The Hubbard chain: Lieb-Wu equations and norm of the eigenfunctions

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Abstract

We argue that the square of the norm of the Hubbard wave function is proportional to the determinant of a matrix, which is obtained by linearization of the Lieb-Wu equations around a solution. This means that in the vicinity of a solution the Lieb-Wu equations are non-degenerate, if the corresponding wave function is non-zero. We further derive an action that generates the Lieb-Wu equations and express our determinant formula for the square of the norm in terms of the Hessian determinant of this action.

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Introduction

Interacting many body systems share universal features. The best known example are the critical exponents which describe the thermodynamic properties near critical points. Two systems that have the same critical exponents belong to the same universality class. In one space dimension there are many systems which are exactly solvable by Bethe ansatz [1, 2, 3]. Each of these systems represents a universality class. The Bethe ansatz provides a unique possibility to obtain exact results for these systems, which are not accessible by perturbative methods.

In this article we address the problem of the calculation of the norm of the Bethe ansatz wave functions of the one-dimensional Hubbard model.

In all cases known so far the norms of Bethe ansatz wave functions are proportional to the determinant of a matrix, which is obtained by linearization of the Bethe ansatz equations around a solution. This assures the non-degeneracy of the Bethe ansatz equations in the vicinity of a solution, if the corresponding wave function does not vanish, and thus provides an important piece of information about the mathematical structure of the Bethe ansatz equations.

The first time a determinant formula for the norm of a Bethe ansatz wave function appeared in the literature was in Gaudin's article [4] on what is nowadays called the Gaudin model. Gaudin's conjecture was later generalized to the XXX and XXZ spin-$\frac{1}{2}$ chains [5] and to the Bose gas with delta interaction [1]. Due to the complicated nature of the Bethe ansatz wave function a proof was not available until the advent of the quantum inverse scattering method, which provided a powerful algebraic reformulation of the Bethe ansatz.

The first proof of norm formulae for a number of important Bethe ansatz solvable systems was presented by one of the authors [6] in 1982. The proof given in [6] is rather general. It relies on the structure of the R-matrix and the existence of an algebraic Bethe ansatz. It applies to the XXX and XXZ spin-$\frac{1}{2}$ chains, to the Bose gas with delta interaction and to a number of other interesting systems. As a corollary follows the norm formula for the Gaudin model (for a direct alternative proof of the norm formula for the Gaudin model see [7]).

In the following years the results of [6] were generalized and confirmed by different methods. Reshetikhin [8] generalized the proof of [6] to the case of a gl_3 invariant R-matrix, i.e. to systems with nested Bethe ansatz. Slavnov proved a formula for the scalar product of a Bethe vector with an arbitrary vector [9]. This formula is valid for models having the same R-matrix as the XXX and XXZ spin-$\frac{1}{2}$ chains. It was recently confirmed by Kitanine, Maillet and Terras who used an algebraic approach based on Drinfel'd twists [10]. Proofs of norm formulae which do not rely on the algebraic Bethe ansatz but on the Knizhnik-Zamolodchikov equation or its quantized version were given by Reshetikhin and Varchenko [11] and by Tarasov and Varchenko [12]. In the latter paper norm formulae for systems with gl_n invariant R-matrices were obtained.

Bethe ansatz solution of the Hubbard model

The Hamiltonian of the one-dimensional Hubbard model on a periodic L-site chain may be written as

$$H = -\sum_{j=1}^{L} \sum_{a=\uparrow,\downarrow} (c_{j,a}^{+} c_{j+1,a} + c_{j+1,a}^{+} c_{j,a}) + U \sum_{j=1}^{L} (n_{j\uparrow} - \tfrac{1}{2})(n_{j\downarrow} - \tfrac{1}{2}) \quad . \tag{1}$$

$c_{j,a}^{+}$ and $c_{j,a}$ are creation and annihilation operators of electrons of spin a at site j (electrons in Wannier states), $n_{j,a} = c_{j,a}^{+} c_{j,a}$ is the corresponding particle number operator, and U is the coupling constant. Periodicity is guaranteed by setting $c_{L+1,a} = c_{1,a}$.

