Theoretical and Mathematical Physics, Vol. 117, No. 3, 1998

ANHARMONIC STATES OF THE ONE-DIMENSIONAL ANISOTROPIC HEISENBERG MODEL WITH FREE BOUNDARY CONDITIONS

S. N. Martynov[1]

States described by anharmonic functions are shown to exist in the one-dimensional anisotropic Heisenberg model with a finite number of spins 1/2 and free boundary conditions. Several such states are determined.

1. Introduction

Solutions of the one-dimensional Heisenberg model are important in magnetism theory because they arise in a variety of problems. In addition, exact solutions of this model provide good criteria for the applicability of many approximation techniques and numerical methods used when exact solutions do not exist. Eigenfunctions and energy eigenvalues in the Heisenberg model, as in any other model, depend essentially on not only the Hamiltonian parameters but also the boundary conditions (BC) imposed on the solutions. Standard cyclical BC [1, 2], which permit using the Bethe ansatz [3], restrict a solution to a periodic function of the coordinate. However, the BC that are usually realized are the free BC under which the border spins of a magnetic chain only interact with one nearest neighbor. The anisotropic open chain was first investigated by Gaudin [2]. The general relations for momenta and phases of an arbitrary number M of flipped spins were found, and the hypothesis that real solutions for momenta exist was advanced. However, the question of what the conditions for the appearance of imaginary solutions k_i are and how to calculate their number remained open. To close this question, we find the complete set of eigenfunctions and energy eigenvalues with $M = 1, 2$ for interchange anisotropy of the "light axis" type.

2. One-magnon solutions

The Hamiltonian of the anisotropic Heisenberg model with a finite number N of spins 1/2 is

$$H = J\sum_n (S_n^z S_{n+1}^z + \Delta(S_n^x S_{n+1}^x + S_n^y S_{n+1}^y)). \tag{1}$$

An exact solution of the corresponding Schrödinger equation can be found in the class of the one-magnon states $M = 1$ with the eigenfunctions

$$\psi(k) = \sum_{n=-(N-1)/2}^{(N-1)/2} a_k(n)\psi(n), \tag{2}$$

where n is the coordinate of the flipped spin, the reference point is in the middle of the magnetic chain, and k is the momentum that parameterizes the solutions. This Schrödinger equation for the amplitudes $a_k(n)$ can be reduced to the system of finite-difference equations

$$2(\varepsilon + 1)a(n) = \Delta(a(n-1) + a(n+1)), \quad -\frac{N-1}{2} < n < \frac{N-1}{2}. \tag{3}$$

[1]Kirenskii Institute for Physics, Siberian Branch, Russian Academy of Sciences, Krasnoyarsk, Russia.

Translated from Teoreticheskaya i Matematicheskaya Fizika, Vol. 117, No. 3, pp. 489–497, December, 1998. Original article submitted May 5, 1998; revised July 6, 1998.

The coordinate n takes integer values for odd N and half-integer values for even N. Hereafter, we omit the subscript k of the $a(n)$ amplitudes for brevity. All formulas for amplitudes are related to eigenstates (1) with k fixed. Energy $\varepsilon = E/J$ is measured in J units w.r.t. the ferromagnetic "vacuum." For free BC, the finite-difference equations for the boundary amplitudes are

$$2\left(\varepsilon + \frac{1}{2}\right)a\left(\pm\frac{N-1}{2}\right) = \Delta a\left(\pm\frac{N-3}{2}\right). \tag{4}$$

The initial inhomogeneous system of finite-difference equations (3) and (4) is equivalent to a homogeneous system if we complete the set of N physical amplitudes $a(n)$, $n \in \big(-(N-1)/2, \ldots, (N-1)/2\big)$, by adding two nonphysical amplitudes related to the physical amplitudes by the two additional conditions

$$a\left(\pm\frac{N-1}{2}\right) = \Delta a\left(\pm\frac{N+1}{2}\right). \tag{5}$$

Adding conditions (5) term-by-term to boundary equations (4), we can reduce the problem to solving the homogeneous finite-difference equation system on which BC (5) are imposed. For $\Delta \neq 1$, these BC are not the mirror-type BC, which ensure the periodicity of solutions of the isotropic Heisenberg model [4]. In an arbitrary finite system, noncyclical BC imply that the physical amplitude of a wave function is identically zero outside the domain of definition. This permits seeking solutions (up to a nonessential phase factor) as real coordinate functions whose symmetries are the symmetries of the problem under consideration.

