

Exact Ground State Energy of Hubbard Rings in the Atomic Limit

W. B. Hodge, N. A. W. Holzwarth, and W. C. Kerr

Department of Physics, Wake Forest University, Winston-Salem, North Carolina 27109-7507

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Making some reasonable assumptions, we derive an expression for the ground state energy of a one-dimensional Hubbard ring in the atomic limit, valid for systems of finite size. In doing so, we show that a straightforward solution to equations derived by Lieb and Wu does not obtain the expected ground state energy in this limit.

For the past forty-odd years the Hubbard model [1] has been used as a minimal model to describe many-body effects in solids. The model incorporates the 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 the on-site Coulomb energy U). The ratio $u = U/t$ is the important dimensionless ratio of the model. Researchers have used the model in combination with the Pauli Exclusion Principle to describe metal-insulator transitions, high-temperature superconductivity, and magnetic states. While the one-dimensional case has been exactly solved, the same can not be said for the properties of the model in higher dimensions [2]. In one dimension, most of the exact knowledge that we have is from Lieb and Wu's solution [3] for the energy eigenvalues and eigenfunctions. Though they obtained exact nonlinear equations that are valid for arbitrary lattice size and electron number, most attention has been paid to solutions of their equations in the thermodynamic limit (number of lattice sites $L \rightarrow \infty$, number of electrons $N \rightarrow \infty$, N/L finite). In this paper we present an exact result, obtained from the Lieb-Wu equations, for another limit, namely the $u \rightarrow \infty$ limit, for Hubbard rings (finite lattices with periodic boundary conditions, in dimension $d = 1$) with $N \leq L$. When these conditions are satisfied, we find that the *exact ground state energy* is

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

It is easy to recover the thermodynamic limit result [4] from this equation. We devote the remainder of this paper to the derivation of this result.

The Hamiltonian of the Hubbard model is [1]

$$\mathcal{H} = -t \sum_{\langle i,j \rangle} c_{i,\sigma}^\dagger c_{j,\sigma} + U \sum_i n_{i,\uparrow} n_{i,\downarrow}, \quad (2)$$

where $c_{i,\sigma}^\dagger$ ($c_{i,\sigma}$) creates (annihilates) an electron with spin σ in the Wannier state localized at lattice site i , and $\langle i,j \rangle$ denotes that a sum is over nearest neighbor sites only. Aside from designating the total number of electrons N , it is often necessary to also specify the electron

spin distribution, with N_\uparrow and N_\downarrow specifying the total number of up and down z -component spin orientations, respectively. In this work, we consider a system described by Eq. (2) in one-dimension with periodic boundary conditions in the limit where $u \rightarrow \infty$, henceforth referred to as the atomic limit. This limit simplifies the Hubbard model considerably, and has been studied previously in the thermodynamic limit [5, 6]; the results presented in this paper, in contrast, are also valid for systems of finite size. In addition to their initial treatment [3], the Lieb-Wu equations used in this paper have been extensively studied [7–9]. We find that there is a problem in the way that these equations are usually handled; we hope that this paper will also serve to illuminate this subtlety.

Applying the Bethe ansatz to the one-dimensional Hubbard model, Lieb and Wu proposed that total energy eigenvalues be written in a form identical to that for independent electrons [3]

$$E = -2t \sum_{j=1}^N \cos k_j; \quad (3)$$

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)

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

and

$$2 \sum_{j=1}^N \tan^{-1} \left[\frac{4}{u} (\lambda_\alpha - \sin k_j) \right] = 2\pi J_\alpha + 2 \sum_{\beta=1}^{N_\downarrow} \tan^{-1} \left[\frac{2}{u} (\lambda_\alpha - \lambda_\beta) \right], \quad (5)$$

where I_j is an integer (half-odd-integer) if N_\downarrow is even (odd), J_α is an integer (half-odd-integer) if $N_\uparrow = N - N_\downarrow$ is odd (even), and $N_\uparrow \geq N_\downarrow$. The λ 's are a set of ordered, unequal real numbers $\lambda_1 < \lambda_2 < \dots < \lambda_{N_\uparrow}$ and the indices j and α run from $1, \dots, N$ and $1, \dots, N_\uparrow$, respectively. Details of the derivation of these equations

are given in Yang's examination of a one-dimensional system with delta function interaction [10] as well as a more recent review of the Hubbard model by Lieb and Wu [11].

The Hubbard Hamiltonian obeys the commutation relations

$$[\mathcal{H}, \mathbf{S}^2] = [\mathcal{H}, S_z] = [\mathcal{H}, S_{\pm}] = 0, \quad (6)$$

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. Because of these relations we require that the energy eigenstates be eigenstates of \mathbf{S}^2 and S_z with quantum numbers S and M_S , respectively.

