Periodic structures on a quantum spin chain

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We find for a discrete anisotropic Heisenberg chain with arbitrary spin value a solution in the form of a coherent spin state with a coherence parameter which changes periodically along the chain. We evaluate the energy and the spin correlators. In the particular cases of uniaxial magnets the solutions obtained describe domain walls.

1. INTRODUCTION

The solution of the problem of finding the energy and the wave function of a one-dimensional spin chain has come a long way from the already classical Bethe Ansatz[1] to the work of Baxter[2] and Faddeev.[3] The gradual broadening of the scope of the problem—from Bethe's isotropic model *XXX* to Baxter's anisotropic *XYZ*—required an appreciable complication of the mathematical apparatus of the theory and the development of a quantal method for inverse scattering. Incidentally, there have appeared in the literature papers[4,5] which contain attempts to solve the quantum problem by traditional methods but they did not get further than the *XXZ* model studied earlier.[6] The present paper also belongs to that class.

We consider the anisotropic *XYZ* model with the Hamiltonian

$$H=-\sum_{n=1}^{N} J_{\alpha\beta} S_n^{\alpha} S_{n+1}^{\beta}, \tag{1.1}$$

where the exchange constant tensor $J_{\alpha\beta}$ is symmetric and triaxial and when it is on principal axes

$$J_3>J_2>J_1>0. \tag{1.2}$$

We assume that the value of the spin

$$\mathbf{S}_n^2=\sigma(\sigma+1) \tag{1.3}$$

is given ($\sigma = 1/2, 1, 3/2, \ldots$).

We look for the wavefunction of the chain in the form[4]

$$\psi=\prod_n \hat{R}_n|0\rangle, \tag{1.4}$$

where $\hat{R}_n$ is the rotation operator for the spin on the nth site, and $|0\rangle$ is the state in which all spins are directed along the z axis (vacuum). We use in Section 2 sphero-conical coordinates to parametrize this operator (the rotation matrix) and the spin state is given by means of the local frame of reference. We solve in Section 3 the Schrödinger equation for the states (1.4) using the addition theorem for elliptical functions and we elucidate the region where the solution obtained is applicable and we give its geometrical interpretation—the end point of the spin vector describes a spherical ellipse. We give in Section 4 a closed expression for the energy of the solution we have obtained, using the boundary conditions, and we evaluate the spin correlators in the various sites in the chain. We consider in Section 5 the limiting cases of an easy-axis and an easy-plane magnetic for which the solution degenerates into domain walls and a "fan." In the conclusion we touch upon some problems which were not elucidated in the main text of the paper and we note, in particular, that the classical ferromagnetic chain is a complete discrete analog of the well known Neumann problem. Some of the results of the present paper were given in a short communication.[7]

2. PARAMETRIZATION OF THE ROTATION MATRIX

The set of states $\hat{R}\,|0\rangle$ forms a complete set of coherent spin states[8] which can be parametrized by a parameter η:

$$\hat{R}(\eta)=\exp(\eta S_+-\bar{\eta} S_-),\quad \eta={}^1/_2\theta e^{i\varphi}, \tag{2.1}$$

where θ and φ are the polar coordinates of the point to which the North pole of the sphere has been transferred and the $S_\pm$ are the circular spin components:

$$S_\pm=S_x\pm iS_y. \tag{2.2}$$

The absence of a third parameter (for instance, one of the Euler angles) is due to the fact that rotation around the z axis forms a stationary sub-group of the vacuum $|0\rangle$ (for details see Ref. 8).

