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Numerical techniques for investigating an excited state of the anisotropic Heisenberg model

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An analysis of the anisotropic Heisenberg model is carried out by solving the Bethe ansatz solution of the model numerically as a function of finite N. A brief introduction to the infinite chain limit is presented and the energy for a few limiting cases of the anisotropy parameter are evaluated. Numerical results for the infinite chain are given which can be compared with the case of finite increasing N. It is shown that the calculation can be extended to the case of an excited state of the model.

1. Introduction

The properties of linear magnetic chains are useful to study because they provide simple yet nontrivial models of many body systems. Linear antiferromagnetic chains exist in crystals and can be studied experimentally. In the case in which the model is described by the Heisenberg Hamiltonian with one anisotropic coupling, the model can be solved exactly using the Bethe ansatz [1–4].

The investigation will be restricted to chains of spins on a lattice with nearest neighbor interactions. The Hamiltonian of the system is taken to be

$$H = \sum_{j=1}^{N} (S_j^x S_{j+1}^x + S_j^y S_{j+1}^y + \rho S_j^z S_{j+1}^z) . \tag{1}$$

Therefore, the Hamiltonian is anisotropic in the z-direction. The spin operator with components S_j^x, S_j^y, and S_j^z is associated with site j, and corresponds to states of spin 1/2 distributed along sites labelled by the index j. Moreover, it is assumed that the sites form a ring and satisfy periodic boundary conditions such that site $(N + 1)$ coincides with site 1.

The completely isotropic problem in which $\rho = 1$ has been investigated by Bethe [1], Hulthen [5], and (1) is the form of the Hamiltonian used by Cloizeaux and Pearson [6]. Bethe was able to classify all the eigenstates of the isotropic Hamiltonian

by means of sets of integers, and to obtain a set of nonlinear, coupled equations which yield the eigenvalues of the system. The isotropic version of the model was investigated by Griffiths [7], and the first extensive treatment of the anisotropic model was given by Cloizeaux and Gaudin [8]. For the sake of completeness, many aspects of the model are reviewed so the numerical work will have context.

Our intention is to investigate the solutions of the anisotropic Hamiltonian and to review the numerical calculation of the ground state energy as a function of the anisotropy parameter. This corresponds to a certain choice of the quantum numbers in the solution of the model. The energy per particle can also be obtained from this. It is shown that the energy can be obtained numerically as a function of N from the Bethe ansatz solution for various values of ρ. For the sake of completeness, an outline of the derivation of the equations for the energy per particle for the infinite chain will be given. The energies calculated from these equations can be compared with the finite N values. In addition to the explicit calculations for finite N, there are results for negative ρ, which were not given in Orbach [3]. It should be noted that the finite N analysis will provide information to treat the infinite limit in a different way. The finite N results can be used in combination with asymptotic analysis, for example extrapolation, to give information about the large N region.

The next step is to use the same basic techniques to calculate the excitation energies which correspond to quantum numbers of a different symmetry for finite N as a function ρ. Some mathematical techniques which are important in the derivations and have not appeared before are included. It is hoped that this will show the methods of this article might be used to study general sets of solutions to the Bethe equations, and that these techniques can be applied to other lattice spin models. For example, let us mention that of particular interest recently in Hamiltonian field theory is the use of finite size scaling. This has been used to extract critical points and critical exponents from the two lowest eigenvalues of the Hamiltonian [8,9]. It may be that by modifying the techniques here enough, one could use these techniques to calculate similar quantities. In fact, the techniques used in this paper have also been used in the study of the one- dimensional Hubbard model [7,10], and the spin Hamiltonian. It is hoped that this work will be of use in encouraging the application of these techniques to other areas.

2. Solution of anisotropic Hamiltonian

The Hamiltonian has been given in (1) and the Hamiltonian H commutes with the component S^z of the total spin operator

$$S^z = \sum_{i=1}^{N} S_i^z .$$

Therefore, it is possible to diagonalize simultaneously H and S^z, so for each eigenstate $|\Psi\rangle$ of H one may write

$$H|\Psi\rangle = E|\Psi\rangle\,,$$

$$S^z|\Psi\rangle = M|\Psi\rangle\,.$$

We know that for $\rho = 1$, H commutes with the total spin S and so for the ground state one has $S = 0$, $M = 0$ and this state is unique. For $\rho > -1$, the ground state should be unique with the value $M = 0$. However, for $\rho < -1$, the ground state should be doubly degenerate with $M = \pm N/2$.

Let us briefly introduce the model, which will establish notation, and give an outline of the solution for finite values of N. Let $|\Psi_F\rangle$ be the ferromagnetic state which corresponds to $M = \frac{1}{2}N$, so that all spins are parallel to each other, that is, $S_j^{\dagger}|\Psi_F\rangle = 0$. One may write

$$H(\rho)|\Psi_F\rangle = \mathcal{E}_F|\Psi_F\rangle\,.$$

Since only the S_j^z operators in H will make a contribution for this state, the energy eigenvalue is given by

$$\mathcal{E}_F(\rho) = \tfrac{1}{4}N\rho\,.$$

By flipping r spins in $|\Psi_F\rangle$, any eigenstate $|\Omega\rangle$ of S^z can be constructed,

$$|\Omega\rangle = \sum_{n_1<n_2<\cdots<n_r} a(n_1,\cdots,n_r)S_{n_1}^{-}\cdots S_{n_r}^{-}|\Psi_F\rangle\,.$$

