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The density of states method for calculating the magnetic properties of a quantum spin chain

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The paper describes and analyzes a method for solving multiparticle quantum-mechanical problems based on the calculation of the density of states of the system as a function of the total energy and the projection of the magnetic moment. The method is applied to the calculation of the properties of a spin chain described by the Heisenberg Hamiltonian. The results are compared with the exact solution for a chain of $N = 16$ spins obtained by the exact diagonalization method. It is shown that in the high-temperature region, the density of states method coincides with the exact solution. At temperatures less than the energy of the exchange interaction, the system is near the edge of the density of states and statistical methods do not work well. Thus, it is shown that the density of states method allows for efficient calculation of the characteristics even for a system with a small number of orderly arranged spins.

Keywords: density of states, spin chain, magnetic susceptibility, heat capacity, Heisenberg Hamiltonian.

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1. Introduction

It is well known that it is impossible to exactly solve most multi-particle quantum mechanics problems due to their high computational complexity. For this reason, various approximate computational methods are widely used [1,2]. All these methods themselves are quite complicated and characterized by limited accuracy and field of application. Therefore, it is still relevant to develop new approximate approaches to solving the multi-particle quantum mechanics problems. One of these approaches is a density of states method.

An idea of the density of states method is to calculate, accurately or approximately, a dependence of the density of states $g(E, M)$ on total energy of the system and its magnetic moment. After that, it is easy to find a partition function and calculate magnetic properties of the system using a standard thermodynamic approach. This approach was first used by Heisenberg in a pioneer study on a nature of ferromagnetism [3]. The interest has been reattracted to the density of states method quite recently, when it was shown that the density of states for spin systems can be quite accurately calculated numerically [4,5]. It was also shown that the density of states for an Ising Hamiltonian could be approximately described analytically way using a central limit theorem [6,7].

The density of states method is attractive due to its comparative simplicity. However, similar to all the approximate methods, it can be applied only in a limited range of parameters of the studied system. The present study was aimed at demonstrating operability and specifying limits of applicability of the method on the example of the multi-particle system as a quantum spin chain with cyclic boundary conditions (a spin ring). This problem was solved by Bethe in 1931 for an isotropic Heisenberg Hamiltonian [8]. The Bethe solution makes it possible to calculate wave functions and energies of states that are close to a ground state. For the other states, this method is reduced to solving a quite complicated system of equations [9]. Therefore, instead of it, a method of numerical diagonalization of a Hamiltonian matrix is often used in the calculations [10]. The spin chains are still actively used as a suitable model object both in theoretical [11] as well as experimental studies [12].

The problem of finding a distribution function for eigenvalues of large matrices is not solved in a general form. It is known for the case of the matrix with normal distribution of its elements that its eigennumbers correspond to a Wigner semicircular distribution [13]. As will be shown below, the eigenvalues of the Heisenberg Hamiltonian for the spin ring, which correspond to a certain projection of the magnetic moment, have a distribution that is close to a normal one. Then, in order to construct the density of states, it is enough to know dependences of the average and dispersions of this normal distribution on the magnetic moment. I. e., unlike a mean field approximation, in the density of states method we consider not only an average value, but dispersion of exchange energy as well.

The article is structured as follows. First, the eigenproblem for the energy for the spin ring will be solved by numerical diagonalization of the Hamiltonian matrix. Based on the obtained energy values, we will calculate numerical values of the first four moments of the distribution function of the density of states in a dependence on the magnetic moment of the system. Then, the average and dispersion of the same distribution will be calculated analytically and results of both the methods will be compared to each other. Using the obtained dependences, the density of states method will be used to calculate values of magnetic susceptibility, the magnetic moment, the average energy and heat capacity for subsequently comparing them with results of the exact solution. The results of the calculations will be taken to conclude on applicability of the density of states method.

2. Exact numerical solution of the problem

In the present study, we consider a chain of N atoms with spin-1/2 and cyclic boundary conditions (the closed spin chain or yje spin ring). Spin interaction is described by the Heisenberg Hamiltonian. We consider that only neighboring spins in the chain interact, while interaction itself is of an antiferromagnetic nature.

$$\hat{\mathbf{H}} = \sum_i J_0 \hat{\mathbf{S}}_i \hat{\mathbf{S}}_{i+1} - g\mu B \sum_i \hat{\mathbf{s}}_{zi} \quad (1)$$

In this expression, J_0 — the constant of exchange interaction, B — the magnetic field, g — the electron g-factor, μ — the Bohr magneton.