The result of the transformation of the spin operators is

$$\tilde{S}_n^{\alpha}=\hat{R}_n^{+}(\eta)S_n^{\alpha}\hat{R}_n(\eta)=R_{n\alpha\beta}S_n^{\beta}. \tag{2.3}$$

The rotation matrix $R_{\alpha\beta}$ is a more convenient object than the operator $\hat{R}$, as it interrelates any vectors and not only spins. They can, in particular, be the coordinate basis vectors $\varepsilon^{(a)}$ and $e^{(a)}$ of the original and the rotated systems:

$$e_\alpha^{(a)}=R_{\alpha\beta}\varepsilon_\beta^{(a)}, \tag{2.4}$$

and it is clear that

$$R_{\alpha\beta}=e_\alpha^{(\beta)}. \tag{2.5}$$

The spin state is thus directly described by giving the local frame of reference—a triad of basis vectors in the given site. From site to site the frame of reference is rotated due to the interaction between neighboring spins.

The usual parametrization of the sphere by polar coordinates leads to cumbersome expressions for $R_{\alpha\beta}$.[9] One

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can reach the maximum simplicity putting for the circular basis vector

$$\mathbf{e}_n^{(+)}=N_n(i,-\mathrm{sn}\,w_n,\mathrm{cn}\,w_n), \tag{2.6}$$

as it occurs in the Schrödinger equation in a decisive manner. One finds the other two basis vectors from (2.6):

$$\mathbf{e}_n^{(-)}=(\mathbf{e}_n^{(+)})^*,\quad \mathbf{e}_n^{(3)}={}^1/_2 i[\mathbf{e}_n^{(+)}\times\mathbf{e}_n^{(-)}]. \tag{2.7}$$

Here $w_n = u_n + iv_n$, and the modulus $\varkappa$ of the elliptical functions will be determined later. One can write the vector $\mathbf{e}_n^{(3)}$ explicitly as follows:

$$\mathbf{e}_n^{(3)}=(s_n'd_n, c_n'c_n, d_n's_n). \tag{2.8}$$

We have used here the notation $s=\mathrm{sn}(u,\varkappa)$, $s'=\mathrm{sn}(v,\varkappa')$, and so on:

$$\varkappa'=(1-\varkappa^2)^{1/2},\quad N_n=(1-s_n'^2d_n^2)^{1/2}. \tag{2.8a}$$

The parameters u, v are none other than the sphero-conical coordinates[10]:

$$x=r\,\mathrm{sn}'\,v\,\mathrm{dn}\,u,\quad y=r\,\mathrm{cn}'\,v\,\mathrm{cn}\,u,\quad z=r\,\mathrm{dn}'\,v\,\mathrm{sn}\,u. \tag{2.9}$$

These coordinates describe the position of the average value of the spin in the state (1.4), since

$$\langle \mathbf{S}_n\rangle=\langle 0|\hat{R}_n^+\mathbf{S}_n\hat{R}_n|0\rangle=\sigma\mathbf{e}_n^{(3)}. \tag{2.10}$$

In other words, $\mathbf{e}_n^{(3)}$ is the same as the classical spin unit vector

3. RECURRENCE RELATIONS

We write the Hamiltonian in the local frame representation[7]:

$$\tilde{H}=-\sum_n \mathcal{J}_{\lambda\mu}{}^n S_n^\lambda S_{n+1}^\mu, \tag{3.1}$$

where

$$\mathcal{J}_{\lambda\mu}{}^n=J_{\alpha\beta}e_{n\alpha}^{(\lambda)}e_{n+1\,\beta}^{(\mu)}. \tag{3.2}$$

Substituting (3.1) into the equation $\tilde{H}|0\rangle=E|0\rangle$ and using the fact that

$$S_n^+|0\rangle=0,\quad S_n^3|0\rangle=\sigma|0\rangle,$$

we get

$$-\sum_n(\mathcal{J}_{++}{}^nS_n^-S_{n+1}^-+\sigma\mathcal{J}_{+3}{}^nS_n^-+\sigma\mathcal{J}_{3+}{}^nS_{n+1}^-+\sigma^2\mathcal{J}_{33}{}^n)|0\rangle$$
$$=E|0\rangle. \tag{3.3}$$

Here

$$\mathcal{J}_{++}{}^n=J_{\alpha\beta}e_{n\alpha}^{(+)}e_{n+1\,\beta}^{(+)},\quad \mathcal{J}_{+3}{}^n=J_{\alpha\beta}e_{n\alpha}^{(+)}e_{n+1\,\beta}^{(3)}. \tag{3.4}$$