Let us assume that $N \leq L$. Then, for the ground state, it is reasonable to assume that the charge momenta are real so that terms of the form $\frac{\sin k_j}{u}$ in Eqs. (4) and (5) vanish in the atomic limit. This assumption would not be valid if $N > L$ since the ground state energy would be linear in u and the k_j 's necessarily complex [8]. As a result, Eq. (5) simplifies to

$$2N \tan^{-1} \left(\frac{4\lambda_{\alpha}}{u} \right) = 2\pi J_{\alpha} + 2 \sum_{\beta=1}^{N_{\downarrow}} \tan^{-1} \left[\frac{2}{u} (\lambda_{\alpha} - \lambda_{\beta}) \right]; \quad (7)$$

by substituting this expression into Eq. (4) we obtain an equation for the charge momenta at $u = \infty$,

$$k_j(N_{\downarrow}, N_{\uparrow}) = \frac{2\pi}{L} \left[I_j + \frac{1}{N} \sum_{\beta}^{N_{\downarrow}} J_{\beta} \right]. \quad (8)$$

For the ground state, Lieb and Wu stated that I_j and J_{α} are consecutive integers (half-odd-integers) centered around the origin [3]. Therefore, if N is even,

$$\sum_{\beta=1}^{N_{\downarrow}} J_{\beta} = 0; \quad (9)$$

otherwise, if N is odd,

$$\sum_{\beta=1}^{N_{\downarrow}} J_{\beta} = \frac{N_{\downarrow}}{2}. \quad (10)$$

Thus, we conclude that

$$k_j(N_{\downarrow}, N_{\uparrow}) = \begin{cases} \frac{2\pi I_j}{L}, & N \text{ even} \\ \frac{2\pi}{L} \left(I_j + \frac{N_{\downarrow}}{2N} \right), & N \text{ odd.} \end{cases} \quad (11)$$

Before examining the validity of the charge momenta obtained in Eq. (11) we first note that in the atomic limit, the ground state energy of a system with $n = L - N$ holes is the same as the ground state energy of a system with n electrons. Therefore, for a system with one hole, that

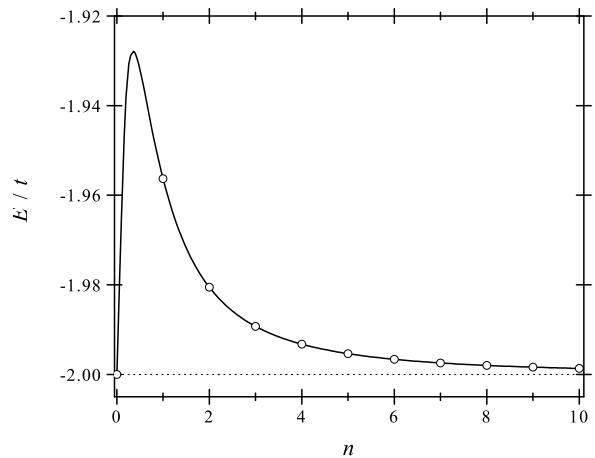


FIG. 1: Plots of the exact ground state energy (dashed line) and lowest energy obtained using the Bethe ansatz charge momenta (solid line) in Eq. (12) at $u = \infty$ for $N = L - 1 = 4n + 1$, as a function of n . The circles denote integer values of the variable n .

is $N = L - 1$, the ground state energy is $E_g = -2t$, independent of the size of the lattice [12]. As an example, assume that $N = L - 1 = 4n + 1$ and $N_{\downarrow} = 2n$, where n is an integer [13]. Then Eq. (11) becomes

$$k_j(2n, 2n + 1) = \frac{2\pi}{4n + 2} \left[j + \frac{n}{4n + 1} \right], \quad (12)$$

where j is an integer. We find the possible energies of the system by using the formula given in Eq. (3); the lowest energy obtained is plotted in Figure 1 as a function of the lattice size. Inspection of this plot reveals that using the charge momenta given in Eq. (12), we do not obtain the predicted exact ground state energy, except in the one-electron case ($n = 0$) and the thermodynamic limit ($n = \infty$). Since we are interested in finite size systems, this is clearly a problem.