With the normalization taken into account, harmonic solutions of homogeneous system (3), (4), (5) that are symmetrical ($^{\mathrm{s}}$) and antisymmetrical ($^{\mathrm{a}}$) w.r.t. the middle of the spin chain $n = 0$ are

$$\begin{aligned} a_k^{\mathrm{s}}(n) &= \sqrt{\frac{2}{N + \frac{\sin(kN)}{\sin k}}}\cos(kn), \\ a_k^{\mathrm{a}}(n) &= \sqrt{\frac{2}{N - \frac{\sin(kN)}{\sin k}}}\sin(kn). \end{aligned} \tag{6}$$

Wave vectors of solutions (6) are determined by BC (5),

$$\cot\frac{kN}{2} = -\frac{1+\Delta}{1-\Delta}\tan\frac{k}{2}, \tag{7}$$

$$\tan\frac{kN}{2} = \frac{1+\Delta}{1-\Delta}\tan\frac{k}{2} \tag{8}$$

for the symmetrical and antisymmetrical solutions respectively. Solutions with the momentum k_j for states with different symmetries are functions (2), which are orthogonal by definition. Solutions with the coinciding symmetries satisfy the orthogonality conditions

$$\frac{\sin\dfrac{N(k+k')}{2}}{\sin\dfrac{k+k'}{2}} \pm \frac{\sin\dfrac{N(k-k')}{2}}{\sin\dfrac{k-k'}{2}} = 0$$

for the corresponding symmetrical and antisymmetrical pairs k and k'. In the domain of definition of physically different solutions $0 \leq k < \pi$, the number of solutions of Eq. (7) is

$$N_{1m}^{\mathrm{s}} = \frac{N}{2} - 1$$

for even N. The number of antisymmetrical harmonic solutions of (8) depends on the number of spinors N and the quantity Δ,

$$N_{1m}^{\mathrm{a}} = \begin{cases} \dfrac{N}{2}, & N < \dfrac{1+\Delta}{1-\Delta}, \\ \dfrac{N}{2} - 1, & N > \dfrac{1+\Delta}{1-\Delta}. \end{cases}$$

For odd N, we obtain

$$N_{1m}^{\mathrm{s}} = \frac{N-1}{2},$$
$$N_{1m}^{\mathrm{a}} = \begin{cases} \dfrac{N-1}{2}, & N < \dfrac{1+\Delta}{1-\Delta}, \\ \dfrac{N-1}{2} - 1, & N > \dfrac{1+\Delta}{1-\Delta}. \end{cases}$$

The case

$$N = \frac{1+\Delta}{1-\Delta}$$

is special. Here, the linear antisymmetrical solution

$$a_l^{\mathrm{a}}(n) = \frac{2\sqrt{3}}{\sqrt{N(N^2-1)}}n \tag{9}$$

with the bottom one-magnon branch energy $\varepsilon_l = \Delta - 1$ arises. Therefore, harmonic one-magnon solutions (6) predict a number of k states less than the initial number N of the independent coordinate functions. The complete set of orthonormal one-magnon functions can be obtained if we enhance exponential function class (6) by adding anharmonic hyperbolic functions possessing the corresponding symmetry; these functions correspond to solutions with imaginary momenta $k = iq$,

$$\begin{aligned} a_q^{\mathrm{s}}(n) &= \sqrt{\frac{2}{N + \dfrac{\sinh(qN)}{\sinh q}}} \cosh(qn), \\ a_q^{\mathrm{a}}(n) &= \sqrt{\frac{2}{\dfrac{\sinh(qN)}{\sinh q} - N}} \sinh(qn). \end{aligned} \tag{10}$$

The corresponding equations for q, which can again be obtained by substituting relations (10) in BC (5), are

$$\coth\frac{qN}{2} = \frac{1+\Delta}{1-\Delta}\tanh\frac{q}{2}, \tag{11}$$
$$\tanh\frac{qN}{2} = \frac{1+\Delta}{1-\Delta}\tanh\frac{q}{2} \tag{12}$$

for the respective symmetrical and antisymmetrical cases. A symmetrical anharmonic solution exists for any N and $\Delta < 1$; antisymmetrical solution equality (12) holds only if the threshold condition

$$N > \frac{1+\Delta}{1-\Delta} \tag{13}$$

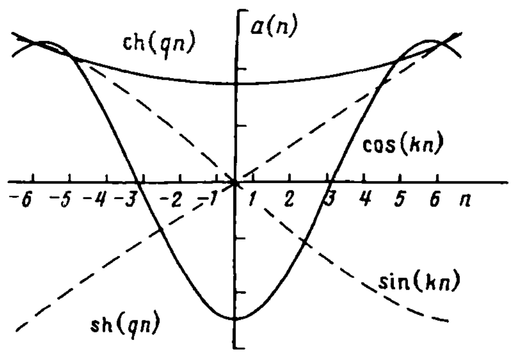

Fig. 1

is satisfied. Therefore, the union of harmonic and anharmonic one-magnon solutions always ensures the completeness of the eigenfunction system for operator (1).

