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Low-Temperature Specific Heat of Spin-1/2 Anisotropic Heisenberg Ring

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Low-temperature specific heat of Heisenberg-Ising ring at $|A|<1$ is calculated by the method of non-linear integral equations. Specific heat in constant magnetic field (C_H) is proportional to temperature (T) at $|2\mu_0H|<(1+A)J$. In particular $\lim_{H \rightarrow 0} \lim_{T \rightarrow 0} C_H/T$ is $2\theta/(3J \sin \theta)$ where $\theta = \cos^{-1} A$, $0 \leq \theta < \pi$. It is conjectured that $\lim_{T \rightarrow 0} \lim_{H \rightarrow 0} C_H/T = \lim_{H \rightarrow 0} \lim_{T \rightarrow 0} C_H/T$ from the result of numerical calculation. Low-temperature specific heat of the one-dimensional X-Y-Z model is proportional to $T^{-3/2} \exp(-\alpha/T)$ in the case of $J_x > J_y > 0$, $J_y \geq J_z > -J_y$.

§ I. Introduction

The Heisenberg-Ising model plays a very important role in the theory of magnetism and quantum fluids. The one-dimensional system of this model can be treated by the method of Bethe's hypothesis. The Hamiltonian is

$$\mathcal{H} = J \sum_{i=1}^N \{S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + A(S_i^z S_{i+1}^z - \frac{1}{4})\} - 2\mu_0 H \sum_{i=1}^N S_i^z, \quad S_{N+1} = S_1. \quad (1 \cdot 1)$$

The ground state energy, magnetic susceptibility ($\lim_{H \rightarrow 0} \lim_{T \rightarrow 0} \chi$) and elementary excitations were obtained by solving linear-integral equations.

We gave a set of non-linear integral equations for the free energy at $|A|<1$ in previous papers,¹⁾ where we used some assumptions about the distribution of quasi-momenta on the complex plane. Though we cannot prove their validity, the high-temperature expansion of free energy is calculated through the second term and we find that it coincides with a known expansion. In Appendix A we will calculate the third term, by which the coincidence is supported. One obtains that the free energy per site is

$$f(T, H) = -T \log \left(2 \operatorname{ch} \frac{\mu_0 H}{T} \right) - \frac{JA}{4} \left(\frac{1}{\operatorname{ch}^2(\mu_0 H/T)} \right) - \frac{J^2}{4T} \left\{ \frac{1+2A^2}{4 \operatorname{ch}^4(\mu_0 H/T)} \right. \\ \left. - \frac{3A^2}{8 \operatorname{ch}^4(\mu_0 H/T)} \right\} + O\left(\frac{1}{T^2}\right) \quad (1 \cdot 2)$$

by calculating $\lim_{N \rightarrow \infty} \{-T \log (\operatorname{Tr} \exp(-\mathcal{H}/T))/N\}$. It was shown in Ref. 1) that this set of equations gives known exact results at zero temperature. So it is quite possible that our assumptions about the distribution of quasi-momenta are correct and that the set of equations gives the exact free energy of one-

dimensional Heisenberg-Ising model.

In § 2 we give the set of integral equations and some other representations of this set. In § 3 we obtain a set of linear integral equations for $\lim_{T \rightarrow 0} C_H/T$ at $J(1+\Delta) > 2\mu_0 H > 0$. We will obtain

$$\lim_{H \rightarrow 0} \lim_{T \rightarrow 0} C_H/T = \frac{2\theta}{3J \sin \theta}, \quad \theta = \cos^{-1} \Delta, \quad 0 \leq \theta < \pi \quad \text{for } J > 0.$$

In § 4 we give a set of non-linear equations for the free energy at $T \ll J$ and $T \sim \mu_0 H$. We calculate numerically the value of $\lim_{T \rightarrow 0} \lim_{H \rightarrow 0} C_H/T$ and find $\lim_{H \rightarrow 0} \lim_{T \rightarrow 0} C_H/T = \lim_{T \rightarrow 0} \lim_{H \rightarrow 0} C_H/T$ within the error of numerical calculation in the case $\Delta = \cos(\pi/3), \cos(\pi/4), \dots, \cos(\pi/10)$. In § 5 the low-temperature free energy of the spin- $\frac{1}{2}$ X-Y-Z ring is calculated through the use of integral equations given in Ref. 1).

§ 2. Mathematical formulation

In this section we give notations of series of numbers and functions which will be used in this paper:

$$\cos \theta = \Delta, \quad p_0 = \pi/\theta, \quad p_1 = 1,$$

$$p_i = p_{i-2} - [p_{i-2}/p_{i-1}] p_{i-1}, \quad \nu_i = [p_{i-1}/p_i],$$

$$m_i = \sum_{i=1}^i \nu_i,$$

$$y_{-1} = 0, \quad y_0 = 1, \quad y_1 = y_1, \quad y_i = \nu_i y_{i-1} + y_{i-2},$$

$$n_j = y_{i-2} + (j - m_i) y_{i-1} \quad \text{for } m_{i-1} \leq j < m_i,$$

$$q_j = (-1)^{i-1} (p_{i-1} + (m_{i-1} - j) p_i) \quad \text{for } m_{i-1} \leq j < m_i, \quad (2.1)$$

$$s_i(x) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{e^{i\omega x}}{2 \operatorname{ch} p_i \omega} = \frac{1}{4p_i} \operatorname{sech} \frac{\pi x}{2p_i},$$

$$d_i(x) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{\operatorname{ch}(p_i - p_{i+1}) \omega \cdot e^{i\omega x}}{2 \operatorname{ch} p_i \omega \operatorname{ch} p_{i+1} \omega}. \quad (2.2)$$

