Some aspects of functional Bethe ansatz

You-Quan Li
Institut für Physik, Universität Augsburg, D-86135 Augsburg, Germany
and Zhejiang Institute of Modern Physics, Zhejiang University, Hangzhou 310027, China
(Received 22 Oct 1999)

The validity of Bethe ansatz wave function without the backward scattering for the problem of impurity in correlated hosts with periodic boundary condition is illustrated by a simple example of quantum mechanics. An long being overlooked point in solving Hubbard model by means of Bethe ansatz is indicated. A possible repairing on the Hamiltonian is suggested so that the well known solution is still valid.

There has been a long and rich history on the study of integrable models in condensed matter physics since Bethe solved the one dimensional Heisenberg model [1]. One of the important examples is the success of Bethe ansatz method to Kondo problem. The exact solution of the Kondo impurity [4] as well as Kondo impurity [5] in correlated electron hosts [3] with quadratic dispersion. In those wave functions, the backward scattering waves are not involved because the periodic boundary condition was imposed. It was argued most recently [7] that the reflection matrices for impurities at edge [8] emulate only forward electron-impurity scattering. In this latter, I show by a simple example of quantum mechanics the validity of Bethe ansatz wave function without backward scattering. By the way, I indicate a long being overlooked point in solving Hubbard model by means of Bethe ansatz, and suggest a choice for repairing the model Hamiltonian so that the well known solution is still valid.

For simplicity, we place a non-magnetic impurity on a circle, if the wave function with backward scattering on the upper patch is assumed as

$$\psi_+(\theta > 0) = Ae^{ik\theta} + Be^{-ik\theta}, \tag{1}$$

then the one on the lower patch should be

$$\psi_-(\theta < 0) = Ae^{ik2\pi e^{ik\theta}} + Be^{-ik2\pi e^{-ik\theta}}. \tag{2}$$

This is due to the circle geometry (see Fig.1), equivalently periodic boundary condition. At the singularity point $\theta = 0$, the wave function is naturally defined by $(\psi_+(0^+) + \psi_-(0^-))/2$. Now we are in the similar situation mathematically for the wave function as for the gauge field in the presence of magnetic monopoles. As is known that a discontinuity relation at $\theta = 0$ for the derivatives of wave function can be obtained from the Schrödinger equation by using Gaussian theorem at the neighborhood of the $\delta$-function singular point, namely,

$$\psi'_+(0^+) - \psi'_-(0^-) = v[\psi_+(0^+) + \psi_-(0^-)], \tag{3}$$

where the prime stands for derivative. Substituting the wave functions (1) and (2) into eq.(3), one can obtain two possible solutions, one is $B/A = -\exp(ik2\pi)$ and the other is

$$e^{ik2\pi} = \frac{v - ik}{v + ik} \tag{4}$$

Because $v = 0$ is the case of a particle moving on a circle without impurity, the coefficient $A$ and $B$ should obviously be independent. The former is not a reasonable solution. If we temporally impose the continuity condition for the wave function at $\theta = 0$, we would get $B/A = \exp(ik2\pi)$. This contradicts not only with the $v = 0$ argument, but also disagrees with the solution of (3). Differing from the relation (3) which can be derived from Schrödinger equation, the continuity condition is not a consequence of the Schrödinger equation. We argue that the continuity condition should no more be imposed at present $\delta$-function singularity point otherwise the present quantum mechanical problem would have no solution. Therefore eq.(4), which is consistent for both $v = \infty$ (i.e., $\psi(0) := (\psi_+(0^+) + \psi_-(0^-))/2 = 0$) and $v = 0$, is the secular equation for the system.

Now let us observe the above example without the help of backward scattering. According to the strategy [4] we define the wave function piece-wisely on the “left” and “right” regions adjacent to the impurity,

$$\Psi(x) = \begin{cases} 
\psi_+(x) = A_+e^{ikx} & x > 0, \\
\psi_-(x) = A_-e^{-ikx} & x < 0. 
\end{cases} \tag{5}$$

The discontinuity relation (3) gives rise to

$$A_- = \frac{v - ik}{v + ik} A_+. \tag{6}$$

From the periodic boundary condition $\Psi(x + L) = \Psi(x)$, explicitly here $\psi_+(x + L) = \psi_-(x)$, we obtain once again the same secular equation (3) as long as $L = 2\pi$, the length of the circle. For $v \to \infty$, the wave function defined at the point $x = 0$ satisfactorily vanishes which
concises with physical picture. The case of \( v = 0 \) gives \( A_+ = A_- \) which is also of consistency.

If the impurity is a Kondo impurity \( V(x) = (JS \cdot S_m + V)\delta(x) \) the same discussion can be made as long as we introduce a two component wave function. We will not show these for the sake of saving pages.

For a Kondo impurity in \( N \) correlated electron host with quadratic dispersion, the secular equation for the spectrum was solved [4,5] on the basis of Bethe ansatz by using the piece-wisely defined wave function without the backward scattering waves. One can see that the secular equation for \( N = 1 \) reduces to the result of the above examples. Conversely, we can imagine a particle moving on the background of the other \( N - 1 \) particles besides the impurity. If employing the picture of the above example, we know that the particle will undergo \( N - 1 \) phase shifts after moving around the circle once due to the scattering with the other “background” potentials caused by the \( N - 1 \) particles. Then we can phenomenally understand the product of the \( N - 1 \) factors in the Bethe ansatz equation for boson system. For fermion system, however, it is too complicated to deduce the Bethe ansatz equation via a vivid description. Whence the literature of Bethe ansatz strategy is necessary and useful.

