An Introduction to Hubbard Rings at $U = \infty$

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(Dated: April 12, 2010)

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 at $U/t = \infty$. This result is valid for an *arbitrary* number of lattice sites L and electrons $N \leq L$. Furthermore, our analysis provides insight into the degeneracy and spin properties of the ground states in this limit.

PACS numbers:

I. INTRODUCTION

For nearly fifty years, the Hubbard model[1] 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, it has provided significant insight into many-body properties of solids such as metal-insulator transitions, high-temperature superconductivity, and magnetic states[2], 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[3,4] who derived a "Bethe anzatz" method[5] for determining eigenvalues and eigenfunctions of the single band, one-dimensional Hubbard model with L lattice sites and N electrons, and obtained an explicit expression for the ground state energy for a half-filled system in the thermodynamic limit ($N = L \to \infty$).

Typical textbooks for courses in condensed matter physics contain relatively little material about the Hubbard model. For example, Ashcroft and Mermin[6] have a one-paragraph qualitative description of the physics of the model plus an end-of-chapter problem involving a two-site Hubbard model representing a hydrogen molecule (the solution to which has been the subject of a published paper[7]). Marder[2] devotes a section of a chapter to the Hubbard model including a presentation of the mean field solution of an infinite one-dimensional system. At larger values of U/t, the mean field solution incorrectly predicts a ferromagnetic ground state and the section concludes with the sentence: "There is no better illustration of the difficulties involved in progressing systematically beyond the one-electron pictures of solids." The more recent textbook by Snoke[8] does not mention the Hubbard model.

Nevertheless, there has been substantial research devoted to analyzing the mathematics and physics of the Hubbard model, particularly in one-dimension. Two recent reviews[9,10] summarize parts of the literature. Much of this literature is very complex, involving the enumeration of special symmetries and the analysis of complicated nonlinear or combinatorial equations. On the other hand, some of the basic ideas behind the analysis and explicit results for some limiting cases are accessible to graduate level instruction and can give students some insight into many-body physics and some exercise in basic quantum mechanical principles for non-trivial systems.

A common problem asked of students in an introductory quantum mechanics course is to determine the energy and degeneracy of the ground state of a system. In the present paper, we present a proof that the exact ground state energy of 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, $U/t \equiv u = \infty$ is

$$E_g = -2t \frac{\sin\left(\frac{\pi N}{L}\right)}{\sin\left(\frac{\pi}{L}\right)}. \tag{1}$$

This simple analytic form is helpful for analysis and numerical studies of the one-dimensional Hubbard model, and our derivation of it provides insight into the nature of the eigenstates of the model. The derivation of Eq. (1) is suitable for an introductory course on solids. We also examine the degeneracy of the ground state for some simple cases.

II. DERIVATION OF GROUND STATE ENERGY

Using second quantized notation, the Hamiltonian of the Hubbard model is[1]

$$\begin{aligned} \mathcal{H} &= \mathcal{H}_{\rm hop}(t) + \mathcal{H}_{\rm int}(U) \\ &= -t \sum_{\langle m,n \rangle} \sum_{\sigma=\uparrow,\downarrow} c^\dagger_{m,\sigma} c_{n,\sigma} + U \sum_m \hat{N}_{m,\uparrow} \hat{N}_{m,\downarrow}, \end{aligned} \tag{2}$$

where $c^\dagger_{m,\sigma}$ ($c_{m,\sigma}$) creates (annihilates) an electron with spin σ in the Wannier state localized at lattice site m, and $\hat{N}_{m,\sigma} = c^\dagger_{m,\sigma} c_{m,\sigma}$. The notation $\langle m,n \rangle$ denotes that a sum is over nearest neighbor sites only. The creation and annihilation operators that appear in Eq. (2) obey the following relations (and their adjoints)

$$\left[c_{m,\sigma}, c^\dagger_{m',\sigma'} \right]_+ = \delta_{m,m'} \delta_{\sigma,\sigma'} \quad \text{and} \tag{3}$$

$$\left[c_{m,\sigma}, c_{m',\sigma'} \right]_+ = 0, \tag{4}$$

where[11] $\left[A,B\right]_\eta \equiv AB + \eta BA$.

