Exact solution of models of one-dimensional magnetic substances with an interaction which goes beyond nearest neighbors

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Exact solutions are derived by means of a Bethe substitution for several models of one-dimensional magnetic substances, including spin-1/2 chains, with an interaction which goes beyond nearest neighbors. The models describe a frustrated state and a ferrimagnetic state.

Several phenomena which have been seen in quasi-one-dimensional conductors cannot be explained on the basis of the models which have been solved. In particular, there is the transition with a vector of $4k_F$. In efforts to describe the entire set of properties of one-dimensional conductors, several investigators have proposed a lattice model of an electron gas in which the interaction goes beyond nearest neighbors (see, for example, Ref. 1 and the bibliography there). I believe that an exact solution of several simpler models could set the stage for the solution of the more general and more complex model proposed in Ref. 1.

In this letter I will discuss three models which can be solved by means of the Bethe substitution. The first model is an isotropic chain of spin-1/2's with an interaction between neighbors which goes beyond nearest neighbors. Its Hamiltonian is

$$\mathcal{H} = J_1 \sum_{n=1}^{N} \vec{\sigma}_n \cdot \vec{\sigma}_{n+1} + J_2 \sum_{n=1}^{N} \vec{\sigma}_n \cdot \vec{\sigma}_{n+2} . \tag{1}$$

The second model is a model of lattice spin-0 fermions:

$$\mathcal{H} = \sum_{n=1}^{N} \left(-(a^+_{n+1} a_n + a^+_n a_{n+1}) + U_1 a^+_{n+1} a_{n+1} a^+_n a_n + U_2 a^+_{n+2} a_{n+2} a^+_n a_n \right). \tag{2}$$

The third model is an Su(2)-invariant magnetic substance with quaternary exchange:

$$\mathcal{H} = \sum_{n=1}^{N} (X^n_{ij} X^{n+1}_{ji} + UX^n_{ij} X^{n+1}_{jk} X^{n+2}_{kp} X^{n+3}_{pi}); \ (X_{ij})_{ab} = \delta_{ia}\delta_{jb} \quad (3)$$

The last of these models is further from reality than the first two, but it is simpler to solve, and it does preserve some nontrivial physics of models (1) and (2). In the case $|U\pi| = +1$, the ground state of this model is a frustrated state, while in the case $|U\pi| > 1$ it is a ferrimagnetic state. The same conclusions would be expected for model (1), so an analysis of the simpler case of model (3) makes it possible to draw certain conclusions about model (1) also, for which I have not yet been able to calculate physical quantities.

Let us examine model (1). The wave function of a single-magnon state is

$$|k\rangle = \sum_n e^{ikn}\sigma^-_n |0\rangle, \qquad \sigma^+_m |0\rangle = 0.$$

Its energy is

$$E(k) = -2[1 + \cos k + U(1+\cos 2k)]. \quad (4)$$

We see a two-magnon function in the form

$$|k_1, k_2\rangle = \sum_{n,m} [f(n-m)e^{ik_1n+ik_2m} + f(m-n)e^{ik_2n+ik_1m}]\sigma^-_n\sigma^-_m |0\rangle. \quad (5)$$

Substituting (5) into the Schrödinger equation $H\psi = E\psi$, we find the system of equations

$$E(k_1, k_2) = E(k_1) + E(k_2) \quad (6a)$$

$$X(z_2 + z_1^{-1}) - S(z_2 + z_1^{-1} + U(z_2^2 + z_1^{-2} - 2))$$

$$= z_2^2 z_1^{-2}(z_1 + z_2^{-1} + U(z_1^2 + z_2^{-2} - 2)) \quad (6b)$$

$$X(z_1 + z_1^{-1} + z_2 + z_2^{-1} - 2 + U(z_1^2 + z_1^{-2} + z_2^2 + z_2^{-2} - 2 - z_1z_2 - z_1^{-1}z_2^{-1}))$$

$$- S(z_1 + z_2^{-1} + U(z_1^2 + z_2^{-2})) = z_2z_1^{-1}(z_2 + z_1^{-1} + U(z_2^2 + z_1^{-2})), \quad (6c)$$

where

$$S = f(2)/f(-2); \quad X = z_2(f(-1)z_1^{-1} + f(1)z_2^{-1})/f(-2), \ z = e^{ik}, \ U = J_2/J_1.$$

Solving system (6), we find the magnon scattering matrix

$$S(z_1, z_2) = -z_2^2P(z_1, z_2)/z_1^2P(z_2, z_1) \quad (7a)$$

$$P(z_1, z_2) = (z_1 + z_2^{-1})(z_1 + z_2^{-1} - 2)$$
$$+ 2U(2 + z_1^2 z_2^{-1} + z_2^2 z_1^{-1} - z_2 - z_1^{-1} - z_2^{-1} - z_1$$
$$+ z_1^3 + z_2^{-3} - z_2^{-2} - z_1^2)$$
$$+ U^2(z_1^2 + z_2^{-2} - 2)(z_1^2 + z_1^{-2} + z_2^2 + z_2^{-2} - z_1 z_2 - z_1^{-1} z_2^{-1}) \quad (7b)$$

Following the standard procedure of the Bethe method,[2] which makes it possible to calculate a multiparticle wave function from a two-particle wave function (there could not be any obstacles to this procedure here since the particles are scalar particles, their scattering matrix is a number, and it thus obviously satisfies the triangle equation), we find the following equations for the eigenvalues of Hamiltonian (1) on a chain with periodic boundary conditions:

$$(z_j)^N = \prod_{k=1}^{M} S(z_j, z_k), \quad (8a)$$

$$E = -2J_1 \sum_{j=1}^{M} (z_j + z_j^{-1} + U(z_j^2 + z_j^{-2} + 1) + 1). \quad (8b)$$

The spin of the system is $S^Z = N/2 - M$.