The eigenvalue problem for the Hubbard Hamiltonian (1) was solved by Lieb and Wu [13] by means of the nested Bethe ansatz (for reviews see [3, 14, 15]). The Hubbard Hamiltonian conserves the number of electrons N and the number of down spins M. The corresponding Schrödinger equation can thus be solved for fixed N and M. Since the Hamiltonian is invariant under a particle-hole transformation and under reversal of all spins, one may set $2M \le N \le L$ [13].

We shall denote the coordinates and spins of the electrons by x_j and a_j, respectively, $x_j = 1, \dots, L$, $a_j = \uparrow, \downarrow$. Then the eigenstates of the Hubbard Hamiltonian (1) may be represented as

$$|N, M\rangle = \frac{1}{\sqrt{N!}} \sum_{x_1,\dots,x_N=1}^{L} \sum_{a_1,\dots,a_N=\uparrow,\downarrow} \psi(x_1,\dots,x_N; a_1,\dots,a_N)\, c_{x_N a_N}^{+} \dots c_{x_1 a_1}^{+} |0\rangle \ . \tag{2}$$

$\psi(x_1,\dots,x_N;a_1,\dots,a_N)$ is the Bethe ansatz wave function. It depends on the relative ordering of the coordinates x_j. Any ordering is related to a permutation Q of the numbers $1,\dots,N$ through the inequality

$$1 \le x_{Q1} \le x_{Q2} \le \dots \le x_{QN} \le L \quad . \tag{3}$$

The set of all permutations of N distinct numbers constitutes the symmetric group S_N. The inequality (3) divides the configuration space of N electrons into $N!$ sectors, which can be labeled by the permutations Q. The Bethe ansatz wave functions in the sector Q are given as

$$\psi(x_1,\dots,x_N;a_1,\dots,a_N) = \sum_{P\in S_N} \mathrm{sign}(PQ)\, \varphi_P(a_{Q1},\dots,a_{QN}) \exp\left(\mathrm{i}\sum_{j=1}^{N} k_{Pj}x_{Qj}\right) \quad . \tag{4}$$

The function $\mathrm{sign}(Q)$ is the sign function (or parity) on the symmetric group, which is -1 for odd permutations and $+1$ for even permutations.

Explicit expressions for the spin dependent amplitudes $\varphi_P(a_{Q1},\dots,a_{QN})$ can be found in [16]. They are of the form of the Bethe ansatz wave functions of an inhomogeneous XXX spin chain,

$$\varphi_P(a_{Q1},\dots,a_{QN}) = \sum_{\pi\in S_M} A(\lambda_{\pi 1},\dots,\lambda_{\pi M}) \prod_{l=1}^{M} F_P(\lambda_{\pi l};y_l) \quad . \tag{5}$$

Here $F_P(\lambda;y)$ is defined as

$$F_P(\lambda;y) = \frac{\mathrm{i}U/2}{\lambda - \sin k_{Py} + \mathrm{i}U/4} \prod_{j=1}^{y-1} \frac{\lambda - \sin k_{Pj} - \mathrm{i}U/4}{\lambda - \sin k_{Pj} + \mathrm{i}U/4} \quad , \tag{6}$$

and the amplitudes $A(\lambda_1,\dots,\lambda_M)$ are given by

$$A(\lambda_1,\dots,\lambda_M) = \prod_{1\le m<n\le M} \frac{\lambda_m - \lambda_n - \mathrm{i}U/2}{\lambda_m - \lambda_n} \quad . \tag{7}$$

In the above equations y_j denotes the position of the jth down spin in the sequence $a_{Q1},\dots,a_{QN}$. The y's are thus 'coordinates of down spins on electrons'. If the number of down spins in the sequence $a_{Q1},\dots,a_{QN}$ is different from M, the amplitude $\varphi_P(a_{Q1},\dots,a_{QN})$ vanishes. An expression for

$\varphi_P(a_{Q1}, \dots, a_{QN})$ using the terminology of the algebraic Bethe ansatz can be found in [20].

