Exact Ground State of the Hubbard Model in One Dimension and Arbitrary Filling at $u = \infty$

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Introduction

Thirty years ago, an exact solution to the Hubbard model in one dimension was found (the Bethe ansatz equations) leading to an exact expression for the energy of a half-filled band in the thermodynamic limit [1]. In this presentation, we return to these solutions, though make no assumptions about the size of the lattice. We show that in the limit where the interaction parameter is infinitely large, straightforward solutions of the Bethe ansatz equations do not, in general, generate the exact ground state energy. We find a new general expression for the ground state energy as a function of the number of particles and lattice sites. This result, which is consistent with numerical tests, requires a modification to the wavevectors obtained using the Bethe ansatz equations.

The Hubbard Hamiltonian

As the simplest model of electron-electron interactions in a lattice, the Hubbard model [2, 3] has elicited much attention since its introduction. The electronic properties of molecules and solids are represented by two competing terms. The first term is a kinetic energy term that arises from the tight-binding model and favors delocalized states; the second represents the electron-electron interactions and favors localized states. Although the Hubbard model oversimplifies both terms by allowing only nearest-neighbor electron hopping and including only electron-electron interactions in the same non-degenerate orbital state, it has enjoyed some success in representing narrow band solids and Mott insulators.

In second quantization, the Hamiltonian representing this model is

$$\mathcal{H}(t,u) = -t\sum_{\langle i,j\rangle} c^{\dagger}_{i\sigma}c_{j\sigma} + ut\sum_i n_{i\uparrow}n_{i\downarrow}, \tag{1}$$

where $c^{\dagger}_{i\sigma}$ ($c_{i\sigma}$) creates (annihilates) an electron with spin σ in the Wannier state localized at site i, t is the electron hopping energy, and u is the dimensionless Coulomb repulsion energy. The sums are over the L lattice sites, with the sum in the one-particle term being restricted to nearest neighbors. Assuming a one-dimensional chain with cyclic boundaries, each site has two nearest neighbors. This Hamiltonian also obeys the spin commutation relations

$$\left[\mathcal{H}, S^{\pm}\right] = 0 \text{ and } \left[\mathcal{H}, \mathbf{S}^2\right] = 0, \tag{2}$$

where S^{+} (S^{-}) is the spin raising (lowering) operator and $\mathbf{S}^2$ is the total spin operator with eigenvalues $S(S+1)$. By using a particle-hole transformation we can assume, without loss of generality, that the number of particles N is such that

$$N \le L. \tag{3}$$

From Eq. (1) we see that the number of particles of each spin, N_σ, is conserved and

$$N_{\uparrow} + N_{\downarrow} = N. \tag{4}$$

In order to obtain all possible energies of our system, we assume that

$$N_{\uparrow} - N_{\downarrow} = \begin{cases} 0, & N \text{ even} \\ 1, & N \text{ odd} \end{cases} \tag{5}$$

The Bethe Ansatz Equations

Bethe's ansatz [4], which was originally applied to the one-dimensional Heisenberg model, has seen use in a variety of related problems including fermions in the presence of a delta function interaction [5, 6], where general solutions were obtained. In 1968, Lieb and Wu derived a similar set of solutions for the Hubbard model in one dimension [1]. We use their results to obtain the ground state energy in the strongly coupled limit ($u = \infty$) for arbitrary filling. We believe the exact method by which we manipulate these equations to be novel.

Applying the Bethe ansatz to the one-dimensional Hubbard model, it was found that the energies could be written in a form reminiscent of that for independent electrons [1]

$$E(N_{\downarrow}, N_{\uparrow}; u) = -2t\sum_{j=1}^{N}\cos k_j. \tag{6}$$

To find the wavevectors, k_j, requires solving the set of coupled nonlinear equations (the Bethe ansatz equations)

$$Lk_j = 2\pi I_j + \sum_{\beta=1}^{N_{\downarrow}}\theta\left(2\sin k_j - 2\lambda_\beta\right), \tag{7}$$

and

$$\sum_{j=1}^{N}\theta\left(2\sin k_j - 2\lambda_\alpha\right) = 2\pi J_\alpha - \sum_{\beta=1}^{N_{\downarrow}}\theta\left(\lambda_\alpha - \lambda_\beta\right), \tag{8}$$

where

$$\theta(x) \equiv -2\tan^{-1}(2x/u), \tag{9}$$

and I_j is an integer (half-odd integer) if $N_{\downarrow}$ is even (odd) and J_α 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 $\lambda_1 < \lambda_2 < ... < \lambda_{N_{\downarrow}}$ and the index j in Eq. (7) runs from $1, ..., N$.