In this paper, we assume that the system described by Eq. (2) is one-dimensional and has periodic boundary conditions (such a system is often referred to as a *Hubbard ring*). These two conditions ensure that each lattice site has exactly two nearest neighbor sites. The site index in Eq. (2) takes values $1 \leq m \leq L$, with indices m and $m+L$ being equivalent. It can be shown (see Problems 1 and 2) that the Hubbard Hamiltonian obeys the relations

$$\left[\mathcal{H}, \mathbf{S}^2\right]_- = 0, \tag{5}$$

$$\left[\mathcal{H}, S_z\right]_- = 0, \tag{6}$$

$$\left[\mathcal{H}, S_\pm\right]_- = 0, \tag{7}$$

where $\mathbf{S}^2$ and S_z are the operators for total spin and z-component of spin, and S_+ and S_- are the spin raising and lowering operators. Due to Eqs. (5) and (6), we choose the energy eigenstates of the Hubbard Hamiltonian to be also simultaneous eigenstates of $\mathbf{S}^2$ and S_z with quantum numbers S and M_S, respectively.

The one-particle hopping term $\mathcal{H}_{\text{hop}}$ favors delocalized states, an observation perhaps not immediately obvious in Eq. (2) since it has been written in the basis of localized Wannier states. We can rewrite this term in a more revealing manner by noting that localized Wannier states and delocalized Bloch states are related by the Fourier transforms

$$c_{m,\sigma} = \frac{1}{\sqrt{L}} \sum_{\nu=1}^{L} e^{+2\pi m\nu i/L} \tilde{c}_{\nu,\sigma} \quad \text{and} \tag{8}$$

$$\tilde{c}_{\nu,\sigma} = \frac{1}{\sqrt{L}} \sum_{m=1}^{L} e^{-2\pi m\nu i/L} c_{m,\sigma}, \tag{9}$$

where $\tilde{c}^\dagger_{\nu,\sigma}$ ($\tilde{c}_{\nu,\sigma}$) creates (annihilates) an electron with spin σ in the Bloch state with quantum number ν, and obeys fermion relations analogous to Eqs. (3) and (4). Using Eq. (8), the Fourier transform of $\mathcal{H}_{\text{hop}}$ is (see Problem 3)

$$\mathcal{H}_{\text{hop}} = -2t \sum_{\nu=1}^{L} \sum_{\sigma=\uparrow,\downarrow} \cos\left(\frac{2\pi\nu}{L}\right) \tilde{N}_{\nu,\sigma}, \tag{10}$$

where $\tilde{N}_{\nu,\sigma} = \tilde{c}^\dagger_{\nu,\sigma}\tilde{c}_{\nu,\sigma}$. In cases where *only* this term in the Hubbard model is important (such as when $U = 0$ *or* when all the electrons' spins are aligned), the Bloch states serve as a natural basis. In those cases, Eq. (2) reduces to a model of independent electrons on a periodic lattice, and it is easy to verify that any N-electron Bloch state

$$|\nu_1, \sigma_1; \cdots; \nu_N, \sigma_N\rangle = \tilde{c}^\dagger_{\nu_1,\sigma_1} \cdots \tilde{c}^\dagger_{\nu_N,\sigma_N} |0\rangle, \tag{11}$$

is an eigenstate of $\mathcal{H}_{\text{hop}}$ with energy

$$E = -2t \sum_{j=1}^{N} \cos\left(\frac{2\pi\nu_j}{L}\right). \tag{12}$$

The disadvantage of using Bloch states as a basis for solving the Hubbard Hamiltonian in Eq. (2) is that they complicate the two-particle interaction term $\mathcal{H}_{\text{int}}$; by introducing this interaction term, the model is no longer one of independent electrons. In their study, 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[5], they found that the total energy eigenvalues have a similar form to those given in Eq. (12) for independent electrons[3]