The wave functions (4) depend on two sets of quantum numbers $\{k_j \,|\, j = 1, \dots, N\}$ and $\{\lambda_l \,|\, l = 1, \dots, M\}$. These quantum numbers may in general be complex. The k_j and λ_l are called charge momenta and spin rapidities, respectively. The charge momenta and spin rapidities satisfy the Lieb-Wu equations (or 'periodic boundary conditions')

$$e^{\mathrm{i}k_j L} = \prod_{l=1}^{M} \frac{\lambda_l - \sin k_j - \mathrm{i}U/4}{\lambda_l - \sin k_j + \mathrm{i}U/4} \quad , \quad j = 1, \dots, N \quad , \tag{8}$$

$$\prod_{j=1}^{N} \frac{\lambda_l - \sin k_j - \mathrm{i}U/4}{\lambda_l - \sin k_j + \mathrm{i}U/4} = \prod_{\substack{m=1 \\ m \neq l}}^{M} \frac{\lambda_l - \lambda_m - \mathrm{i}U/2}{\lambda_l - \lambda_m + \mathrm{i}U/2} \quad , \quad l = 1, \dots, M \quad . \tag{9}$$

The states (2) are joint eigenstates of the Hubbard Hamiltonian (1) and the momentum operator (cf. [17]) with eigenvalues

$$E = -2 \sum_{j=1}^{N} \cos k_j + \frac{U}{4}(L - 2N) \quad , \quad P = \left(\sum_{j=1}^{N} k_j \right) \bmod 2\pi \quad . \tag{10}$$

The eigenfunctions (4) are antisymmetric with respect to interchange of any two charge momenta k_j and symmetric with respect to interchange of any two spin rapidities λ_l. They are antisymmetric with respect to simultaneous exchange of spin and space coordinates of two electrons, and hence respect the Pauli principle.

An action for the Lieb-Wu equations

Let us rewrite the Lieb-Wu equations (8), (9) in logarithmic form,

$$k_j L - \mathrm{i} \sum_{l=1}^{M} \ln \left(\frac{\mathrm{i}U + 4(\lambda_l - \sin k_j)}{\mathrm{i}U - 4(\lambda_l - \sin k_j)} \right) = 2\pi n_j^c \ , \tag{11}$$

$$\mathrm{i} \sum_{j=1}^{N} \ln \left(\frac{\mathrm{i}U + 4(\lambda_l - \sin k_j)}{\mathrm{i}U - 4(\lambda_l - \sin k_j)} \right) - \mathrm{i} \sum_{m=1}^{M} \ln \left(\frac{\mathrm{i}U + 2(\lambda_l - \lambda_m)}{\mathrm{i}U - 2(\lambda_l - \lambda_m)} \right) = 2\pi n_l^s \ . \tag{12}$$

Here the logarithm is defined in the cut complex plane, where the cut is along the real axis from $-\infty$ to zero. n_j^c in equation (11) is integer, if M is even and half odd integer, if M is odd. Similarly, n_l^s in (12) is integer, if $N - M$ is odd, half odd integer, if $N - M$ is even.

In order to formulate our norm conjecture we shall introduce certain functions connected to the logarithmic form (11), (12) of the Lieb-Wu equations. We shall start with the definition

$$\Theta_U(x) = \mathrm{i} \int_0^x dy \, \ln \left(\frac{\mathrm{i}U + 4y}{\mathrm{i}U - 4y} \right) \quad . \tag{13}$$

In terms of this function the Lieb-Wu equations (11), (12) read

$$k_j L - \sum_{l=1}^{M} \Theta'_U(\lambda_l - \sin k_j) - 2\pi n_j^c \;=\; 0 \quad , \tag{14}$$

$$\sum_{j=1}^{N} \Theta'_U(\lambda_l - \sin k_j) - \sum_{m=1}^{M} \Theta'_{2U}(\lambda_l - \lambda_m) - 2\pi n_l^s \;=\; 0 \quad . \tag{15}$$

Here the primes denote derivatives with respect to the argument. The left hand side of these equations can be easily integrated with respect to the variables $\sin k_j$ and λ_l, yielding the action

$$\begin{aligned} \mathcal{S} \;=\; & \sum_{j=1}^{N} (k_j \sin k_j + \cos k_j) L \\ & + \sum_{j=1}^{N} \sum_{l=1}^{M} \Theta_U(\lambda_l - \sin k_j) - \frac{1}{2} \sum_{l,m=1}^{M} \Theta_{2U}(\lambda_l - \lambda_m) \\ & - 2\pi \sum_{j=1}^{N} n_j^c \sin k_j - 2\pi \sum_{l=1}^{M} n_l^s \lambda_l \quad . \end{aligned} \tag{16}$$