Equation (3.3) will be satisfied if

$$\mathcal{J}_{++}{}^n=0, \tag{3.5a}$$

$$\mathcal{J}_{+3}{}^n+\mathcal{J}_{3+}^{n-1}=0. \tag{3.5b}$$

There are just the equations for the rotation of the frame of reference which we discussed above. In the parametrization chosen the first one is satisfied immediately by virtue of the theorem for the addition of elliptical functions[11]:

$$\mathrm{cn}\,a\,\mathrm{cn}\,b+dn(a-b)\,\mathrm{sn}\,a\,\mathrm{sn}\,b=\mathrm{cn}(a-b). \tag{11}$$

Comparing (3.6) with Eq. (3.5a) written in the form

$$J_3\,\mathrm{cn}\,w_n\,\mathrm{cn}\,w_{n+1}+J_2\,\mathrm{sn}\,w_n\,\mathrm{sn}\,w_{n+1}=J_1,$$

we find

$$w_{n+1}-w_n=q=\mathrm{const}, \tag{3.7}$$

where

$$\mathrm{dn}\,q=J_2/J_3,\quad \mathrm{cn}\,q=J_1/J_3. \tag{3.8}$$

Hence we find the elliptical modulus

$$\varkappa^2=\frac{1-\mathrm{dn}^2 q}{1-\mathrm{cn}^2 q}=\frac{J_3^2-J_2^2}{J_3^2-J_1^2}. \tag{3.9}$$

By virtue of inequality (1.2) we have $0\leqslant\varkappa^2\leqslant1$. The ordering (1.2) of the exchange constants corresponds in the phase diagram to a dashed triangle the boundaries of which correspond to the XZZ model (vertical line) and the XXZ model (bisectrix), i.e., to uniaxial magnets. The intersection of the boundary when the relations between the exchange constants is changed leads to a rearrangement of the state (Fig. 1).

The parameter q is not determined uniquely by Eqs. (3.8): it can be real or purely imaginary. In the second case $J_1>J_2>J_3$ and we obtain a solution in another part of the diagram that is symmetric with regard to the triangle with respect to the point Q. Using the fact that $w=u+iv$ we note that this symmetry reduces to the substitution $u\rightleftarrows v$. In what follows we assume in accordance with (1.2) that q is real and positive.

The solution of Eq. (3.7):

$$w_n=qn+w_0, \tag{3.10}$$

means that

$$u_n=qn+u_0,\quad v_n=v_0=\mathrm{const}. \tag{3.11}$$

In other words, one of the sphero-conical coordinates v is fixed. As it is given by the intersection of an elliptical cone with the sphere $r^2=1$, i.e., a spherical ellipse, the axis of the local frame (the vector $\mathbf{e}_n^{(3)}$) traces on the sphere just this line (Fig. 2). The distribution of the spin axes along the sites of the chain is a scan of the spherical ellipse.

There are no additional restrictions imposed by Eq.

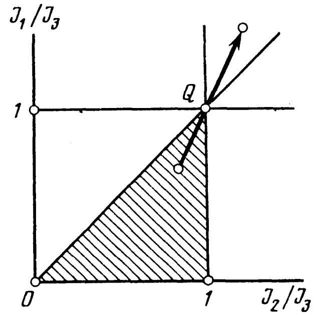

FIG. 1.

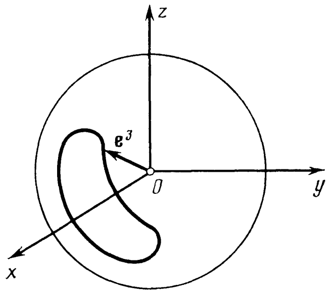

FIG. 2.