A state of the spin system can be characterized by the full magnetic moment and a projection of the magnetic moment onto a certain direction. It is convenient when this direction is selected to be an axis z, which is co-directional with the external magnetic field. Since the spin projections x, y and z are not observed simultaneously, it is convenient to transform the Hamiltonian by transiting to ladder operators

$$\hat{\mathbf{S}}^{+} = \hat{\mathbf{S}}_x + i\hat{\mathbf{S}}_y; \quad \hat{\mathbf{S}}^{-} = \hat{\mathbf{S}}_x - i\hat{\mathbf{S}}_y. \quad (2)$$

It is convenient to select states of the kind $\Psi_i = |\uparrow\uparrow \ldots \downarrow\downarrow\rangle$ as basic wave functions and to group them by a value of the projection of the magnetic moment onto the axis z. Then, by subsequently acting with the operator $\hat{\mathbf{H}}$ on the spin wave functions, one can obtain the Hamiltonian matrix of the size 2^N, [14], where each matrix element is

$$H_{ij} = \langle \Psi_i | \hat{\mathbf{H}} | \Psi_j \rangle. \quad (3)$$

This matrix has a unit structure, wherein each unit corresponds to its value of the projection of the magnetic moment onto the axis z. The energy eigenvalues that correspond to a specific magnetic moment were calculated by unit-by-unit diagonalization of the Hamiltonian matrix. The calculations were accelerated by using a technique of parallel computations using the CUDA platform and the Julia language software. The largest size of the system, whose density of states could be calculated, was $N = 16$. Limitation of the spin number is related to available memory volume: the Hamiltonian matrix has the size $(2^N)^2$. The exact solution of the problem can be used for testing the solution obtained by the density of states method.

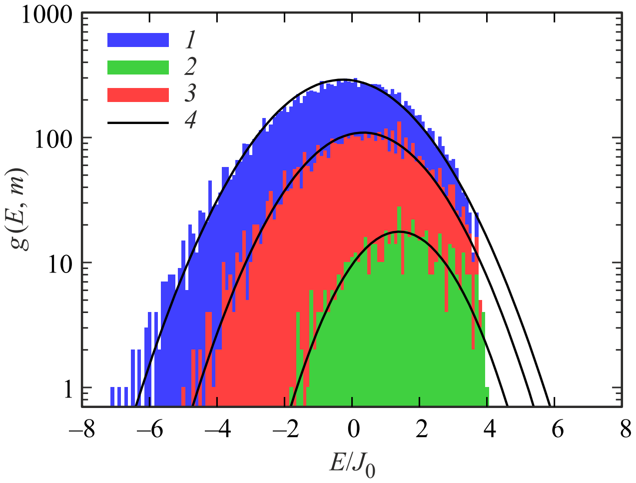

Figure 1. Density of states $g(E, m)$ for the spin ring of the $N = 16$ spins, which is calculated by numerical diagonalization, for the various values of the magnetic moment: *1* — $m = 0$; *2* — $m = 3/8$; *3* — $m = 5/8$. The black line *4* corresponds to the equation (11).

For each fixed value of the magnetic moment, we have constructed the density of a number of the states $g(E, m)$ in a dependence on the system energy and the nondimensionalized magnetic moment per one spin $m = 2M/g\mu N$ and calculated moments of distribution. Figure 1 shows a histogram of distribution of the energy states of the system of $N = 16$ spins for three values of m. It can be noted that at the fixed m the distribution of the number of the energy states is close to the normal one. In order to compare the real distribution with the normal one, we have calculated the first four moments of distribution. Figure 2 dots (1) — the average energy $\overline{E}$, (2) — dispersion $\sigma^2 = \overline{(E - \overline{E})^2}$, (3) — the skewness $S = \overline{(E - \overline{E})^3}/\sigma^3$ and (4) — the kurtosis $K = \overline{(E - \overline{E})^4}/\sigma^4 - 3$.

The skewness and the kurtosis are close to 0, as must be the case for the normal distribution. The significant difference from 0 is observed only for m, which are close to 1. It means that even for the small N the distribution of the total exchange energy is close to the normal one. With an increase of N, a number of summands in the total energy will be increased, therefore, by virtue of the central limit theorem the distribution of the number of the energy states will tend to the normal distribution.

3. Density of states method for the spin chain

As shown above, at the fixed value of the magnetic moment the density of the number of the energy states $g(E, m)$ can be approximately described by the normal distribution. This distribution is characterized by the average

