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Complete Solution of the One-Dimensional Hubbard Model

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We show how to construct a complete set of eigenstates of the Hamiltonian of the one-dimensional Hubbard model on a finite lattice of even length L. This is done by using the nested Bethe ansatz *and* the SO(4) symmetry of the model.

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The one-dimensional Hubbard model has been known to be exactly solvable since the work of Lieb and Wu of 1968 [1]. In their paper, a large set of eigenfunctions of the Hamiltonian were found by using the nested Bethe ansatz (BA) [2,3]. These eigenfunctions are normalizable and mutually orthogonal (this became especially clear from the results in [4]). However, the issue of whether this set of eigenfunctions is actually *complete* has not been considered until recently.

By a complete set of eigenstates we mean a set that forms a basis in the Hilbert space of the model. A complete set of eigenstates for the Hubbard model on a lattice of L sites contains 4^L independent states.

In a recent paper [5], we used the SO(4) symmetry of the Hubbard model (which had been explored in [6,7]) to show that the BA is not complete. This was done by showing that by acting on the BA states with the SO(4) generators, one can find eigenstates that are outside the BA.

In this Letter we show how to construct a complete set of eigenstates of the one-dimensional Hubbard model. This will be done as follows. We will first construct all BA states of a special type, which we call regular BA states. We will then generate additional states by acting with the SO(4) generators on the regular Bethe ansatz states. We will show that the number of eigenstates obtained in this way is 4^L, which is precisely the dimension of the Hilbert space. Since all the eigenstates considered are orthogonal, this will show that we constructed a basis.

The Hamiltonian of the Hubbard model on a one-dimensional finite lattice of even length L is given by

$$H=-\sum_{i=1}^{L}\sum_{\sigma=1,-1}(c_{i,\sigma}^\dagger c_{i+1,\sigma}+c_{i+1,\sigma}^\dagger c_{i,\sigma}) +U\sum_{i=1}^{L}(n_{i,1}-\tfrac{1}{2})(n_{i,-1}-\tfrac{1}{2}). \tag{1}$$

Here the $c_{i,\sigma}$ are canonical Fermi operators on the lattice, with anticommutation relations given by $\{c_{i,\sigma}^\dagger,c_{j,\tau}\}=\delta_{i,j}\delta_{\sigma,\tau}$. They act in a Fock space with the pseudovacuum $|0\rangle$ defined by $c_{i,\sigma}|0\rangle=0$. The operator $n_{i,\sigma}=c_{i,\sigma}^\dagger c_{i,\sigma}$ is the number operator for electrons with spin σ on site i.

The model is invariant under spin rotations, with the corresponding SU(2) generators given by

$$\zeta=\sum_{i=1}^{L}c_{i,1}^\dagger c_{i,-1},\quad \zeta^\dagger=(\zeta)^\dagger,\quad \zeta_z=\frac{1}{2}\sum_{i=1}^{L}(n_{i,-1}-n_{i,1}). \tag{2}$$

(Note that ζ_z equals *minus* the third component of the total spin.) It has been found [6] that for even L the model has a second SU(2) invariance, generated by

$$\eta=\sum_{i=1}^{L}(-1)^i c_{i,1}c_{i,-1},\quad \eta^\dagger=\sum_{i=1}^{L}(-1)^i c_{i,-1}^\dagger c_{i,1}^\dagger,$$
$$\eta_z=\frac{1}{2}\sum_{i=1}^{L}(n_{i,-1}+n_{i,1})-\frac{L}{2}. \tag{3}$$

The raising operator $\eta^\dagger$ of this second SU(2) creates a pair of two opposite-spin electrons on the same site, with momentum π. Combining the two SU(2)'s, which commute with the Hamiltonian and with one another, leads to an SO(4) invariance of the one-dimensional Hubbard model [7].

The Hamiltonian (1) was analyzed in [1] using the "nested" BA [2]. This analysis resulted in a large number of eigenstates of the Hamiltonian, which are characterized by momenta k_i and rapidities Λ_α, where $i=1,2,\ldots,M+N$ and $\alpha=1,2,\ldots,M$ for an eigenstate with a total number of N spin-up and M spin-down electrons. Imposing periodic boundary conditions on the BA wave functions leads to the following equations:

$$e^{ik_jL}=\prod_{\alpha=1}^{M}\frac{\sin(k_j)-\Lambda_\alpha-U/4i}{\sin(k_j)-\Lambda_\alpha+U/4i},\quad j=1,2,\ldots,M+N,$$
$$\prod_{j=1}^{M+N}\frac{\sin(k_j)-\Lambda_\alpha-U/4i}{\sin(k_j)-\Lambda_\alpha+U/4i}=-\prod_{\beta=1}^{M}\frac{\Lambda_\beta-\Lambda_\alpha-U/2i}{\Lambda_\beta-\Lambda_\alpha+U/2i},\quad \beta=1,2,\ldots,M. \tag{4}$$

The total number of solutions to (4) is less than 4^L, so that the BA alone does not lead to a complete set of eigenstates.