We define the following functions,

$$D_{ji}(x) = \begin{cases} (1 - 2\delta_{j,m_{i-1}}) \delta_{j,i+1} s_i(x) + \delta_{j,i-1} s_i(x) & \text{for } m_{i-1} \leq j \leq m_i - 2, \\ (1 - 2\delta_{j,m_{i-1}}) \delta_{j,i+1} s_i(x) + \delta_{ji} d_i(x) + \delta_{j,i-1} s_{i+1}(x) & \text{for } j = m_i - 1, \end{cases} \quad (2.3)$$

$$\alpha_j(x) = \int_{-\infty}^{\infty} \frac{\operatorname{ch}(p_0 - 1 - j) \omega}{\operatorname{ch}(p_0 - 1) \omega} e^{i\omega x} \frac{d\omega}{2\pi} = \frac{1}{p_0 - 1} \left\{ \operatorname{ch} \frac{\pi x}{2(p_0 - 1)} \sin \frac{\pi(p_0 - 1 - j)}{2(p_0 - 1)} \right\}$$

$$\times \left\{ \operatorname{ch} \frac{\pi x}{p_0 - 1} + \cos \frac{\pi(p_0 - 1 - j)}{p_0 - 1} \right\}^{-1} \quad \text{for } j = 1, 2, \dots, \nu_1 - 1, \quad (2.4a)$$

$$\beta(x) = \int_{-\infty}^{\infty} \frac{e^{i\omega x}}{2 \operatorname{ch}(p_0 - 1) \omega} \frac{d\omega}{2\pi} = \frac{1}{4(p_0 - 1)} \operatorname{sech} \frac{\pi x}{2(p_0 - 1)}, \quad (2.4b)$$

$$B_{jl}(x) = \begin{cases} \alpha_{|j-l|} + 2\alpha_{|j-l|+2} + \cdots + 2\alpha_{j+l-2} + \alpha_{j+l} & \text{for } j \neq l, \\ 2\alpha_2 + 2\alpha_4 + \cdots + 2\alpha_{2l-2} + \alpha_{2l} & \text{for } j = l, \end{cases} \quad (2.4c)$$

$$C_j(x) = s_2^* B_{j,\nu_1-1}(x) + \delta_{j,\nu_1-1} s_2(x), \quad (2.4d)$$

$$a_j(x) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{\sinh q_j \omega e^{i\omega x}}{\sinh p_0 \omega} = \frac{\sin(\pi q_j/p_0)}{2p_0(\operatorname{ch}(\pi x/p_0) + \cos(\pi q_j/p_0))}. \quad (2.4e)$$

When θ/π is an irrational number and $0 < \theta < \pi/2$, the set of integral equations is

$$\ln \eta_j = -As_1(x)\delta_{j1}/T + \sum_{i=1}^{\nu_1} D_{ji}^* \ln(1+\eta_i), \quad j=1, 2, \dots,$$

$$\lim_{j \rightarrow \infty} \frac{\ln \eta_j}{n_j} = \frac{2\mu_0 H}{T}, \quad A = 2\pi J \sin \theta / \theta, \quad (2.5a)$$

and the free energy per site is

$$f(T, H) = -A \int_{-\infty}^{\infty} s_1(x) a_1(x) dx - T \int_{-\infty}^{\infty} s_1(x) \ln(1+\eta_1(x)) dx. \quad (2.5b)$$

Equations (2.5a) can be transformed as follows:

$$\begin{aligned} \ln \eta_j &= -\frac{A}{T} \alpha_j(x) + \sum_{i=1}^{\nu_1-1} B_{ji}^* \ln(1+\eta_i^{-1}) + C_j^* \ln(1+\eta_{\nu_1}) \quad \text{for } 1 \leq j < \nu_1, \\ \ln \eta_{\nu_1} &= \frac{A}{T} \beta(x) - \sum_{i=1}^{\nu_1-1} C_i^* \ln(1+\eta_i^{-1}) + \sum_{i>\nu_1} D_{ri}^* \ln(1+\eta_i) - s_2^* C_{\nu_1-1}^* \ln(1+\eta_{\nu_1}), \\ \ln \eta_j &= \sum_{i=\nu_1}^{\infty} D_{ji}^* \ln(1+\eta_i) \quad \text{for } j > \nu_1, \\ \lim_{j \rightarrow \infty} \frac{\ln \eta_j}{n_j} &= \frac{2\mu_0 H}{T}. \end{aligned} \quad (2.6a)$$

The expression for free energy (2.5b) can be transformed as follows:

$$\begin{aligned} f(T, H) &= -A \int_{-\infty}^{\infty} s_1(x) (\alpha_1(x) - \alpha_1(x)) dx - T \sum_{j=1}^{\nu_1-1} \int_{-\infty}^{\infty} \alpha_j(x) \ln(1+\eta_j^{-1}(x)) dx \\ &\quad - T \int_{-\infty}^{\infty} \beta(x) \ln(1+\eta_{\nu_1}(x)) dx. \end{aligned} \quad (2.6b)$$

By taking the limit in Eqs. (2.5), we obtain integral equations, when θ/π is a rational number. In this case the number of unknown functions becomes finite. Equations (2.5) and (2.6) are useful for the discussion of the low-temperature properties in the antiferromagnetic case ($J > 0$) and ferromagnetic case ($J < 0$), respectively.

§ 3. Low-temperature expansion of the free energy at $\mu_0 H \gg T$

Assume that $\ln \eta_i \gg 1$ for $J > 0$, $i \geq 2$ and $2\mu_0 H \gg T$. The term $\ln(1+\eta_i)$ in

(2.5a) is replaced by $\ln \eta_j$ and one obtains

$$\begin{aligned}\ln \eta_j(x) = & \int_{-\infty}^{\infty} dx' \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{\operatorname{sh} q_j \omega e^{i\omega(x-x')}}{\operatorname{sh} q_1 \omega} \ln(1 + \eta_1(x')) \\ & + \left(n_j - \frac{q_j}{q_1}\right) \frac{2\mu_0 H}{T} + \sum_{l=2}^{\infty} O(\eta_l^{-1}), \quad j=2, 3, \dots.\end{aligned}\quad (3.1a)$$

Substituting the case $j=2$ of this equation into the case $j=1$ of (2.5a), we have

$$\begin{aligned}T \ln \eta_1 = & -\frac{2\pi J \sin \theta}{\theta} s_1(x) + \frac{\pi \mu_0 H}{\pi - \theta} + \int_{-\infty}^{\infty} R_+(x-x') T \ln(1 + \eta_1(x')) dx' \\ & + O\left(T \exp\left(-\frac{2\pi \mu_0 H}{T(\pi-\theta)}\right)\right),\end{aligned}\quad (3.1b)$$

where

$$R_+(x) = \int_{-\infty}^{\infty} \frac{\operatorname{sh}(p_0-2)\omega e^{i\omega x}}{2\operatorname{ch} \omega \operatorname{sh}(p_0-1)\omega} \frac{d\omega}{2\pi}. \quad (3.1c)$$

At $J<0$, $1>\Delta\geq 0$ we assume that $\ln \eta_j \gg 1$ for $j>\nu_1$. Then we have

$$\begin{aligned}T \ln \eta_j(x) = & T \int_{-\infty}^{\infty} d\omega \int_{-\infty}^{\infty} dx' \frac{\operatorname{sh} q_j \omega e^{i\omega(x-x')}}{\operatorname{sh} q_{\nu_1} \omega} \ln(1 + \eta_{\nu_1}(x')) \\ & + \left(n_j - \frac{q_j}{q_{\nu_1}}\right) 2\mu_0 H + \sum_{l=\nu_1}^{\infty} O(T\eta_l^{-1}) \quad \text{for } j>\nu_1.\end{aligned}\quad (3.2a)$$