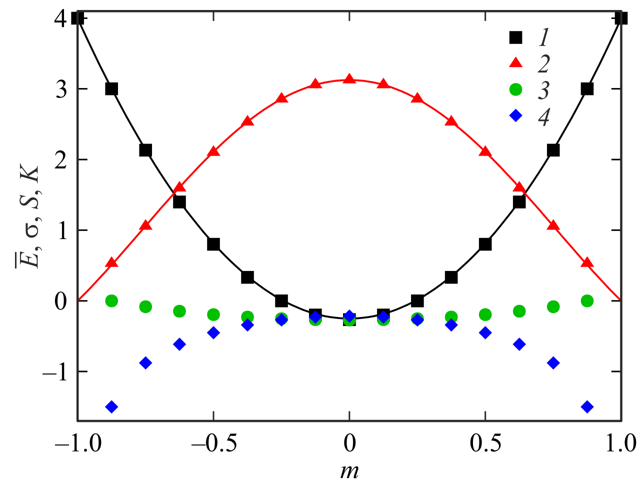

Figure 2. Dependence of the average energy $\overline{E}$ (*1*), dispersion σ^2 (*2*), the skewness S (*3*) and the kurtosis K (*4*) on the magnetic moment m. The solid lines mark the dependences of the average energy and dispersion, which are calculated according to the formulas (5) and (6).

energy $\overline{E}(m)$ and dispersion $\sigma(m)$, which can be calculated analytically.

The two-spin system can be in four states. In the state $|\uparrow\uparrow\rangle$ the projection of the magnetic moment is $+1$, while the energy is $+1/4$, and in the state $|\downarrow\downarrow\rangle$ the projection of the magnetic moment is -1, while the energy is $+1/4$. There are also two states with a zero projection of the magnetic moment. In the symmetric state $\frac{|\uparrow\downarrow\rangle+|\downarrow\uparrow\rangle}{\sqrt{2}}$, the system has the energy of $+1/4$, while in the antisymmetric state $\frac{|\uparrow\downarrow\rangle-|\downarrow\uparrow\rangle}{\sqrt{2}}$ the system energy is $-3/4$.

If the average moment of the system is m, then each separate spin is directed upward at the probability $(1+m)/2$ and downward at the probability $(1-m)/2$. Then, among all the N pairs of the adjacent spins the chain will on average have $N(1+m)^2/4$ pairs in the state $|\uparrow\uparrow\rangle$, $N(1-m)^2/4$ pairs in the state $|\downarrow\downarrow\rangle$, while the other $2N(1-m)(1+m)/4$ pairs of the spins will be equally distributed between the two states with the zero projection of the magnetic moment. The average energy of these states is $-1/4$. By taking into account these considerations, the average exchange energy of the system of $N \gg 1$ spins can be written as

$$\begin{aligned}\overline{E} &= NJ_0\overline{\hat{\mathbf{S}}_i\hat{\mathbf{S}}_{i+1}}\\ &= NJ_0\frac{1}{4}\left(\frac{(1+m)^2}{4}+\frac{(1-m)^2}{4}-2\frac{(1-m)(1+m)}{4}\right)\\ &= \frac{1}{4}NJ_0m^2. \qquad (4)\end{aligned}$$

For the system of a small number of spins, there are also corrections of about $1/N$. Probability of appearance of the states $|\uparrow\uparrow\rangle$ and $|\downarrow\downarrow\rangle$ with co-directional spins in the chain of randomly oriented spins turns out to be somewhat less, while probability of appearance of the states with anti-directional spins in it turns out to be higher

$$\overline{E} = \frac{1}{4}NJ_0\left(m^2+\frac{m^2}{N}-\frac{1}{N}+O\left(\frac{1}{N^2}\right)\right). \qquad (5)$$

With similar reasoning, considering possible states for four spins based on combinatorics considerations, we calculate dispersion of the exchange energy. For the sake of brevity, we omit the the calculations and write only an answer

$$\sigma^2 = \overline{E^2}-\overline{E}^2 = \frac{1}{16}NJ_0^2\Bigg(3-4m^2+m^4 + \frac{2-6m^2+4m^4}{N}+O\left(\frac{1}{N^2}\right)\Bigg). \qquad (6)$$

When calculating the density of states, we take into account all states with equal statistical weight, which is equivalent to simple calculation of the spectrum of the quantum system with taking into account level degeneracy multiplicity. Correlations between the spins will be taken into account below, when a statistical weight is calculated for each state according to the Gibbs distribution.

It is interesting to compare the expressions obtained for the average energy and dispersion in a dependence on m with the results of the exact numerical calculation. Solid lines of Figure 2 mark dependences calculated by the formulas (5) and (6) for $N = 16$ spins. It is clear that there is good compliance between the analytical expressions and the exact results shown by dots.

Thus, the density of states can be written as

$$g(E,m) = \binom{N}{\frac{N(1+m)}{2}}\frac{1}{\sqrt{2\pi}\sigma(m)}\exp\left(-\frac{\left(E-\overline{E}(m)\right)^2}{2\sigma^2(m)}\right). \qquad (7)$$

In this expression, $N(1+m)/2$ is the number of upward-directed spins, therefore, m takes discrete values so that the number of the spins is an integer. But for large N, one can transit to continuous distribution by m.

