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Exact results of a hard-core interacting system with a single impurity

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The quantum-mechanical problem of a many-particle system with a single impurity in one dimension, interacting by a $\delta$ function, is solved. The wave function for a bosonic system and the related secular equation for the spectrum are obtained. The energy per length is calculated in the thermodynamic limit.

The quantum-mechanical problem of particles in one dimension with $\delta$-function interaction was studied in Refs. 1–5. In Ref. 3, the strategy now referred to as the "Bethe ansatz" was successfully applied to this problem. In order to obtain the secular equation for the spectrum, periodic boundary condition is imposed so that the particles were thought of as situated on a circle. Subsequently, some other kind of boundary conditions were taken into account, such as the case of particles being enclosed in an infinitely deep potential well, the case of Ref. 7 with a modification by the addition of an infinitely deep and very narrow well at one end of the interval or, recently, the case of particles being enclosed in a well of finite depth. As a mathematical consideration, Ref. 10 had generalized the above problem to the extent within the finite Coxeter group.

In the series of a line of studies on exact solutions of the above mentioned quantum-mechanical problem, as far as we are aware, attention has largely been concentrated on the replacement of boundary conditions which are used to determine the secular equation. In this paper we consider a system of $N$ particles and a single impurity. We find the Bethe ansatz wave function of the system and the secular equation for the spectrum. As a result, the wave function is a sum of nondiffractive waves over the permutation group $S_N$ and defined piecewise on separate regions. These regions are specified by the permutation group $S_{N+1}$ instead of $S_N$. The energy per length of the system is calculated in the thermodynamic limit. The problem involved in this paper differs from that of the Kondo Hamiltonian which was ever diagonalized in Refs. 11 and 12.

The Hamiltonian of a system of $N$ particles and a single impurity, interacting by a $\delta$ function, reads

$$ H = -\frac{\hbar^2}{2m} \sum_{i=1}^{N} \frac{\partial^2}{\partial x_i^2} - \frac{\hbar^2}{2m} \frac{\partial^2}{\partial x_i' \partial x_i} + u \sum_{j=1}^{N} \delta(x_i - x_j) $$

$$ + \nu \sum_{i=1}^{N} \delta(x_i - x_i'), $$

where $x'$ stands for the coordinate of the impurity and $x_i$ for that of the $i$th particle. For simplicity, we start discussion with the convention $\mu = m'/m$, $\hbar = 1$, $m = 1$. The Hamiltonian (1) is invariant under the action of whole coordinate translation, so the total momentum of the system is conserved.

The continuity of wave functions and their derivatives is determined by the Schrödinger equation on the basis of the properties of the potential in the Hamiltonian. In order to conveniently obtain the boundary condition arising from the $\delta$-function terms in (1), we make a scalar transformation $x' \rightarrow x_0 = \sqrt{\mu} x'$. With this transformation, we can combine the first and second terms of (1) so that they become a
standard Laplace operator in an \((N+1)\) dimensional Euclidean space \(\mathbb{R}^{N+1}\) with Cartesian coordinates \((x_0,x_1,x_2,...,x_N)\). Thus, the Schrödinger equation takes the following form:

\[
H = -\frac{1}{2} \sum_{i=0}^{N} \frac{\partial^2}{\partial x_i^2} + \frac{1}{2\mu} \left( \frac{\partial}{\partial y_0} - \sum_{i=1}^{N} \frac{\partial}{\partial y_i} \right)^2 + u \sum_{j=1}^{N} \delta(y_j - y_j)
\]

\[
+ v \sum_{i=1}^{N} \delta(y_i),
\]

where the summation of the “kinetic energy” starts from \(l=0\) instead of \(l=1\).