Different one-magnon solutions with the minimal values of k and q for $N = 10$ and $\Delta = 0.9$ are depicted in Fig. 1. To clarify threshold condition (13), the functions are taken not normalized but passing through the same boundary points (5). For the given N and Δ, an antisymmetrical anharmonic solution cannot pass through these points and through the inversion center and is therefore absent. To obtain such a solution, either a larger N or a smaller Δ must be chosen. Then, the first antisymmetrical harmonic solution $a \sim \sin(kn)$ disappears.

3. Two-magnon solutions

For $M = 2$, the symmetry restrictions imposed on the eigenfunction amplitudes,

$$\psi(k_1, k_2) = \sum_{n_1 < n_2} a(n_1, n_2)\psi(n_1, n_2), \tag{14}$$

can be reduced to the evenness restrictions for the corresponding amplitudes w.r.t. the flipped-spin coordinate inversion,

$$a(n_1, n_2) = \pm a(-n_2, -n_1).$$

Hereafter, we omit the amplitude subscripts k_1 and k_2 for brevity. All the amplitudes $a(n_1, n_2)$ are related to the fixed pair k_1, k_2, which parameterizes each two-magnon solution. The plus sign corresponds to the functions with a symmetrical amplitude distribution w.r.t. the center, and the minus sign corresponds to the antisymmetrical distribution. The inhomogeneous system of finite-difference equations for amplitudes can be reduced to the homogeneous system

$$2(\varepsilon + 2)a(n_1, n_2) = \Delta(a(n_1 + 1, n_2) + a(n_1 - 1, n_2) + a(n_1, n_2 + 1) + a(n_1, n_2 - 1)), \quad n_1 < n_2, \tag{15}$$

if we complete the set of physical amplitudes $a(n_1 < n_2)$,

$$n_1, n_2 \in \left(-\frac{N-1}{2}, \ldots, \frac{N-1}{2}\right),$$

by adding $3N - 2$ nonphysical amplitudes $a(n, n)$, $a(-(N+1)/2, n_2)$, $a(n_1, (N+1)/2)$, on which the BC

$$\begin{aligned} a\left(-\frac{N-1}{2}, n_2\right) &= \Delta a\left(-\frac{N+1}{2}, n_2\right), \\ a\left(n_1, \frac{N-1}{2}\right) &= \Delta a\left(n_1, \frac{N+1}{2}\right), \end{aligned} \tag{16}$$

$$2a_{k_1 k_2}(n_1, n_1 + 1) = \Delta\left(a_{k_1 k_2}(n_1, n_1) + a_{k_1 k_2}(n_1 + 1, n_1 + 1)\right) \tag{17}$$

are imposed. The procedure, completely analogous to the isotropic case [4], equates the total numbers of amplitudes and equations; the solution is therefore unique. Because the amplitudes are real, we obtain the relation for the harmonic solutions

$$a^{\mathrm{s,a}}(n_1,n_2) = C(k_1,k_2)\Big(\cos\big(k_1(n_1+\delta_1)\big)\cos\big(k_2(n_2-\delta_2)\big) \pm \cos\big(k_2(n_1+\delta_2)\big)\cos\big(k_1(n_2-\delta_1)\big)\Big). \tag{18}$$

The phase shifts $\delta_1 = \delta(k_1)$ and $\delta_2 = \delta(k_2)$ determine the maxima of the wave function, which are equal to $N/2$ in the case of the mirror-like BC [4] (the isotropic Heisenberg model). In the anisotropic case, these shifts are determined from BC (16), which result in the equations

$$\delta_i = \delta_i' + \frac{N}{2}, \qquad \cot(k_i\delta_i') = \frac{1+\Delta}{1-\Delta}\tan\frac{k_i}{2}, \quad i=1,2. \tag{19}$$