In the same way as is used in the preceding paragraph, we obtain

$$\ln \eta_j = -\frac{A}{T} \alpha_j(x) + \sum_{l=1}^{\nu_1-1} B_l^* \ln(1 + \eta_l^{-1}) + C_j^* \ln(1 + \eta_{\nu_1}), \quad (3.2b)$$

$$\ln \eta_{\nu_1} = +\frac{A}{T} \beta(x) - \sum_{l=1}^{\nu_1-1} C_l^* \ln(1 + \eta_l^{-1}) + \int_{-\infty}^{\infty} R_-(x-x') \ln(1 + \eta_{\nu_1}) dx' + \frac{\pi \mu_0 H}{\theta T}, \quad (3.2c)$$

where

$$R_-(x) = \int_{-\infty}^{\infty} \frac{\operatorname{sh}(2-p_0)\omega e^{i\omega x}}{2\operatorname{ch}(p_0-1)\omega \cdot \operatorname{sh} \omega} \frac{d\omega}{2\pi}. \quad (3.2d)$$

Considering $-A/T \gg 1$ and $C_j^* \ln(1 + \eta_{\nu_1}) \sim \mu_0 H/T$, we have $\ln \eta_j \gg 1$, $j=1, 2, \dots, \nu_1-1$.

From Eq. (2.6b) we have

$$f(T, H) - f(0, 0) = -T \int_{-\infty}^{\infty} \beta(x) \ln(1 + \eta_{\nu_1}(x)) dx + \sum_{j=1}^{\nu_1-1} O(T\eta_j^{-1}). \quad (3.2e)$$

Considering that $f(T, H)$ is invariant under the transformation $(J, \Delta) \rightarrow (-J, -\Delta)$, we have from Eqs. (3.1), (3.2) and (2.5b)

$$\varepsilon_1(x) = \frac{2\pi J \sin \theta}{\theta} \frac{1}{4} \operatorname{sech} \frac{\pi x}{2} + \frac{\pi \mu_0 H}{\pi - \theta} + T \int_{-\infty}^{\infty} R(x-x') \ln(1 + \exp(\varepsilon_1(x')/T)) dx', \quad (3.3a)$$

$$R(x) = \int_{-\infty}^{\infty} \frac{d\omega e^{i\omega x}}{2\pi} \frac{\operatorname{sh}(\pi - 2\theta)\omega}{2\operatorname{ch}\omega \operatorname{sh}(\pi - \theta)\omega}, \quad (3.3b)$$

$$f(T, H) = -\frac{2\pi J \sin \theta}{\theta} \int_{-\infty}^{\infty} \frac{1}{4} \operatorname{sech} \frac{\pi x}{2} \cdot \frac{\theta}{2\pi} \frac{\sin \theta}{\cosh \theta x - \cos \theta} dx - T \int_{-\infty}^{\infty} \frac{1}{4} \operatorname{sech} \frac{\pi x}{2} \ln(1 + \exp(\varepsilon_1(x)/T)) + O\left(T \exp\left(-\frac{2\pi \mu_0 H}{(\pi - \theta)T}\right)\right), \quad (3.3c)$$

where θ is determined by

$$\Delta = \cos \theta, \quad 0 \leq \theta \leq \pi \quad (3.3d)$$

for $|\Delta| \leq 1$ and $J > 0$, $2\mu_0 H \gg T$. This set of equations is equivalent to

$$\begin{aligned} \varepsilon_1(x) = & -\frac{2\pi J \sin \theta}{\theta} a_1(x) + 2\mu_0 H \\ & + T \int_{-\infty}^{\infty} a_2(x-x') \ln(1 + \exp(-\varepsilon_1(x')/T)) dx', \end{aligned} \quad (3.4a)$$

$$a_j(x) = \frac{\theta}{2\pi} \frac{\sin j\theta}{\operatorname{ch} \theta x - \cos j\theta}, \quad j=1, 2, \quad (3.4b)$$

$$f(T, H) = -\mu_0 H - T \int_{-\infty}^{\infty} a_1(x) \ln(1 + \exp(-\varepsilon_1(x)/T)) dx. \quad (3.4c)$$

a) Case $J > 0$, $J(1+\Delta) > 2\mu_0 H$

We put the solution of (3.4a) at $T=0$ as $\varepsilon_1^{(0)}(x)$, which satisfies

$$\varepsilon_1^{(0)}(x) = -\frac{2\pi J \sin \theta}{\theta} a_1(x) + 2\mu_0 H - \int_{\varepsilon_1^{(0)}(x') < 0} a_2(x-x') \varepsilon_1^{(0)}(x') dx'. \quad (3.5)$$

Function $\varepsilon_1^{(0)}$ is a monotonically increasing function of x^2 and is $2\mu_0 H$ in the limit $x \rightarrow \pm \infty$ because $a_1(\infty)$ and $a_2(\infty)$ are zero. It is clear that if $-(2\pi J \sin \theta/\theta) \times a_1(0) + 2\mu_0 H < 0$ (namely, $J(1+\Delta) > 2\mu_0 H$), $\varepsilon_1^{(0)}(x)$ has necessarily two zeros $\pm K$, $K > 0$. Using $\varepsilon_1^{(0)}(K) = 0$ and (3.5), one can calculate $2\mu_0 H$ from K :

$$2\mu_0 H = \frac{2\pi J \sin \theta}{\theta} \cdot \frac{V(K)}{Z(K)}, \quad (3.6a)$$

where

$$V(x) + \int_{-K}^K a_2(x-x') V(x') dx' = a_1(x), \quad (3.6b)$$

$$Z(x) + \int_{-K}^K a_2(x-x') Z(x') dx' = 1. \quad (3.6c)$$

If $T \ll J(1+A) - 2\mu_0 H$, $\varepsilon_1(x)$ has two zeros even at finite T and we put these zeros $\pm K'$, $K' > 0$. From (3.4a) and (3.5) we have

$$\begin{aligned} \varepsilon_1(x) - \varepsilon_1^{(0)}(x) + \int_{-K'}^K a_2(x-x') (\varepsilon_1 - \varepsilon_1^{(0)})(x') dx' \\ = \int_{K'}^K a_2(x-x') \varepsilon_1(x') dx' + \int_{-K}^{-K'} \dots \\ + T \int_{-\infty}^{\infty} a_2(x-x') \ln \left(1 + \exp \left(- \frac{|\varepsilon_1(x')|}{T} \right) \right) dx'. \end{aligned} \quad (3.7)$$

