard Hamiltonian which are also eigenstates of \( \mathbf{S}^2 \) and \( S_z \) with quantum numbers \( S \) and \( M_S \), respectively.

The use of the charge momenta relations in Eq. (10) does not take this spin symmetry into account. In order to include this symmetry in the Bethe ansatz formulation, we consider the relationships between systems having different spin configurations. We assume that the energy eigenfunctions \( \psi(N_{\uparrow}, N_{\downarrow}) \) are known

\[
\mathcal{H}\psi(N_{\uparrow}, N_{\downarrow}) = E\psi(N_{\uparrow}, N_{\downarrow}),
\]

and are simultaneously eigenfunctions of \( \mathbf{S}^2 \) with total spin quantum number \( S \). Applying the spin-raising operator \( S_{\uparrow} \) to Eq. (15), one of two things occurs: either the eigenfunction \( \psi(N_{\uparrow}, N_{\downarrow}) \) is annihilated if it has minimal total spin quantum number \( S = \frac{1}{2}(N_{\uparrow} - N_{\downarrow}) \), or we obtain the eigenvalue equation

\[
\mathcal{H}\psi(N_{\uparrow} - 1, N_{\downarrow} + 1) = E\psi(N_{\uparrow} - 1, N_{\downarrow} + 1),
\]

where \( E \) is the same energy that appears in Eq. (15). Therefore, the set of eigenvectors and eigenvalues that solves Eq. (10) is a subset of the set of eigenvectors and eigenvalues that solves Eq. (15). This process can be
repeated to span all of the possible related spin configurations corresponding to the same energy eigenvalue $E(M, M') = E(N_1, N_1)$, where the possible values of $(M, M')$ are determined from limits of the raising operations to be $0 \leq M \leq N_1$, $N_1 \leq M' \leq N$, and $M + M' = N$.

In determining the ground state energy of our system, we are not actually constructing the eigenstate wavefunctions, but searching for the minimum energy represented by Eq. (3) through the use of the charge momenta in Eq. (3). We write the charge momenta configurations corresponding to the same energy eigenvalue where the values of the momenta $\mu$ are consistent with the modified Bethe ansatz charge equation which is realized when $\frac{j}{L} = \frac{2 \pi}{\sqrt{2}}$.

This expression has a minimum when

$$k_j(N_1, N_1) = \begin{cases} \frac{2\pi I_j}{L}, & N \text{ even} \\ \frac{2\pi}{L} \left( I_j + \frac{M}{2N} \right), & N \text{ odd.} \end{cases} \quad (17)$$

where $0 \leq M \leq N_1$.

With this modified result, we now minimize the system energy in Eq. (3). We write the charge momenta appearing in Eq. (3) in a general form consistent with Eq. (17)

$$k_j = \frac{2\pi}{L} \left( j + j_0 \right), \quad (18)$$

where the $j$’s are positive integers and $j_0$ is a real number. With this choice of charge momenta $k_j$, Eq. (3) can be summed as a geometric series resulting in the energy equation

$$E = -2t \sum_{j=1}^{N} \cos \left[ \frac{2\pi}{L} \left( j + j_0 \right) \right]$$

$$= -2t \frac{\sin \left( \pi N / L \right)}{\sin \left( \pi / L \right)} \cos \left[ \frac{2j_0 + N + 1}{L} \pi \right]. \quad (19)$$

This expression has a minimum when

$$j_0 = -\frac{N + 1}{2}. \quad (20)$$

Now we must check whether this mathematical minimum is consistent with the modified Bethe ansatz charge momenta $k_j(N_1, N_1)$ given by Eq. (17). First consider the case of $N$ even. For this case Eq. (20) is a half-odd-integer and $I_j(M) = j + j_0$ must be a half-odd-integer, which is realized when $M$ is odd. Since for all even $N > 0$, there is at least one choice of odd $M$ in the range $0 \leq M \leq N/2$, this case is consistent with the modified Bethe ansatz solution. Now consider the case of $N$ odd. For this case, Eq. (20) must be an integer and $I_j(M) + M/(2N) = j + j_0$ must be an integer, which is realized when $M = 0$. To summarize all of these possibilities we conclude that the charge momenta corresponding to the ground state can be chosen using consecutive integers $j$ centered at the origin of the form

$$k_j(N_1, N_1) = \begin{cases} \frac{2\pi}{L} \left( j + \frac{1}{2} \right), & N \text{ even} \\ \frac{2\pi j}{L}, & N \text{ odd,} \end{cases} \quad (21)$$

Using these charge momenta, and minimizing Eq. (3), we obtain the ground state energy expression in Eq. (1). This concludes our derivation.