(3.5b) on the parameters w, $\varkappa$. It is the same as the Landau-Lifshitz equation for a classical chain of spins considered as unit vectors. The reason for this agreement is clear and consists in the choice of the solution (1.4) in the form of coherent spin states which are the quantum analog of the classical system.[8]

4. ENERGY AND CORRELATIONS

Satisfying the compensation (3.5) we get from the Schrödinger Eq. (3.3) the energy of the given state:

$$E=-\sigma^2\sum_n J_{\alpha\beta}e_{n\alpha}^{(3)}e_{n+1\,\beta}^{(3)}. \tag{4.1}$$

Substituting the components of the basis vector (2.8) we find the expression

$$E=-\sigma^2\sum_n (J_1\,\mathrm{sn}^2\,v d_n d_{n+1}+J_2\,\mathrm{cn}^2\,v c_n c_{n+1}+J_3\,\mathrm{dn}^2\,v s_n s_{n+1}), \tag{4.2}$$

which reminds us of the expressions of Baxter and Faddeev but with a different parametrization. More important differences consist in the fact that we consider the case of arbitrary (and not only 1/2) spin and do not impose periodic boundary conditions.

Using Eq. (3.6) and one similar to it[11]

$$\mathrm{dn}\,a\,\mathrm{dn}\,b+\varkappa^2\,\mathrm{cn}(a-b)\,\mathrm{sn}\,a\,\mathrm{sn}\,b=\mathrm{dn}(a-b) \tag{4.3}$$

all elliptic functions in (4.2) reduce to the sines:

$$E=-\sigma^2 J_3\sum_n(\mathrm{cn}\,q\,\mathrm{dn}\,q+\varkappa^2\,\mathrm{sn}^2\,q s_n s_{n+1}). \tag{4.4}$$

Remarkably, this expression can be summed and provides thereby an answer to one of Baxter's questions (about the transformation of his expression for the energy to another form). To do this we must use the Jacobi identity[11]:

$$\varkappa^2\,\mathrm{sn}\,q\,\mathrm{sn}\,A\,\mathrm{sn}(A+q)=E(q)+E(A)-E(A+q), \tag{4.5}$$

where

$$E(u)=\int_0^u \mathrm{dn}^2\,t\,dt \tag{4.6}$$

is an elliptical integral of the second kind. Putting $A=u_n=qn+u_0$ we have

$$E=-\sigma^2 J_3 N[\mathrm{cn}\,q\,\mathrm{dn}\,q+\mathrm{sn}\,qE(q)]+\sigma^2 J_3\,\mathrm{sn}\,q[E(u_N)-E(u_1)]. \tag{4.7}$$

In this formula we can split off the homogeneous part with density

$$\varepsilon=\frac{E}{N}=-\sigma^2 J_3\left\{\mathrm{cn}\,q\,\mathrm{dn}\,q+\mathrm{sn}\,q\left[E(q)-\frac{qE(K)}{K}\right]\right\}, \tag{4.8}$$

where $E(K)$ and, K are complete elliptical integrals of the second and first kind.

The remaining dependence in (4.7) on the boundary conditions means (by virtue of the variational principle) that when solution (1.4) exists it is necessary to fix the state of the spins at the end points of the chain (e.g., by an external magnetic field) or to give periodic boundary conditions.

The parameter q reduces to an elliptical integral of the first kind:

$$q=F(\varphi,\varkappa),\quad \cos\varphi=J_1/J_3. \tag{4.9}$$

It is important to emphasize that the energy is independent of v [this is already clear from (4.4)]—of the parameter determining the "eccentricity" of the spherical ellipse. This degeneracy is manifested by the presence of an additional integral which [for the solution (1.4)] commutes with the Hamiltonian. Strictly speaking, it is just the existence of this extra integral, and with it of a dynamical symmetry group, which is the primary case of the complete integrability of the chain problem.