and the corresponding eigenvalue of S^z is

$$M = \tfrac{1}{2}(N - 2r)\,.$$

The task now is to determine the coefficients $a(n_1,\cdots,n_r)$ in order to give an eigenstate of H with eigenvalue E

$$H|\Omega\rangle = E|\Omega\rangle\,.$$

If we define ϵ by setting

$$\epsilon = (E - \mathcal{E}_F)/N$$

then by substituting $|\Omega\rangle$ it is found that the eigenvalue problem is equivalent to the difference equation

$$\sum[a(n_1',\cdots,n_r') - \rho a(n_1,\cdots,n_r)] = 2N\epsilon a(n_1,\cdots,n_r)$$

with $n_1 < \cdots < n_r$. In this equation, a term of $a(n_1',\cdots,n_r')$ is obtained by changing one number n of $a(n_1,\cdots,n_r)$ by one unit and summing over all possible combinations which come from it. The coefficients can be expressed in terms of r wavenumbers k_α, $\alpha = 1,\cdots,r$, and phases $\psi_{\alpha\beta}$ associated with each pair of wavenumbers k_α and k_β. The form of the ansatz is

$$a(n_1,\cdots,n_r) = \sum_P \exp\left(i\sum_\alpha k_{P\alpha}n_\alpha + \frac{i}{2}\sum_{\alpha<\beta}\psi_{P\alpha P\beta}\right),$$

where P is any permutation of the set of numbers $(1, \cdots, r)$. This is Bethe's ansatz form for the solution.

In terms of the wavenumbers k_α, the energy per particle ϵ, which will be referred to as the energy, is given by

$$\epsilon = N^{-1} \sum_\alpha (\cos k_\alpha - \rho) . \tag{2}$$

A relation implicit in the eigenvalue problem gives an equation which determines $\psi_{\alpha\beta}$ as follows:

$$\cot(\tfrac{1}{2}\psi_{\alpha\beta}) = \rho \left(\frac{\cot(\frac{1}{2}k_\alpha) - \cot(\frac{1}{2}k_\beta)}{(1+\rho) - (1-\rho)\ \cot(\frac{1}{2}k_\alpha)\ \cot(\frac{1}{2}k_\beta)} \right) . \tag{3}$$

Since the spin system is cyclic, the coefficients $a(n_1, \cdots, n_r)$ must satisfy the following boundary condition equations

$$a(n_1, n_2, \cdots, n_r) = a(n_2, \cdots, n_r, n_1 + N)$$

and after some algebra with the ansatz, these imply the following equations for the k_α:

$$N k_\alpha = 2\pi \lambda_\alpha + \sum_\beta \psi_{\alpha\beta} . \tag{4}$$

The total wavevector is directly related to the λ_α since

$$K = \sum_\alpha k_\alpha = 2\pi N^{-1} \sum_\alpha \lambda_\alpha .$$

A numerical solution of the system (3) and (4), which corresponds to the ground state quantum numbers, will be treated first. A second choice of the λ_α will then be investigated. These correspond to an excitation of the system which is different from the ground state.

3. Quantum numbers and variables as $\rho \to 0$

The behaviour of the variables will be discussed in the neighborhood of $\rho = 0$. In particular, the behaviour of the quantities k_α and $\psi_{\alpha\beta}$ when $\rho \to +0$ will be discussed first. The equations which determine the wavenumbers (4) come from the periodic boundary conditions, where $\psi_{\alpha\beta}$ is determined by (3).

If one supposes that near $\rho = 0$, the set of k_α vary between $\pi/2$ and $3\pi/2$, then the set $k_\alpha/2$ varies between $\pi/4$ and $3\pi/4$, and so the product of functions $(1-\rho)\ \cot(k_\alpha/2)\ \cot(k_\beta/2)$ should never exceed one, and ought to be less than one. Taking into account the fact that the cotangent is decreasing on $(0, \pi)$ one has from (3)

$$\cot(\tfrac{1}{2}\psi_{\alpha\beta}) \to -0\ \mathrm{sign}(k_\alpha - k_\beta)$$

and therefore

$$\psi_{\alpha\beta} \to -\pi \operatorname{sign}(k_\alpha - k_\beta) .$$

Since the $\psi_{\alpha\beta}$ goes to a constant, the k_α can be evaluated from (4) by writing the sum over β explicitly as follows:

$$\sum_{\beta\neq\alpha} \psi_{\alpha\beta} = \sum_{1\leqslant\beta<\alpha} \psi_{\alpha\beta} + \sum_{\alpha<\beta\leqslant N/2} \psi_{\alpha\beta} .$$

The first sum on the right can be done by assuming the set of k_α are monotonic so that $k_\beta < k_\alpha$ for $\beta < \alpha$ to give in the limit $\rho \to +0$

$$\sum_{1\leqslant\beta<\alpha} \psi_{\alpha\beta} = -\pi(\alpha - 1) .$$

The second sum is given by

$$\sum_{\alpha<\beta\leqslant N/2} \psi_{\alpha\beta} = \pi\left(\frac{N}{2} - \alpha\right) .$$

Therefore

$$\sum_{\beta\neq\alpha} \psi_{\alpha\beta} = \pi\frac{N}{2} - 2\pi\alpha + \pi .$$

Setting

$$\lambda_\alpha = 2\alpha - 1 \tag{5}$$

in (4) for the ground state, where $\alpha = 1, \cdots, N/2$, gives the result

$$k_\alpha(+0) = \frac{\pi}{2} + \frac{\pi}{N}(2\alpha - 1) . \tag{6}$$

As conjectured, for the limit $\rho = +0$, the k_α vary roughly between $\pi/2$ and $3\pi/2$ as expected.