To establish a relation between the SO(4) symmetry and the BA, it is useful to define "regular" BA states (for finite L), to be denoted by $|\psi_{M,N}\rangle$, by the properties that $N-M\geq 0$, $M+N\leq L$ (less than half or half filling), and that all k_i

and Λ_α are finite. In [5], we established the following remarkable property of the regular BA eigenstates of the Hamiltonian: They are all *lowest weight states* of the SO(4) algebra (2),(3), i.e.,

$$\eta|\psi_{M,N}\rangle=0,\quad \zeta|\psi_{M,N}\rangle=0\,. \tag{5}$$

Since the SO(4) commutes with the Hamiltonian, this means that we can generate an SO(4)-multiplet of eigenstates by acting with the raising operators $\eta^\dagger$ and $\zeta^\dagger$ on $|\psi_{M,N}\rangle$. Since

$$\begin{aligned}\eta_z|\psi_{M,N}\rangle&=\tfrac{1}{2}(M+N-L)|\psi_{M,N}\rangle\,,\\ \zeta_z|\psi_{M,N}\rangle&=\tfrac{1}{2}(M-N)|\psi_{M,N}\rangle\,,\end{aligned} \tag{6}$$

a state $|\psi_{M,N}\rangle$ has spin $\eta=\frac{1}{2}(L-M-N)$ with respect to the η-pairing SU(2) algebra and spin $\zeta=\frac{1}{2}(N-M)$ with respect to the ζ SU(2) algebra. The dimension of the corresponding SO(4) multiplet is therefore given by

$$\begin{aligned}\dim_{M,N}&=(2\eta+1)(2\zeta+1)\\ &=(L-M-N+1)(N-M+1)\,.\end{aligned} \tag{7}$$

The states in this multiplet, which are of the form $(\eta^\dagger)^\alpha(\zeta^\dagger)^\beta|\psi_{M,N}\rangle$, are all mutually orthogonal.

We now observe that (i) states obtained by acting with the SO(4) are not lowest weight states, and are thus, as a consequence of (5), outside the *regular* BA, and (ii) all the states that are not highest or lowest weight states for both SU(2) algebras are outside the BA. The statement (ii) shows that the BA is not complete. An example [5] of a state that is outside the BA is $\eta^\dagger|0\rangle=\sum_{j=1}^{L}(-1)^j c_{j,-1}^\dagger c_{j,1}^\dagger|0\rangle$.

Counting regular BA states means counting inequivalent solutions of the equations (4). Following Takahashi [8], we will first distinguish different types of solutions $\{k_i,\Lambda_\alpha\}$ of (4). The idea is that for a solution $\{k_i,\Lambda_\alpha\}$, the set of all the k_i's and Λ_α's can be split into (three) different kinds of subsets (strings), which are (i) a single real momentum k_i; (ii) m Λ_α's that combine into a string-type configuration ("Λ strings"), and this includes the case $m=1$, which is just a single real Λ_α; (iii) $2m$ k_i's and m Λ_α's that combine into a different string-type configuration ("k-Λ strings"). The configurations (ii) and (iii) are bound states.

Let us now consider a solution that splits into M_m copies of a Λ string of size m, M'_m copies of a k-Λ string of size m (containing $2m$ k_i's and m Λ_α's), and M_e additional single k_i's. Clearly, we have

$$M+N=M_e+2\sum_{m=1}^{\infty}mM'_m,\quad M=\sum_{m=1}^{\infty}m(M_m+M'_m)\,. \tag{8}$$

How many solutions of this type exist?

The idea is that each of the basic strings in a solution can be characterized by the position of its center on the real momentum or rapidity axis. Because of the periodic boundary conditions, this position has to be chosen from a discrete set. We will denote the centers for the size-m Λ strings by Λ_α^m, $\alpha=1,2,\ldots,M_m$, those for the size-m k-Λ strings by $\Lambda_\alpha'^m$, $\alpha=1,2,\ldots,M'_m$, and we will denote the unpaired momenta by k_j, $j=1,2,\ldots,M_e$.