For large N, one can use the Stirling's formula and expand the factorials in a binomial coefficient

$$\binom{N}{\frac{N(1+m)}{2}} = \frac{\sqrt{2\pi N}}{\pi N\sqrt{1-m^2}}\frac{2^N}{(1-m)^{(1-m)N/2}(1+m)^{(1+m)N/2}}. \qquad (8)$$

for the sake of brevity, we introduce a designation

$$p(m) = \ln 2 - \frac{1-m}{2}\ln(1-m) - \frac{1+m}{2}\ln(1+m) \qquad (9)$$

then the binomial coefficient can be written as

$$\binom{N}{\frac{N(1+m)}{2}} = \sqrt{\frac{2}{\pi N}}\frac{1}{\sqrt{1-m^2}}\exp\left(Np(m)\right). \qquad (10)$$

Further on, it will be convenient to nondimensionalize the energy to J_0 and transit from the total energy of the system to nondimensionalized energy per one spin $e = E/NJ_0$. For brevity, we also introduce a nondimensionalized mean-square error $s = \sigma/\sqrt{N}J_0$. In this notation, the density of states will be written as

$$g(e, m) = \frac{N}{2\pi s(m)(1 - m^2)} \exp\left(Np(m) - \frac{N\left(e - \overline{e}(m)\right)^2}{2s^2(m)}\right). \tag{11}$$

Below, for the sake of brevity, we will often omit explicit indication in the formulas that the average energy and dispersion are functions of m. Now, let us consider the spin chain, in which the density of states is described by the expression (11). Let the system have the temperature T and be in the external magnetic field B. Probability of the system being in a certain state will be described by the Gibbs distribution with the energy $E - g\mu BNm/2$. Here, as above, E designates only the exchange energy of the system. For convenience, we introduce the dimensionless temperature $t = kT/J_0$ and the dimensionless magnetic field $\beta = g\mu B/2J_0$. In this notation, we can write an expression for a density of probability of the system having the energy e and the magnetic moment m at the temperature t and in the external magnetic field β

$$f(e, m, t, \beta) = \frac{1}{Z(t, \beta)} \frac{N}{2\pi s(1 - m^2)} \times \exp\left(Np(m) - \frac{N(e - \overline{e})^2}{2s^2} - \frac{N(e - \beta m)}{t}\right). \tag{12}$$

Here, Z is a partition function that can be calculated as

$$Z(t, \beta) = \int_{-\infty}^{\infty} de \int_{-1}^{1} dm \frac{N}{2\pi s(1 - m^2)} \times \exp\left(N\left(p(m) - \frac{(e - \overline{e})^2}{2s^2} - \frac{(e - \beta m)}{t}\right)\right). \tag{13}$$

The integral over the energy is calculated analytically

$$Z(t, \beta) = \int_{-1}^{1} \sqrt{\frac{N}{2\pi}} \frac{1}{1 - m^2} \times \exp\left(N\left(p(m) + \frac{\beta m}{t} + \frac{s^2}{2t^2} - \frac{\overline{e}}{t}\right)\right) dm. \tag{14}$$

The integral over the magnetic moment can be calculated numerically, while at high N the method of steepest descent can be used (the Laplace's method).

When knowing the expression for the density of probability $f(e, m, t, \beta)$ and the partition function, one can calculate system parameters such as the average magnetic moment, magnetic susceptibility, the average energy and heat capacity in a dependence on the magnetic field and the temperature. The formula (12) is also useful for clarifying an issue of the influence of the spin correlations on the density of states. It directly follows from this that the density of states corresponds to the density of probability at an infinitely high temperature. Therefore, the spin correlations shall not be taken into account when calculating the density of states.

In case of low m, i.e. in case of weak magnetic fields, one can obtain an analytical expression for the partition function without integrals. For this, we use an approximate expression for the binomial coefficient that is valid provided that $m \ll 1$

$$\binom{N}{\frac{N(1+m)}{2}} \approx 2^N \sqrt{\frac{2}{\pi N}} \exp\left(-\frac{Nm^2}{2}\right). \tag{15}$$

For the density of states, we obtain the expression

$$\tilde{g}(e, m) = \frac{2^N}{\pi s} \exp\left(-\frac{Nm^2}{2} - \frac{N(e - \overline{e})^2}{2s^2}\right). \tag{16}$$

Here, a tilde above the density of states shows that the expression is valid only for $m \ll 1$. Further on, similar to the way it was done above, we introduce the density of probability $\tilde{f}(e, m, t, \beta)$ and the partition function

$$\tilde{Z}(t, \beta) = \int_{-\infty}^{\infty} de \int_{-1}^{1} dm \frac{2^N}{\pi s} \times \exp\left(-N\left(\frac{m^2}{2} + \frac{(e - \overline{e})^2}{2s^2} + \frac{(e - \beta m)}{t}\right)\right). \tag{17}$$