The first and the second terms of r.h.s. are of the order of $(K-K')^2$. The third term is

$$\frac{\pi^2 T^2}{6\varepsilon_1^{(0)'}(K')} (a_2(x-K') + a_2(x+K')) (1 + O(T)). \quad (3.8)$$

From Eq. (3.7) one can see

$$K - K' = O(T^2).$$

Equation (3.7) can then be written as

$$\begin{aligned} \varepsilon_1(x) - \varepsilon_1^{(0)}(x) + \int_{-K}^K a_2(x-x') (\varepsilon_1(x') - \varepsilon_1^{(0)}(x')) dx' \\ = \frac{\pi^2 T^2}{6\varepsilon_1^{(0)'}(K)} (a_2(x-K) + a_2(x+K)) + O(T^3), \end{aligned} \quad (3.9a)$$

or

$$\varepsilon_1(x) - \varepsilon_1^{(0)}(x) = \frac{\pi^2 T^2}{6\varepsilon_1^{(0)'}(K)} U(x) + O(T^3), \quad (3.9b)$$

where $U(x)$ is defined by

$$U(x) + \int_{-K}^K a_2(x-x') U(x') dx' = a_2(x-K) + a_2(x+K). \quad (3.9c)$$

Using Eq. (3.4c) we have

$$\begin{aligned} f(T, H) - f(0, H) &= -T \int_{-\infty}^{\infty} a_1(x) \ln \left(1 + \exp \left(- |\varepsilon_1(x)| / T \right) \right) \\ &\quad + \int_{-K'}^{K'} a_1(x) \varepsilon_1(x) dx' - \int_{-K}^{-K'} a_1(x) \varepsilon_1^{(0)}(x) dx \\ &= -\frac{\pi^2 T^2}{6\varepsilon_1^{(0)'}(K)} \left[2a_1(K) - \int_{-K}^K a_1(x) U(x) dx \right] + O(T^3). \end{aligned} \quad (3.10a)$$

The bracket of the r.h.s. is $2V(K)$, where $V(x)$ is defined in (3.6b). Differentiating (3.5) and using partial integration, we have

$$\varepsilon_1^{(0)'}(x) = \frac{2\pi J \sin \theta}{\theta} \cdot W(x), \quad (3.10b)$$

$$W(x) + \int_{-K}^K a_2(x-x') W(x') dx' = -\frac{d}{dx} a_1(x). \quad (3.10c)$$

Then we have

$$f(T, H) = f(0, H) - \frac{\pi \theta T^2}{6J \sin \theta} \cdot \frac{V(K)}{W(K)} + O(T^3). \quad (3.11)$$

In the limit $K \rightarrow \infty$ ($H \rightarrow 0$) we can calculate $V(K)/W(K)$.

By the Fourier transformation (3.6b) and (3.10c), we have

$$V(x) - \int_K^\infty (R(x-x') + R(x+x')) V(x') dx' = \frac{1}{4} \operatorname{sech} \frac{\pi x}{2}, \quad (3.12a)$$

$$W(x) - \int_K^\infty (R(x-x') + R(x+x')) W(x') dx' = \frac{d}{dx} \left(\frac{1}{4} \operatorname{sech} \frac{\pi x}{2} \right). \quad (3.12b)$$

Considering that the inhomogeneous terms are $\frac{1}{2}e^{-\pi x/2}$ and $e^{-\pi x/2}/\pi/4$ at $x \gg 1$ and that $R(x)$ becomes zero at $x \rightarrow \infty$, we have

$$\frac{V(K)}{W(K)} = \begin{cases} \frac{2}{\pi} + O(e^{-\pi K}) + O(e^{-2\pi \theta K / (\pi - \theta)}) = \frac{2}{\pi} + O\left(\left(\frac{\mu_0 H}{J}\right)^2\right) \\ \quad + O\left(\left(\frac{2\mu_0 H}{J}\right)^{4\theta/(\pi-\theta)}\right) & \text{for } -1 < \Delta < 1, \\ \frac{2}{\pi} + O(e^{-\pi K}) + O(K^{-2}) = \frac{2}{\pi} + O\left(\left(\frac{\mu_0 H}{J}\right)^2\right) + O\left(\left(\ln\left(\frac{\mu_0 H}{J}\right)\right)^{-2}\right) \\ & \text{for } \Delta = 1. \end{cases} \quad (3.13)$$

Using the relation $C_H = -\partial/\partial T(T^2(\partial/\partial T)(f/T))$, we have

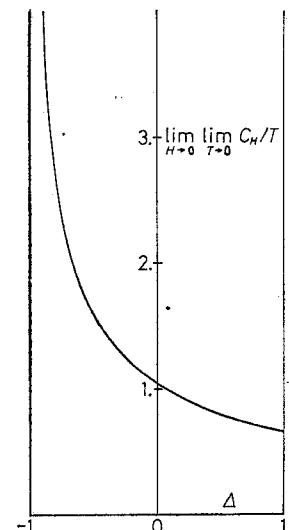
$$\lim_{H \rightarrow 0} \lim_{T \rightarrow 0} C_H/T = \frac{2\theta}{3J \sin \theta}. \quad (3.14)$$

At $\Delta = 1$, $\lim_{H \rightarrow 0} \lim_{T \rightarrow 0} C_H/T$ is $2/3J$. This coincides with Yamada's result calculated from the Fermi liquid theory, and with Johnson and McCoy's⁸⁾ calculation. At $\Delta = 0$, (3.14) is $\pi/3J$. This coincides with the known result for the $X-Y$ model.⁴⁾ In the limit $\Delta \rightarrow -1$, (3.14) becomes infinity.

b) Case $J > 0$, $2\mu_0 H \geq J(1+\Delta)$, $1 \geq \Delta > -1$

The third term of (3.4a) is of the order of $T^{3/2} \exp((-2\mu_0 H + J(1+\Delta))/T)$. Substituting (3.4a) into (3.4c), we have

Fig. 1. The coefficient of T -linear low-temperature specific heat in the limit $T \rightarrow 0$ and $H \rightarrow 0$. In the limit $\Delta \rightarrow -1$, $\lim_{H \rightarrow 0} \lim_{T \rightarrow 0} C_H/T$ diverges as $(1+\Delta)^{-1/2}$.



$$\begin{aligned} f(T, H) = & -\mu_0 H - \frac{T^{3/2}}{\pi} \sqrt{\frac{2}{J}} \int_0^\infty \ln(1 + \exp\left(\frac{-2\mu_0 H + J(1+\Delta)}{T}\right) \\ & \times \exp(-x^2)) dx (1 + O(T)) + O\left(T^{1/2} \exp\left(\frac{-2\mu_0 H + J(1+\Delta)}{T}\right)\right). \end{aligned} \quad (3.15a)$$