After removing the \(\delta\)-function terms from the left-hand side to the right-hand side of (2), one takes the integration of (2) over a “Gauss box” that is cut into halves by either the hyperplane \(\{x_i = 0\mid i=1,2,...,N\}\) or \(\{x_i/x_0 = \sqrt{\mu} = 0\mid i=1,2,...,N\}\). With the help of the Gauss integral theorem, we obtain the discontinuity relations for the derivatives of the wave function along the normal of a hyperplane \(\alpha = \{x_i(x) = 0\}\), where \(\alpha\) stands for the normal vector and \(\alpha(x)\) stands for a scalar product of two vectors \(\alpha\) and \(x = (x_0,x_1,x_2,...,x_N)\), i.e.,

\[
\lim_{\epsilon \to 0^+} \{ \alpha \cdot \nabla [\psi(x(\alpha) + \epsilon\alpha) - \psi(x(\alpha) - \epsilon\alpha)] \} = 2c \psi(x(\alpha)),
\]

where \(c = u\) for \(\alpha = e_1 - e_j\) and \(c = v\) for

\[
\alpha = e_i - \frac{1}{\sqrt{\mu}} x_0 (i = 1,2,\ldots,N); \quad \nabla = \sum_{i=0}^{N} e_i \frac{\partial}{\partial x_i}; \quad x_0(\alpha) \in \mathcal{P}_\alpha,
\]

and \(\{e_i\}\) is the standard orthogonal basis.

It is convenient to discuss the present problem in the frame of reference of the impurity. This requires a coordinate transformation \((x_0,x_1,x_2,...,x_N) \rightarrow (y_1,y_2,y_3,...,y_N)\) given by

\[
y_0 = x' = 1/\sqrt{\mu} x_0, \quad y_i = x_i - x' = x_i - 1/\sqrt{\mu} x_0.
\]

It results that

\[
\frac{\partial}{\partial x_0} = \frac{1}{\sqrt{\mu}} \left( \frac{\partial}{\partial y_0} - \sum_{i=1}^{N} \frac{\partial}{\partial y_i} \right)
\]

and

\[
\frac{\partial}{\partial x_i} = \frac{\partial}{\partial y_i}.
\]

Obviously,

\[
\frac{\partial}{\partial y_0} = \sum_{i=1}^{N} \frac{\partial}{\partial x_i} + \frac{\partial}{\partial x'}
\]

is just the operator of total momentum (apart from a factor \(-i\)). In terms of these coordinates \((y_0,y_1,y_2,...,y_N)\), the Hamiltonian (1) and the discontinuity relation (3) become

\[
H = -\frac{1}{2} \sum_{i=1}^{N} \frac{\partial^2}{\partial y_i^2} + \frac{1}{2\mu} \left( \frac{\partial}{\partial y_0} - \sum_{i=1}^{N} \frac{\partial}{\partial y_i} \right)^2 + u \sum_{j=1}^{N} \delta(y_j - y_j)
\]

\[
+ v \sum_{i=1}^{N} \delta(y_i),
\]

\[
\lim_{\epsilon \to 0^+} \left( \frac{\partial}{\partial y_i} - \frac{\partial}{\partial y_j} [\psi(y(x) + \epsilon\alpha) - \psi(y(x) - \epsilon\alpha)] \right) = 2u \psi(y(x)),
\]

and

\[
\lim_{\epsilon \to 0^+} \left( \frac{\partial}{\partial y_i} - \frac{\partial}{\partial y_j} [\psi(y(x') + \epsilon\alpha') - \psi(y(x') - \epsilon\alpha')] \right) = 2v \psi(y(x')),
\]

where \(\alpha\) stands for the normal vector of the hyperplane \(\{y_{i \neq j}=0\}\) and \(\alpha'\) for that of the hyperplane \(\{y_j = 0\}\). Clearly, (4) is invariant under the translation of \(y_0 \rightarrow y_0 + \epsilon\) or under any permutation of the coordinates \(y_i\) for \(i=1,2,\ldots,N\). Because of the translational invariance of \(y_0\), we may set \(\psi(y_0,y_1,...,y_N) = e^{ik_0 y_0} \psi(y_1,...,y_N)\), where \(k_0\) is a constant, i.e., the total momentum is conserved. Then the Schrödinger equation is reduced to a differential equation for \(\Phi(y_1,y_2,...,y_N)\). On the domain \(\mathbb{R}^N \setminus \mathcal{P}_\beta\) it becomes