To address this issue, we begin with the following claim: *All of the possible $k_j(M, M')$ defined in Eq. (11), where $0 \leq M \leq N_{\downarrow}$, $N_{\uparrow} \leq M' \leq N$, and $M + M' = N$ are possible charge momenta for a system described by given values of N_{\uparrow} and N_{\downarrow} .* To prove this claim, we use the spin-raising commutation relation given in Eq. (6). Let us assume that the energy eigenfunctions $\psi(N_{\downarrow}, N_{\uparrow})$ are known

$$\mathcal{H}\psi(N_{\downarrow}, N_{\uparrow}) = E\psi(N_{\downarrow}, N_{\uparrow}), \quad (13)$$

and are also simultaneous eigenfunctions of \mathbf{S}^2 . Applying the spin-raising operator S^+ to Eq. (13) one of two things occurs. The eigenfunction $\psi(N_{\downarrow}, N_{\uparrow})$ is annihilated if it has minimal total spin quantum number $S = \frac{1}{2}(N_{\uparrow} - N_{\downarrow})$; otherwise, we obtain the eigenvalue equation

$$\mathcal{H}\psi(N_{\downarrow} - 1, N_{\uparrow} + 1) = E\psi(N_{\downarrow} - 1, N_{\uparrow} + 1), \quad (14)$$

where E is the same energy that appears in Eq. (13). Therefore, the set of eigenenergies that solves Eq. (14) is a subset of the set of eigenenergies that solves Eq. (13).

For the system described in Eq. (13), we expect to use the charge momenta defined in Eq. (11) with quantum numbers N_{\downarrow} and N_{\uparrow} . However, if we use charge momenta with quantum numbers $M = N_{\downarrow} - 1$ and $M' = N_{\uparrow} + 1$, any energies we calculate are also valid energies for this system. We find that varying M and M' results in energies different than those found when using the quantum numbers N_{\downarrow} and N_{\uparrow} of the desired system. The question then is: *can the energies found in this manner be lower than the lowest energy calculated using the given quantum numbers of the system?* The answer is, *yes*. To prove this, we look more closely at the sum given in Eq. (3).

We write the charge momenta appearing in Eq. (3) in a general form consistent with Eq. (11)

$$k_j = \frac{2\pi}{L} (j + j_0), \quad (15)$$

where the j 's are positive integers and j_0 is a real number. Writing Eq. (3) as a geometric series results in the energy equation

$$\begin{aligned} E &= -2t \sum_{j=1}^N \cos \left[\frac{2\pi}{L} (j + j_0) \right] \\ &= -2t \frac{\sin(\pi N/L)}{\sin(\pi/L)} \cos \left[\frac{(2j_0 + N + 1)\pi}{L} \right]; \end{aligned} \quad (16)$$

this expression has a minimum when

$$j_0 = -\frac{N+1}{2}. \quad (17)$$

Equations (16) and (17) indicate that for an odd (even) number of electrons, the lowest possible energy is obtained when $j + j_0$ is an integer (half-odd-integer) and the charge momenta $k_j(M, M')$ are centered around the origin. For an odd number of electrons, we accomplish this by letting $M = 0$; for an even number of electrons, we accomplish this by letting M be odd so that I_j is a half-odd-integer. With these assumptions, we conclude that the charge momenta corresponding to the ground state are

$$k_j(N_{\downarrow}, N_{\uparrow}) = \begin{cases} \frac{2\pi}{L} \left(j + \frac{1}{2} \right), & N \text{ even} \\ \frac{2\pi j}{L}, & N \text{ odd}, \end{cases} \quad (18)$$

where the j 's are integers and not necessarily the same as in Eq. (15); for the ground state, they are consecutive integers centered around the origin. Since these charge momenta minimize Eq. (16), the ground state energy is given by Eq. (1), which concludes our derivation.

The electron-hole symmetry of the ground state energy is also evident by replacement of N with $L - N$ in Eq. (1). Furthermore, it is easy to show that Eq. (1) is consistent with the lower bound calculation to the ground state energy found by Trugman [14]. In Figure 2 a comparison between the lowest energies found using Eqs. (3) and (11), and the energy found using Eq. (1) is shown for $L = 10$ and $L = 15$ at various lattice densities.