Consider the limit from the other direction $\rho \to -0$. In this case, the behaviour of the phases is somewhat different. Since the sign of ρ is opposite in this limit, requiring that (3) give the $\psi_{\alpha\beta}$

$$\cot(\tfrac{1}{2}\psi_{\alpha\beta}) \to +0 \operatorname{sign}(k_\alpha - k_\beta) ,$$

$$\psi_{\alpha\beta} \to \pi \operatorname{sign}(k_\alpha - k_\beta) .$$

The sum over β in (4) can be done in the same way to give

$$\sum_{\beta\neq\alpha} \psi_{\alpha\beta} = 2\pi\alpha - \pi - \frac{N}{2}\pi .$$

Suppose it is required that k_α be continuous at $\rho = 0$ as ρ goes to zero from either the right or the left, that is

$$k(+0) = k(-0)\,.$$

Let λ'_α be the set of quantum numbers for the region $-1 < \rho < 0$, then applying continuity gives the following equation:

$$\frac{N}{2}\pi + \pi(2\alpha - 1) = 2\pi\lambda'_\alpha + 2\pi\alpha - \pi - \frac{N}{2}\pi\,.$$

Solving this equation for the λ'_α, one obtains

$$\lambda'_\alpha = \frac{N}{2}\,.$$

In order to describe the ground state for $\rho \geqslant 1$, the same set of λ_α given in (5) are used as in the domain $0 \leqslant \rho \leqslant 1$ to calculate the energy.

Given the wavevectors at $\rho = 0$, the energy for N finite can be found by substituting (6) into (2). The sum over α can be done by writing the sines in terms of complex exponentials and then summing the geometric series. One obtains

$$\epsilon_N(0) = -\frac{1}{N \sin\frac{\pi}{N}}$$

for finite N.

4. Calculations for finite N

To carry out the calculation, the region $\rho > 0$ will be treated first. To calculate the energy for $\rho > 0$, the set of λ_α given by (5) are used to define the ground state and (6) is used to initialize the wavevectors in a small region just to the right of the origin. Of course these are only the approximate values for the wavevectors close to 0, however, the calculation will produce the correct ones. If ρ is initialized to a small positive number in this interval, the set of eqs. (3) and (4) can be solved numerically by a straightforward Newton–Raphson iteration technique to calculate the exact values for the set of k_α at the corresponding value of ρ. The energy can be calculated from (2). With these values to initialize the variables, the parameter ρ can be incremented by a small amount and the exact values of the variables at the new ρ can be evaluated. If this is continued, the wavevectors, and consequently the energy, and the energy per particle, can be calculated essentially as continuous functions of ρ out to large values of ρ. The results of the numerical calculation over a range of ρ are shown in table 1.

The calculation for $-1 < \rho < 0$ proceeds in exactly the same way by using (6) to initialize the wavevectors just to the left of the origin, where the wavevectors are continuous through $\rho = 0$. However, in this region, the quantum numbers which define the state are given by $\lambda'_\alpha = N/2$ for each α. In this case, the parameter ρ is decreased by small amounts until the neighbourhood to the right of $\rho = -1$ is reached. At this value, the ground state becomes doubly degenerate and the energy

Table 1
Values of ϵ as a function of ρ from 0.1 to 2.0 for particle numbers of $N = 6, 10, 14, 34$ and 50.

ρ	$N = 6$	$N = 10$	$N = 14$	$N = 34$	$N = 50$
0.1	−0.3696	−0.3593	−0.3565	−0.3541	−0.3539
0.2	−0.4064	−0.3955	−0.3925	−0.3900	−0.3897
0.3	−0.4437	−0.4321	−0.4290	−0.4264	−0.4261
0.4	−0.4814	−0.4693	−0.4660	−0.4632	−0.4629
0.5	−0.5196	−0.5069	−0.5034	−0.5005	−0.5002
0.6	−0.5582	−0.5449	−0.5413	−0.5383	−0.5380
0.7	−0.5973	−0.5834	−0.5797	−0.5765	−0.5761
0.8	−0.6368	−0.6223	−0.6184	−0.6151	−0.6148
0.9	−0.6767	−0.6617	−0.6577	−0.6542	−0.6539
1.0	−0.7171	−0.7015	−0.6973	−0.6938	−0.6934
1.1	−0.7579	−0.7418	−0.7375	−0.7338	−0.7334
1.2	−0.7991	−0.7825	−0.7781	−0.7744	−0.7740
1.3	−0.8407	−0.8237	−0.8192	−0.8154	−0.8265
1.4	−0.8827	−0.8653	−0.8607	−0.8569	−0.8668
1.5	−0.9251	−0.9074	−0.9028	−0.8990	−0.9077
1.6	−0.9679	−0.9500	−0.9453	−0.9416	−0.9728
1.7	−1.0110	−0.9930	−0.9883	−0.9848	−1.0256
1.8	−1.0545	−1.0364	−1.0318	−1.0284	−1.0805
1.9	−1.0984	−1.0802	−1.0757	−1.0726	−1.1224
2.0	−1.1426	−1.1244	−1.1201	−1.1173	−1.1987

becomes proportional to ρ. Results from the numerical calculations are shown in table 2. For the cases $N = 6$, 10 and 14, the calculation has been continued down to a value of $\rho = -0.999$ and the following values for energy have been obtained, $\epsilon = -0.00030$ for $N = 6$, -0.00027 for $N = 10$ and -0.00026 for $N = 14$.

