Transformation of the Bethe Equations for Finite Cycles into Secular Polynomials in Energy

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The study of spin Hamiltonians is facilitated by the use of the Bethe equations. Up to now, these equations were primarily used for the study of the energy of the lowest state of a given symmetry. In this paper, we would like to show that there is a technique by which these equations for finite cycles can be transformed into an algebraic equation for the energy in which the coefficients are polynomials in the coupling constant, or just numbers. From this algebraic equation, we can get all energies of a given symmetry in a straightforward way. [S0031-9007(96)00513-3]

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Lattice spin models are of great importance both in solid state physics as well as in quantum chemistry and, therefore, they have been the subject of considerable investigation over the years. For infinite chains, it is often possible to get an exact result. However, there are many physically interesting quantities, namely, those that occur in statistical physics, which are not possible to calculate analytically. Consequently, many authors have studied finite chains and calculated physical properties using extrapolation. For these studies, it is necessary to know all the states of the given symmetry. One technique which is frequently used is the direct diagonalization of the Hamiltonian, while the use of the Bethe equations for cyclic chains [1] has been primarily *limited just to the lowest state of the given symmetry*. In fact, for this lowest state numerical results can be obtained by iteration, while excited states of the given symmetry are much more difficult to extract from the Bethe equations. Further details can be found in Refs. [2–6].

Direct diagonalization was proposed by Hulthén [7] for the case of the isotropic Hamiltonian for $N = 2$, 4, 6, 8, and 10 member systems. Here he studied the ground and excited states of A and B type symmetry. Orbach [8] has calculated energies by direct diagonalization for all states $N = 4$, 6, 8, and 10, while Klein and Seitz [9] calculated the energies up to $N = 12$. Orbach as well as Bonner and Fischer [10] have calculated quantities for the anisotropic model. It is interesting to note that Majumdar, Krishan, and Mubayi [11] considered hidden symmetry for the anisotropic case while Hashimoto [12] has calculated some excited states for the Heisenberg Hamiltonian.

The main purpose of this Letter is to demonstrate that it is possible to obtain from the Bethe equations the energy of all excited states in the form of polynomials in terms of energy and the coupling constant in the Hamiltonian. The energies of these excited states are input data for the calculation of the partition function and other thermodynamic quantities. We would like to return to the original paper of Bethe and show that energies can also be obtained in closed form as polynomials in the energy and coupling constants of the Hamiltonian. We outline a unified program for the calculation of these polynomials. We shall study two important classes of models which will be referred to as A and B. First, we shall describe these models.

(A) First of all, we have already developed a substantial set of results for the isotropic Heisenberg Hamiltonian. Our technique is the transformation of the Bethe equations to a system of algebraic equations which can be solved using the Gröbner method [13] and in which symmetric functions can be introduced for simplifying the equations when N becomes larger.

(B) These results have been extended to the study of the anisotropic spin Hamiltonian which contains a single anisotropy parameter ρ [14]. Much the same holds here as in the case of the isotropic model. The modified Bethe equations can be transformed into a set of algebraic equations which depend on the anisotropy parameter.

To begin with, let us write down the equations for all of the model Hamiltonians which are relevant to the Letter. The spin Hamiltonian up to an additive and multiplicative constant will assume the general form for cyclic chains

$$H_S = \sum_{i=1}^{N} [\mathbf{S}_i \cdot \mathbf{S}_{i+1} + (\rho - 1) S_i^z S_{i+1}^z - \rho/4]. \quad (1)$$

From this anisotropic Hamiltonian, one obtains the isotropic Hamiltonian for $\rho = 1$, the XY Hamiltonian for $\rho = 0$, and finally the Ising model for $\rho = \infty$ after proper rescaling. The Bethe equations for the anisotropic model are presented in a slightly modified form, which avoids complex numbers and which is convenient for our purposes,

$$2N\tan^{-1}(2\tau_\alpha) = 2\pi d_\alpha + 2\sum_{\beta=1}^{M}\phi_{\alpha\beta}\,, \tag{2}$$

where

$$\phi_{\alpha\beta} = \tan^{-1}\left(\frac{\rho[\tau_\alpha - \tau_\beta]}{2[(1+\rho)/4 - (1-\rho)\tau_\alpha\tau_\beta]}\right). \tag{3}$$

The energy is found from the equation

$$E = \sum_{\alpha=1}^{M}\left(-\frac{2}{1+4\tau_\alpha^2} + 1 - \rho\right). \tag{4}$$

The equations for the isotropic case are found by letting $\rho = 1$. In the isotropic case, the Bethe equations can be expressed as

$$2\sum_{j=1}^{N}\tan^{-1}(2\tau_\alpha) = 2\pi d_\alpha + 2\sum_{\gamma=1}^{M}\tan^{-1}(\tau_\alpha - \tau_\gamma)\,. \tag{5}$$

Here, $M = N/2$.