One could also evaluate the energy differently by averaging the Hamiltonian:

$$E=\langle H\rangle=-\sum_n J_{\alpha\beta}\langle S_n^\alpha S_{n+1}^\beta\rangle, \tag{4.10}$$

which requires the calculation of the correlator of neighboring spins. Because

$$\langle S_n^\alpha S_{n+1}^\beta\rangle=R_{\alpha\lambda}{}^n R_{\beta\mu}^{n+1}\langle 0|S_n^\lambda S_{n+1}^\mu|0\rangle,$$

and because the spins on different sites commute, we get

$$\langle 0|S_n^\lambda S_{n+1}^\mu|0\rangle=\sigma^2\delta_{\lambda 3}\delta_{\mu 3}, \tag{4.11}$$

so that

$$E=-\sigma^2\sum_n J_{\alpha\beta}e_{n\alpha}^{(3)}e_{n+1\,\beta}^{(3)}.$$

Naturally we returned to Eq. (4.1). Incidentally we obtained a result for the correlator

$$\langle S_n^\alpha S_m^\beta\rangle=\sigma^2 e_{n\alpha}^{(3)}e_{m\beta}^{(3)}. \tag{4.12}$$

It is clear from Eq. (2.8) that the correlator of any pair of spins depends periodically on the number m for fixed n. We must note that the period of the correlator of the transverse spin components is twice the period of the longitudinal correlator as $\mathrm{dn}\,x$ in contrast to $\mathrm{cn}\,x$ and $\mathrm{sn}\,x$ has the period $2K(\varkappa)$ rather than $4K(\varkappa)$.

In the evaluation of the spin fluctuation we must consider the quantity

$$\langle S_n^\alpha S_n^\beta\rangle=\sigma^2 e_{n\alpha}^{(3)}e_{n\beta}^{(3)}+2\sigma e_{n\alpha}^{(+)}e_{n\beta}^{(-)}. \tag{4.13}$$

In particular,

$$\langle (S_n^z)^2\rangle=\sigma^2(d's_n)^2+2\sigma(c'^2c_n^2+s'^2d'^2s_n^2d_n^2)/[1-(s'd_n)^2] \tag{4.14}$$

[we bear in mind that $s_n = \mathrm{sn}(qn+q_0)$, $s' = \mathrm{sn}(v, \varkappa')$, and so on]. This means that the correlators, as one should expect, depend on the parameter v, with respect to which the energy is degenerate.

5. "WALLS AND "FANS"

Here we consider the behavior of the solution at the boundary of the triangle (Fig. 1). On the bisectrix ($J_1 = J_2 < J_3$) we have an easy-axis type magnet and on the vertical ($J_2 = J_3 > J_1$) an easy plane type magnetic.

In the first case the elliptical modulus $\varkappa = 1$ and in the second case $\varkappa = 0$. It is well known that in those cases the elliptical functions reduce to elementary functions

$$\mathrm{sn}(u,1)=\mathrm{th}\,u,\quad \mathrm{cn}(u,1)=\mathrm{dn}(u,1)=1/\mathrm{ch}\,u, \tag{5.1}$$

$$\mathrm{sn}(u,0)=\sin u,\quad \mathrm{cn}(u,0)=\cos u,\quad \mathrm{dn}(u,0)=1. \tag{5.2}$$

The solution for the easy-axis magnet thus becomes nonperiodic; more precisely, its period tends to infinity. If we consider a sufficiently long chain this will be a domain wall type solution. Indeed, the averaged spin component equals

$$\langle \mathbf{S}_n\rangle=\sigma\mathbf{e}_n^{(3)}=\left(\frac{\sin v}{\mathrm{ch}\,u_n},\ \frac{\cos v}{\mathrm{ch}\,u_n},\ \mathrm{th}\,u_n\right)\sigma, \tag{5.3}$$

i.e., the projection on the easy axis changes from $-\sigma$ to $+\sigma$ according to the relation $\tanh(qn+q_0)$ which is typical for a domain wall. The parameter q determines the thickness of the wall and equals, according to (3.8)

$$q=\mathrm{Arch}(J_3/J_1). \tag{5.4}$$

The transverse components of the spin depend on the parameter v and in all cases the spin rotates in a plane containing the easy z axis.