The limit $\rho = -1$ is characterized by the fact that all the values of k_α become equal, in fact, one should have $k_\alpha = \pi$. As an example, at $\rho = -0.999$ one obtains numerically the following values for the three wavevectors when $N = 6$, $k_1 = 3.1069, k_2 = 3.1415, k_3 = 3.1762$, respectively.

Table 2
Values of ϵ as a function of ρ from -0.1 to -0.9 for particle numbers of $N = 6, 10, 14, 34$ and 50.

ρ	$N = 6$	$N = 10$	$N = 14$	$N = 34$	$N = 50$
−0.1	−0.2974	−0.2883	−0.2859	−0.2838	−0.2836
−0.2	−0.2620	−0.2536	−0.2514	−0.2494	−0.2492
−0.3	−0.2272	−0.2195	−0.2174	−0.2156	−0.2154
−0.4	−0.1928	−0.1859	−0.1840	−0.1824	−0.1822
−0.5	−0.1591	−0.1529	−0.1512	−0.1498	−0.1496
−0.6	−0.1259	−0.1206	−0.1191	−0.1178	−0.1177
−0.7	−0.0934	−0.0890	−0.0878	−0.0867	−0.0866
−0.8	−0.0615	−0.0582	−0.0573	−0.0565	−0.0564
−0.9	−0.0303	−0.0285	−0.0279	−0.0273	−0.0200

5. Limit of the infinite chain

An integral can be obtained for the energy in the limit $N \to \infty$, and it will briefly be outlined how this is accomplished, and then three limiting cases can be examined. The numerical results of the calculation can be compared to the analytical results.

For $-1 < \rho < 1$, define

$$\rho = \cos\gamma, \quad 0 < \gamma < \pi,$$

$$\tanh(\tfrac{1}{2}\theta_\alpha) = \tan(\tfrac{1}{2}\gamma)\cot(\tfrac{1}{2}k_\alpha),$$

$$\cot(\tfrac{1}{2}\psi_{\alpha\beta}) = \cot\gamma\tanh(\tfrac{1}{2}\theta_\alpha - \tfrac{1}{2}\theta_\beta),$$

$$-\pi < \psi_{\alpha\beta} < \pi.$$

When $N \to \infty$, k_α becomes a continuous function $k(x)$. In the same way, $\psi_{\alpha\beta}$ becomes the function $\psi(x, x')$ and these equations pass into a corresponding set which depend continuously on the variables $k(x)$ and $\psi(x, x')$. Passing to the continuous limit these equations become

$$\tanh(\tfrac{1}{2}\theta) = \tan(\tfrac{1}{2}\gamma)\cot(\tfrac{1}{2}k), \tag{7}$$

$$\cot(\tfrac{1}{2}\psi(x, x')) = \cot\gamma\tanh\left(\frac{\theta}{2} - \frac{\theta'}{2}\right). \tag{8}$$

Consequently, the energy of the corresponding state can be expressed in terms of the integral

$$\epsilon = \frac{1}{4\pi}\int_0^{2\pi} (\cos(k(x)) - \rho)\, dx \tag{9}$$

and (4) becomes an integral equation

$$k(x) = x + \frac{1}{4\pi}\int_0^{\infty} \psi(x, x')\, dx'. \tag{10}$$

The auxillary variable θ_α becomes a continuous function $\theta(x)$, and differentiating both sides of this equation with respect to x, realizing that ψ is discontinuous at $x = x'$, and finally introducing the function $f(\theta)$ defined by

$$\frac{dx}{d\theta} = -f(\theta),$$

the integral equation in terms of $f(\theta)$ is given by

$$\frac{\partial k}{\partial\theta} = -\frac{1}{2}f(\theta) + \frac{1}{4\pi}\int_{-\infty}^{\infty} \frac{\partial\psi(x, x')}{\partial\theta} f(\theta)\, d\theta \tag{11}$$

such that $\partial\psi(x,x')/\partial\theta$ denotes the continuous part of the derivative of $\psi(x,x')$. It may be assumed that $\theta(x)$ decreases from $+\infty$ to $-\infty$ when x increases from 0 to 2π. Differentiating (8) with respect to θ one obtains using $\cosh^2 v = (\cosh 2v + 1)/2$,

$$\frac{\partial\psi}{\partial\theta} = -\frac{\sin 2\gamma}{\cosh(\theta-\theta') - \cos 2\gamma}.$$

The derivative of k is given by

$$\frac{\partial k}{\partial\theta} = -\frac{\sin\gamma}{\cosh\theta - \cos\gamma}$$

and so the integral equation can be written as

$$f(\theta) + \frac{1}{2\pi}\int_{-\infty}^{\infty} \frac{\sin 2\gamma}{\cosh(\theta-\theta') - \cos 2\gamma} f(\theta')d\theta' = \frac{2\sin\gamma}{\cosh\theta - \cos\gamma}.$$

Introducing the Fourier transform of $f(\theta)$,

$$f(\theta) = \int_{-\infty}^{\infty} e^{i\omega\theta} a(\omega)\, d\omega.$$

the integral over θ' can be done by using the following result:

$$\frac{1}{2\pi}\int_{-\infty}^{\infty} \frac{\exp(i\omega\theta')}{\cosh(\theta-\theta') - \cos\Gamma} d\theta' = \frac{e^{i\omega\theta}\sinh\omega(\pi-\Gamma)}{\sin\Gamma\sinh\omega\pi}. \tag{12}$$