$$E = -2t \sum_{j=1}^{N} \cos k_j. \tag{13}$$

The so-called charge momenta k_j, however, do not have the simple form $2\pi\nu_j/L$ given in Eq. (12) for independent electrons. To find the charge momenta requires solving the set of coupled nonlinear equations (the Lieb-Wu equations)

$$Lk_j = 2\pi I_j + 2\sum_{\beta=1}^{N_\downarrow} \tan^{-1}\left[\frac{4}{u}\left(\sin k_j - \lambda_\beta\right)\right], \tag{14}$$

and

$$2\sum_{j=1}^{N} \tan^{-1}\left[\frac{4}{u}\left(\lambda_\alpha - \sin k_j\right)\right] = 2\pi J_\alpha + 2\sum_{\beta=1}^{N_\downarrow} \tan^{-1}\left[\frac{2}{u}\left(\lambda_\alpha - \lambda_\beta\right)\right]. \tag{15}$$

Henceforth, we assume that $N \leq L$ and $N_\uparrow - N_\downarrow = 0\ (+1)$ if N is even (odd). The parameter I_j, where $1 \leq j \leq N$, is an integer (half-odd-integer) if $N_\downarrow$ is even (odd). The parameter J_α, where $1 \leq \alpha \leq N_\downarrow$, is an integer (half-odd-integer) if $N_\uparrow = N - N_\downarrow$ is odd (even). The $\lambda' s$ are a set of ordered, unequal real numbers $\lambda_1 < \lambda_2 < ... < \lambda_{N_\downarrow}$. Details of the derivation of these equations are given in Yang's examination of a one-dimensional system with delta function interaction[12] as well as a more recent review of the Hubbard model by Lieb and Wu[4]. While the derivation of these equations is quite challenging, Karbach *et al.*[13,14] provide an excellent introduction to the Bethe ansatz for the Heisenberg model.

In Figure 1, some of the lowest energy eigenvalues of the Hubbard Hamiltonian are plotted as a function of u for the case $N = L = 6$. Even for such a small system, the low-energy spectrum is quite complex for finite u. However, in the infinite-u limit, disparate energy curves asymptotically approach the same limiting energy level. This limit, which represents a highly correlated system, simplifies the mathematical properties of the Hubbard model considerably. For the remainder of this paper, we will focus on this limit, exclusively.

Since we are considering the case where $N \leq L$, it is reasonable to assume that the charge momenta for the

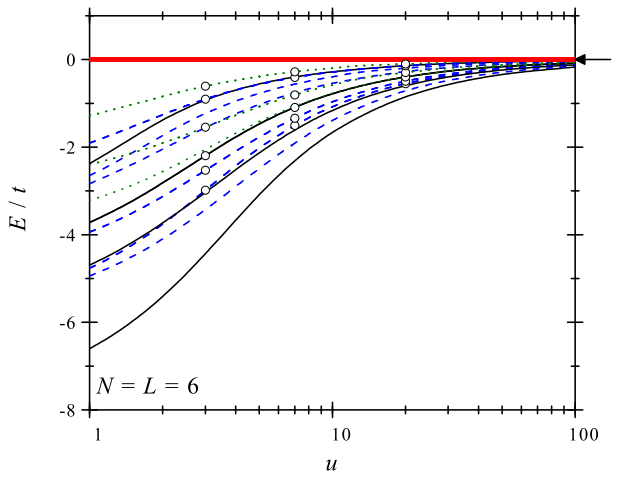

FIG. 1: Plot of the lowest energies as a function of u for $N = L = 6$. A thick (red) line represents a maximal spin $S = N/2$ state; a dotted (green) curve represents a $S = (N-2)/2$ state; a dashed (blue) curve represents a $S = (N-4)/2$ state; a solid (black) curve represents a $S = (N-6)/2 = 0$ state. Symbols denote a doubly degenerate energy. The arrow marks the energy obtained by Eq. (1).

ground state are real so that terms of the form $(\sin k_j)/u$ in Eqs. (14) and (15) vanish in this limit. (Obviously, this assumption is not valid if $N > L$ since the ground state energy is necessarily linear in u, making the k_j's necessarily complex[15,16].) As a result, Eq. (15) simplifies to

$$2N \tan^{-1}\left(\frac{4\lambda_\alpha}{u}\right) = 2\pi J_\alpha + 2\sum_{\beta=1}^{N_\downarrow} \tan^{-1}\left[\frac{2}{u}\left(\lambda_\alpha - \lambda_\beta\right)\right]. \tag{16}$$