The $u = \infty$ Limit

By assuming that the wavevectors corresponding to the ground state are real and taking the $u = \infty$ limit, we can ignore all terms of the form $\sin k_j/u$ in Eqs. (7) and (8) (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. As a result, Eqs. (7) and (8) become

$$Lk_j = 2\pi I_j - \sum_{\beta=1}^{N_{\downarrow}}\theta\left(2\lambda_\beta\right), \tag{10}$$

and

$$-N\theta\left(2\lambda_\alpha\right) = 2\pi J_\alpha - \sum_{\beta=1}^{N_{\downarrow}}\theta\left(\lambda_\alpha - \lambda_\beta\right), \tag{11}$$

and we obtain a simple expression for the wavevectors

$$k_j = \frac{2\pi}{L}\left[I_j + \frac{1}{N}\sum_{\beta=1}^{N_{\downarrow}} J_\beta\right]. \tag{12}$$

There appear to be four cases that must be examined. The first two occur if N is even; then $N_{\downarrow}$ and $N - N_{\downarrow}$ are either both even or both odd. In either case,

$$\sum_{\beta=1}^{N_{\downarrow}} J_\beta = 0, \tag{13}$$

since the $J_\alpha' s$ are consecutive integers (or half-odd integers) centered around the origin. The remaining two cases occur if N is odd in which case the sum in Eq. (12) is dependent upon $N_{\downarrow}$

$$\sum_{\beta=1}^{N_{\downarrow}} J_\beta = \frac{N_{\downarrow}}{2}. \tag{14}$$

Using these results, Eq. (12) becomes

$$k_j(N_{\downarrow}, N_{\uparrow}, L) = \begin{cases} \dfrac{2\pi I_j}{L}, & N \text{ even} \\[2ex] \dfrac{2\pi}{L}\left(I_j + \dfrac{N_{\downarrow}}{2N}\right), & N \text{ odd} \end{cases}, \tag{15}$$

where $I_j = j$ ($I_j = j + \frac{1}{2}$) when $N_{\downarrow}$ is even (odd).

We expect the ground state of a system to be described by the set of k_j's defined in Eq. (15), consistent with the system's parameters, that minimizes Eq. (6). As an example, let us examine the case of one hole ($N = L - 1$), which has a well known solution, namely that the ground state energy at $u = \infty$ is $-2t$ [7], independent of the size of the lattice. Let us assume that $N = L - 1 = 4n + 1$ and $N_{\downarrow} = 2n$, where n is an integer. Then Eq. (15) becomes

$$k_j(2n, 2n+1, 4n+2) = \frac{2\pi}{4n+2}\left[j + \frac{n}{4n+1}\right], \tag{16}$$

where j is an integer and lies in the interval $[-2n, 2n+1]$. Energies are found using the energy formula given in Eq. (6); the ground state corresponds to the lowest set of k_j's and is shown in Figure 1. This plot shows that our solution to the Bethe ansatz equation does not obtain the predicted exact ground state energy, except in the one-electron case ($n = 0$) and the thermodynamic limit ($n = \infty$). In response to this dilemma, we offer the following:

Theorem. *All possible $k_j(M, M', L)$ defined in Eq. (15), where $0 \le M \le N_{\downarrow}$, $N_{\uparrow} \le M' \le N$, and $M + M' = N$ are valid wavevectors for a system described by $N_{\uparrow}$, $N_{\downarrow}$, and L.*