The momenta k_1 and k_2 of each solution are related by Eq. (17), which establishes a one-to-one correspondence between k_1 and k_2, i.e., two-magnon solutions to the anisotropic one-dimensional Heisenberg model depend on a single parameter. We obtain two systems of equations

$$\begin{gathered}\frac{\sin 2k_1\delta_1}{\sin k_1}(1-\Delta\cos k_1) \pm \frac{\sin 2k_2\delta_2}{\sin k_2}(1-\Delta\cos k_2) = 0,\\ \frac{\sin k_1(2\delta_1-1)}{\sin k_1} \pm \frac{\sin k_2(2\delta_2-1)}{\sin k_2} = 0,\end{gathered} \tag{20}$$

where $\delta_{1,2}$ satisfy Eqs. (19), for the respective symmetrical and antisymmetrical solutions.

When considering real solutions k_i, it is convenient to exclude phases (19) and write the equations for the total ($K = k_1 + k_2$) and relative ($q = (k_1 - k_2)/2$) momenta. We obtain

$$\begin{aligned}&\tan\left(\frac{KN}{2}\right)\sin\left(\frac{K}{2}\right)\left(2\cos\frac{K}{2} - \Delta(3-\Delta^2)\cos q\right) + \Delta^2 - 1+\\ &\qquad + 2\cos^2\frac{K}{2} + 2\Delta^2\cos^2 q - \Delta(3+\Delta^2)\cos\left(\frac{K}{2}\right)\cos q = 0,\\ &\tan(qN)\sin(q)\left(2\cos q - \Delta(3-\Delta^2)\cos\frac{K}{2}\right) + \Delta^2 - 1+\\ &\qquad + 2\cos^2 q + 2\Delta^2\cos^2\frac{K}{2} - \Delta(3+\Delta^2)\cos\left(\frac{K}{2}\right)\cos q = 0\end{aligned} \tag{21}$$

for the symmetrical solutions and

$$\begin{aligned}&\cot\left(\frac{KN}{2}\right)\sin\left(\frac{K}{2}\right)\left(\Delta(3-\Delta^2)\cos q - 2\cos\frac{K}{2}\right) + \Delta^2 - 1+\\ &\qquad + 2\cos^2\frac{K}{2} + 2\Delta^2\cos^2 q - \Delta(3+\Delta^2)\cos\left(\frac{K}{2}\right)\cos q = 0,\\ &\cot(qN)\sin(q)\left(\Delta(3-\Delta^2)\cos\frac{K}{2} - 2\cos q\right) + \Delta^2 - 1+\\ &\qquad + 2\cos^2 q + 2\Delta^2\cos^2\frac{K}{2} - \Delta(3+\Delta^2)\cos\left(\frac{K}{2}\right)\cos q = 0\end{aligned} \tag{22}$$

for the antisymmetrical solutions.

Equations (20) are invariant w.r.t. changing the signs of k_i and transposing them (correspondingly, w.r.t. changing the signs of and transposing K and q in (20) and (21)). All physically different solutions of (20) and (21) lie inside the interval $0 \le K, q < \pi$. Except for the real solutions K and q, these equations have solutions in which one of these momenta is imaginary. Because of the equation symmetry under transpositions of K and q, we can obtain all physically different solutions of this type keeping K real and q imaginary. These solutions correspond to the bounded Bethe complexes $k_1 = k_2^*$ for which Eqs. (20) and (21) for K and $q' = -iq$ remain real. In the coordinates $R = (n_1 + n_2)/2$ and $r = n_1 - n_2$, the Bethe complex amplitudes are

$$a_B^{\mathrm{s}}(R,r) = C(K,q')\Big(\cos(KR)\cosh\big(q'(r+N+2\,\mathrm{Re}(\delta')) + K\,\mathrm{Im}(\delta')\big) + \\ + \cosh(2q'N)\cos\Big(\frac{K}{2}(r+N+2\,\mathrm{Re}(\delta')) + 2q'\,\mathrm{Im}(\delta')\Big)\Big),$$

$$a_B^{\mathrm{a}}(R,r) = C(K,q')\Big(\sin(KR)\sinh\big(q'(r+N+2\,\mathrm{Re}(\delta')) + K\,\mathrm{Im}(\delta')\big) + \\ + \sinh(2q'N)\sin\Big(\frac{K}{2}(r+N+2\,\mathrm{Re}(\delta')) + 2q'\,\mathrm{Im}(\delta')\Big)\Big)$$

for the respective symmetrical and antisymmetrical complexes where $\delta' = \delta_1' = (\delta_2')^*$.