Following [8], we now write the following equations for the centers k_j, Λ_α^m, and $\Lambda_\alpha'^m$. They follow from (4) and the form of the "idealized" string solutions (we write $N_e=M+N$ and $M'=\sum_{m=1}^{\infty}mM'_m$):

$$\begin{aligned}
&k_jL=2\pi I_j-\sum_{n=1}^{\infty}\sum_{\alpha=1}^{M_n}\theta\left(\frac{\sin k_j-\Lambda_\alpha^n}{nU}\right)-\sum_{n=1}^{\infty}\sum_{\alpha=1}^{M'_n}\theta\left(\frac{\sin k_j-\Lambda_\alpha'^n}{nU}\right),\\
&\sum_{j=1}^{N_e-2M'}\theta\left(\frac{\Lambda_\alpha^n-\sin k_j}{nU}\right)=2\pi J_\alpha^n+\sum_{(m,\beta)}\Theta_{nm}\left(\frac{\Lambda_\alpha^n-\Lambda_\beta^m}{U}\right),\\
&L\left[\sin^{-1}\left(\Lambda_\alpha'^n+in\frac{U}{4}\right)+\sin^{-1}\left(\Lambda_\alpha'^n-in\frac{U}{4}\right)\right]=2\pi J_\alpha'^n+\sum_{j=1}^{N_e-2M'}\theta\left(\frac{\Lambda_\alpha'^n-\sin k_j}{nU}\right)+\sum_{(m,\beta)}\Theta_{nm}\left(\frac{\Lambda_\alpha'^n-\Lambda_\beta'^m}{U}\right),
\end{aligned} \tag{9}$$

where

$$\theta(x)=2\tan^{-1}(4x)\,,$$

$$\Theta_{nm}(x)=\begin{cases}\theta\left(\dfrac{4x}{|n-m|}\right)+2\theta\left(\dfrac{4x}{|n-m|+2}\right)+\cdots+2\theta\left(\dfrac{4x}{n+m-2}\right)+\theta\left(\dfrac{4x}{n+m}\right) & \text{for } n\neq m\,,\\[2ex] 2\theta(2x)+\cdots+2\theta\left(\dfrac{2x}{n-1}\right)+\theta\left(\dfrac{2x}{n}\right) & \text{for } n=m\,.\end{cases} \tag{10}$$

The I_j, J_α^n, and $J_\alpha'^n$ are integer or half integer according to the following prescriptions: I_j is integer (half integer) if $\sum_m(M_m+M'_m)$ is even (odd); the J_α^n are integer (half integer) if N_e-M_n is odd (even); the $J_\alpha'^n$ are integer (half integer) if $L-(N_e-M_n')$ is odd (even). According to [8], we have the following inequalities:

$$|J_a^n| \le \frac{1}{2}\left(N_e-2M'-\sum_{m=1}^{\infty} t_{nm}M_m-1\right),$$
$$|J_a'^n| \le \frac{1}{2}\left(L-N_e+2M'-\sum_{m=1}^{\infty} t_{nm}M_m'-1\right), \tag{11}$$

where $t_{nm}=2\min(n,m)-\delta_{nm}$.

In order to enumerate the different solutions of the system (9), it is sufficient (according to [8-10]) to enumerate all possible sets of nonrepeating (half) integers I_j, J_a^n, and $J_a'^n$ satisfying (11). (In the context of the XXX Heisenberg model, it has been known since Bethe [11] that the actual distribution of the different types of solutions can be different from the one implied by this counting: For example, some of the predicted complex two-string solutions do not occur, but their absence is compensated for by the existence of additional pairs of real solutions [with repeating (half) integers]. Still, the counting of solutions according to [9,10] gives the correct result for the total number of states.)

From (11) we read off that the number of allowed values for the (half) integers corresponding to each of the strings are (i) L for a free k_i, (ii) $N_e-2M'-\sum_{m=1}^{\infty}t_{nm}M_m$ for a Λ string of length n, and (iii) $L-N_e+2M'-\sum_{m=1}^{\infty}t_{nm}M_m'$ for a k-Λ string of length n. The total number of ways to choose the (half) integers in a solution with multiplicities M_e, M_m, and M_m' is therefore given by

$$n(M_e,\{M_m\},\{M_m'\}) = \binom{L}{M_e}\prod_{n=1}^{\infty}\binom{N_e-2\sum_{m=1}^{\infty}mM_m'-\sum_{m=1}^{\infty}t_{nm}M_m}{M_n}\prod_{n=1}^{\infty}\binom{L-N_e+2\sum_{m=1}^{\infty}mM_m'-\sum_{m=1}^{\infty}t_{nm}M_m'}{M_n'}. \tag{12}$$

The total number of solutions of (4) with given numbers N and M is now obtained by summing $n(M_e,\{M_m\},\{M_m'\})$ over all the M_e, M_m, and M_m', under the constraints (8).

