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Numerical Calculation of Thermodynamic Quantities of Spin-1/2 Anisotropic Heisenberg Ring

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Thermodynamic quantities such as specific heat and magnetic susceptibility are calculated numerically for the one-dimensional spin-1/2 Heisenberg-Ising model at $\Delta=0$, ±0.5, $\pm1/\sqrt{2}$. We use a set of nonlinear integral equations which is derived from the Bethe ansatz and from some assumptions on the distribution of quasi-momenta. In the same way we calculate the specific heat of the one-dimensional X-Y-Z model in zero field, putting various values into the coupling constants (J_x, J_y, J_z).

§ 1. Introduction and methods of numerical calculation

In a previous paper[1)] we gave integral equations for the free energy of one-dimensional spin-$\frac{1}{2}$ Heisenberg-Ising model at $|\Delta|<1$ in the magnetic field which is parallel to anisotropy axis and for the free energy of the X-Y-Z model in zero field. The Hamiltonians of these models are

$$\mathcal{H}=J\sum_{i=1}^{N}\{S_i^xS_{i+1}^x+S_i^yS_{i+1}^y+\Delta(S_i^zS_{i+1}^z-\tfrac{1}{4})\}-2\mu_0H\sum_{i=1}^{N}S_i^z \tag{1a}$$

and

$$\mathcal{H}=\sum_{i=1}^{N}\{J_xS_i^xS_{i+1}^x+J_yS_i^yS_{i+1}^y+J_zS_i^zS_{i+1}^z\} \tag{1b}$$

under the condition $|J_x|<J_y<J_z$. The set of integral equations given in the paper[1)] can be reduced to those with finite unknown functions, when π/θ or K_l/ζ is a rational number. Here, θ, ζ and l are defined by

$$\Delta=\cos\theta,\quad \mathrm{cn}(2\zeta, l)=J_x/J_z\quad \text{and}\quad \mathrm{dn}(2\zeta, l)=J_y/J_z\,. \tag{1c}$$

K_l is a complete elliptic integral of the first kind with modulus l. In this paper we carry out numerical calculations in the case of π/θ or K_l/ζ being an integer 3 or 4, putting J or J_z into ±1. We obtain the free energy, energy, entropy, specific heat and magnetic susceptibility of the Heisenberg-Ising model at $\mu_0H=0$ as functions of temperature. Magnetization curves (M-H curves) of this model at fixed temperature are also calculated. The specific heat of the X-Y-Z model is calculated as a function of temperature.

In the case of $\Delta=\cos(\pi/n)$ $(n=3, 4, \cdots)$, the set of integral equations is

$$\ln(1+\eta_0(x)) = -2nJ\sin(\pi/n)T^{-1}\delta(x),$$

$$\ln\eta_j(x) = s_1 * \ln(1+\eta_{j-1}(x))(1+\eta_{j+1}(x));\, j=1, 2, \cdots, n-3,$$

$$\ln\eta_{n-2}(x) = s_1 * \ln(1+\eta_{n-3}(x))\left(1+2\,\mathrm{ch}\,\frac{n\mu_0 H}{T}\kappa(x)+\kappa^2(x)\right),$$

$$\ln\kappa(x) = s_1 * \ln(1+\eta_{n-2}(x)). \tag{2a}$$

The free energy per site at temperature T and magnetic field H is given by

$$f(T,H) = f(0,0) - T\int_{-\infty}^{\infty} s_1(x)\ln(1+\eta_1(x))\,dx, \tag{2b}$$

where

$$s_1(x) = (1/4)\,\mathrm{sech}(\pi x/2) \quad \text{and} \quad s_1 * g(x) = \int_{-\infty}^{\infty} s_1(x-x')g(x')\,dx'.$$

We transform this set of equations as follows: Putting $t=\sin^{-1}(\mathrm{th}(\pi x/2))$, $\ln(1+\eta_j)=h_j$, $\ln(1+\kappa\exp(n\mu_0 H/T))=h_{n-1}$ and $\ln(1+\kappa\exp(-n\mu_0 H/T))=h_n$, and considering that the h_j's are symmetric functions of t, we have

$$h_0(t) = -2nJ\sin(\pi/n)T^{-1}\delta(t),$$

$$h_j(t) = F\left(\int_0^{\pi/2} S(t,t')(h_{j-1}(t')+h_{j+1}(t'))\,dt'\right);\, j=1, 2, \cdots, n-3,$$