In the expression for the partition function, first we calculate the integral over the energy

$$\tilde{Z}(t, \beta) = 2^N \sqrt{\frac{2}{\pi N}} \int_{-1}^{1} dm \times \exp\left(N\left(-\frac{m^2}{2} + \frac{\beta m}{t} - \frac{\overline{e}}{t} + \frac{s^2}{2t^2}\right)\right). \tag{18}$$

Then, we put explicit expressions for the dependence of the average energy and dispersion on m, neglect a small summand that is proportional to m^4 and transit to integration from minus infinity to infinity. Then the integral over m will also be calculated analytically

$$\tilde{Z}(t, \beta) = \frac{2^{N+2} t}{N\sqrt{4t^2 + 2t + 1}} \exp\left(\frac{2N\beta^2}{4t^2 + 2t + 1} + \frac{3N}{32t^2}\right). \tag{19}$$

4. Calculation of magnetic properties of the spin chain

Using the formula for the density of probability (12), we can find the average magnetic moment of the system in a dependence on the magnetic field and the temperature. We will calculate numerically since when taking into account small corrections of about $1/N$ the expressions for the average energy and dispersion are quite cumbersome

$$\overline{m}(t,\beta) = \frac{1}{Z}\int_{-\infty}^{\infty} de \int_{-1}^{1} dm \, \frac{Nm}{2\pi s(1-m^2)} \times \exp\left(N\left(p(m) - \frac{(e-\overline{e})^2}{2s^2} - \frac{(e-\beta m)}{t}\right)\right). \quad (20)$$

The integral over the energy is calculated analytically

$$\overline{m}(t,\beta) = \frac{1}{Z}\sqrt{\frac{N}{2\pi}}\int_{-1}^{1} \frac{m}{1-m^2} \times \exp\left(N\left(p(m) + \frac{\beta m}{t} + \frac{s^2}{2t^2} - \frac{\overline{e}}{t}\right)\right) dm. \quad (21)$$

Generally, the obtained integral is calculated numerically. But in the weak magnetic fields, when the expansion (15) is true, one can obtain an explicit expression for the average magnetic moment

$$\tilde{\overline{m}}(t,\beta) = \frac{4\beta t}{4t^2+2t+1}. \quad (22)$$

In order to compare with the results obtained by the density of states method, the magnetic moment was found by exact diagonalization by the following formula:

$$\overline{m}(t,\beta) = \frac{\sum_j m_j \exp(-\frac{e_j - m_j\beta}{t})}{\sum_j \exp(-\frac{e_j - m_j\beta}{t})}. \quad (23)$$

Here, it is summed over all the 2^N states of the system.

Figure 3 compares the dependence of the average magnetic moment on the magnetic field, which is calculated by the exact solution for the $N = 16$ spins (the solid line), by the formula (21) (the red dashed line), as well as by the approximate formula (22) that is valid for small m (the thin green line). The calculations have been carried out for the three values of the dimensionless temperature, $t_1 = 0.5$, $t_2 = 1.5$ and $t_3 = 3.0$. It is clear that the formula (21) well coincides with the exact calculation and a small deviation at m that is close to unity is related to the fact that the Stirling's formula used in derivation of the formula (8) is only valid for relatively high numbers. When approaching $m = 1$, the magnitude $N(1-m)/2$ tends to zero, therefore, the expansion (8) becomes inappropriate. The approximate formula (22) well coincides with the exact solution at small m, but when $m \geq 0.4$ it starts diverging from the exact result.

In the zero magnetic field, we can obtain the explicit expression for the dependence of magnetic susceptibility on the temperature. In this case, we use the expression (22) for the average magnetic moment

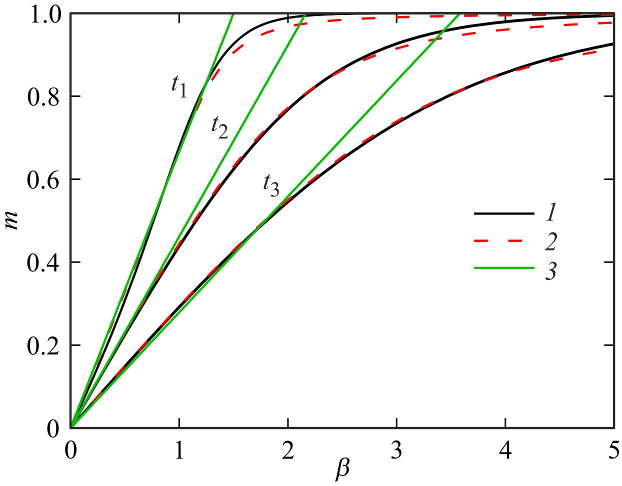

Figure 3. Dependence of the average magnetic moment on the magnetic field, which is calculated for the three various values of the temperature $t_1 = 0.5$, $t_2 = 1.5$ and $t_3 = 3.0$. The black line (the curve *1*) is calculated by the exact solution, the red dashed line (the curve *2*) — the formula (21), the green line (the curve *3*) — the formula (22).