Additional confirmation of Eq. (1) was obtained by direct diagonalization of the Hubbard Hamiltonian in the $u \to \infty$ limit. Furthermore, it is easy to show that Eq. (1) is consistent with previously found lower bounds to the ground state energy. In Fig. 2 a comparison between the lowest energies found using Eqs. (3) and (10), and the energy found using Eq. (1) is shown for $L = 10$ and $L = 15$ at various lattice densities. On this scale, the error introduced by using Eq. (10) is small but non-trivial.

In addition to the analysis presented above, there are other possible ways to find the ground state energies from the Lieb-Wu equations. Instead of restricting the $J_\alpha$’s to be consecutive integers or half-odd-integers centered around the origin as assumed in the above derivation of Eq. (1), it is also possible to find energies (including the ground state energy) using Eqs. (3) and (10) but with non-consecutive $J_\alpha$’s. In Table I we list several examples of this situation. In all cases we have investigated, the ground state energies determined in this way are consistent with Eq. (1). One might hope that such an approach could generate excited states in addition to the ground

| $L$ | $N$ | $E_g/t$ | $N_1$ ($N_1$) | $J_\alpha$ | $E_{\text{min}}/t$ |
|-----|-----|--------|----------------|----------|----------------|
| 4   | 2   | -3.46410 | 2 (2) | $-\frac{1}{2}, \frac{1}{2}$ | -3.00000 |
| 6   | 3   | -2.00000 | 2 (3) | 0, 1 | -1.1 - 2.00000 |
| 7   | 4   | -4.49396 | 2 (2) | $-\frac{1}{2}, \frac{3}{2}$ | -4.04892 |
| 8   | 5   | -3.60388 | 2 (3) | 0, 1 | -3.54596 |
| 8   | 6   | -2.00000 | 2 (4) | $-\frac{1}{2}, \frac{3}{2}$ | -1.80194 |
| 10  | 7   | 49396 $2 \pm 2$ | $-\frac{1}{2}, \frac{3}{2}$ | -1.91115 |
| 10  | 8   | 49396 $2 \pm 2$ | $-\frac{1}{2}, \frac{3}{2}$ | -1.97766 |
| 10  | 9   | 49396 $2 \pm 2$ | $-\frac{1}{2}, \frac{3}{2}$ | -2.00000 |

TABLE I: Examples of minimum energies obtained using Eqs. (3) and (10) and particular choices of the $J_\alpha$ parameters. The ground state energies $E_g$ were found using Eq. (1) and verified by exact diagonalization.
FIG. 3: Plot of the lowest energies as a function of $u$ for (top) $N = L = 5$ and (bottom) $N = L = 6$. A thick (red) line represents a maximal spin $S = N/2$ state; a dotted (green) curve represents a $S = (N - 2)/2$ state; a dashed (blue) curve represents a $S = (N - 4)/2$ state. In the bottom plot, a solid (black) curve represents a $S = (N - 6)/2 = 0$ state. Symbols denote a doubly degenerate energy. Arrows mark the energies obtained by Eq. (1).

FIG. 4: Plot of the lowest energies as a function of $u$ for (top) $N = L - 1 = 5$ and (bottom) $N = L - 1 = 6$, using the same line (color) style as Figure 3. The degeneracy of the ground state in the atomic limit is given by Eqs. (28) (top) and (33) (bottom).

III. NUMERICAL EXAMPLES

In order to understand the results presented here, we consider some specific examples. Throughout this section, we assume, without loss of generality, that $N_\uparrow - N_\downarrow = 0$ (+1) if $N$ is even (odd). For ground states in the atomic limit, the probability of two electrons occupying the same lattice site vanishes. Therefore, there are only two configurations for a lattice site: vacant (henceforth referred to as a hole) or singly occupied. In general, for a system of $n$ holes, the ground state is highly degenerate, with a degeneracy denoted by $d^{(n)}$.

We begin our examination with the simplest case (half-filling) where the number of holes is zero. For any half-filled system in the atomic limit, the ground states have energy $E_g = 0$. The degeneracy of the ground states is the number of possible ways of filling $N = L$ holes with $N$ indistinguishable spin-1/2 particles

$$d^{(0)} = \frac{N!}{N_\uparrow!N_\downarrow!}.$$  (22)

In Figure 3 the energies of these $d^{(0)}$ states, that become the ground states in the atomic limit, are plotted as a function of $u$ for two small half-filled systems: $N = 5$ and $N = 6$. Results were obtained by exact diagonalization. In either case, the degeneracy of the ground state in the atomic limit is given by Eq. (22): for $N = 5$,
Turbed Hamiltonian. The unperturbed we use perturbation theory, taking any ground states in the atomic limit for $E_{\text{tem}}$ is given by the number \( N \). According to Eq. (1), the energy of the ground states is

\[ E_{\text{tem}} = \frac{1}{2} \left( \sum_{i \neq j} t_{ij} \delta_{\sigma_i \sigma_j} + \sum_{i} \delta_{\sigma_{i+1} \sigma_i} \right) \]