In order to illustrate the application of the above mentioned methods, we shall present the isotropic case for $N = 14$ in detail. This case is complicated enough to show all aspects of the problem, but small enough to be presented here. There are seven τ_α variables such that $\tau_4 = 0$ and the remaining ones are antisymmetric. This means that $\tau_{8-\alpha} = -\tau_\alpha$, $\alpha = 1,2,3$. With these assumptions, the number of independent τ_α reduces to three. These variables are determined by the three equations

$$\begin{aligned}14\tan^{-1}(2\tau_\alpha) = \pi d_\alpha &+ \tan^{-1}(\tau_\alpha) \\ &+ \sum_{\gamma=1}^{3}[\tan^{-1}(\tau_\alpha - \tau_\gamma) \\ &+ \tan^{-1}(\tau_\alpha + \tau_\gamma)]\,,\end{aligned} \tag{6}$$

Here $\alpha = 1,2,3$, and the d_α are positive integers. When the inverse tangents are combined using the identity

$$\tan^{-1}(u) + \tan^{-1}(v) = \tan^{-1}\left(\frac{u+v}{1-uv}\right) + k\pi \tag{7}$$

and introducing the notation $x = \tau_1^2$, $y = \tau_2^2$, and $z = \tau_3^2$, then we get for $\alpha = 1$ from Eq. (6) the following expression:

$$\begin{aligned}X = &-21 - 23(y+z) - 25yz + [978 + 1429(y+z) + 1976yz]x + [-3873 - 13\,416(y+z) - 29\,744yz]x^2 \\ &+ [-20\,904 + 2288(y+z) + 109\,824yz]x^3 + [-11\,440 + 73\,216(y+z) - 36\,608yz]x^4 \\ &+ [49\,920 + 49\,920(y+z) - 133\,120yz]x^5 + [88\,320 - 34\,816(y+z) + 45\,056yz]x^6 \\ &+ [55\,296 - 28\,672(y+z)]x^7 + 12\,288x^8.\end{aligned} \tag{8}$$

We denote the other equations for $\alpha = 2,3$ by Y and Z, respectively. Y is obtained from X by interchanging x and y and keeping z fixed. Similarly, Z is obtained from Y by interchanging y and z and keeping x fixed. Consequently, X is symmetric in y and z, Y is symmetric in x and z, and Z is symmetric in x and y. By adding these three functions together, we obtain an equation

$$F = X + Y + Z = 0\,, \tag{9}$$

which is symmetric in x, y, and z. Next, we introduce the functions

$$G_x = (Y - Z)/(y - z)\,, \tag{10}$$

$$G_y = (Z - X)/(z - x)\,, \tag{11}$$

$$G_z = (X - Y)/(x - y)\,. \tag{12}$$

It can be shown that the function

$$G = G_x + G_y + G_z = 0 \tag{13}$$

is a second independent symmetric function in x, y, and z. Finally,

$$H = \frac{G_x - G_y}{x - y} + \frac{G_y - G_z}{y - z} + \frac{G_z - G_x}{z - x} = 0 \tag{14}$$

is a third symmetric equation. The functions F, G, and H are complicated, but can be simplified by the introduction of the new variables described next.

Since we have a system of three equations which are symmetric in their variables, it is reasonable to introduce new unknowns defined as the coefficients of the polynomial

$$w^3 + Pw^2 + Qw + R = 0\,, \tag{15}$$

where the roots are just the above variables such that $P = -x - y - z$, $Q = xy + yz + xz$, and $R = -xyz$ are three elementary symmetric functions. The equations F, G, and H will simplify after substituting these variables. After applying the Gröbner elimination scheme [13], we obtain a polynomial of degree 20 for P. The variable Q can be expressed through the polynomial in P and finally, one gets R as a polynomial in P.

The energy is a rational symmetric function of the variables x, y, and z. Therefore, it can be expressed in terms of P, Q, and R:

$$E = -\frac{4(3 - 8P + 16Q)}{1 - 4P + 16Q - 64R} - 2\,. \tag{16}$$

If we substitute into this expression Q and R in terms of P, the energy is expressed as a ratio of two rational functions of P. With the use of the resultant, it is then easy to obtain from this equation and the polynomial in P another polynomial which gives directly the energy. This procedure has been carried out also for $N = 6$ to 14. In principle, one is able to calculate it for $N = 16, 18,$ and so on; however, we are working on a more efficient algorithm.