One can revisit the problem by taking account the backward scattering in the Bethe ansatz wave function, i.e.,

\[
\psi(x) = \sum_{P \in W_B} A(P; Q^{(i)}) e^{i(Pk_x)} \text{ for } x \in C(Q^{(i)}).
\]

where \( W_B \) stands for the Weyl group of \( B_N \) Lie algebra; \( a := (a_{Q1}, a_{Q2}, \ldots, a_{QN}) \), \( a_j \) denotes the spin component of the \( j \)th particle; \( Pk \) represents the image of a given \( k := (k_1, k_2, \ldots, k_N) \) by a mapping \( P \in W_B \), i.e., either permutating or adding a minus sign; \( \langle Pk|Qx \rangle = \sum_{j=1}^N \langle Pk_j|Qx \rangle \) and \( C(Q^{(i)}) := \{ |Qx \rangle_1 < |Qx \rangle_2 \ldots < |Qx \rangle_i < 0 \ldots < |Qx \rangle_N, Q \in S_N \}. \)

Although there are more coefficients \( A \)'s in this case, the Schrödinger equation is sufficiently satisfied by the same electron-impurity S-matrix. Of course, the argument \( (Pk)_i \) in the S-matrix \( S^{Q_i,0}(Pk)_i \) takes not only any of the \( k \)'s in \( \{ k_1, k_2, \ldots, k_N \} \) but also those with an additional minus sign. However, due to the property

\[
S^{Q_i,0}[-(Pk)_i] = [S^{Q_i,0}(Pk)_i]^{-1},
\]

one is able to obtain the same set of independent equations for the spectrum as in ref. [10] at the integrable sector. For open boundary condition, of cause, the backward scattering wave is necessary. Away from the integrable sector, the backward scattering plays an essential role. The dynamical backward scattering in a system of nonintegrable Kondo impurity was shown [10] to influence the properties of the system. Although the existence of impurity breaks infinitesimal translation symmetry, the symmetry of translation with a finite distance \( L \) remains for periodic boundary condition [10]. This may help to understand the validity of Bethe ansatz wave function without backward scattering for an integrable Kondo impurity.

Let us turn to a long-being overlooked point in solving Hubbard model [10],

\[
H = \sum_{i,a} -t(C_{i,a}^+ C_{i+1,a} + C_{i+1,a}^+ C_{i,a}) + U \sum_{i} n_{i\uparrow} n_{i\downarrow}.
\]

The spin states are denoted either by \( a = \pm 1/2, \pm 1/2 \) or by \( \uparrow \) and \( \downarrow \). The correct first quantized version of the Hamiltonian [8] in the Hilbert space of \( N \) particles, in stead, should be

\[
H = -\sum_{j=1}^N \Delta_j + U \sum_{i,j} \delta_{a_i, a_j} \delta_{x_i, x_j},
\]

The second term is spin-dependent which had not been noticed for a long period, so the result of ref. [11] can not be employed to present case directly. The original model, however, can be repaired. The antisymmetry property of fermion permutation always requires the wave function to be null when \( x_i = x_j \) and \( a_i = a_j \). This can be explicitly verified even if the wave function is piece-wisely defined.

Consequently, the Hamiltonian (8) is allowed to have an additional term \( \sum_{i,j} \delta_{a_i, a_j} \delta_{x_i, x_j} \) for arbitrary parameter \( V \) without changes in physical observables. Thus, strictly speaking, the Lieb-Wu solution [10] was solved from the Hamiltonian (8) after repairing the second term to be

\[
U \sum_{i,a,b} n_{i\alpha} n_{i\beta}.
\]

Fortunately, the spectrum obtained in ref. [10] is still valid without changes due to the above mentioned equivalence relation.

The work is supported by AvH-Stiftung, also supported by NSFC-19975040 and EYFC98.

[1] H. Bethe, Z. Physik 71, 205 (1931).
[2] N. Andrei, K. Furuya, and J.H. Lowenstein, Rev. Mod. Phys. 55, 331 (1983).
[3] A.M. Tsvelick, and P.B. Wiegmann, Adv. in Phys. 32, 453 (1983).
[4] Y.Q. Li, and Z.S. Ma, Phys. Rev. B52, R13071 (1995).
[5] Y.Q. Li, and P.A. Bares, Phys. Rev. B56, R11384 (1997).
[6] P. Fendley, A.W.W. Ludwig, and H. Saleur, Phys. Rev. Lett. 74, 3005 (1995).
[7] A.A. Zvyagin, and H. Johannesson, Phys. Rev. Lett. 81, 2751 (1998).
[8] Y.P. Wang, and J. Voit, Phys. Rev. Lett. 77, 4934 (1996).
[9] H.D. Lee, and J. Toner, Phys. Rev. Lett. 69, 3378 (1992); A. Furusaki, and N. Nagosa, Phys. Rev. Lett. 72, 892 (1994); P. Fröjd, and H. Johannesson, Phys. Rev. Lett. 75, 300 (1995).
[10] E.H.Lieb, and F.Y.Wu, Phys. Rev. Lett. 20, 1445 (1968).
[11] C. N. Yang, Phys. Rev. Lett. 19, 1312 (1967).
FIG. 1. The circle is separated by an impurity into upper patch $\theta > 0$ and lower patch $\theta < 0$, on which the wave function of a single particle is defined piece-wisely. Both forward and backward waves are indicated by dot-lines. The relations between the coefficients in eq.(1) and eq.(4) are obvious from the figure.