It is not difficult to verify that in the case $U = 0$ the substitution $z = (\lambda + i)/(\lambda - i)$ makes matrix (7) a function of the rapidity difference $\lambda_j - \lambda_k$ and puts Eqs. (7) and (8) in their customary form[2]:

$$\left(\frac{\lambda_\alpha + i}{\lambda_\alpha - i}\right)^N = \prod_{\beta=1}^{M} \left(\frac{\lambda_\alpha - \lambda_\beta + 2i}{\lambda_\alpha - \lambda_\beta - 2i}\right). \quad (9)$$

In the case $J_1 = 0$ ($U \to \infty$), magnetic substance (1) decomposes into two magnetic substances which are independent of each other and which each have a number of spins $N/2$. In this case the substitution $Z^2 = (\lambda + i)/(\lambda - i)$ sends (7) and (8) into two independent equations for the rapidities $\{\lambda_\alpha\}$ and $\{\lambda'_\alpha\}$. These equations become the same as Eq. (9) when we replace N by $N/2$ and when we insert a coefficient of $(-1)^{N/2}$ on the left side of one of these equations.

For other values of U, there is apparently no similar change of variables. A case of this sort has been seen previously in the theory of integrable systems.[3]

The procedure for solving model (2) differs in no fundamental way from that for solving model (1). The scattering matrix is of the same form as (7a), but with

$$P(z_1, z_2) = (z_1 + z_2^{-1} - U_1)(z_1 + z_2^{-1} - U_2) - U_2 z_2/z_1 (z_1 + z_2^{-1}). \quad (10)$$

The solution for model (3) has in principle already been given in the literature (Ref. 4, for example), although no one has discussed its physical properties. The situation is that the fourth term in Hamiltonian (3) is an integral of motion of an XXX Heisenberg chain. Specifically, it is the second derivative of the logarithm of its transfer matrix.[4] The solution of model (3) is therefore described by Eqs. (9), but with a different energy:

$$E = -\frac{4}{\pi}\sum_{\alpha=1}^{M}\left(\frac{1}{1+\lambda_\alpha^2} + U\frac{d^2}{d\lambda_\alpha^2}\frac{1}{1+\lambda_\alpha^2}\right) \qquad (11)$$

(for simplicity, I am assuming $J = \pi/4$).

The thermodynamic equations are essentially the same as those for an *XXX* chain, (5). The free energy of the system is

$$F = -T\int d\lambda \frac{1}{2\cosh \pi\lambda}\ln(1+e^{\epsilon_1(\lambda)/T}), \qquad (12)$$

and the functions $\epsilon_j(\lambda)$ satisfy the infinite system of nonlinear equations

$$\epsilon_j(\lambda) = Ts * \ln(1+e^{\epsilon_{j-1}(\lambda)/T})(1+e^{\epsilon_{j+1}(\lambda)/T}) - \delta_{j,1}\left[\frac{(1+\pi U)}{2}(\cosh \pi\lambda)^{-1} - \pi U(\cosh \pi\lambda)^{-3}\right], \qquad (13a)$$

$$\lim_{j\to\infty} \epsilon_j/j = H$$

$$s * f(\lambda) = \int_{-\infty}^{+\infty} d\lambda'(2\cosh\pi(\lambda-\lambda'))f(\lambda') \qquad (13b)$$

(H is the magnetic field).

In the case $|\pi U| < 1$ the ground state of the model is the same as a state of an *XXX* chain; it is antiferromagnetic ($S^Z = 0$). In the case $|\pi U| > 1$ the ground state is ferrimagnetic ($0 < S^Z < N/2$). In this case all of the $\epsilon_j(\lambda)$ are greater than zero at $T = 0$ except $\epsilon_1(\lambda)$, which is less than zero if $|\lambda| > Q$, where Q is found from the equation

$$\epsilon_1(\lambda) + \int_{-\infty}^{+\infty} R(\lambda-\lambda')\epsilon_1(\lambda')d\lambda' = -\frac{(1+\pi U)}{2}(\cosh \pi\lambda)^{-1} + \pi U(\cosh \pi\lambda)^{-3},$$

$$\epsilon_1(\pm Q) = 0. \qquad (14)$$

$$R(\omega) = (1+e^{|\omega|})^{-1}.$$

In the case $\pi U = 1$, the function $\epsilon_1(\lambda)$ vanishes at only a single point (frustration): $\epsilon_1(\lambda) \approx -2\pi^2\lambda^2$ ($|\lambda| \ll 1$). The heat capacity in the limit $T \to 0$ in this case is

$$C = AT^{1/2} + \frac{\pi}{6}T.$$

With a further increase in U, the term in the heat capacity, which is linear in T, decreases by a factor of two.

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