This theorem is a direct result of Eq. (2). To prove it, we assume that *all* of the wavefunctions $\psi(N_{\downarrow}, N_{\uparrow}, L)$, where N_σ satisfies Eq. (5), are known

$$\mathcal{H}\psi(N_{\downarrow}, N_{\uparrow}, L) = E\psi(N_{\downarrow}, N_{\uparrow}, L). \tag{17}$$

Applying the spin-raising operator S^{+} to Eq. (17) and using the commutation relation given in Eq. (2) results in either the wavefunction being annihilated or the eigenvalue equation

$$\mathcal{H}\psi(N_{\downarrow}-1, N_{\uparrow}+1, L) = E\psi(N_{\downarrow}-1, N_{\uparrow}+1, L). \tag{18}$$

Therefore, the set of energies defined in Eq. (18) is a subset of the set of energies defined in Eq. (17).

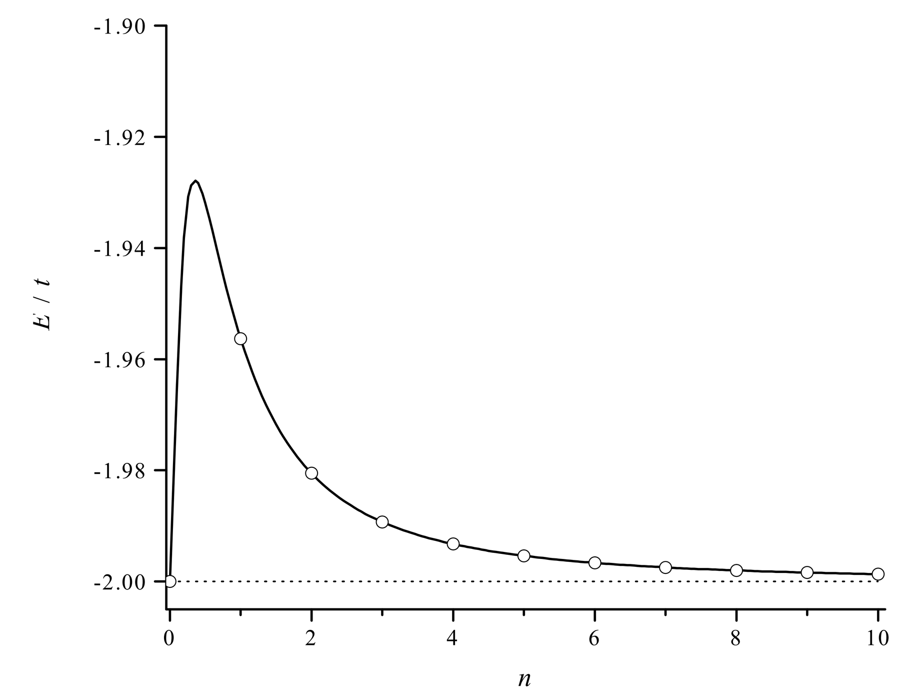

Figure 1: Plots of the exact ground state energy (dotted line) and energy obtained using the Bethe ansatz solutions in Eqs. (6) and (16) (solid line) at $u = \infty$ for $N = L - 1 = 4n + 1$, as a function of n. The discrete points at which symbols are placed correspond to integer particle numbers.