The integral equation then becomes

$$\int_{-\infty}^{\infty} d\omega a(\omega) e^{i\omega\theta}\left(1 + \frac{\sinh(-2\omega\gamma + \pi\omega)}{\sinh\omega\pi}\right) = \frac{2\sin\gamma}{\cosh\theta - \cos\gamma}.$$

Multiplying both sides of this equation by $e^{-i\omega/\theta}$ and integrating from $-\infty$ to $+\infty$ with respect to θ using (12) one obtains

$$a(\omega) = \frac{2\sinh\omega(\pi-\gamma)}{\sinh\omega\pi + \sinh(\omega\pi - 2\omega\gamma)} = \operatorname{sech}\omega\gamma$$

and substituting this result for $a(\omega)$ back into the integral for $f(\theta)$ it is found that the integral can be done in closed form to give

$$f(\theta) = \frac{\pi}{\gamma}\operatorname{sech}\frac{\theta\pi}{2\gamma}.$$

Since $\cos k(x) = (1 - 2\sin^2 k(x))/2$, using (10) and identities, the energy can be written as

$$\epsilon = -\frac{\sin^2\gamma}{4\pi}\int_{-\infty}^{\infty} \frac{f(\theta)}{\cosh\theta - \cos\gamma} d\theta.$$

Introducing the Fourier transform of $f(\theta)$ and carrying out the integral over θ, the energy per particle is

$$\epsilon = -\frac{1}{2}\sin\gamma \int_{-\infty}^{\infty} \frac{\sinh\omega(\pi-\gamma)}{\sinh\omega\pi\cosh\omega\gamma}\,d\omega\,.$$

Expanding the hyperbolic sine, one arrives at the final result for $0 \leqslant \rho \leqslant 1$:

$$\epsilon = -\sin\gamma \int_{0}^{\infty} \left(1 - \frac{\tanh\omega\gamma}{\tanh\omega\pi}\right) d\omega\,.$$

The particular limits $\rho = 0$ and $\rho = 1$ can be evaluated explicitly from this equation and in order to compare with the case of finite N, it is useful to do so. To obtain $\rho = 0$, set $\gamma = \pi/2$ and so it follows that

$$\epsilon(0) = -\frac{1}{2}\int_{0}^{\infty} \cosh^2(\omega\pi/2)\,d\omega = -\frac{1}{\pi}\,.$$

Exactly the same result is obtained if one takes $\epsilon_N(0)$ and calculates the limit $N \to \infty$. To obtain $\rho = 1$, set $v = \omega\gamma$ so that $\epsilon(\rho)$ can be written as

$$\epsilon(\rho) = -\frac{\sin\gamma}{\gamma}\int_{0}^{\infty}\left(1 - \frac{\tanh v}{\tanh(v/\gamma)}\right)dv\,.$$

Taking the limit $\gamma \to 0$ gives $\epsilon(1)$

$$\epsilon(1) = -\int_{0}^{\infty}(1-\tanh v)dv = -2\int_{0}^{\infty}\frac{dv}{e^{2v}+1} = -\ln 2\,.$$

Since $\lambda_\alpha = N/2$ for $-1 < \rho < 0$, it can be shown that the integral equation corresponds exactly with the previous integral equation, and so the calculation of $f(\theta)$ is performed in exactly the same way. It is then very easy to obtain the energy per particle at $\rho = -1$ for the infinite limit where $\gamma = \pi$, and one obtains

$$\epsilon(-1) = 0\,. \tag{13}$$

For $\rho \geqslant 1$ set $\rho = \cosh\gamma$, the integral equation is exactly the same as (11) however since $\rho > 1$ the derivatives are found from the continuations of (7) and (8) which are valid for $\rho > 1$,

$$\tan(\tfrac{1}{2}\phi) = \tanh(\tfrac{1}{2}\gamma)\cot(\tfrac{1}{2}k)\,,$$

$$\cot(\tfrac{1}{2}\psi(x,x')) = \coth\gamma\tan(\tfrac{1}{2}\phi - \tfrac{1}{2}\phi')\,.$$

The integral equation which determines $g(\phi)$ is therefore

$$g(\phi) + \frac{\sinh 2\gamma}{2\pi}\int_{-\pi}^{\pi}\frac{g(\phi')}{\cosh 2\gamma - \cos(\phi-\phi')}d\phi' = \frac{2\sinh\gamma}{\cosh\gamma - \cos\phi}\,.$$

Notice that if one makes the replacement $\phi \to \phi + 2\pi$ in this equation, it follows that $g(\phi) = g(\phi + 2\pi)$ so $g(\phi)$ is 2π periodic, and can therefore be expanded in a 2π periodic Fourier series as follows

$$g(\phi) = \sum_{n=-\infty}^{\infty} a_n e^{in\phi}\,.$$

Using the integral

$$\frac{1}{2\pi}\int_{-\pi}^{\pi}\frac{\exp(in\phi')}{\cosh\gamma-\cos(\phi-\phi')}d\phi' = e^{in\phi}\frac{\exp(-|n|\gamma)}{\sinh\gamma}, \tag{14}$$

it is found that

$$a_n = \frac{1}{\cosh n\gamma}.$$

Substituting $g(\phi)$ with a_n given above, the energy per particle is given in this region by

$$\epsilon = -\sinh\gamma\left(\sum_{n=1}^{\infty}(1-\tanh n\gamma)+\tfrac{1}{2}\right).$$

Values for the energy can be obtained from this by simply adding terms when $\rho > 1$. Values for ϵ as a function of ρ for the case $N = \infty$ as calculated from the integral and this series expansion for ϵ are given for certain values of ρ in table 4. Using Thiele with five points as a function of N, it can be shown that the finite chain results in the first table tend to those of the infinite chain as N becomes large.