At $2\mu_0 H - J(1+\Delta) \gg T$, (3.15a) is

$$f(T, H) = -\mu_0 H - T^{3/2} \frac{1}{\sqrt{2\pi J}} \exp\left(-\frac{2\mu_0 H - J(1+\Delta)}{T}\right) [1 + O(T)], \quad (3.15b)$$

and we have

$$C_H = \frac{1}{\sqrt{2\pi J}} \frac{(2\mu_0 H - J(1+\Delta))^2}{T^{3/2}} \exp\left(-\frac{2\mu_0 H - J(1+\Delta)}{T}\right) [1 + O(T)]. \quad (3.15c)$$

At $2\mu_0 H = J(1+\Delta)$ one obtains from (3.15a)

$$f(T, H) = -\mu_0 H - T^{3/2} \frac{1}{\sqrt{2\pi J}} \zeta\left(\frac{3}{2}\right) \left(1 - \frac{1}{\sqrt{2}}\right) (1 + O(T^{1/2})), \quad (3.15d)$$

$$C_H = \frac{3}{4} \frac{1}{\sqrt{2\pi}} \left(1 - \frac{1}{\sqrt{2}}\right) \zeta\left(\frac{3}{2}\right) \sqrt{\frac{T}{J}} (1 + O(T^{1/2})), \quad (3.15e)$$

where ζ is Riemann's zeta function. It is remarkable that the low-temperature specific heat is proportional to $T^{1/2}$ and that the coefficient does not depend on Δ at $2\mu_0 H = J(1+\Delta)$.

§ 4. Case $\mu_0 H \sim T$ and $T \ll J$

a) Case $J > 0, 1 \geq \Delta \geq 0$

Equations (2.5) are transformed as

$$\ln \eta_j(x) = -\frac{A}{4T} \operatorname{sech} \frac{\pi x}{2} \delta_{j1} + \int_0^\infty \{D_{j1}(x-x') + D_{j1}(x+x')\} \ln(1 + \eta_1(x')) dx',$$

$$\lim_{j \rightarrow \infty} \frac{\ln \eta_j}{n_j} = \frac{2\mu_0 H}{T},$$

$$f(T, H) - f(0, 0) = -2T \int_0^\infty \frac{1}{4} \operatorname{sech} \frac{\pi x}{2} \ln(1 + \eta_1(x)) dx.$$

Putting $x \rightarrow x + (2/\pi) \ln(A/2T)$ and $T \rightarrow 0$, we have a set of non-linear integral equations which determines the T^2 order term of free energy as follows:

$$\ln \eta_j = -\delta_{j1} e^{-\pi x/2} + \sum_{l=1}^{\infty} D_{jl}^* \ln(1 + \eta_l), \quad j = 1, 2, \dots, \quad (4.1a)$$

$$\lim_{j \rightarrow \infty} \frac{\ln \eta_j}{n_j} = y, \quad (4.1b)$$

$$C(y) = \int_{-\infty}^{\infty} e^{-\pi x/2} \ln(1 + \eta_1(x)) dx, \quad (4.1c)$$

$$f(T, H) - f(0, 0) = -\frac{2\theta T^2}{\pi J \sin \theta} C\left(\frac{2\mu_0 H}{T}\right) + O(T^4). \quad (4.1d)$$

When π/θ is a rational number, one can reduce this set of equations to that with finite unknowns. Therefore the numerical method is available for the calculation of $C(x)$. Especially when $\pi/\theta=3$, the set of integral equations is

$$\ln \eta_1 = -e^{-\pi x/2} + s_1 * \ln(1 + 2\operatorname{ch}(3y/2) \cdot \kappa + \kappa^2),$$

$$\ln \kappa = s_1 * \ln(1 + \eta_1).$$

In order to determine $\lim_{T \rightarrow 0} \lim_{H \rightarrow 0} C_H/T$, it is sufficient to calculate $C(0)$. From the numerical calculation, we have $C(0)=0.5235378$. This value is very near to $\pi/6=0.5235987\cdots$. When $\pi/\theta=\nu$ is an integer larger than 3, we have

$$\ln \eta_1 = -e^{-\pi x/2} + s_1 * \ln(1 + \eta_2),$$

$$\ln \eta_j = s_1 * \ln(1 + \eta_{j-1}) (1 + \eta_{j+1}), \quad 2 \leq j < \nu - 2,$$

$$\ln \eta_{\nu-2} = s_1 * \ln(1 + \eta_{\nu-3}) \left(1 + 2 \operatorname{ch}\left(\frac{\nu y}{2}\right) \cdot \kappa + \kappa^2\right),$$

$$\ln \kappa = s_1 * \ln(1 + \eta_{\nu-2}).$$

The results of our numerical calculation of $C(0)$ at $A=\cos(\pi/\nu)$, $\nu=3, 4, \dots, 10$ are shown in Table I.

In this calculation the number of unknown functions is $\nu-1$. An unknown function is represented by 40 unknown numbers. This set of non-linear equations is solved by the method of iteration through the use of computer NEAC 500. These values are very near to $\pi/6$. We can regard the small deviations from $\pi/6$ as numerical errors. It is very plausible that $C(0)$ is $\pi/6$ for any value of A and that $\lim_{T \rightarrow 0} \lim_{H \rightarrow 0} C_H/T$ is $2\theta/3J \sin \theta$, that is, $\lim_{T \rightarrow 0} \lim_{H \rightarrow 0} C_H/T = \lim_{H \rightarrow 0} \lim_{T \rightarrow 0} C_H/T$.

b) Case $J<0$, $1>A \geq$

At $x \gg p_0 - 1$, it is clear that

$$\alpha_j(x) = \frac{1}{p_0 - 1} \sin \frac{\pi(p_0 - 1 - j)}{2(p_0 - 1)} \cdot e^{-\pi x/2(p_0 - 1)},$$

$$\beta(x) = \frac{1}{2(p_0 - 1)} e^{-\pi x/2(p_0 - 1)},$$

from (2.4a) and (2.4b). Using these equations, we have the following integral

Table I. Numerical calculation of $C(0)$.