$$h_{n-2}(t) = F\left(\int_0^{\pi/2} S(t,t')\left\{h_{n-3}(t')+h_{n-1}(t')+h_n(t')\right\}dt'\right),$$

$$h_{n-1}(t) = F\left(\int_0^{\pi/2} S(t,t')h_{n-2}(t')\,dt' + \frac{n\mu_0 H}{T}\right),$$

$$h_n(t) = F\left(\int_0^{\pi/2} S(t,t')h_{n-2}(t')\,dt' - \frac{n\mu_0 H}{T}\right), \tag{3a}$$

$$f(T,H) = f(0,0) - \frac{T}{\pi}\int_0^{\pi/2} h_1(t)\,dt, \tag{3b}$$

where

$$S(t,t') = \frac{1}{\pi}\cdot\frac{\cos t}{1-\sin^2 t\,\sin^2 t'}, \tag{3c}$$

$$F(x) = \ln(1+\exp x). \tag{3d}$$

In order to obtain energy (e), entropy (S), specific heat (C), magnetization (m) and magnetic susceptibility (χ) per site, we use the following thermodynamic identities:

$$e = -T^2\frac{\partial}{\partial T}(T^{-1}f(T,H)),\ S = T^{-1}(e-f),\ C = \frac{\partial e}{\partial T},\ m = \mu_0^{-1}\frac{\partial f}{\partial H}$$

$$\text{and}\quad \chi = \frac{\partial^2 f(T,H)}{\partial H^2}. \tag{4}$$

From Eqs. (3b) and (4) we see

$$e=f(0,0)+T^2\pi^{-1}\int_0^{\pi/2}(\partial h_1(t)/\partial T)dt\,.$$

Thus for the calculation of e we are sufficient to obtain $u_j(t)=T^2\partial h_j(t)/\partial T$, the equations of which are derived from the differentiation of Eqs. (3):

$$u_0(t)=2Jn\sin(\pi/n)\delta(t)\,,$$

$$u_j(t)=(1-e^{-h_j(t)})\int_0^{\pi/2}S(t,t')\,(u_{j-1}(t')+u_{j+1}(t'))dt'\,;j=1,\cdots,n-3\,,$$

$$u_{n-2}(t)=(1-e^{-h_{n-2}(t)})\int_0^{\pi/2}S(t,t')\,\Big\{u_{n-3}(t')+u_{n-1}(t')+u_n(t')\Big\}dt'\,,$$

$$u_{n-1}(t)=(1-e^{-h_{n-1}(t)})\left(\int_0^{\pi/2}S(t,t')u_{n-2}(t')dt'-n\mu_0H\right),$$

$$u_n(t)=(1-e^{-h_n(t)})\left(\int_0^{\pi/2}S(t,t')u_{n-2}(t')dt'+n\mu_0H\right). \tag{5}$$

These equations are coupled linear integral equations for $u_j(t)$, inhomogeneous terms of which are the r.h.s. of the first equation and the last terms of last two equations. In the same way, for obtaining the specific heat, magnetization and magnetic susceptibility, one derives from Eqs. (3) sets of equations for

$$(\partial/\partial T)T^2(\partial h_j(t)/\partial T),\quad \partial h_j(t)/\partial H \quad\text{and}\quad \partial^2 h_j(t)/\partial H^2.$$

These are all linear integral equations with the same homogeneous terms and with different inhomogeneous terms from those of Eqs. (5). At the first stage of the numerical calculation, we solve nonlinear integral equations (3a) for given temperature and magnetic field. Then substituting the value of $h_j(t)$ into (5), we solve this set of linear integral equations for $u_j(t)$. Functions

$$(\partial/\partial T)T^2(\partial/\partial T)(h_j(t)/T),\quad \partial h_j(t)/\partial H \quad\text{and}\quad \partial^2 h_j(t)/\partial H^2$$

are also calculated in a similar way. Though, of course, these thermodynamic quantities can be calculated by numerical differentiation of $f(T,H)$, we do not adopt this method because it sometimes causes large numerical errors.