This unperturbed degeneracy is

\[ N = \begin{cases} 4 & \text{for } N = 5; \\ 6 & \text{for } N = 6 \end{cases} \]

It is odd, first. Then, it is easy to show that the number of connected arrangements in each spin configuration is

\[ C = NL = N(N+1); \quad (27) \]

this expression is valid provided that $N_{\sigma} \neq 0$ and $N_{\uparrow}/N_{\downarrow}$ and its inverse are not integers for $N_{\sigma} > 1$. With the assumption that $N_{\uparrow} = N_{\downarrow} + 1$, this expression is necessarily valid for an odd number of electrons. Therefore, the number of distinct spin configurations is

\[ \frac{D}{C} = \frac{(N-1)!}{N_{\uparrow}!N_{\downarrow}!} = d^{(1)}; \quad (28) \]

the last equality will be shown below.
Returning to Eq. (29), we factor the first-order correction as
\[ \mathcal{W}_{kl}^{(1)} = -2t(k)\mathcal{H}_{\text{hop}}(-\frac{1}{2}) |\ell\rangle; \] (29)
the lowest eigenvalue of \( \mathcal{W}_{kl}^{(1)} \) corresponds to the maximum eigenvalue of the dimensionless operator \( \mathcal{H}_{\text{hop}}(-\frac{1}{2}) \). By appropriately choosing the unperturbed basis defined in Eq. (23), it can be shown that if \( N \) is odd, then each row and column of \( \mathcal{H}_{\text{hop}}(-\frac{1}{2}) \) consists of only two nonzero elements, which have the value \( \frac{1}{2} \). Therefore,
\[ \langle k |\mathcal{H}_{\text{hop}}(-\frac{1}{2}) |\ell\rangle \geq 0, \] (30)
and the sum of the elements in every row or column is 1
\[ \sum_{|k\rangle} \langle k |\mathcal{H}_{\text{hop}}(-\frac{1}{2}) |\ell\rangle = 1 \] (31)
and
\[ \sum_{|\ell\rangle} \langle k |\mathcal{H}_{\text{hop}}(-\frac{1}{2}) |\ell\rangle = 1. \] (32)

Nonnegative matrices that satisfy either Eq. (31) or Eq. (32) are known as stochastic matrices\(^{22}\) and are well studied. These matrices describe the transitions of a Markov chain; their elements are the transition probabilities that a system will jump from one state to another. Equations (31) and (32) state that the total probability of transition is unity. By the Perron-Frobenius theorem\(^{22}\), the maximal eigenvalue of these matrices is always 1, with the corresponding unnormalized eigenstate being the unity vector, whose elements are all 1.

Since each block is a stochastic matrix, we conclude that the ground state is \( d^{(1)} \)-fold degenerate. Furthermore, from Eq. (29), the energy of the ground state is \(-2t\), in agreement with Eq. (1). For the case \( N = L - 1 = 5 \) and \( N_1 = N_1 + 1 = 3 \), Eq. (28) predicts that in the atomic limit, \( d^{(1)} = 2 \), which is confirmed in Figure 3. For small values of \( u > 0 \), the ground state energy is two-fold degenerate. As we increase \( u \), an energy crossing occurs in the vicinity \( u \approx 100 \) and a different state becomes the ground state. As \( u \to \infty \), this state converges to the energy of the lowest-energy maximal spin state, which is \(-2t\). In the atomic limit, the higher energy states plotted in Figure 3 have energy \(-1.95630\); this result corresponds to the case of \( n = 1 \) in Figure 1 which was obtained by using the charge momenta in Eq. (16). This was identified as the ground state in the atomic limit in Ref. 21.

For an even number of electrons, the situation is slightly more complicated, since Eq. (27) is not valid for every spin configuration. Particular spin configurations may have additional periodicities that decrease the number of connected states in that configuration. However, with our assumption that \( N_f = N_1 \), we find that if \( N_\sigma \) is prime, then there is only one spin configuration which does not obey Eq. (27). This configuration contains all

![FIG. 6: Possible one-dimensional spin arrangements for \( N = L - 1 = 7 \) and \( N_1 = 3 \). Arrangements (1) through (4) each represent a different spin configuration for this system; arrangements (5) and (5) represent the fifth and final spin configuration. Arrangements (1) through (4) are disconnected from one another and from arrangements (5) and (5); arrangements (5) and (5) are connected to one another.](image)

the states defined in Eq. (24) where every pair of electron neighbors have opposite spin (a one-hole antiferromagnetic chain). Obviously, the number of connected states in this spin configuration is \( 2L \). Therefore, the degeneracy is
\[ d^{(1)} = \frac{D - 2L}{C} + 1 = \frac{(N - 1)!}{N_1!N_1!} - \frac{2}{N} + 1. \] (33)

For the case of \( N = L - 1 = 6 \) and \( N_\sigma = 3 \) (shown in Figure 1), \( d^{(1)} = 4 \).