ν	A	$C(0)$
3	0.500000	0.5235378
4	0.707107	0.5233042
5	0.809017	0.5230769
6	0.866025	0.5229287
7	0.900969	0.5228421
8	0.923880	0.5227903
9	0.939693	0.5227562
10	0.951057	0.5227310

equations for T^2 order term of free energy at $\mu_0 H \sim T$ and $T \ll |J|$:

$$\begin{aligned} \ln \eta_j &= 2 \sin \frac{\pi(p_0 - 1 - j)}{2(p_0 - 1)} e^{-\pi x/2(p_0 - 1)} + \sum_{i=1}^{v_1-1} B_{ji}^* \ln(1 + \eta_i^{-1}) \\ &\quad + C_j^* n(1 + \eta_{v_1}) \quad \text{for } 1 \leq j \leq v_1 - 1, \end{aligned} \quad (4.2a)$$

$$\begin{aligned} \ln \eta_{v_1} &= -e^{-\pi x/2(p_0 - 1)} - \sum_{j=1}^{v_1-1} C_j^* \ln(1 + \eta_j^{-1}) - s_2^* C_{v_1-1}^* \ln(1 + \eta_{v_1}) \\ &\quad + \sum_{i>v_1} D_{v_1 i}^* \ln(1 + \eta_i), \end{aligned} \quad (4.2b)$$

$$\ln \eta_j = \sum_{i=v_1}^{\infty} D_{ji}^* \ln(1 + \eta_i) \quad \text{for } j > v_1, \quad (4.2c)$$

$$\lim_{j \rightarrow \infty} \frac{\ln \eta_j}{n_j} = y, \quad (4.2d)$$

$$\begin{aligned} C(y) &= \sum_{a=1}^{v_1-1} \sin \frac{\pi(p_0 - 1 - j)}{2(p_0 - 1)} \int_{-\infty}^{\infty} e^{-\pi x/2(p_0 - 1)} \ln(1 + \eta_j^{-1}) dx \\ &\quad + \int_{-\infty}^{\infty} e^{-\pi x/2(p_0 - 1)} \ln(1 + \eta_{v_1}) dx, \end{aligned} \quad (4.2e)$$

$$f(T, H) - f(0, 0) = -\frac{2(\pi - \theta)}{\pi |J| \sin \theta} \frac{T^2}{T} C\left(\frac{2\mu_0 H}{T}\right) + O(T^4). \quad (4.2f)$$

The author believes that $C(0)$ is $\pi/6$ in this case also, though numerical calculation is not yet done.

§ 5. The X-Y-Z model in zero field

In this section we consider the low-temperature specific heat of the X-Y-Z model in zero field. The Hamiltonian is

$$\mathcal{H} = \sum_{i=1}^N J_x S_i^x S_{i+1}^x + J_y S_i^y S_{i+1}^y + J_z S_i^z S_{i+1}^z, \quad S_{N+1} = S_1. \quad (5.1)$$

a) Case $0 \leq J_x \leq J_y < J_z$

Equations (4.10), (4.13) and (4.16) of Ref. 1) are written as

$$\epsilon_1 = -A s_1(x) + T D_{12}^* \ln(1 + \eta_1) + T D_{11}^* \ln(1 + \exp(\epsilon_1/T)), \quad (5.2a)$$

$$\ln \eta_j = D_{j1}^* \ln(1 + \exp(\epsilon_1/T)) + \sum_{i=2}^{\infty} D_{ji}^* \ln(1 + \eta_i), \quad j \geq 2, \quad (5.2b)$$

$$\lim_{j \rightarrow \infty} \frac{\ln \eta_j}{n_j} = 0, \quad (5.2c)$$

$$f(T) = f(0) - T \int_{-q}^q \ln(1 + \exp(\epsilon_1(x)/T)) s_1(x) dx, \quad (5.2d)$$

$$A = \pi J_z \operatorname{sn} 2\zeta/\zeta, \quad (5.2e)$$

$$\mathbf{D}_{jl}(x) = \begin{cases} (1 - 2\delta_{j,m_{i-1}})\delta_{j,l+1}\mathbf{s}_i(x) + \delta_{j,l-1}\mathbf{s}_i(x) & \text{for } m_{i-1} \leq j < m_i - 1, \\ (1 - 2\delta_{j,m_{i-1}})\delta_{j,l+1}\mathbf{s}_i(x) + \delta_{jl}\mathbf{d}_i(x) + \delta_{j,l-1}\mathbf{s}_{i+1}(x) & \text{for } j = m_i - 1. \end{cases} \quad (5.2f)$$

The first term of the r.h.s. of (5.2b) is of the order of $T \exp(-A\mathbf{s}_1(Q)/T)$. From Eqs. (5.2b) and (5.2c) we have

$$\eta_2 = 3 + O(\sqrt{T} \exp(-A\mathbf{s}_1(Q)/T)) \quad (5.3a)$$

and from (5.2a)

$$\varepsilon_1(x) = -A\mathbf{s}_1(x) + T \ln 2 + O(T^{3/2} \exp(-A\mathbf{s}_1(Q)/T)). \quad (5.3b)$$

Substituting this into (5.2d), we have

$$f(T) = f(0) - 2T^{3/2}\mathbf{s}_1(Q)\sqrt{\frac{2\pi}{A\mathbf{s}_1''(Q)}} \exp(-A\mathbf{s}_1(Q)/T) \{1 + O(T)\}. \quad (5.4a)$$

Using

$$\mathbf{s}_1(x) = \frac{K_{k'}}{2\pi} \operatorname{dn}(K_{k'}x; k),$$

we have

$$\mathbf{s}_1(Q) = \frac{K_{k'}}{2\pi} k', \quad \mathbf{s}_1''(Q) = \frac{K_{k'}^3}{2\pi} k^2 k', \quad (5.4b)$$

where k' is $\sqrt{1-k^2}$ and $K_{k'}$ is the complete elliptic integral of the first kind with modulus k' , k being determined by

$$\frac{K_k}{K_{k'}} = \frac{K_{k'}}{\zeta}, \quad \frac{J_y}{J_z} = \operatorname{dn}(2\zeta, l), \quad \frac{J_x}{J_z} = \operatorname{cn}(2\zeta, l), \quad (5.4c)$$

with $0 \leq \zeta \leq K_l/2$.