Thus, introducing the abbreviation $\mathrm{s}_j = \sin k_j$, we can write the Lieb-Wu equations as extremum condition for $\mathcal{S}$,

$$\frac{\partial \mathcal{S}}{\partial \mathrm{s}_j} = 0 \quad , \quad j = 1, \dots, N \quad , \quad \frac{\partial \mathcal{S}}{\partial \lambda_l} = 0 \quad , \quad l = 1, \dots, M \quad . \tag{17}$$

We shall use the action $\mathcal{S}$ below in order to formulate our norm conjecture. A similar action was first introduced by Yang and Yang in the context of the Bose gas with delta interaction [18].

There is an interesting alternative way to write the Lieb-Wu equations. Let us define

$$\chi_j = k_j - \frac{1}{L}\sum_{l=1}^{M}\Theta'_U(\lambda_l - \sin k_j) - \frac{M\pi}{L} \quad , \tag{18}$$

$$\varphi_l = \frac{1}{N}\sum_{j=1}^{N}\Theta'_U(\lambda_l - \sin k_j) - \frac{1}{N}\sum_{m=1}^{M}\Theta'_{2U}(\lambda_l - \lambda_m) - \frac{(N-M+1)\pi}{N}, \tag{19}$$

where $j = 1, \dots, N$ and $l = 1, \dots, M$. In terms of these new variables the Lieb-Wu equations (8), (9) become

$$e^{\mathrm{i}\chi_j L} = 1 \quad , \quad j = 1, \dots, N \quad , \quad e^{\mathrm{i}\varphi_l N} = 1 \quad , \quad l = 1, \dots, M \quad . \tag{20}$$

This suggests to interpret the χ_j and φ_l as the momenta of charge and spin degrees of freedom.

The norm formula

The square of the norm of the wave function (4) is by definition

$$\| \psi \|^2 = \sum_{x_1,\dots,x_N=1}^{L} \sum_{a_1,\dots,a_N=\uparrow,\downarrow} |\psi(x_1,\dots,x_N; a_1,\dots,a_N)|^2 \quad . \tag{21}$$

Note that the normalization in (2) is such that

$$\langle N, M | N, M \rangle = \| \psi \|^2 \quad . \tag{22}$$

We suggest the following formula for the square of the norm of the Hubbard wave function (4),

$$\begin{aligned} \| \psi \|^2 \;&=\; (-1)^{M'} N! \left(\frac{U}{2}\right)^M \prod_{j=1}^{N} \cos k_j \prod_{1\le j<k\le M} \left(1 + \frac{U^2}{4(\lambda_j - \lambda_k)^2}\right) \cdot \\ &\quad \cdot \det \begin{pmatrix} \dfrac{\partial^2 \mathcal{S}}{\partial \mathrm{s}^2} & \dfrac{\partial^2 \mathcal{S}}{\partial \mathrm{s} \partial \lambda} \\ \dfrac{\partial^2 \mathcal{S}}{\partial \lambda \partial \mathrm{s}} & \dfrac{\partial^2 \mathcal{S}}{\partial \lambda^2} \end{pmatrix} \quad . \end{aligned} \tag{23}$$

Here M' is the number of pairs of complex conjugated k_j's in a given solution of the Lieb-Wu equations. The determinant on the right hand side of (23) is the determinant of an $(N+M) \times (N+M)$-matrix. This matrix consists of four blocks with matrix elements

$$\left(\frac{\partial^2 \mathcal{S}}{\partial \mathrm{s}^2}\right)_{mn} = \frac{\partial^2 \mathcal{S}}{\partial \mathrm{s}_m \partial \mathrm{s}_n} = \delta_{m,n} \left\{ \frac{L}{\cos k_n} + \sum_{l=1}^{M} \frac{U/2}{(U/4)^2 + (\lambda_l - \mathrm{s}_n)^2} \right\} \quad ,$$
$$m, n = 1, \dots, N \quad , \tag{24}$$

$$\left(\frac{\partial^2 \mathcal{S}}{\partial \lambda \partial \mathrm{s}}\right)_{mn} = \left(\frac{\partial^2 \mathcal{S}}{\partial \mathrm{s} \partial \lambda}\right)_{nm} = \frac{\partial^2 \mathcal{S}}{\partial \lambda_m \partial \mathrm{s}_n} = - \frac{U/2}{(U/4)^2 + (\lambda_m - \mathrm{s}_n)^2} \quad ,$$
$$m = 1, \dots, M \quad , \quad n = 1, \dots, N \quad , \tag{25}$$