By substituting this expression into Eq. (14) we obtain an equation for the charge momenta at $u = \infty$,

$$k_j(N_\downarrow, N_\uparrow) = \frac{2\pi}{L}\left[I_j + \frac{1}{N}\sum_{\beta}^{N_\downarrow} J_\beta\right]. \tag{17}$$

In order to analyze the ground state, one possibility[3,4] is to choose I_j and J_α to be consecutive integers (or half-odd-integers) centered around the origin. With this choice, if N is even,

$$\sum_{\beta=1}^{N_\downarrow} J_\beta = 0; \tag{18}$$

otherwise, if N is odd,

$$\sum_{\beta=1}^{N_\downarrow} J_\beta = \frac{N_\downarrow}{2}. \tag{19}$$

With this assumption, the charge momenta take the form

$$k_j(N_\downarrow, N_\uparrow) = \begin{cases} \dfrac{2\pi I_j}{L}, & N \text{ even} \\ \dfrac{2\pi}{L}\left(I_j + \dfrac{N_\downarrow}{2N}\right), & N \text{ odd.} \end{cases} \tag{20}$$

Equation (20) is of the general form

$$k_j = \frac{2\pi}{L}\left(j + j_0\right), \tag{21}$$

where j is an integer and j_0 is a real number. With this choice of charge momenta k_j, Eq. (13) can be summed as a geometric series resulting in the energy equation

$$\begin{aligned} E &= -2t\sum_{j=1}^{N} \cos\left[\frac{2\pi}{L}\left(j + j_0\right)\right] \\ &= -2t\frac{\sin\left(\pi N/L\right)}{\sin\left(\pi/L\right)} \cos\left[\frac{\left(2j_0 + N + 1\right)\pi}{L}\right], \end{aligned} \tag{22}$$

which has a minimum when

$$j_0 = -\frac{N+1}{2}. \tag{23}$$

The special value of j_0 given in Eq. (23) results in the minimum energy obtainable for the general class of wave vectors given in Eq. (21). By inspection, this choice of j_0 is not the same as that in Eq. (20); in fact, there is no reason to expect *a priori* that it would be. However, the charge momenta can be chosen to be consistent with Eqs. (21) *and* (23) by utilizing Eq. (7). We begin by assuming that the energy eigenfunctions of $\mathcal{H}$ are known; for a particular choice of $N_\uparrow$ and $N_\downarrow$, each eigenfunction $\psi(N_\downarrow, N_\uparrow)$ satisfies the eigenvalue equation

$$\mathcal{H}\psi(N_\downarrow, N_\uparrow) = E\psi(N_\downarrow, N_\uparrow), \tag{24}$$

and has a definite spin quantum number S. Applying the spin-raising operator S_+ to Eq. (24), one of two things occurs: either the eigenfunction $\psi(N_\downarrow, N_\uparrow)$ is annihilated if it has minimal total spin quantum number $S = \frac{1}{2}\left(N_\uparrow - N_\downarrow\right)$, or we obtain the eigenvalue equation

$$\mathcal{H}\psi(N_\downarrow - 1, N_\uparrow + 1) = E\psi(N_\downarrow - 1, N_\uparrow + 1), \tag{25}$$

where, due to Eq. (7), E is the same energy that appears in Eq. (24). Therefore, the set of eigenvectors and eigenvalues that solves Eq. (25) is a subset of the set of eigenvectors and eigenvalues that solves Eq. (24). This process can be repeated to span all of the possible related spin configurations corresponding to the same energy eigenvalue $E(M, M') = E(N_\downarrow, N_\uparrow)$, where the possible values of (M, M') are determined from limits of the raising operations to be $0 \le M \le N_\downarrow$, $N_\uparrow \le M' \le N$, and $M + M' = N$. This argument suggests that Eq. (20)

can be modified to take the form:

$$k_j(N_\downarrow, N_\uparrow) = \begin{cases} \dfrac{2\pi I_j}{L}, & N \text{ even}, \\ \dfrac{2\pi}{L}\left(I_j + \dfrac{M}{2N}\right), & N \text{ odd}. \end{cases} \tag{26}$$

where $0 \leq M \leq N_\downarrow$.