b) Case $0 \leq -J_x < -J_y < -J_z$

In the same way as Eqs. (2.5) were transformed into Eqs. (2.6), Eqs. (5.2) are transformed as follows:

$$\varepsilon_j(x) = -A\alpha_j(x) + \sum_{l=1}^{\nu_1-1} \mathbf{B}_{jl}^* T \ln(1 + \exp(-\varepsilon_l/T)) + \mathbf{C}_j^* T \ln(1 + \exp(\varepsilon_{\nu_1}/T)) \quad \text{for } 1 \leq j < \nu_1, \quad (5.5a)$$

$$\begin{aligned} \varepsilon_{\nu_1}(x) = A\beta(x) - \sum_{l=1}^{\nu_1-1} \mathbf{C}_l^* T \ln(1 + \exp(-\varepsilon_l/T)) + \sum_{l>\nu_1} \mathbf{D}_{\nu_1 l}^* T \ln(1 + \eta_l) \\ - \mathbf{s}_2^* \mathbf{C}_{\nu_1-1}^* T \ln(1 + \exp(\varepsilon_{\nu_1}/T)), \end{aligned} \quad (5.5b)$$

$$\ln \eta_j = \sum_{l>\nu_1}^{\infty} \mathbf{D}_{jl}^* \ln(1 + \eta_l) + \mathbf{D}_{j,\nu_1}^* \ln(1 + \exp(\varepsilon_{\nu_1}/T)) \quad \text{for } j > \nu_1, \quad (5.5c)$$

$$\lim_{j \rightarrow \infty} \frac{\ln \eta_j}{n_j} = 0, \quad (5.5d)$$

$$f(T) = f(0) - T \sum_{j=1}^{\nu_1-1} \int_{-Q}^Q \alpha_j(x) \ln(1 + \exp(-\varepsilon_j/T)) dx \\ - T \int_{-Q}^Q \beta(x) \ln(1 + \exp(\varepsilon_{\nu_1}/T)) dx, \quad (5.5e)$$

where α_j , β , B_{jl} , C_j and D_{jl} are defined by

$$\alpha_j(x) = \sum_{j=-\infty}^{\infty} \alpha_j(x+2jQ), \quad \beta(x) = \sum_{j=-\infty}^{\infty} \beta(x+2jQ), \dots$$

and $f(0)$ is the ground state energy per site. One can show

$$\beta(x) = \frac{K_{k'}}{2\pi(p_0-1)} \operatorname{dn}\left(\frac{K_{k'}x}{p_0-1}, k\right), \quad \alpha_j(x) = \beta(x+i(p_0-1-j)) \\ + \beta(x-i(p_0-1-j)) = \frac{K_{k'}}{\pi(p_0-1)} \operatorname{dn}\left(\frac{K_{k'}x}{p_0-1}, k\right) \operatorname{dn}\left(\frac{K_{k'}(p_0-1-j)i}{p_0-1}, k\right) \\ \times \left(1 - k^2 \operatorname{sn}^2\left(\frac{K_{k'}x}{p_0-1}, k\right) \operatorname{sn}^2\left(\frac{K_{k'}(p_0-1-j)i}{p_0-1}, k\right)\right)^{-1},$$

where k is defined by

$$\frac{K_k}{K_{k'}} = \frac{K_k}{K_l - \zeta}, \quad \frac{J_y}{J_z} = \operatorname{dn}(2\zeta, l), \quad \frac{J_x}{J_z} = \operatorname{cn}(2\zeta, l). \quad (5.6)$$

Functions $\alpha_j(x)$ and $\beta(x)$ have the minimum at $x=Q$ and

$$\alpha_j(Q) = \frac{K_{k'}k'}{\pi(p_0-1)} \operatorname{sn}\left(\frac{K_{k'}j}{p_0-1}, k'\right), \\ \alpha_j''(Q) = \frac{K_{k'}^3k'}{\pi(p_0-1)^3} \operatorname{sn}\left(\frac{K_{k'}j}{p_0-1}, k'\right) \left(1 + k'^2 - 2k'^2 \operatorname{sn}^2\left(\frac{K_{k'}j}{p_0-1}, k'\right)\right), \\ \beta(Q) = \frac{K_{k'}k'}{2\pi(p_0-1)}, \quad \beta''(Q) = \frac{K_{k'}^3k^2k'}{2\pi(p_0-1)^3}. \quad (5.7)$$

From (5.5c) and (5.5b) we have

$$\eta_{\nu_1+1} = 3 + O(\exp(A\beta(Q)/T)). \quad (5.8)$$

Substituting this into (5.5a) and (5.5b), we have

$$\varepsilon_j(x) = -A\alpha_j(x) + O(T \exp(A\beta(Q))) + O(T \exp(A\alpha_1(Q))) \\ \text{for } j=1, 2, \dots, \nu_1-1,$$

$$\varepsilon_{\nu_1}(x) = A\beta(x) + T \ln 2 + O(T \exp(A\beta(Q))) + O(T \exp(A\alpha_1(Q))). \quad (5.9)$$

From (5.5e) one has

$$f(T) = f(0) - 2T^{3/2} \beta(Q) \sqrt{\frac{2\pi}{-A\beta''(Q)}} \exp(A\beta(Q)/T) \{1 + O(T)\}$$

$$-T^{3/2}\alpha_1(Q)\sqrt{\frac{2\pi}{A\alpha_1''(Q)}} \exp(A\alpha_1(Q)/T) \{1+O(T)\}. \quad (5.10)$$

At $\text{sn}(K_{k'}/(\rho_0-1), k') > \frac{1}{2}$ the second term of (5.10) is dominant because of $\beta(Q) < \alpha_1(Q)$. It is interesting that the energy gap appearing in specific heat cannot be analytically continued as a function of $\rho_0 = K_l/\zeta$ at $\rho_0 = 1 + K_{k'}/(\text{sn}^{-1}(\frac{1}{2}, k'))$.

It is well known that $f(T)$ is invariant under the transformation $(J_x, J_y, J_z) \rightarrow (J_x, -J_y, -J_z)$. Then we restrict ourselves to the case $J_z > J_y \geq |J_x|$. The energy gap appearing in specific heat is

$$\frac{J_z \text{sn}(2\zeta, l) K_{k'} k'}{2\zeta} \quad \text{for } \frac{K_l - \zeta}{\zeta} \geq \frac{\text{sn}^{-1}(\frac{1}{2}, k')}{K_{k'}}, \quad (5.11a)$$

$$\frac{J_z \text{sn}(2\zeta, l) K_{k'} k'}{\zeta} \text{sn}\left(\frac{(K_{k'}(K_l - \zeta)}{\zeta}, k'\right) \quad \text{for } \frac{K_l - \zeta}{\zeta} \leq \frac{\text{sn}^{-1}(\frac{1}{2}, k')}{K_{k'}} \quad (5.11b)$$

where k , l and ζ are defined by (5.4c) in the condition $0 \leq \zeta \leq K_l$.

The low-temperature free energy, at $J_z = J_y > 0$ and $J_y \geq J_x > -J_y$, is obtained if we put $\mu_0 H = 0$ in Eqs. (4.1) and (4.2). Then the specific heat is proportional to T at low-temperature. But we cannot obtain low-temperature free energy at $J_z \geq J_y = -J_x > 0$.