For the *X-Y-Z* model in zero field, the set of integral equations in the case of $K_l/\zeta=n$ is the same as Eqs. (2), if we replace the r.h.s. of the first equation by $-n\pi J_zT^{-1}K_l^{-1}\,\mathrm{sn}(2K_l/n,\,l)\delta(x)$, μ_0H by zero, $s_1(x)$ by $s_1(x)=K_{k'}/\pi\times\mathrm{dn}(K_k'x,k')$, $s_1*g(x)$ by $\int_{-Q}^{Q}s_1(x-x')g(x')dx'$ and r.h.s. of (2b) by $f(0,0)-T\times\int_{-Q}^{Q}s_1(x)\ln(1+\eta_1(x))dx$, where Q and k are determined by

$$Q=K_k/K_k'=nK_l'/K_l.$$

Putting $t=\mathrm{am}(K_k'x,k')$, which is the elliptic amplitude function, we find that in Eqs. (3) $S(t,t')$ is replaced by

$$S(t,t')=\frac{1}{\pi}\cdot\frac{\sqrt{1-k^2\sin^2t}}{1-k^2\sin^2t\,\sin^2t'}\,. \tag{6}$$

Then we obtain a set of equations similar to Eqs. (3). The procedure of calculating the energy and specific heat is essentially the same as that for the Heisenberg-Ising model.

§ 2. Results and discussion

We have calculated the free energy, energy, entropy, specific heat and magnetic susceptibility per site in zero magnetic field as functions of temperature for the one-dimensional Heisenberg-Ising model at $\Delta=0$, ± 0.5, $\pm 1/\sqrt{2}$ and $J>0$.

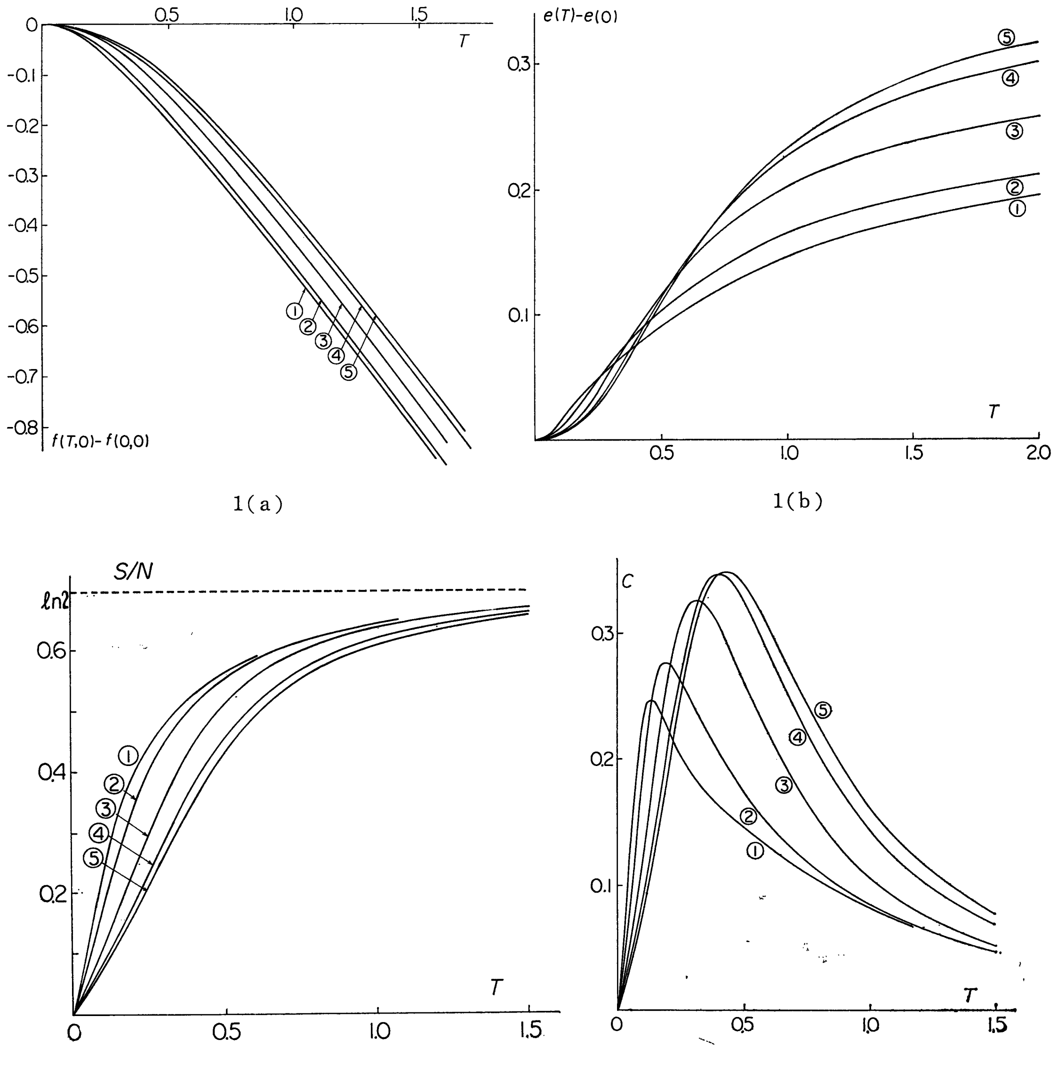
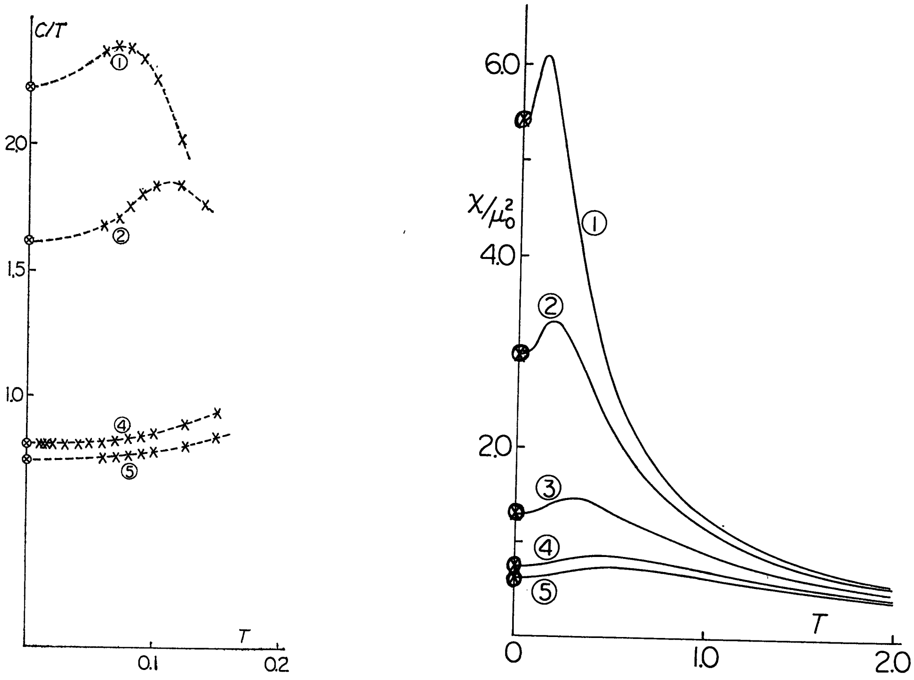