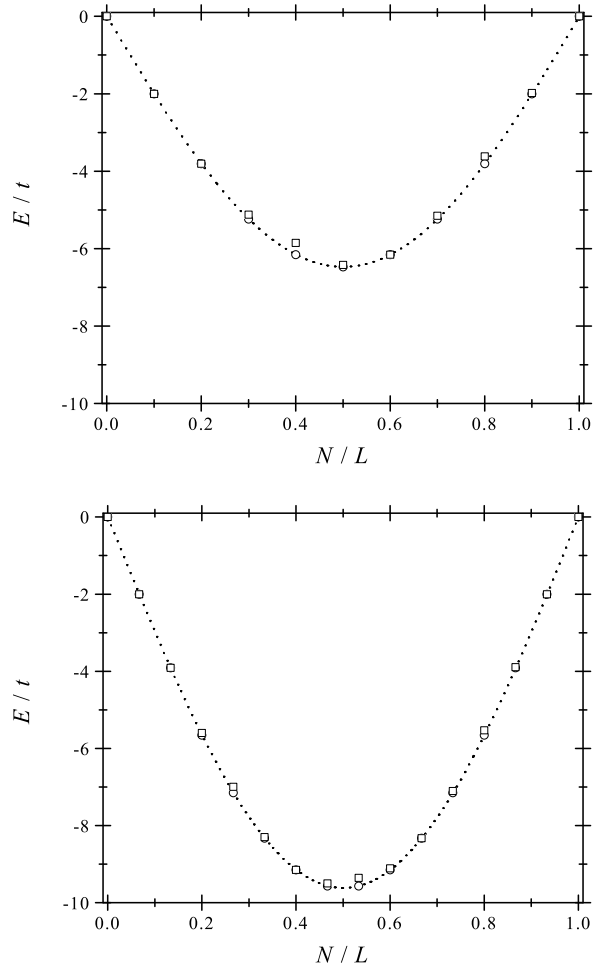


FIG. 2: Plots of the exact ground state energy (circles) using Eq. (1) and energy obtained using the unmodified Bethe ansatz solutions in Eqs. (3) and (11) (squares) at $u = \infty$ for $L = 10$ (top) and $L = 15$ (bottom) as a function of the chain density N/L . The dotted line connecting the circles is obtained by treating N as a continuous variable.

It has been shown by previous authors that for an odd number of electrons in the atomic limit, exactly one of the ground states (not counting the trivial $2S_{\max} + 1 = N + 1$ degeneracy) has maximal total spin [15]. To prove this we note that the entire energy spectrum of states with maximal total spin can be obtained by considering only states with all aligned spins, that is $M_S = \pm \frac{N}{2}$. The solutions to the Hubbard model in this case are indepen-

dent electrons in the Bloch basis; the minimum energy of this system is

$$E_{\min}(0, N) = E_{\min}(N, 0) = \begin{cases} -2t \left[1 + 2 \sum_{j=1}^{\frac{N}{2}-1} \cos\left(\frac{2\pi j}{L}\right) + \cos\left(\frac{\pi N}{L}\right) \right] = E_g \cos\left(\frac{\pi}{L}\right), & N \text{ even} \\ -2t \left[1 + 2 \sum_{j=1}^{\frac{N-1}{2}} \cos\left(\frac{2\pi j}{L}\right) \right] = E_g, & N \text{ odd} \end{cases} \quad (19)$$

L	N	$E_g(t)$	$N_{\uparrow} (N_{\downarrow})$	J_{α}	$E_{\min}(t)$
6	4	-3.46410	2 (2)	$-\frac{1}{2}, \frac{1}{2}$	-3
				$-\frac{1}{2}, \frac{1}{2}$	-3.34607
				$-\frac{1}{2}, \frac{1}{2}$	-3.46410
	5	-2	3 (2)	0, 1	-1.95630
7				-1, 1	-2
				$-\frac{1}{2}, \frac{1}{2}$	-4.04892
	4	-4.49396	2 (2)	$-\frac{1}{2}, \frac{1}{2}$	-4.38129
				$-\frac{1}{2}, \frac{1}{2}$	-4.49396
				0, 1	-3.54596
	5	-3.60388	3 (2)	-1, 1	-3.60388
			3 (3)	-1, 0, 1	-2
	6	-2	4 (2)	$-\frac{1}{2}, \frac{1}{2}$	-1.80194
				$-\frac{1}{2}, \frac{1}{2}$	-1.91115
				$-\frac{1}{2}, \frac{1}{2}$	-1.97766
				$-\frac{1}{2}, \frac{1}{2}$	-2

TABLE I: Examples of minimum energies obtained using Eqs. (3) and (8) and particular choices of the J_{α} parameters. The ground state energies E_g were found using Eq. (1) and were verified by exact diagonalization.

where E_g is the energy given in Eq. (1). Therefore, for an odd number of electrons, there exists a state with maximal total spin quantum number that is one of the degenerate ground states of the system in the atomic limit. For an even number of electrons, the minimum energy of a state with maximal total spin is above the ground state energy.

In deriving Eq. (1), we began by restricting the J_{α} 's to be consecutive integers or half-odd-integers centered around the origin. Then, by noting that the Hubbard Hamiltonian commutes with the operators S_{\pm} , we obtained the ground state solution. We note, however, that it is possible to find states, by using Eqs. (3) and (8) but with non-consecutive J_{α} 's, that give the minimum energy predicted by Eq. (1). In Table I we list several examples of this situation. The method presented in this paper, while successful in finding the ground state energy, can

not be used to determine all of the excited states of the model. However, for L even, Essler *et al.* [16] derived a method for finding the complete solution, using an additional SU(2) invariance of the model.

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 [4, 14].

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