6. Excited state

The notation of des Cloizeaux and Gaudin [8] for the excitation energy will first be reviewed here. In the limit $N \to \infty$, one calculates the excitation energy $\eta(\rho, M, q)$ which is defined by the equation

$$\eta(\rho, M, q) = \lim_{N\to\infty}(E(\rho, M, q) - E_{AF}(\rho)).$$

Consequently, for finite cycles, one has

$$\eta(\rho, M, q) = N(\epsilon(\rho, M, q) - \epsilon_{AF}(\rho)), \tag{15}$$

where $\epsilon_{AF}(\rho)$ is the value of ϵ which corresponds to the ground state. By solving

Table 3
Values of ϵ as a function of N at fixed $\rho = \pm 0.00001$ calculated numerically. Theoretically, it is found that $\epsilon_\infty(0) = -1/\pi \doteq 0.31830$.

N	$\epsilon(0.00001)$	$\epsilon(-0.00001)$	$\epsilon_N(0)$
6	−0.33333	−0.33332	−0.33333
10	−0.32361	−0.32360	−0.32360
14	−0.32100	−0.32099	−0.32099
34	−0.31876	−0.31875	−0.31876
50	−0.31852	−0.31851	−0.31851

Table 4
Selected values of ϵ as a function of ρ for the case $N = \infty$ calculated from the integral for $\rho < 1$ and from the series for $\rho > 1$.

ρ	ϵ
0.3	−0.4259
0.4	−0.4627
0.5	−0.4999
0.6	−0.5377
0.7	−0.5759
0.8	−0.6145
1.0	−0.6931
1.1	−0.7331
1.2	−0.7736
1.3	−0.8146
1.4	−0.8562
1.5	−0.8984
1.6	−0.9411
1.7	−0.9844
1.8	−1.0282
1.9	−1.0725
2.0	−1.1172

the coupled Bethe ansatz equations for the given set of λ_α, the value of $\epsilon(\rho)$ can be calculated using (4), and then the excitation energy is calculated from (5).

To determine the excitation energy η, the integers λ_α which characterize the given state must be specified. For the ground state, these integers are given as $\lambda_\alpha = 2\alpha - 1$, for $\alpha = 1, \cdots, N/2$. For the state which is referred to as $|\rho, 0, q\rangle$ in [8], the quantum numbers are given as follows:

$$\lambda_\alpha = 2\alpha - 2\,, \quad 1 \leqslant \alpha \leqslant n\,,$$

$$\lambda_\alpha = 2\alpha - 1\,, \quad n \leqslant \alpha \leqslant N/2\,, \tag{16}$$

Here, n is an integer. A fixed number n of these quantum numbers will differ by one unit from the ground state values. The spin wave vector q is determined by n through the equation

$$|q| = \frac{2\pi n}{N}\,.$$

Given these quantum numbers, the system (2) and (3) can be solved as a function of ρ. Quantum numbers for other excitations have been discussed by Griffiths [7]. This is done for finite values of N. By taking a number of values for the pair of integers n and N, the ratio can be adjusted so that we are working at a fixed value of q for increasing N. This means we take a finite value of n and calculate the corresponding λ_α. Of course, q becomes a continuous variable as $N \to \infty$.

7. Calculations

The quantum numbers are determined by eq. (16). Consider, as an example, the case in which $N = 6$, and let us take $n = 1$. This gives the value $|q| = \pi/3$. Then the set of quantum numbers which is used to solve (2) and (3) is the set given by $\{0, 3, 5\}$ where in contrast, the ground state quantum numbers are given by $\{1, 3, 5\}$.

The numerical analysis is just an extension of that used for the ground state. The Bethe equations, which were presented in the introduction, can be solved numerically for a given set of quantum numbers using a Newton method algorithm once initial values for the variables k_α have been determined. This is the main point we would like to emphasize in this article. The variables k_α can be initialized at $\rho = 0$ for this state. To do this, consider first the ground state. For the ground state, it has been shown [8] that the set of k_α can be determined analytically at $\rho = 0$, and are given by the expression

$$k_\alpha = \frac{\pi}{2} + (2\alpha - 1)\frac{\pi}{N}.$$

Using these values to initialize the calculation at $\rho = 0$, the system can be solved by iterating in the first n quantum numbers while keeping ρ fixed near zero. That is, we begin with the set of ground state values, and then increment the first n of them in a direction such that they have been changed to the point at which the first n of the λ_α are equal to the numbers given in (16). At each small change in the quantum numbers, a corresponding set of k_α is calculated by means of the iterative Newton algorithm. These k_α will initialize the variables at the next increment.

Once this is carried out, a set of k_α which correspond to the λ_α in (16) and $\rho = 0$ are obtained. Now keeping the quantum numbers fixed, ρ can be varied away from zero to obtain the energy as a function of ρ for the new state.

Similarly, the k_α can be calculated for $-1 < \rho < 0$ where the quantum numbers which are used for this state are given as follows:

$$\lambda'_\alpha = \frac{N}{2} - 1, \quad 1 \leqslant \alpha \leqslant n,$$

$$\lambda'_\alpha = \frac{N}{2}, \quad n < \alpha \leqslant \frac{N}{2}.$$

The k_α which correspond to these for $\rho = 0^-$ can be calculated in exactly the same way as the set for $\rho = 0^+$, and then this set of momenta is used to initialize the calculation as ρ is decreased toward $\rho = -1$.