\[
\left( -\frac{1}{2} \sum_{i=1}^{N} \frac{\partial^2}{\partial y_i^2} + \frac{1}{2\mu} \left( \sum_{i=1}^{N} \frac{\partial}{\partial y_i} - iK \right)^2 \right) \psi(y_1,y_2,...,y_N) = E \psi(y_1,y_2,...,y_N),
\]

where \(\{\mathcal{P}_\beta\}\) stands for the set of hyperplanes \(\{y_{i \neq j}=0\}\) and \(\{y_j = 0\}\) for \(i,j=1,2,\ldots,N\). Obviously these hyperplanes partition \(\mathbb{R}^N\) into finitely many regions and a wave function must be a piecewise continuous function defined respectively on separate regions. The regions into which the hyperplanes \(\{y_{i \neq j}=0\}\mid i,j=1,2,\ldots,N\}\) partition \(\mathbb{R}^N\) can be specified by elements of a permutation group \(S_N\). In other words, different regions have different orders for the coordinates \((y_1,y_2,...,y_N)\) if their components are arranged from large value to small ones, e.g., \(y_1 > y_2 > y_3 > \cdots > y_N\), \(y_2 > y_1 > y_3 > \cdots > y_N\), etc. Moreover, each of such regions is partitioned into \(N+1\) separate regions by the other type of hyperplanes \(\{y_j = 0\}\). For example, the region \(y_1 > y_2 > \cdots > y_N\), is partitioned into the regions \(0 > y_1 > y_2 > \cdots > y_N\), \(y_1 > 0 > y_2 > \cdots > y_N\), \(y_1 > 0 > y_2 > \cdots > y_N\), \(y_1 > y_2 > 0 \cdots > y_N\), etc. These regions can be specified by a permutation group \(S_N\). It is easy to find a special solution for (7), i.e., a plane wave solution \(\Psi_k(y) = e^{ik y_0}\), here \(k(y) = k_1 y_1 + k_2 y_2 + \cdots + k_N y_N\). The corresponding energy is

\[
E = \frac{1}{2} \sum_{i=1}^{N} k_i^2 + \frac{1}{2\mu} \left( \sum_{i=1}^{N} k_i - K \right)^2
\]

or more neatly,
\[ E = \frac{1}{2} \sum_{i=1}^{N} k_i^2 + \frac{1}{2 \mu} \lambda^2, \quad (8) \]

where a parameter \( \lambda = K - \sum_{i=1}^{N} k_i \) is introduced.

Because of the permutational invariance of the Hamiltonian (4), we look for solutions of the Bethe ansatz form:

\[ \varphi_\sigma(y) = \sum_{\sigma \in S_N} A(\sigma, \sigma) e^{i(\sigma k \cdot y)}, \quad (9) \]

where \( \sigma k \) stands for the image of a given \( k = (k_1, k_2, \ldots, k_N) \) by a permutation \( \sigma \in S_N \) and the coefficients \( A(\sigma, \sigma) \) are functionals on \( S_N \). It is worthwhile to mention that the summation in (9) is taken over the permutation group \( S_N \) whereas the various regions on which the wave function is defined are specified by elements of \( S_{N+1} \). This is different from the Bethe-Yang ansatz. As far as the Bethe ansatz solution (9) is concerned, the boundary condition (6) becomes

\[ \left( \frac{\partial}{\partial y_i} - \frac{\lambda}{\mu} \right) \varphi(y)|_{y_i = 0^+} - \varphi(y)|_{y_i = 0^-} = 2v \varphi(y)|_{y_i = 0}. \quad (10) \]

For a bosonic system, the wave function is supposed to be symmetric under any permutation of the coordinates. Because any element of permutation group \( S_N \) can be expressed as a product of the neighboring interchanges \( \sigma_1 : (y_1, y_2, \ldots, y_N) \rightarrow (y_2, y_3, \ldots, y_1) \), \( i = 1, 2, \ldots, N-1 \), it follows that \( (\sigma \sigma_i \sigma^{-1} \sigma) \varphi = \varphi \). Since \( \varphi \) is a scalar function, \( (\sigma \varphi) = \varphi \) well defined by \( \varphi(\sigma^{-1} \cdot y) \). Thus both sides of the equation can be written out using (9). In terms of the evident identity \( (\sigma k | \sigma^{-1} \cdot y) = (\sigma k | y) \) and the rearrangement theorem of group theory, we obtain the following consequence:

\[ A(\sigma, \sigma, \sigma) = A(\sigma_i, \sigma, \sigma), \quad \text{for } i = 1, 2, \ldots, N-1. \quad (11) \]