Real and complex-conjugate solutions k_i of the anisotropic open chain with $\Delta < 1$ neither exhaust all possible solutions of Eqs. (20) nor produce the complete set of eigenfunctions of Hamiltonian (1). Equations (20) admit solutions in which one of the momenta k_i or both these momenta are purely imaginary. In the former case, mixed states (m-states) appear whose wave function amplitudes are expressed via a superposition of harmonic (trigonometric) and hyperbolic functions,

$$a_{\mathrm{m}}^{\mathrm{s,a}}(n_1,n_2) = C(k_1,k_2)\Big(\cos\big(k_1(n_1+\delta_1)\big)\cosh\big(|k_2|(n_2-\delta_1)\big) \pm \cosh\big(|k_2|(n_1+\delta_2)\big)\cos\big(k_1(n_2-\delta_1)\big)\Big).$$

In the latter case, pure anharmonic states (a-states) appear whose amplitudes are expressed only via the hyperbolic functions,

$$a_{\mathrm{a}}^{\mathrm{s}}(n_1,n_2) = C(k_1,k_2)\Big(\cosh\big(|k_1|(n_1+\delta_1)\big)\cosh\big(|k_2|(n_2-\delta_2)\big) + \\ + \cosh\big(|k_2|(n_1+\delta_2)\big)\cosh\big(|k_1|(n_2-\delta_1)\big)\Big),$$

$$a_{\mathrm{a}}^{\mathrm{a}}(n_1,n_2) = C(k_1,k_2)\Big(\cosh\big(|k_1|(n_1+\delta_1)\big)\sinh\big(|k_2|(n_2-\delta_2)\big) + \\ + \sinh\big(|k_2|(n_1+\delta_2)\big)\cosh\big(|k_1|(n_2-\delta_1)\big)\Big).$$

For the amplitudes $a_{\mathrm{a}}^{\mathrm{a}}(n_1,n_2)$, BC (16) imply that for the phase δ_2,

$$\delta_2 = \delta_2' + \frac{N}{2}, \qquad \tanh(|k_2|\delta_2') = -\frac{1+\Delta}{1-\Delta}\tanh\frac{k_2}{2}$$

instead of (19).

4. One- and two-magnon state energies

In Fig. 2, the energy spectrum, which depends on the total real momentum $K = \mathrm{Re}\big(\sum k_i\big)$, is depicted for $N = 10$ and $\Delta = 0.9$ for the obtained solutions. One-magnon states are labelled by small circles (black are symmetrical and white are antisymmetrical states). Squares correspond to two-magnon solutions (again,

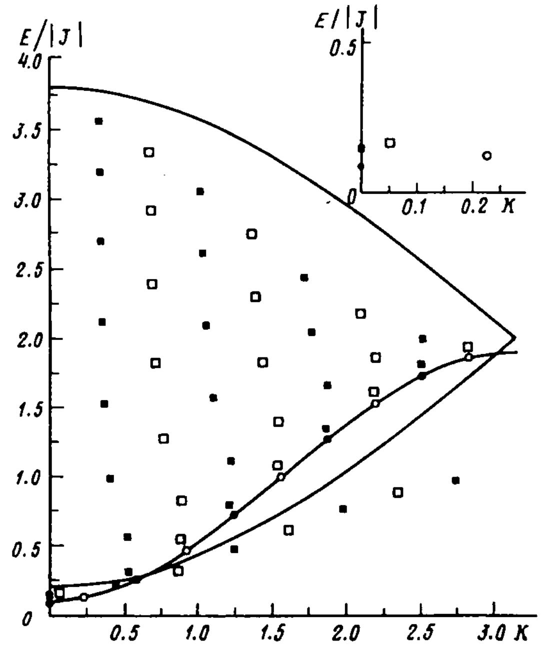

Fig. 2

black are symmetrical and white are antisymmetrical states). The one-magnon energies correspond to one anharmonic and $N-1$ harmonic solutions,

$$\varepsilon_{\mathrm{h}}^{(1)} = \Delta \cos k - 1,$$
$$\varepsilon_{\mathrm{a}}^{(1)} = \Delta \cosh q - 1.$$

The last is the energy of the symmetrical anharmonic solution. In this case, threshold condition (13) is not satisfied and the antisymmetrical a-state is absent. Because $\cosh q \geq 1$, anharmonic-solution energies for the ferromagnetic exchange $J < 0$ are below the branch of harmonic energies. At the same time, the symmetrical anharmonic state has the minimum energy (the first excited state). This follows from the wave function form (see Fig. 1): the state energy decreases as the magnetization distribution (wave function amplitude) becomes more homogeneous along the chain. The distribution of levels in our problem is completely analogous to the distribution of particle levels in a potential well; the latter depends on the number of the wave function nodes.