$$\left(\frac{\partial^2 \mathcal{S}}{\partial \lambda^2}\right)_{mn} = \frac{\partial^2 \mathcal{S}}{\partial \lambda_m \partial \lambda_n} =$$
$$\delta_{m,n} \left\{ \sum_{j=1}^{N} \frac{U/2}{(U/4)^2 + (\lambda_n - \mathrm{s}_j)^2} - \sum_{l=1}^{M} \frac{U}{(U/2)^2 + (\lambda_n - \lambda_l)^2} \right\}$$
$$+ \frac{U}{(U/2)^2 + (\lambda_m - \lambda_n)^2} \quad , \quad m, n = 1, \dots, M \quad . \tag{26}$$

The norm is thus proportional to the Hessian determinant of the action $\mathcal{S}$ regarded as a function of the charge momenta k_j and spin rapidities λ_l. Recalling the formulation (17) of the Lieb-Wu equations we see that a solution is non-degenerate (locally unique for fixed values of n_j^c and n_l^s), if the norm of the corresponding wave function does not vanish. In other words, all eigenstates of the Hubbard Hamiltonian (1) correspond to non-degenerate solutions of the Lieb-Wu equations.

Another interesting form of the norm formula is obtained by expressing the Hessian determinant in equation (23) in terms of the momenta of elementary charge and spin excitations χ_j and φ_l,

$$\| \psi \|^2 = (-1)^{M'} N! L^N N^M \left(\frac{U}{2}\right)^M \prod_{1 \le j < k \le M} \left(1 + \frac{U^2}{4(\lambda_j - \lambda_k)^2}\right) \cdot$$
$$\cdot \frac{\partial(\chi_1, \dots, \chi_N; \varphi_1, \dots, \varphi_M)}{\partial(k_1, \dots, k_N; \lambda_1, \dots, \lambda_M)} \quad . \tag{27}$$

The norm is proportional to the Jacobian of the transformation from the set of charge momenta and spin rapidities k_j, λ_l to the set of momenta of charge and spin degrees of freedom χ_j, φ_l.

Let us list our arguments in support of (23):

(i) Our experience with other Bethe ansatz solvable models [6, 7, 8, 12] shows that norm formulae for Bethe ansatz wave functions are generically of the form (23).

(ii) It is easy to see that (23) is valid for $M = 0$ and arbitrary N.

(iii) We verified (23) for $N = 2$, $N = 3$ and $M = 1$. The calculation is lengthy and involves highly non-trivial cancellations based on the Lieb-Wu equations.

(iv) We verified (23) for arbitrary N and M in the limit $U \to \infty$. This limit requires rescaling of the spin rapidities, $\lambda_j = \Lambda_j U/2$. The remaining non-trivial factor in the expression for the norm reduces to the case of the XXX spin-$\frac{1}{2}$ chain, and the result of [6] can be applied.

(v) We calculated (for arbitrary N and M) the leading order term of the norm in the large L limit. This term is proportional to L^N and fixes the prefactor in (23).

Finally we would like to point out two applications of the norm formula (23). The string hypothesis for the Hubbard model [19] together with the SO(4) symmetry [20] predicts the correct number of eigenstates of the Hubbard Hamiltonian [21]. This fact is sometimes called combinatorial completeness. For some Bethe ansatz solvable models there exists an alternative proof of completeness which avoids the string hypothesis [22]. An important ingredient of this proof is a norm formula similar to (23).

Over the past two decades a programme was developed for calculating exactly temperature correlation functions of Bethe ansatz solvable models [2]. In the thermodynamic limit the correlation functions are represented as determinants of Fredholm integral operators of a certain form. The determinant representation is a powerful tool for studying the properties of the correlation functions analytically. It enabled, in particular, the exact calculation of long and short distance asymptotics for a number of Bethe ansatz solvable models. The calculation of the norm of the Bethe ansatz wave function is an important step towards a determinant representation for correlation functions of the Hubbard model at finite coupling. For the special case of infinite repulsion a determinant representation was recently obtained in [23].

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