It can be shown that if we define γ through the equation

$$\rho = \cos\gamma,$$

then, in the limit of the infinite chain, $N \to \infty$, the excitation energy is given by the equation

$$\eta(\rho, 0, q) = \frac{\pi \sin\gamma}{2\gamma} |\sin q|, \quad -1 < \rho < 1. \tag{17}$$

Numerical results for small cycles can be compared to results which are obtained from this equation for the infinite cycle.

8. Results

It has been found that for each of the finite rings which have been studied with this technique, a finite, well-defined solution for the set of k_α and corresponding ϵ is obtained as ρ is varied between -1 and $+1$. The initial values for the variables are calculated using the procedure outlined earlier, and the corresponding value of q is taken to agree with that calculated for the finite N case. The ground state energy can be calculated using a similar procedure. These values are used to calculate the excitation energies. The values for the excitation energies for the infinite chain are calculated from equation (17). The numerical results are reported in tables 5 to 7.

There are some other interesting features of this particular solution to the Bethe equations we mention. It is also found that one of the k_α, in particular k_1, tends numerically to zero as ρ approaches 1. In the solution of (2) and (3), this means that the function $\cot(k_1/2)$ becomes singular. It is possible to approach arbitrarily close

Table 5
Excitation energy $\eta = N|\epsilon - \epsilon_g|$ for the anisotropic Heisenberg model as a function of ρ where ϵ_g is the ground state energy. The quantum numbers are as given in the text, and $|q| = \pi/3$.

ρ	$N = 6$	$N = 18$	$N = \infty$
0.1	1.0499	0.9920	0.9203
0.2	1.0999	1.0393	0.9732
0.3	1.1502	1.0874	1.0249
0.4	1.2008	1.1349	1.0754
0.5	1.2520	1.1818	1.1250
0.6	1.3039	1.2285	1.1736
0.7	1.3567	1.2751	1.2213
0.8	1.4105	1.3218	1.2683
0.9	1.4656	1.3689	1.3146
−0.1	0.4492	0.7106	0.8100
−0.2	0.3969	0.6534	0.7521
−0.3	0.3428	0.5940	0.6919
−0.4	0.2865	0.5320	0.6289
−0.5	0.2273	0.4667	0.5625
−0.6	0.1645	0.3971	0.4914
−0.7	0.0968	0.3214	0.4140
−0.8	0.0216	0.2362	0.3267
−0.9	0.0667	0.1327	0.2203

Table 6
Excitation energy $\eta = N|\epsilon - \epsilon_g|$ for the anisotropic Heisenberg model as a function of ρ where ϵ_g is the ground state energy. The quantum numbers are given, and $|q| = \pi/4$.

ρ	$N = 8$	$N = 16$	$N = \infty$
0.1	0.8077	0.7920	0.7514
0.2	0.8497	0.8328	0.7946
0.3	0.8913	0.8730	0.8368
0.4	0.9328	0.9128	0.8781
0.5	0.9745	0.9523	0.9185
0.6	1.0165	0.9917	0.9582
0.7	1.0590	1.0310	0.9972
0.8	1.1023	1.0705	1.0356
0.9	1.1467	1.1105	1.0734
−0.1	0.4978	0.5912	0.6613
−0.2	0.4532	0.5446	0.6140
−0.3	0.4068	0.4962	0.5649
−0.4	0.3584	0.4456	0.5135
−0.5	0.3074	0.3923	0.4592
−0.6	0.2531	0.3354	0.4012
−0.7	0.1942	0.2735	0.3380
−0.8	0.1282	0.2038	0.2667
−0.9	0.0490	0.1192	0.1799

Table 7
Excitation energy $\eta = N|\epsilon - \epsilon_g|$ for the anisotropic Heisenberg model as a function of ρ where ϵ_g is the energy of the ground state. The quantum numbers are given and $|q| = \pi/5$.

ρ	$N = 10$	$N = 20$	$N = \infty$
0.1	0.6538	0.6457	0.6246
0.2	0.6891	0.6803	0.6605
0.3	0.7239	0.7144	0.6956
0.4	0.7584	0.7480	0.7299
0.5	0.7929	0.7812	0.7635
0.6	0.8275	0.8141	0.7965
0.7	0.8624	0.8469	0.8289
0.8	0.8980	0.8798	0.8608
0.9	0.9345	0.9131	0.8923
−0.1	0.4632	0.5129	0.5497
−0.2	0.4253	0.4740	0.5104
−0.3	0.3859	0.4335	0.4696
−0.4	0.3448	0.3912	0.4268
−0.5	0.3014	0.3466	0.3817
−0.6	0.2552	0.2990	0.3335
−0.7	0.2049	0.2472	0.2810
−0.8	0.1483	0.1887	0.2217
−0.9	0.0800	0.1177	0.1495

Table 8
Momenta for two values of N near $\rho = 1$. The three lowest momenta are presented for each N.