The case of two holes in the atomic limit is much more complex, and the methods used for one hole are not applicable. In Figure 5 the lowest energies of two small two-hole systems, \( N = L - 2 = 5 \) and \( N = 6 \), are plotted as a function of \( u \). In general, the low-lying energies in Figure 5 show a striking similarity to the one-hole energies plotted in Figure 4. Again, we find that in the case \( N = L - 2 = 5 \), there is an exchange of ground states in the vicinity \( u \approx 100 \).

IV. DISCUSSION AND CONCLUSIONS

The form of the ground state energy given by Eq. (1) and its derivation provides additional insight into the nature of the eigenstates of the one-dimensional Hubbard model in the atomic limit. The form of the energy Eq. (1) shows that there is an electron-hole symmetry in the ground state energy such that the energy of a system with \( N \) electrons is identical to a system with \( L - N \) electrons, corresponding to \( L - N \) and \( N \) holes, respectively. In the course of deriving Eq. (1), we used Eq. (12) to show that for an odd number of electrons, \( N \),
at half-filling \((N = L)\), the maximal total electron spin configuration has the ground state energy given in Eq. \(\ref{eq:1}\) for any system size \(L \geq N\). The conclusion that for an odd number of electrons in the atomic limit, exactly one of the ground states (not counting the trivial \(2S_{\text{max}} + 1 = N + 1\) degeneracy) has maximal total spin has also been discussed by previous authors. If \(N\) is even (except for the case of half-filling), the minimum energy of a state with maximal total spin is above the ground state energy, as shown in Eq. \(\ref{eq:1}\).

Numerical results illustrate the asymptotic behavior of the energies of the ground state and low-lying excited states as \(u \to \infty\). In all the cases presented, the absolute error per particle of the \(u = \infty\) energy given in Eq. \(\ref{eq:1}\) to the exact energy of the ground state at \(u = 100\) is less than 0.03\% per particle.

Due to its rich structure and relative simplicity, there is an impressive literature devoted to solutions of the one-dimensional Hubbard model. To the best of our knowledge, Eq. \(\ref{eq:1}\) and the derivation presented here has not appeared in the previous literature. On the other hand, there are closely related works. For example, Kotrla\(^\text{14}\) extended the approach of Caspers and Iske\(^\text{12}\) to consider the \(u \to \infty\) limit of the one dimensional Hubbard model from the view point of enumeration of all possible single occupancy states of the system. The analysis of the minimum energy configuration results in an expression that is equivalent to our Eq. \(\ref{eq:1}\) although the explicit analytic form is not given. Another related result is by Schadschneider\(^\text{15}\), who augments the electron hopping term of the original Hubbard model in Eq. \(\ref{eq:2}\) with a bond-charge interaction with strength parameter \(X\). When \(X = t\), the number of doubly occupied sites becomes a conserved quantity. The energies of the modified Hamiltonian are determined. In the limit as \(u \to \infty\), the ground state energy of that model is the same as Eq. \(\ref{eq:1}\). However, this is for \(X = t, u \to \infty\), whereas our result is for \(X = 0, u \to \infty\). Recently, Kumar\(^\text{15}\) considered the fixed boundary solutions of a one-dimensional Hubbard system in the infinite \(u\) limit. For this case, the Lieb-Wu analysis is not applicable and the energy spectrum is quite different. Kumar was able to find the analogue of Eq. \(\ref{eq:1}\) for the fixed boundary case.

More detailed analysis has been devoted to case where \(L\) is even which for periodic boundary conditions allows for bipartite symmetry. Essler et al.\(^\text{6}\) derive a method for finding all of the energy eigenstates by augmenting the Bethe ansatz using generators associated with the SO(4) symmetry of the system. Their results are presumably consistent with those in this paper, though they do not explicitly evaluate their equations in the \(u \to \infty\) limit. Lieb and Wu\(^\text{2}\) and Goldbaum\(^\text{2}\) prove the existence of ground state solutions to the Bethe ansatz equations for the restricted case of even \(N = L\) and odd \(N_{\text{e}} = N/2\), and show that the ground state is non-degenerate. It should be noted that in this case, the ground state is unique only for finite values of \(u\); in general, at \(u = \infty\) the ground state is degenerate. Figure \(\ref{fig:3}\) illustrates this for the case \(N = L = 6\): for \(u < \infty\) the ground state is non-degenerate and has \(S = 0\); at \(u = \infty\), \(d^0 = 20\).

In summary, we have derived an expression for the ground state energy of a Hubbard ring in the atomic limit for even and odd integer \(L\). This expression agrees with exact diagonalization energies obtained for several small systems, and is consistent with limiting results reported in the literature\(^\text{16,20}\).

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