Substituting (9) into the boundary condition (10) and using the continuity condition for the wave function on the hyperplanes, we obtain the following relation (when \( y_i \) is nearest to zero among all \( \{y_j, j = 1, 2, \ldots, N\} \)):

\[ A(\sigma, \sigma, \sigma) = -\frac{v - i[(\sigma k) - (\lambda/\mu) \cdot \sigma]}{v + i[(\sigma k) - (\lambda/\mu) \cdot \sigma]} A(\sigma, \sigma, \sigma), \quad (12) \]

where \( \sigma \in S_{N+1} \) but \( \sigma \in S_N \). The relations (11) and (12) relate \( A \) coefficients between different regions, so we direct our attention to one of the regions, e.g., \( y_1 > y_2 > \cdots > y_N > 0 \).

Because the region with \( y_1 < y_2 < \cdots < y_i \) is next to the region with \( y_1 < y_2 < \cdots < y_N \) the boundary condition (5) and the continuity condition for the wave function on the hyperplanes give a relation between \( \varphi_\sigma(y) \) and \( \varphi_{\sigma_i}(y) \) \( i = 1, 2, \ldots, N-1 \). After writing out the relation in detail we obtain the following:

\[ i[(\sigma k)_i - (\sigma k)_{i+1}]A(\sigma, \tau) - A(\sigma, \sigma, \tau) = A(\sigma, \sigma, \sigma) \]

\[ + A(\sigma, \sigma, \sigma) = 2uA(\sigma, \tau) + A(\sigma, \sigma, \sigma). \quad (13) \]

With the help of (11) this relation gives

\[ A(\sigma, \sigma, \tau) = -Y(\cdot k)A(\sigma, \sigma, \tau), \]

\[ Y(\cdot k) = \frac{u - i[(\cdot k) - (\cdot k)_{i+1}]}{u + i[(\cdot k) - (\cdot k)_{i+1}]} \quad \text{for } i = 1, 2, \ldots, N - 1 \]

As a result, all the \( A \) coefficients are determined up to an overall scalar factor by using (14) repeatedly. The consistency of successive use of (14) is guaranteed because the \( Y \)'s in (14) satisfy the Yang-Baxter equation.

In the above we have obtained the Bethe ansatz solution of the Schrödinger equation on the basis of boundary conditions arising from \( \delta \) functions in the Hamiltonian. Now we turn to determine the secular equation of the spectrum \( \{k\} \). Suppose the system is situated on a circle of length \( L \), the wave function must obey the periodic boundary condition \( \varphi(y_1, \ldots, y_N) = \varphi(y_1, \ldots, y_N) \). If \( y = (y_1, \ldots, y_i, \ldots, y_N) \) is a point in the region specified by \( \tau \in S_{N+1} \), as a result of periodicity, \( y' = (y_1, \ldots, y_i, \ldots, y_N) \) must be a point on another region specified by \( \gamma = \tau \sigma \in S_{N+1} \), where \( \gamma = \sigma_i \Delta \) and \( \Delta = \sigma_{N-1} \cdots \sigma_1 \sigma_i \). Then the requirement of the periodic boundary condition is explicitly written as \( \varphi_\gamma(y') = \varphi(y) \). After writing this relation in terms of the Bethe ansatz solution (9), we find that the periodic boundary condition is guaranteed as long as the relation \( A(\sigma, \sigma) e^{-i(\cdot k)_{1}\cdot L} = A(\sigma, \tau) \) is imposed. This implies the following equation after using (11), (12), and (14) repeatedly,

\[ e^{i(\cdot k)_{1}\cdot L} = (-1)^N \frac{v - i[(\cdot k) - (\cdot k)_{i+1}]}{v + i[(\cdot k) - (\cdot k)_{i+1}]} \prod_{j=1}^{N} \frac{u - i[(\cdot k) - (\cdot k)_{j}]}{u + i[(\cdot k) - (\cdot k)_{j}]}. \quad (15) \]

As (15) holds for any \( \sigma \in S_N \), \( (\cdot k) \) will take \( k_1, k_2, \ldots, k_N \), respectively. So (15) represents \( N \) distinct equations.