$$\chi = \frac{\partial \overline{M}}{\partial B} = \frac{g^2\mu^2 N}{4J_0}\frac{\partial \overline{m}}{\partial \beta}. \quad (24)$$

In the expression for the average magnetic moment, the magnetic field is included in the exponent in the expression for the density of probability (12) and in the partition function (13). When explicitly calculating the derivative of the formula (21) by the magnetic field, we obtain a useful relationship

$$\chi = \frac{g^2\mu^2 N^2}{4J_0 t}\left(\overline{m^2} - \overline{m}^2\right) = \frac{\overline{M^2} - \overline{M}^2}{kT}. \quad (25)$$

In the zero magnetic field, the average magnetic moment is zero, then we obtain $\chi = \overline{M^2}/kT$, which is a known result for susceptibility in the weak magnetic field. Besides, magnetic susceptibility in the zero magnetic field can be explicitly calculated by differentiating the expression for the average magnetic moment (22) by the magnetic field.

$$\chi = \frac{g^2\mu^2 N}{4J_0}\frac{\partial \overline{m}}{\partial \beta} = \frac{g^2\mu^2 N}{4J_0}\frac{4t}{4t^2+2t+1}. \quad (26)$$

It is convenient to analyze not susceptibility itself, but inverse magnetic susceptibility, since in a case of the free spins, which is described by the Curie law, inverse magnetic susceptibility linearly depends on the temperature. In the expression for inverse susceptibility, we transit to the dimensional temperature T

$$\frac{1}{\chi} = \frac{4kT + 2J_0}{g^2\mu^2 N} + \frac{J_0^2}{g^2\mu^2 NkT}. \quad (27)$$

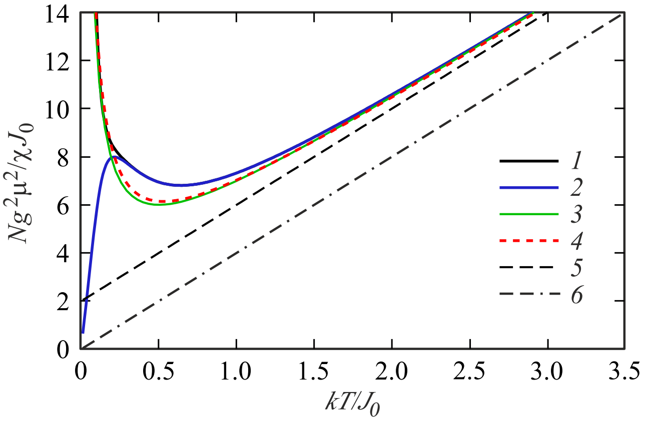

Figure 4. Inverse dimensionless magnetic susceptibility in a dependence on the dimensionless temperature. *1* — the result of the exact numerical calculation for the $N = 16$ spins; *2* — the result of the exact numerical calculation for the $N = 15$ spins; *3* — the density of states method, decomposition at small m, the formula (27); *4* — the density of states method, the derivative of the magnetic moment (21) by the magnetic field; *5* — the Curie-Weiss law; *6* — the Curie law.

The obtained dependence of inverse susceptibility on the temperature is shown in Figure 4. The figure also shows the dependences that are obtained by the exact numerical calculation for the spin rings of the 15 and 16 spins. Magnetic susceptibility was calculated by a method of numerical differentiation of the average magnetic moment by the field. It is clear that at the high temperatures both the dependences behave in the same way, but at the low temperatures there is a significant difference between the dependences for even and odd N. For even N, the spins are paired, as a result of which the total magnetic moment and magnetic susceptibility tend to zero. For odd N, the magnetic moment is always non-zero, therefore, magnetic susceptibility is high. It is essential that at the high temperatures the formula (27) much better describes results of the exact numerical calculation than just the Curie law for susceptibility of free electrons ($1/\chi = 4kT/g^2\mu^2N$) or the Curie-Weiss law ($1/\chi = (4kT + 2J_0)/g^2\mu^2N$), which are plotted by the dashed line. The dependence of inverse susceptibility for the spin chain on the temperature in the zero magnetic field was numerically calculated in the study [10]. Our results that are obtained by the method of exact diagonalization of the Hamiltonian very well agree with results obtained in the study [10].