It is now a simple problem to verify that Eq. (26) satisfies Eq. (23). First, we consider the case of N even. For this case Eq. (23) is a half-odd-integer and $I_j = j + j_0$ must be a half-odd-integer, which occurs 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. (23) must be an integer and $I_j + M/2N = j + j_0$ must also be an integer, which occurs 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

$$k_j(N_\downarrow, N_\uparrow) = \begin{cases} \dfrac{2\pi}{L}\left(j + \dfrac{1}{2}\right), & N \text{ even}, \\ \dfrac{2\pi j}{L}, & N \text{ odd}. \end{cases} \tag{27}$$

Using these charge momenta, and minimizing Eq. (13), we obtain the ground state energy expression in Eq. (1). This concludes our derivation.

III. DEGENERACY OF THE GROUND STATE

In the previous section, we derived an expression for the energy of the ground state at $u = \infty$. The simplicity of this derivation and the resulting formula itself is appealing to an introductory examination of the Hubbard model. However, this formula says nothing of the degeneracy of the ground state. Naturally, the question arises, *is the ground state at $u = \infty$ degenerate*? Examination of Figure 1 reveals that, at least for the case of $N = L = 6$, the answer is *highly so*.

We begin with an observation: at $u = \infty$, 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[17]. In general, for a system of h holes, the ground state is highly degenerate, with a degeneracy denoted by $d^{(h)}$. In this section, we examine two special cases, that of half filling ($h = 0$) and of one hole ($h = 1$).

A. Half filling

We begin our examination with the simplest case (half-filling) where the number of holes is zero, $h = 0$; that is, $N = L$. From Eq. (1), we find that for *any* half-filled system, the energy of the ground state at $u = \infty$ is $E_g = 0$. The degeneracy of the ground state is the number of possible ways of filling $N = L$ holes with N indistinguishable spin-1/2 particles

$$d^{(0)} = \frac{N!}{N_\uparrow! N_\downarrow!}. \tag{28}$$

In Figure 1, the energies of the $d^{(0)}$ states are plotted as a function of u for the small half-filled system $N = L = 6$. Results were obtained by exact diagonalization. In this case, the degeneracy of the ground state at $u = \infty$ is given by Eq. (28): for $N = 6$, $d^{(0)} = 20$. We note that in this case, one of the ground states is characterized as having maximal total spin. This state is easily distinguished by having an energy that is independent of the coupling parameter u (see Problem 7).

B. One hole

Next, we introduce one hole and examine its effect. From Eq. (1), we note that *all* one-hole Hubbard rings, regardless of their size, have the same ground state energy, namely $E_g = -2t$. In order to determine the degeneracy, we use perturbation theory, taking $\mathcal{H}_{\rm int}$ as the unperturbed Hamiltonian and treating $\mathcal{H}_{\rm hop}$ as a perturbation. The *unperturbed* ground states $|i\rangle$ are degenerate and have zero energy

$$\mathcal{H}_{\rm int}(U \to \infty)|i\rangle = E_i^{(0)}|i\rangle = 0. \tag{29}$$

This *unperturbed degeneracy* D is given by the number of possible ways of filling L holes with $N = L - 1$ indistinguishable spin-1/2 particles

$$D = \frac{(N+1)!}{N_\uparrow! N_\downarrow!}. \tag{30}$$

The first order correction to the ground state energy is the lowest eigenvalue of the matrix

$$\mathcal{W}^{(1)}_{k\ell} = \langle k|\mathcal{H}_{\rm hop}(t)|\ell\rangle. \tag{31}$$

At $u = \infty$, higher order corrections to the ground state energy vanish (see Problem 8); the lowest energy eigenstates of the perturbation matrix in Eq. (31) are the exact ground states in this limit. Furthermore, we observe that this perturbation matrix *can* be put in block diagonal form, by appropriate ordering of the states from Eq. (29). To prove this assertion we must more closely examine the unperturbed ground states.