Fig. 1. (Figure captions are printed on the next page)



1(e) 1(f)

Fig. 1. Various thermodynamic quantities as functions of temperature of the Heisenberg-Ising model in the case of zero field and $J=1$. Here ①, ②, ③, ④ and ⑤ correspond to $\Delta=-0.707$, -0.500, 0, 0.500 and 0.707, respectively.

1(a) Free energy minus ground state energy per site.

1(b) Energy minus ground state energy per site.

1(c) Entropy per site.

1(d) Specific heat per site.

1(e) C/T. Symbols ⊗ denote theoretical values predicted in Ref. 3). Symbol × are numerically calculated values.

1(f) Magnetic susceptibility. Symbols ⊗ denote theoretical values at zero temperature given by Yang and Yang.[4)]

The case $\Delta=0$ corresponds to the isotropic X-Y model and the method of calculation of its thermodynamic quantities is well known.[2)] Equations (2) or (3) are applicable only to the cases $\Delta=0.5, 1/\sqrt{2}, \cdots$. Then for the analysis of the cases $\Delta=-0.5$ and $-1/\sqrt{2}$, we use the fact that $f(T,H)$ is invariant under the transformation $(J,\Delta)\rightarrow(-J,-\Delta)$. Specific heat behaves as $aT+bT^3$ at $T\ll J$ and the coefficient a coincides with the result of the latest paper:[3)]

$$\lim_{H\rightarrow 0}\lim_{T\rightarrow 0} C/T=2\theta/3J\sin\theta\,. \tag{7a}$$

It behaves as cT^{-2} at $T\gg J$ and has the maximum at $T\sim J$. Magnetic susceptibility behaves as $a+bT^2$ at $T\ll J$ and as μ_0^2/T at $T\gg J$. The value of a coincides with the susceptibility at $T=0$ which was calculated by Yang and Yang:[4)]

$$\lim_{H\to 0}\lim_{T\to 0}\chi = 4\theta\mu_0^2/J(\pi-\theta)\sin\theta\,. \tag{7b}$$

Magnetic susceptibility has the maximum at $T\sim J$, the position of which approaches zero if $\Delta\to -1$. Though the values of $\lim_{T\to 0}\lim_{H\to 0} C/T$ and $\lim_{T\to 0}\lim_{H\to 0}\chi$ have not been analytically calculated, the numerical results shown in Figs. 1(e) and 1(f) coincide with (7a) and (7b), respectively.