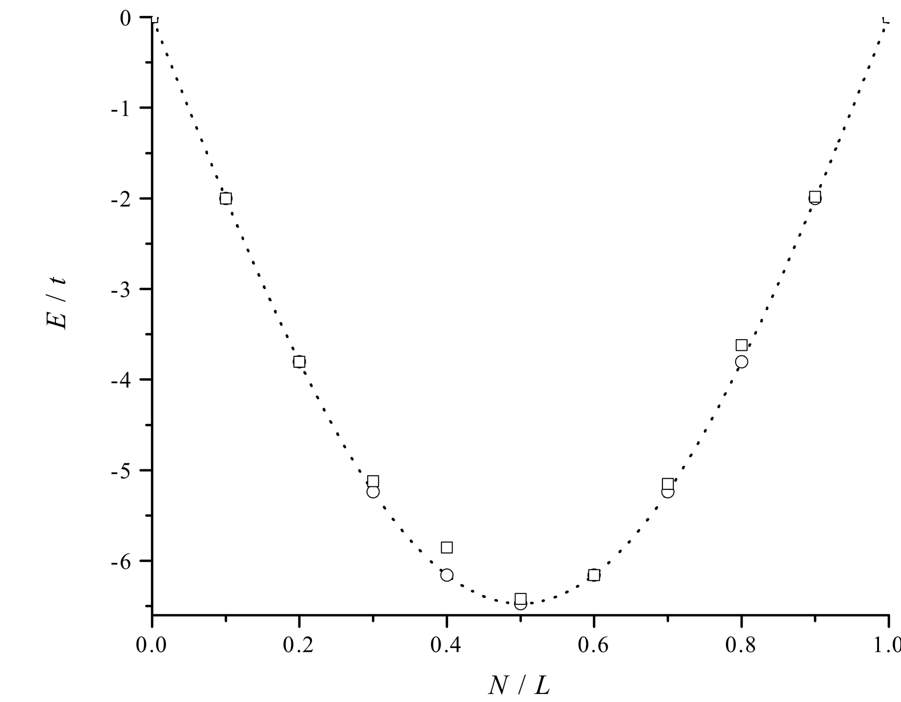

Figure 2: Plots of the exact ground state energy (dotted line) using Eq. (20) and energy obtained using the unmodified Bethe ansatz solutions in Eqs. (6) and (15) (squares) at $u = \infty$ for $L = 10$ as a function of the chain density N/L. The discrete points at which the symbols are placed correspond to integer particle numbers.

Question. *Using the Bethe ansatz solutions, is the set of energies defined in Eq. (18) a subset of the set of energies defined in Eq. (17)?*

It can be shown that the answer to this question is, *no*. By using our theorem, we conclude that the wavevectors corresponding to the ground state are

$$\boxed{k_j(N_{\downarrow}, N_{\uparrow}) = \begin{cases} \dfrac{2\pi}{L}\left(j + \dfrac{1}{2}\right), & N \text{ even} \\[2ex] \dfrac{2\pi j}{L}, & N \text{ odd} \end{cases}. \tag{19}}$$

Using this result, we calculate the ground state energy of a system with arbitrary filling at $u = \infty$ to be

$$\boxed{E(N, L) = -2t\frac{\sin\left(\dfrac{\pi N}{L}\right)}{\sin\left(\dfrac{\pi}{L}\right)}, \tag{20}}$$

In the thermodynamic limit, $\sin(\pi/L) \to \pi/L$ and Eq. (20) is consistent with the ground state energy found previously in this limit [8]. Furthermore, it is easy to show that Eq. (20) is consistent with the lower bound calculation to the ground state energy for all L [9].

Aside from the energy, the wavevectors defined in Eq. (19) tell us something about the properties of the ground state. When N is odd, the corresponding wavevectors are the same as those for independent electrons. Due to the short-range nature of the interaction term in Eq. (1), the easiest way to ensure that the electrons act independently at *any* $u > 0$ (which $u = \infty$ certainly satisfies), is by forcing all of them to have aligned spins. Then the Pauli principle disallows any two electrons from occupying the same lattice site and the electron-electron interaction term vanishes. The above argument is valid for *any* system with N odd and $N \le L$ and, since states with all electron spins aligned must have maximal total spin, we conclude with a few observations about the ground state.

Observation 1. *For an odd number of electrons, there exists exactly one state with maximal total spin that is a ground state at $u = \infty$.*

Observation 2. *For an even number of electrons, there exists no state with maximal total spin that is a ground state at $u = \infty$.*

Conclusions

We found that the wavevectors obtained by solving the Bethe ansatz equations in the limit when $u = \infty$ did not agree with the expected results. As a solution to this problem, we argued that the number of particles of each spin must be varied in order to obtain the desired ground state. Using this method, we have obtained an expression for the exact ground state energy of a system with arbitrary filling at $u = \infty$. In the thermodynamic limit, our result is in agreement with previous work.

References

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