Harmonic two-magnon solutions have the energies

$$\varepsilon_{\mathrm{h}}^{(2)} = \Delta(\cos k_1 + \cos k_2) - 2,$$

whose number is diminished by N in comparison with the isotropic case [4]. This is because N m- and a-solutions appear. In our example, only one symmetrical a-solution, which possesses the minimum energy among all the two-magnon solutions, exists (this solution is on the axis $K = 0$ in the insert in Fig. 2). An antisymmetrical a-solution arises when anisotropy increases to $\Delta \approx 0.8$ (for $N = 10$) and one of the antisymmetrical m-solutions (the one that is closest to the axis $K = 0$ in the insert in Fig. 2) disappears. Energies of mixed and anharmonic solutions are respectively

$$\varepsilon_{\mathrm{m}}^{(2)} = \Delta(\cos k_1 + \cosh |k_2|) - 2,$$
$$\varepsilon_{\mathrm{a}}^{(2)} = \Delta(\cosh |k_1| + \cosh |k_2|) - 2.$$

The Bethe complexes compose the lower branch of two-magnon solutions,

$$\varepsilon_{\mathrm{B}}^{(2)} = 2\Delta \cos K \cosh |q| - 2.$$

5. Discussion

The general relations for momenta and phases of the exponential Bethe functions [2] produce one-magnon ($M = 1$) solutions (6)–(8) after the corresponding transformations. Admitting the imaginary momenta k, we obtain anharmonic states, which are needed to complete the eigenfunction set to the total number of N. The number of anharmonic states (one or two) depends on the relation between the anisotropy and the number of spins, and their energies are the lowest in the spectrum. The linear solution appearing at $N = (1 + \Delta)/(1 - \Delta)$ cannot be obtained from a finite number of exponential functions. This means that the exponential functions do not necessarily produce the total eigenfunction set.

Already for $M = 2$, it is difficult to obtain the explicit form of functions and equations for momenta by solving general relations (2). Using the symmetrized real wave functions, we can give a mathematically simple and physically clear analysis of the number and types of possible solutions. For the exchange anisotropy $\Delta < 1$ (of the "light axis" type) and under the free BC, the number of real-k_i solutions reduces, and, correspondingly, N imaginary-k_i solutions appear. Anisotropy $\Delta > 1$ (of the "light plane" type) does not admit such solutions. In the latter case, the ground state is degenerate w.r.t. the basic plane direction, and the excited-state wave functions need a separate investigation. For an anisotropy $\Delta < 1$, the number of the bounded Bethe complexes is not changed although it depends nontrivially on the spin number [5, 6]. The total number of states is equal to the initial state number $C_N^2 = N(N - 1)/2$, all the states are one-parametric, and there are no states with coinciding momenta. For the ferromagnetic exchange, the a-state energies lie below the bottom of the energy zone of two-magnon harmonic states, and the m-state energies constitute the lower two-magnon branch spreading over the one-magnon branch in Fig. 2. The m-state momenta k_j are close to the one-magnon momenta but not equal to them as in the isotropic case. This means that resonance transitions $\Delta M = 1$ occur with $\Delta K \neq 0$, and because $\Delta K \ll \pi/N$ in the present case, it is just this branch that gives the macroscopic probability for transitions in a homogeneous resonance field $W_n \sim N$.

REFERENCES

1. Yu. A. Izyumov and Yu. N. Skryabin, *Statistical Mechanics of Magnetically Ordered Systems* [in Russian], Nauka, Moscow (1987); English transl., Plenum, New York (1988).
2. M. Gaudin, *La fonction d'onde de Bethe*, Masson, Paris (1983).
3. H. A. Bethe, *Z. Phys.*, **71**, 205 (1931).
4. S. N. Martynov, *Theor. Math. Phys.*, **113**, 1484 (1997).
5. K. Isler and M. B. Paranjape, *Phys. Lett. B*, **319**, 209 (1993).
6. S. N. Martynov, *Phys. Lett. A*, **219**, 329 (1996).