Taking the logarithm of (15), we have a system of coupled transcendental equations,

\[ k_j = I_j \left( \frac{2 \pi}{L} \right) - \frac{2}{L} \tan^{-1} \left( \frac{k_j - \lambda/\mu}{u} \right) + \sum_{i=1}^{N} \tan^{-1} \left( \frac{k_j - k_i}{u} \right), \quad (16) \]

where the choice of range for \( \tan^{-1} \) is \( (-\pi, \pi) \), and \( I_j \) takes integer values or half integer values accordingly as \( N \) is even or odd. Equation (16) is the secular equation for the spectrum and the \( I_j \) play the role of the quantum numbers. As a result of periodicity, the total momentum is quantized, i.e., \( K = n(2 \pi/L) \), \( n \) is an integer. In particular, when \( \mu = 1 \), the secular equation recover the known result\(^3\) of \( N+1 \) particles. From (8) we learned that eigenstates related to \( \{k_1, k_2, \ldots, k_N\} \) and those related to \( \{\lambda, k_2, \ldots, k_N\} \), \( \{k_1, \lambda, \ldots, k_N\} \), etc., have the same energy for \( \mu = 1 \). However, the \( (N+1) \) fold degeneracy is broken by the replacement of a particle by an impurity.

Although the transcendental equation is difficult to solve, we are able to do some meaningful calculations for \( N \rightarrow \infty \), i.e., the thermodynamic limit. Suppose that \( \{k_1, k_2, \ldots, k_N\} \) is a self-consistent solution set of (16). Consider the function
\[ I(k) = \frac{1}{2\pi} \left( kL + 2 \left[ \sum_{i=1}^{N} \tan^{-1} \left( \frac{k - k_i}{v} \right) \right] \right), \]  

which is a monotonically increasing function of \( k \). Clearly, when \( I(k) \) passes through one of the quantum numbers \( I_j \), the corresponding \( k \) is equal to \( k_j \), one of the roots. However, there may exist some integer (or half integer) values for which the corresponding \( k \) is not in the set \( \{k_1, k_2, \ldots, k_N\} \), then such a \( k \) is called a "hole." A smooth, positive-definite density (per length) describing the distribution of roots and holes is naturally defined as

\[ \rho(k) = \frac{1}{L} \frac{dI(k)}{dk}. \]

Differentiating (17) we get an expression for \( \rho(k) \). In the thermodynamic limit (i.e., sufficiently large \( N \)) one can make a replacement, namely, \( \lim_{N \to \infty} \sum_{i=1}^{N} f(k_i) = \int dk \rho(k) f(k) \) 

\[ - \sum_{j=1}^{m} f(h_j), \]  

where \( h_1, h_2, \ldots, h_m \) are positions of holes. Then we have

\[ \rho(k) = \frac{1}{2\pi} \left[ \frac{1}{\pi L} \frac{u}{v^2 + (k - \lambda/\mu)^2} \right] - \sum_{j=1}^{m} \frac{u}{u^2 + (k - h_j)^2} \]

\[ + \int dk' \rho(k') \frac{u}{u^2 + (k - k')^2}. \]

This can be solved by means of the Fourier transformation technique. After some calculations, one gets the density of roots and holes as a Fourier integral. Then the energy per length of the system is obtained as

\[ E = \frac{\lambda^2}{2\mu L} + \frac{1}{4\pi} \int \frac{k^2 e^{-i k \xi}}{1 - e^{-i \xi}} \left( \delta(\xi) - \sum_{j=1}^{m} e^{i \xi h_j} \right) d\xi dk. \]

for repulsive case \( u, v > 0 \).

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