In Figure 2 we show several unperturbed ground states defined in Eq. (29) for the case $N = L - 1 = 7$ and $N_\downarrow = 3$. With periodic boundary conditions, the state depicted in (5′) can be obtained from arrangement (5) by repeatedly moving electrons one at a time to nearest neighbor sites with the provision that all intermediate states contain no doubly occupied lattice sites; the

same cannot be said for states (1) through (4). Therefore, states (5) and (5′) are said to be *connected* to each other and *disconnected* from states (1) through (4). In fact, states (1) through (5) represent the five distinct *spin configurations* for that system. To indicate that the unperturbed ground states can be sorted into different spin configurations, we write them as $|\alpha, i_\alpha\rangle$, where the integer α denotes to which spin configuration the state belongs, and i_α is an arbitrary state label. Since states in different spin configurations are disconnected,

$$\langle \alpha', i'_{\alpha'} | \mathcal{H}_{\rm hop} | \alpha, i_\alpha \rangle = 0, \quad \text{if } \alpha \neq \alpha'. \tag{32}$$

Therefore, the first order perturbation matrix is block diagonal, with the number of blocks being the number of distinct spin configurations for that system.

In general, the number of blocks is a complicated function that depends upon our choice of N and L. We treat the simplest case, when N is odd; a restricted case for even N is given as Suggested Problem 10. When N is odd, it is easy to show that the number of connected arrangements in each spin configuration is

$$\mathcal{C} = NL = N(N+1); \tag{33}$$

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

$$\frac{D}{\mathcal{C}} = \frac{(N-1)!}{N_\uparrow! N_\downarrow!} = d^{(1)}; \tag{34}$$

the last equality will be shown below.

Returning to Eq. (31), we factor the first-order correction as

$$\mathcal{W}^{(1)}_{k\ell} = -2t \langle k | \mathcal{H}_{\rm hop}\left(-\tfrac{1}{2}\right) | \ell \rangle; \tag{35}$$

the lowest eigenvalue of $\mathcal{W}_{(1)}$ corresponds to the maximum eigenvalue of the dimensionless operator $\mathcal{H}_{\rm hop}(-\frac{1}{2})$. By appropriately choosing the unperturbed basis defined in Eq. (29), it can be shown that if N is odd, then each row and column of $\mathcal{H}_{\rm hop}(-\frac{1}{2})$ consists of only two nonzero elements, which have the value $\frac{1}{2}$. Therefore,

$$\langle k | \mathcal{H}_{\rm hop}\left(-\tfrac{1}{2}\right) | \ell \rangle \geq 0, \tag{36}$$

and the sum of the elements in every row or column is 1:

$$\sum_{|k\rangle} \langle k | \mathcal{H}_{\rm hop}\left(-\tfrac{1}{2}\right) | \ell \rangle = 1, \tag{37}$$

and

$$\sum_{|\ell\rangle} \langle k | \mathcal{H}_{\rm hop}\left(-\tfrac{1}{2}\right) | \ell \rangle = 1. \tag{38}$$

Nonnegative matrices that satisfy either Eq. (37) or Eq. (38) are known as *stochastic matrices*[18] 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 (37) and (38) state that the total probability of transition is unity. By the Perron-Frobenius theorem[18], 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.

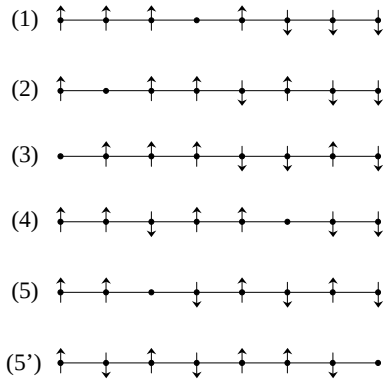

FIG. 2: Possible one-dimensional spin arrangements for $N = L - 1 = 7$ and $N_\downarrow = 3$. Arrangements (1) through (4) each represent a different spin configuration for this system; arrangements (5) and (5′) represent the fifth and final spin configuration. Arrangements (1) through (4) are disconnected from one another and from arrangements (5) and (5′); arrangements (5) and (5′) are connected to one another.