Every solution to (4) gives us a regular BA state, which comes with an entire multiplet of eigenstates of the Hamiltonian, the dimension $\dim_{M,N}$ of which is given in (7). The full number of eigenstates that are obtained from the BA *and* the SO(4) symmetry is therefore given by

$$N_{\text{eigenstates}} = \sum_{\substack{M\ge 0\\ N-M\ge 0\\ M+N\le L}}\sum_{N\ge 0}\left[\sum_{\substack{M_e=0\\ M+N=M_e+2\sum_{m=1}^{\infty}mM_m'\\ N-M=M_e-2\sum_{m=1}^{\infty}mM_m}}^{\infty}\sum_{M_m=0}^{\infty}\sum_{M_m'=0}^{\infty} n(M_e,\{M_m\},\{M_m'\})\right]\dim_{M,N}. \tag{13}$$

We will now outline how to prove that for even L the sum in (13) equals 4^L. We first recall two identities which have been used to prove completeness for the XXX Heisenberg model [9,10]:

$$\sum_{\substack{M_m=0\\ \sum_{m=1}^{\infty}mM_m=M_X}}^{\infty}\prod_{n=1}^{\infty}\binom{L_X-\sum_m t_{nm}M_m}{M_n} = \binom{L_X}{M_X}-\binom{L_X}{M_X-1} \tag{14}$$

and

$$\sum_{M_X=0}^{[L_X/2]}\left[\binom{L_X}{M_X}-\binom{L_X}{M_X-1}\right](L_X-2M_X+1)=2^{L_X}. \tag{15}$$

The first of these equations gives the number of regular BA states (defined by $M_X\le[L_X/2]$) for the Heisenberg XXX spin chain on a lattice of length L_X with M_X overturned spins. Formula (15) shows completeness: The total number of states in the SU(2) extended BA is equal to 2^{L_X}, which is the dimension of the Hilbert space of the model.

The summations over the multiplicities M_m and over the difference $N-M$ in the Hubbard model are precisely of the type (14) and (15), after the substitution $M_X\to\frac{1}{2}(M_e-N+M)$ and $L_X\to M_e$. (Under these summations the total number of electrons $M+N$, denoted by N_e, is fixed.) The summation that remains after this spin summation is

$$N_{\text{eigenstates}} = \sum_{N_e=0}^{L}(L-N_e+1)\left[\sum_{\substack{M_e=0\\ N_e=M_e+2\sum_{m=1}^{\infty}mM_m'}}^{N_e}\sum_{M_m'=0}^{\infty} 2^{M_e}\binom{L}{M_e}\prod_{n=1}^{\infty}\binom{L-N_e+\sum_{m=1}^{\infty}(2m-t_{nm})M_m'}{M_n'}\right]. \tag{16}$$

For evaluating this sum we will use a "summation device" which is similar to the one discussed by Takahashi in the Appendix of [9]. We will only sketch the idea here and present the details of this derivation elsewhere [12]. The main idea for the summation procedure is that one identifies the result of the summation as the coefficient of a certain power of a variable x in the Laurent expansion of a suitable function. This function is then worked out as an infinite product of factors, which arise upon the successive summations over the numbers M'_m, $m=1,2,\ldots,\infty$. After a rather long derivation this leads to

$$N_{\text{eigenstates}}=\frac{1}{2\pi i}\oint\frac{dx}{x^{L+1}}(1+2x)^L\sum_{E=0}^{L}(E+1)x^E[f(x)]^{-E-1}, \tag{17}$$

where the contour of integration is a small circle around the origin. The function $f(x)$ is given by $f(x)=\prod_{l=1}^{\infty}(1-U_l^{-1})$ and the functions $U_l(x)$ are determined by the recursion relation $U_{l+1}U_{l-1}=(1-U_l)^2$ and the initial values $U_1(x)=x^{-2}$ and $U_2(x)=(1-x^2)^2/x^4$. The two initial conditions determine the solution of the recursion relation uniquely, and we find that $2f(x)=1+(1-4x^2)^{1/2}$. After substituting this solution into (17) we obtain

$$N_{\text{eigenstates}}=4^L. \tag{18}$$

Thus we find that the number of eigenstates of the Hubbard model constructed by the SO(4) extension of the BA coincides with the dimension of the space of all electron configurations. This means that these states form a complete set of eigenstates.

We can also obtain a closed expression for the number of regular BA states for given numbers M and N of spin-down and spin-up electrons:

$$\binom{L}{N}\left[\binom{L}{M}+\binom{L}{M-2}\right]-\left[\binom{L}{N+1}+\binom{L}{N-1}\right]\binom{L}{M-1}. \tag{19}$$

This formula is the close analog of the result (14) for the XXX Heisenberg model.

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