Magnetization curves for various temperatures are also calculated at $\Delta = \pm\frac{1}{2}$. The magnetization curve for zero temperature has a kink at $2\mu_0 H$

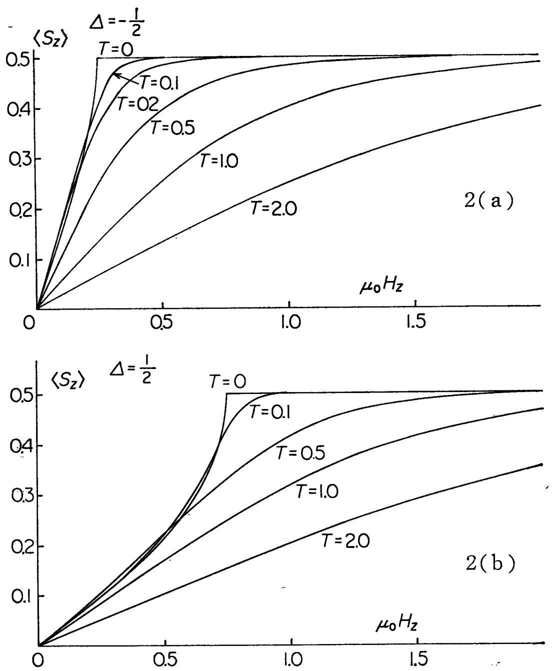


Fig. 2. Magnetization curves of the Heisenberg-Ising model for various temperatures.
2(a) $\Delta=-0.5$.
2(b) $\Delta=0.5$.

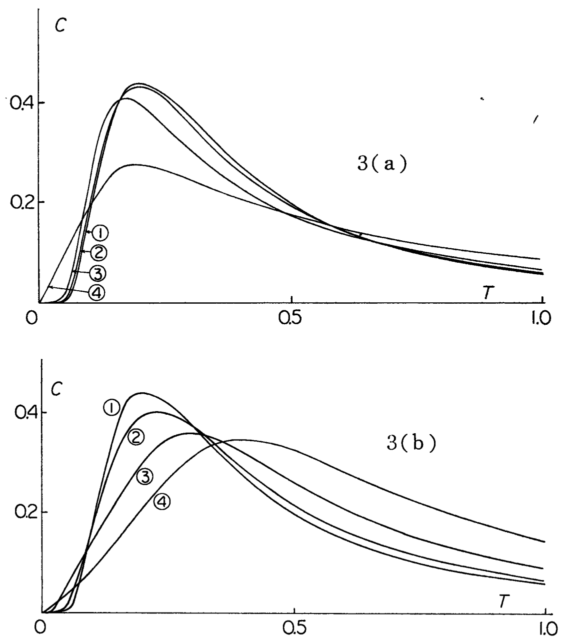


Fig. 3. Specific heat of one-dimensional X-Y-Z model in zero field.
3(a) Case $K_l/\zeta=3$ and $J_z=1$. The values of (J_x, J_y) are (0, 0) for ①, (0.182, 0.223) for ②, (0.342, 0.519) for ③, and (0.5, 1) for ④.
3(b) Case $K_l/(K_l-\zeta)=3$ and $J_z=1$. The values of (J_x, J_y) are (0, 0) for ①, (−0.182, 0.223) for ②, (−0.342, 0.519) for ③, and (−0.5, 1) for ④. Thermodynamic quantities in this case can be calculated from those in the case $K_l/\zeta=3$ and $J_z=-1$, because the free energies in both cases are the same.

$=J(1+\Delta)$. This singularity disappears at finite temperatures.

The specific heat of the X-Y-Z model is shown in Figs. 3(a) and 3(b). The line ① corresponds to the Ising model, and the line ④ to the Heisenberg-Ising model. The characteristic fact at $J_y \neq J_z$ is that specific heat behaves as $T^{\alpha}\exp(-\alpha/T)$, therefore all the derivatives by T become zero at $T\to 0$. The value of α is given theoretically in the Ref. 3). In the limit $l\to 0$ (namely $J_y=J_z$), the value of α becomes zero and the specific heat curve shows T-linear dependence in the region $J_z \gg T \gg \alpha$.

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