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 at $u = \infty$. 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 the same as the energy of a system with $L-N$ electrons, corresponding to $L - N$ and N holes, respectively.

Due to its rich structure and relative simplicity, there is an impressive literature devoted to solutions of the one-dimensional Hubbard model. Several authors[19–21] have derived results equivalent to Eq. (1) in the thermodynamic limit. Considering both finite and infinite systems, Kotrla[22] extended the approach of Caspers and Iske[23] to consider the $u \to \infty$ limit of the one dimensional Hubbard model from the viewpoint 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. (1) although the explicit analytic form is not given. Equation (1) also appeared

in a paper by Kusmartsev[24] that considers the response of a Hubbard ring to a magnetic flux. Another related result is by Schadschneider[25], who augments the electron hopping term of the original Hubbard model in Eq. (2) with a bond-charge interaction with strength parameter X. This change produces an analytically solvable model that is equivalent to the Hubbard model at $u = \infty$.

Recently, Kumar[26] 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. He was able to find the analogue of 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[4]. Essler *et al.*[27,28] 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 $u = \infty$ limit. Lieb and Wu[4] and Goldbaum[29] prove the existence of ground state solutions to the Bethe ansatz equations for the restricted case of even $N = L$ and odd $N_\sigma = N/2$, 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 1 illustrates this for the case $N = L = 6$: for $u < \infty$ the ground state is nondegenerate and has $S = 0$; at $u = \infty$, $d^0 = 20$.

Suggested Problems

1. Show that in second quantized notation, the total spin operator $\mathbf{S}^2$ is given by (in units where $\hbar = 1$)

$$\mathbf{S}^2 = \frac{1}{2}\hat{N} + \frac{1}{4}\left(\hat{N}_\uparrow - \hat{N}_\downarrow\right)^2 + \sum_{n,m} c^\dagger_{n,\uparrow} c^\dagger_{m,\downarrow} c_{m,\uparrow} c_{n,\downarrow},$$

   where $\hat{N}_\sigma = \sum_n \hat{N}_{n,\sigma}$ is the number operator for particles with spin σ.

2. Use the result of Problem 1 to verify that the Hubbard Hamiltonian commutes with the total spin operator $\mathbf{S}^2$.

3. Using the Fourier transform in Eq. (8), derive the expression given in Eq. (10) for $\mathcal{H}_{\text{hop}}$.

4. Verify the energy equation in Eq. (22).

5. Starting from Eq. (12), show that if $N = L$ or if N is odd, the lowest energy eigenvalue for a system of spinless independent fermions is the same as Eq. (1).

6. Explain why the result in Problem 5 leads to the following conclusion: if $N = L$ or N is odd, the ground state of a Hubbard ring at $u = \infty$ necessarily includes one (and *only* one, up to the trivial M_S spin degeneracy) state of maximal total spin.

7. Explain why the energy of any Hubbard state with maximal total spin is independent of the dimensionless parameter u.

8. Verify the statement after Eq. (31) that the higher order corrections to the ground state energy vanish.

9. Prove Eq. (33) and show that it is valid only if $N_\sigma \neq 0$ and $N_\uparrow/N_\downarrow$ (and its inverse) are not integers for $N_\sigma > 1$.

10. When N is even, Eq. (33) is no longer valid for every spin configuration. Particular spin configurations may have additional periodicities that decrease the number of connected states in that configuration. However, if $N_\uparrow = N_\downarrow$, where N_σ is prime, then there is only one spin configuration which does not obey Eq. (33). From this observation, show that the degeneracy of the ground state at $u = \infty$ for this case is

$$d^{(1)} = \frac{(N-1)!}{N_\uparrow! N_\downarrow!} - \frac{2}{N} + 1. \tag{39}$$

Acknowledgements

The computations were performed on the DEAC cluster, a resource supported in part by Wake Forest University.

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