5. Average energy of the system and heat capacity

Let us calculate the average energy of the spin chain in the magnetic field. The total energy of the system in question consists of exchange energy and energy of interaction with the external magnetic field. First, we find an average of only an exchange part of the energy E.

$$\overline{E}(t,\beta) = \frac{N^2 J_0}{Z(t,\beta)2\pi} \int_{-\infty}^{\infty} de \int_{-1}^{1} dm \frac{e}{s(1-m^2)} \times \exp\left(N\left(p(m) - \frac{(e-\overline{e})^2}{2s^2} - \frac{(e-\beta m)}{t}\right)\right). \quad (28)$$

The integral over the energy is calculated analytically

$$\overline{E}(t,\beta) = \frac{NJ_0}{Z(t,\beta)} \sqrt{\frac{N}{2\pi}} \int_{-1}^{1} \frac{\overline{e} - \frac{s^2}{t}}{1-m^2} \times \exp\left(N\left(p(m) + \frac{\beta m}{t} + \frac{s^2}{2t^2} - \frac{\overline{e}}{t}\right)\right) dm. \quad (29)$$

Integration over the magnetic moment can be carried out numerically. Now, we return to the total energy of the spin chain $\overline{E} - B\overline{M}$. Taking into account the expression for the average magnetic moment (21), we obtain

$$\overline{E} - B\overline{M} = \frac{NJ_0}{Z(t,\beta)} \sqrt{\frac{N}{2\pi}} \int_{-1}^{1} \frac{\overline{e} - \frac{s^2}{t} - m\beta}{1-m^2} \times \exp\left(N\left(p(m) + \frac{\beta m}{t} + \frac{s^2}{2t^2} - \frac{\overline{e}}{t}\right)\right) dm. \quad (30)$$

For the case when $m \ll 1$, we use an approximate expansion of the binomial coefficient (15), which allows analytically calculating the average exchange energy.

$$\tilde{\overline{E}}(t,\beta) = \frac{2^N NJ_0}{\tilde{Z}(t,\beta)} \sqrt{\frac{2}{\pi N}} \int_{-1}^{1} \left(\overline{e} - \frac{s^2}{t}\right) \times \exp\left(N\left(-\frac{m^2}{2} + \frac{\beta m}{t} - \frac{\overline{e}}{t} + \frac{s^2}{2t^2}\right)\right) dm. \quad (31)$$

Taking into account smallness of m, we omit the summand of the order of m^4 in the expression for dispersion and transit to integration over the entire real number axis. We also put the explicit expressions for the dependence of the average energy and dispersion on m

$$\tilde{\overline{E}}(t,\beta) = \frac{2^N NJ_0}{\tilde{Z}(t,\beta)} \sqrt{\frac{2}{\pi N}} \int_{-\infty}^{\infty} \left(\frac{m^2}{4} - \frac{3-4m^2}{16t}\right) \times \exp\left(N\left(-\frac{m^2}{2} + \frac{\beta m}{t} - \frac{m^2}{4t} + \frac{3-4m^2}{32t^2}\right)\right) dm. \quad (32)$$

After integration over m we obtain

$$\tilde{\overline{E}}(t,\beta) = \frac{J_0(t^2+t)}{4t^2+2t+1}\left(1 + \frac{32\beta^2 t^2}{(4t^2+2t+1)^2}\right) - \frac{3NJ_0}{16t}. \quad (33)$$

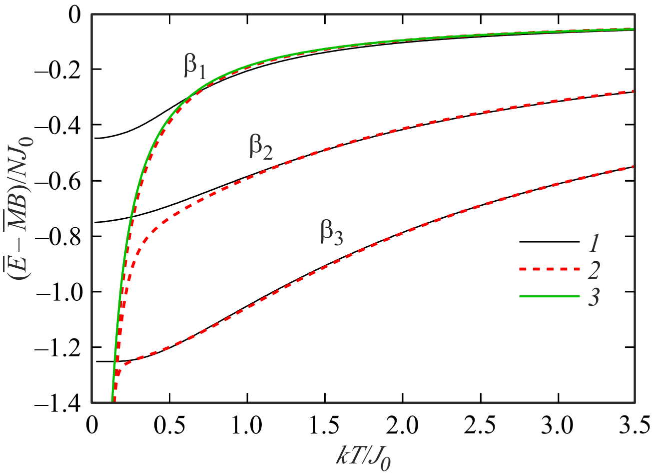

Figure 5. Dependence of the average energy of the spin chain on the temperature in the magnetic fields $\beta_1 = 0, \beta_2 = 1, \beta_3 = 1.5$. *1* — the exact solution, *2* — the formula (30), *3* — the approximate analytical expression (34).