The energy of the domain wall is independent of its type (i.e., of v) and, according to (4.7) equals

$$E_{\mathrm{dw}}=\sigma^2 J_3\,\mathrm{th}\,q\,(\mathrm{th}\,u_N-\mathrm{th}\,u_1), \tag{5.5}$$

as the elliptical integral (4.6) in that case reduces to an elementary one: $E(u) = \tanh u$. For an infinite chain

$$E_{\mathrm{dw}}=2\sigma^2(J_3^2-J_1^2)^{1/2}. \tag{5.6}$$

Gochev[5] did obtain this formula earlier.

We now turn to an easy plane type magnetic. From (5.2) and (2.8) we have

$$\langle \mathbf{S}_n\rangle=\sigma\left(\mathrm{th}\,v,\ \frac{\cos u_n}{\mathrm{ch}\,v},\ \frac{\sin u_n}{\mathrm{ch}\,v}\right).$$

This means that the spin component along the difficult axis is fixed by the parameter v and in the easy plane it rotates with an "angular velocity" $q = \arccos(J_1/J_3)$ per step along the chain. We call this solution a fan; it is completely analogous to the precessional rotation of a top.

The energy density of the fan equals

$$\varepsilon_{\mathrm{EP}}=-\sigma^2 J_1, \tag{5.7}$$

which follows immediately from (4.4) when $\varkappa = 0$. The degeneracy with respect to energy of the states manifests itself here in that $\varepsilon_{\mathrm{EP}}$ is independent of the spread angle of the fan.

We indicate finally that the spherical ellipse in the easy-axis magnet is degenerate in the meridian joining the north and the south poles of the sphere. The spin rotates by 180° in the plane of this meridian.

In the easy-plane magnet the ellipse turns out to be a circle—the parallel around the difficult axis. The energy is independent of the lattitude on which this parallel is drawn and also of the longitude on which the meridian in the easy-axis case is positioned. To give these quantities it is necessary to fix the second integral of the motion.

For a qualitative representation of the properties of the solution in the general case when $\varkappa \neq 0$ we can use a mixture of the properties of the wall and the fan. In particular, when $\varkappa$ is close to unity and $v = 0$ the solution gives a model of a band domain structure—several domain walls fit onto a finite length chain.

6. CONCLUSION

The solution obtained in the present paper for a quantal anisotropic Heisenberg chain has a number of features on which we must dwell.

Firstly, the solution is practically independent of the magnitude of the spin: the spin enters trivially merely into the expressions for the energy and the correlators [this property reflects the coherent nature of the solution (1.4)]. We thereby obtained a certain class of solutions with fixed energies for anisotropic chains with arbitrary (and in the limit of large σ, classical) spin. Not a single solution was previously known for such chains.

Secondly, as we have already noted, periodic boundary conditions need not be satisfied; we thereby go beyond the framework of the inverse scattering method[3] in which boundary effects are lost such as those which are responsible for the existence of domain walls.

Thirdly, it is well known that in the continuum classical limit the (stationary) Landau-Lifshitz equation describes the motion of a point on a sphere with a quadratic potential (the so-called Neumann problem[12]). This is completely integrable, i.e., it possesses three independent integrals of motion which are in involution with the Hamiltonian. The discrete Eq. (3.5b) turns out also to have three "integrals"—expressions which are algebraic in $\mathbf{e}_n^{(3)}$ and which are independent of the number of the site. The anisotropic chain described by Eq. (3.5b) is thus the discrete analog of the Neumann problem which retains all important properties of the latter. In particular, this explains the success of the sphero-conical parametrization (2.8)—the variables in the Hamilton-Jacobi equation in the Neumann problem separate just in the sphero-conical coordinates.[12]

One can use the solution as a zeroth approximation for a perturbation theory solution of problems connected with the inclusion of a weak external field or for taking into account anisotropy which is not of an exchange nature. The problem of the possibility of constructing "excited" states on the solution (1.4) and also the symmetry aspect of the "random" degeneracy with respect to the parameter v are of interest.

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