The secular polynomial for the $N = 14$ ground state ${}^1A_{1g}$ takes the form

$$\begin{aligned} &E^{20} + 90E^{19} + 3791E^{18} + 99\,330E^{17} + 1\,814\,739E^{16} + 24\,559\,806E^{15} + 255\,298\,049E^{14} + 2\,085\,639\,739E^{13} \\ &+ 13\,587\,286\,107E^{12} + 71\,206\,008\,153E^{11} + 301\,436\,293\,156E^{10} + 1\,030\,976\,495\,948E^{9} + 2\,838\,437\,223\,906E^{8} \\ &+ 6\,241\,247\,040\,767E^{7} + 10\,819\,799\,727\,199E^{6} + 14\,501\,443\,108\,368E^{5} + 14\,591\,509\,201\,376E^{4} \\ &+ 10\,536\,885\,559\,363E^{3} + 5\,072\,469\,026\,424E^{2} + 1\,420\,272\,996\,516E + 166\,552\,673\,007 = 0\,. \end{aligned} \tag{17}$$

Here E is in the same units as Orbach's [8], which in turn is different by a factor of 2 from the one used by Hulthén.

The ${}^1B_{2u}$ state is described by two complex τ_α which we write as $2\tau^\pm = \pm i$. This introduces a slight modification into the equations. The resulting equations can be combined in the same way as for the ground state using the identity above. The quantum numbers are integers and the τ_α will satisfy the antisymmetry constraint. This procedure has been carried out for $N = 6$ to 14, and the secular polynomial for the ${}^1B_{2u}$ state for $N = 14$ has the form

$$\begin{aligned} &E^{15} + 70E^{14} + 2249E^{13} + 43\,972E^{12} + 584\,760E^{11} + 5\,598\,792E^{10} + 39\,837\,921E^{9} + 214\,308\,613E^{8} \\ &+ 877\,805\,606E^{7} + 2\,734\,052\,369E^{6} + 6\,412\,755\,365E^{5} + 11\,103\,818\,047E^{4} + 13\,711\,066\,334E^{3} \\ &+ 11\,371\,319\,099E^{2} + 5\,648\,846\,224E^{1} + 1\,263\,484\,747 = 0\,. \end{aligned} \tag{18}$$

The size of these polynomials is in agreement with those of Klein and Seitz when hidden symmetry is taken into account. This is described in the note at the end of their paper [15].

Finally, we shall briefly describe our results on the *anisotropic* Hamiltonian which are based on the generalization of the first section. Calculations for $N = 6$ and 8 have been done. The Bethe equations have been transformed into algebraic equations, and the calculated polynomial for $N = 8$ is given in Table I. Let us mention that our compact results permit us to decide that Jain *et al.* [16] are indeed obtaining a level crossing for $N = 8$. To go further does not represent any conceptual difficulty.

TABLE I. Secular polynomial $E^7 + \sum_{n=0}^{6} c_n E^n$ for anisotropic model, $N = 8$.

n	c_n
0	$88\rho^3 - 376\rho^5 + 288\rho^7$
1	$125\rho^2 - 934\rho^4 + 984\rho^6$
2	$56\rho - 891\rho^3 + 1388\rho^5$
3	$8 - 411\rho^2 + 1054\rho^4$
4	$-92\rho + 467\rho^3$
5	$-8 + 121\rho^2$
6	17ρ

These days, the open chains with constant β, and open and closed chains with alternating β, as well as the two dimensional Heisenberg Hamiltonian are the subject of intensive research. We are working on the implementation of some ideas presented in this Letter on these Hamiltonians which are topical today.

In conclusion, we would like to stress the simplicity and compactness of these results. It should be emphasized that it has been shown that analytic studies of the Bethe equations represent a valuable complement to the contemporary large scale calculations based on a direct diagonalization of the Hamiltonian. Let us mention that even on the topics treated in this Letter, we have presented only exploratory calculations which fit into the format of this communication. All work reported was made possible by the systematic use of the symbolic manipulation language Maple [17].

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Note added in proof.—See also *The Many-Body Problem—An Encyclopedia of Exactly Solved Models in One Dimension* Ref. [18] and Adams and Loustaunau, *An Introduction to Gröbner Bases* Ref. [19].

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