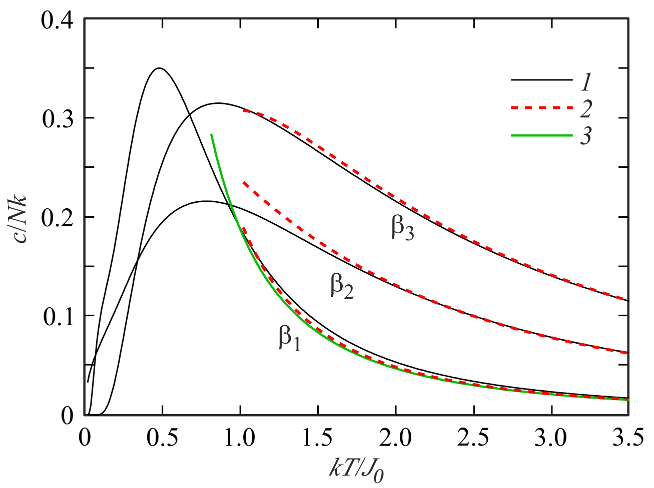

Figure 6. Dependence of heat capacity of the spin chain on the temperature in the magnetic fields $\beta_1 = 0, \beta_2 = 1, \beta_3 = 1.5$. *1* — the exact solution, *2* — the density of states method, the formula (36), *3* — the approximate analytical solution by the formula (38).

For high N, we keep only the last summand and the expression will be strongly simplified. Besides, in the magnetic field we also take into account the energy of interaction of the magnetic moment of the chain with the field

$$\tilde{\overline{E}} - B\tilde{\overline{M}} \approx -\frac{3NJ_0}{16t} - \frac{4J_0N\beta^2 t}{4t^2 + 2t + 1}. \quad (34)$$

Similar to the average magnetic moment, the average exchange energy for the method of exact diagonalization was calculated by the formula:

$$\overline{E}(t, \beta) = NJ_0 \frac{\sum_j e_j \exp(-\frac{e_j - m_j\beta}{t})}{\sum_j \exp(-\frac{e_j - m_j\beta}{t})}. \quad (35)$$

The dependence of the total energy of the spin chain $\overline{E} - B\overline{M}$ on the temperature is shown in Figure 5 for the three values of the magnetic field. The solid black lines mark a result of the exact calculation, the red dashed line marks the calculations by the density of states method and the green line marks an approximate dependence that is calculated with taking into account expansion in the weak magnetic field. It is clear that the theoretical dependence well coincides with the exact calculation within the temperature range $t \geq 1$. At the lower temperatures, the density of states method provides a significant divergence from the exact result due to the fact that the system is near an edge of the density of states. The approximate formula well coincides with the theoretical dependence for $\beta = 0$, while for the strong fields there is a significant divergence.

Heat capacity of the spin ring in the magnetic field can be calculated as a derivative of the total energy by the temperature.

$$c(t, \beta) = \frac{\partial(\overline{E} - B\overline{M})}{\partial T}. \quad (36)$$

In a specific case of low m and high N, we obtain

$$c(t, \beta) = \frac{\partial(-\frac{3NJ_0}{16t} - J_0N\beta\frac{4\beta t}{4t^2+2t+1})}{\partial t}\frac{k}{J_0}, \quad (37)$$

$$c(t, \beta) = Nk\left(\frac{3}{16t^2} + \frac{4\beta^2(4t^2 - 1)}{(4t^2 + 2t + 1)^2}\right). \quad (38)$$

We underline again that the last expression is only valid at low m, i. e. in the weak magnetic fields, and when $N \gg 1$.

The dependence of heat capacity of the spin chain on the temperature is shown in Figure 6 for the three values of the magnetic field. The solid black lines mark a result of the exact calculation, which is obtained numerical differentiation of the average energy by the temperature, the red dashed line marks the calculations by the density of states method (36) and the green line marks an approximate dependence (38) that is calculated with taking into account expansion in the weak magnetic field. It is clear from the figure that at the high temperatures $t \geq 1$ the density of states method quite well describes the dependence of heat capacity on the temperature. But at the smaller temperatures, the dependence is strongly different from the exact solution and is not plotted.

6. Conclusion

In conclusion, we note that the density of states method can be successfully used for describing even the small ($N = 16$) systems without spatial disorder such as the spin chains. Significant differences from the exact solution are manifested at the low temperatures ($kT < J_0$), when a maximum of the density of probability is shifted to a boundary of the density of energy states. In this area, the distribution of the energy states can no longer be considered to be the normal one. The deviation from the exact calculation can also be manifested in the strong magnetic field, when the average magnetic moment m is close to 1. In this case, the number of the system states with this magnetic moment becomes small, specifically, when $m = 1$, the system has just one state, therefore, the statistics laws can not be applied. In the other cases, i. e. at the comparatively high temperature and in the not too strong magnetic field, the density of states method allows finding system characteristics by numerical integration or analytically in the approximation $m \ll 1$.

Conflict of interest

The authors declare that they have no conflict of interest.

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