	$N = 6\ \rho = 0.99$	$N = 20\ \rho = 0.999$
k_1	0.0134396	0.0019152
k_2	3.5106817	1.3661808
k_3	4.8534589	2.2480143

to the value $\rho = 1$ and obtain a well defined energy which approaches the value predicted by (17) as N becomes large. A well-defined numerical solution has not been found for $\rho > 1$ with N finite for the set of quantum numbers given above. Some values for the sets of k_α for particular values of finite N are presented in table 8. There are a total of three momenta for the case $N = 6$ and only the three lowest values of the ten momenta for $N = 20$ are given. For the finite rings near $\rho = -1$, the three momenta approach the same value. For example, when $N = 6$ the three momenta are given as follows: $k_1 = 2.8278, k_2 = 2.8278, k_3 = 2.7218$.

Appendix

EVALUATION OF INTEGRALS

To evaluate the integral (12), define the function

$$f(z) = \frac{e^{i\omega z}}{\cosh z + c}$$

and integrate this function around a contour C_R with one vertex at $(R, i\pi)$ such that it is symmetric under reflection about the real and imaginary axes. Using the identity $\cosh(x \pm i\pi) = -\cosh x$ one obtains

$$\int_{C_R} \frac{e^{i\omega z}}{\cosh z + c} dz = -(e^{\pi\omega} - e^{-\pi\omega}) \int_{-R}^{R} \frac{e^{i\omega x}}{\cosh x - c} dx + e^{i\omega R} \int_{-\pi}^{\pi} \frac{e^{-\omega y}}{\cosh(R + iy) + c} i dy - e^{-i\omega R} \int_{-\pi}^{\pi} \frac{e^{-\omega y}}{\cosh(R - iy) + c} i dy .$$

Introduce the variable $c = \cos\lambda$ where $0 < \lambda < \pi$ so that $c \in (-1, 1)$. There will be two poles inside the rectangle at $z_j = \pm iy_0$ such that the denominator vanishes at $\pm iy_0$, that is

$$\cosh(\pm iy_0) = -\cos\lambda$$

or

$$\cos y_0 = \cos(\pi - \lambda)$$

and $y_0 = \pi - \lambda$ will give complex z_j on the imaginary axis contained inside the contour.

Evaluating the residues, one obtains

$$2\pi i \sum Res(f, z_j) = -4\pi \frac{\sinh \omega(\pi - \lambda)}{\sin \lambda} .$$

Therefore

$$2\pi \frac{\sinh \omega(\pi - \lambda)}{\sin \lambda} = \sinh \pi\omega \int_{-R}^{R} \frac{e^{i\omega x}}{\cosh x - \cos \lambda} dx + e^{i\omega R} \int_{-\pi}^{\pi} \frac{e^{-\omega y}}{\cosh(R + iy) + c} idy - e^{-i\omega R} \int_{-\pi}^{\pi} \frac{e^{-\omega y}}{\cosh(R - iy) + c} idy$$

since

$$\left| e^{\pm i\omega R} \int_{-\pi}^{\pi} \frac{e^{-\omega y}}{\cosh(R \pm iy) + c} idy \right| \leqslant \frac{2\pi e^{|\omega|\pi}}{\sinh R - |c|} .$$

Also $\sinh R \to \infty$ as $R \to \infty$. Thus, the contributions from the vertical segments vanish as $R \to \infty$ and this gives the result.

To evaluate (14), it suffices to consider the following integral for $n \geqslant 0$:

$$I_n = 2 \int_C \frac{z^n e^{in\varphi}}{2a + z^{-1} + z} \frac{dz}{iz} .$$

Here, C is the unit circle in the complex plane. The denominator vanishes at the roots of the polynomial

$$z^2 + 2az + 1 = 0 ,$$

where $a = \cosh \Phi$. These roots are given by

$$z_{1,2} = -a \pm \sqrt{a^2 - 1}$$

and if $a > 1$, only the upper root is inside the circle. Evaluating the residues one obtains

$$Res(z_1, f) = \frac{z_1^n}{(z_1 - z_2)} = \frac{(-1)^n e^{-2n\Phi}}{2 \sinh 2\Phi} .$$

Therefore

$$I_n = e^{in\varphi}(2\pi) \frac{(-1)^n e^{-2n\Phi}}{\sinh 2\Phi} .$$

References

[1] H. Bethe, Z. Physik 71 (1931) 205.
[2] F. Woynarovich, J. Phys. A: Math. Gen. 15 (1982) 2985.

[3] E. Lieb and D. Mattis, *Mathematical Physics in One Dimension* (Academic Press, New York, 1966);
R. Orbach, Phys. Rev. 112 (1958) 309; 115 (1959) 1181.
[4] B.S. Shastry, S.S. Jha and V. Singh, *Exactly Solvable Problems in Condensed Matter and Relativistic Field Theory*, Vol. 242 (Springer, 1985).
[5] L. Hulthen, Arkiv. Mat. Astron. Fys. A26 (1938) 1.
[6] J. des Cloizeaux and J.J. Pearson, Phys. Rev. 128 (1962) 2131.
[7] R. Griffiths, Phys. Rev. 133 (1964) A768;
R. Orbach, Phys. Rev. 112 (1959) 309.
[8] J. des Cloizeaux and M. Gaudin, J. Math. Phys. 7 (1966) 1384.
[9] P. Bracken and J. Čížek, Int. J. Quant. Chem. 53 (1995) 467.
[10] M. Henkel, J. Phys. A: Math. Gen. 20 (1987) 995.
[11] F.C. Alcaraz, M.N. Barber, M.T. Batchelor, R.J. Baxter and G.R.W. Quispel, J. Phys. A: Math. Gen. 20 (1987) 6397.
[12] F. Woynarovich, J. Phys. C15 (1982) 85, 95.