§ 6. Summary and discussion

For the Heisenberg-Ising ring, $f(0, 0)$ and $\lim_{H \rightarrow 0} \lim_{T \rightarrow 0} \chi$ were obtained by Yang and Yang,⁶⁾ and des Cloizeaux and Gaudin.⁶⁾ In Table II these quantities are given as functions of $\theta (\Delta = \cos \theta)$ at $J > 0$. An interesting feature is that these quantities are analytic as functions of Δ at $-1 < \Delta < 1$.

Table II. Analytic expression of physical quantities at $J > 0$ and $0 \leq \theta < \pi$.

$\lim_{H \rightarrow 0} \lim_{T \rightarrow 0} \chi$	$\lim_{H \rightarrow 0} \lim_{T \rightarrow 0} C_H/T$	The ground state energy per site
$\frac{4\theta\mu_0^2}{J(\pi-\theta)\pi\sin\theta}$	$\frac{2\theta}{3J\sin\theta}$	$-J\sin\theta \int_{-\infty}^{\infty} \frac{\text{sh}(\pi-\theta)\omega}{2\text{ch}\theta\omega \text{sh}\pi\omega} d\omega$

We can discuss the low-temperature properties by considering a few kinds of excitations when $\mu_0 H \gg T$, because other excitations have a finite energy gap. On the other hand in the case $H=0$, we must consider all kinds of excitations, because the energy gap vanishes. Therefore, integral equations for low-temperature thermodynamics have many unknown functions.

- a) *Relations between the results for $|\Delta| \geq 1$ and those for $|\Delta| < 1$*

Gaudin⁷⁾ gave a set of integral equations for H-I ring at $\Delta \geq 1$ which included author's set for $\Delta = 1$ ⁸⁾ as a special case. His set of equations is equivalent to the following set:

$$\varepsilon_1(x) = -As_1(x) + s_1^* T \ln(1 + \exp(\varepsilon_1(x)/T)), \quad (6.1a)$$

$$\varepsilon_j(x) = s_1^* T \ln(1 + \exp(\varepsilon_{j-1}/T)) (1 + \exp(\varepsilon_{j+1}/T)), \quad (6.1b)$$

$$\lim_{j \rightarrow \infty} \frac{\varepsilon_j(x)}{j} = 2\mu_0 H, \quad (6.1c)$$

$$f(T, H) = f(0, 0) - T \int_{-Q}^Q s_1(x) \ln(1 + \exp(\varepsilon_1(x)/T)) dx, \quad (6.1d)$$

where

$$s_1(x) = \sum_{j=-\infty}^{\infty} \frac{1}{4} \operatorname{sech} \frac{\pi}{2} (x - 2jQ) = \frac{K_k}{2\pi} \operatorname{dn}(K_k x; k), \quad (6.1e)$$

$$Q = \frac{\pi}{\emptyset}, \quad \frac{K_k}{K_{k'}} = Q, \quad (6.1f)$$

and \emptyset is determined by $\operatorname{ch} \emptyset = 4$. Johnson and McCoy⁹⁾ calculated the low-temperature free energy using these equations.

At $J > 0, 0 < 2\mu_0 H < As_1(Q), A > 1$ one obtains

$$\begin{aligned} \varepsilon_1(x) &= -As_1(x) + T \ln(2\operatorname{ch}(\mu_0 H/T)) + O(T \exp(-\varepsilon_1(Q)/T)), \\ \varepsilon_j(x) &= T \ln \left(\left(\frac{\operatorname{sh}(j\mu_0 H/T)}{\operatorname{sh}(\mu_0 H/T)} \right)^2 - 1 \right) + O(T \exp(-\varepsilon_1(Q)/T)) \quad \text{for } j > 1. \end{aligned} \quad (6.2a)$$

Then one has

$$f(T, H) = f(0, 0) - T^{3/2} s_1(Q) \sqrt{\frac{2\pi}{As_1''(Q)}} \exp(-As_1(Q)/T) 2 \operatorname{ch} \frac{\mu_0 H}{T} (1 + O(T)). \quad (6.2b)$$

At $J > 0, J(1+A) > 2\mu_0 H > As_1(Q), A \geq 1$ we can treat the problem in the same way as § 3, and obtain

$$\varepsilon_1(x) = -\frac{2\pi J \operatorname{sh} \emptyset}{\emptyset} a_1(x) + 2\mu_0 H + \int_{-Q}^Q a_2(x-x') T \ln(1 + \exp(-\varepsilon_1(x')/T)) dx', \quad (6.3a)$$

where

$$a_j(x) = \frac{\emptyset}{2\pi} \cdot \frac{\operatorname{sh} j\emptyset}{\operatorname{ch} j\emptyset - \cos \emptyset x}, \quad j = 1, 2. \quad (6.3b)$$

These correspond to Eqs. (3.4a) and (3.4b). The free energy is given by

$$f(T, H) - f(0, H) = -\frac{\pi \emptyset T^2}{6J \operatorname{sh} \emptyset} \frac{V(K)}{W(K)} + O(T^3) \quad (6.4a)$$

and K is determined by

$$2\mu_0 H = \frac{2\pi J \operatorname{sh} \emptyset}{\emptyset} \cdot \frac{V(K)}{Z(K)}, \quad (6.4b)$$

where

$$W(x) + \int_{-\kappa}^{\kappa} a_2(x-x') W(x') dx' = a_1(x), \quad (6.4c)$$

$$V(x) + \int_{-\kappa}^{\kappa} a_2(x-x') V(x') dx' = -\frac{d}{dx} a_1(x), \quad (6.4d)$$

$$Z(x) + \int_{-\kappa}^{\kappa} a_2(x-x') Z(x') dx' = 1. \quad (6.4e)$$

The second term of (3.11) and (6.4a) are analytic functions of θ^2 and \emptyset^2 , respectively. Putting $\emptyset^2 \rightarrow -\theta^2$ one finds that (6.4a), (6.4b) and $A = \operatorname{ch} \emptyset$ analytically continue to (3.11), (3.6a) and $A = \cos \theta$ as functions of θ^2 , respectively. Then one finds that $\lim_{T \rightarrow 0} C_H/T$ is analytic as a function of A at $A=1, H \neq 0$.

At $J > 0, A \geq 1, 2\mu_0 H \geq J(1+A)$ one has

$$\varepsilon_f(x) = -\frac{J \operatorname{sh} \emptyset \operatorname{sh} j\emptyset}{\operatorname{ch} j\emptyset - \cos \emptyset x} + 2j\mu_0 H + O(T^{-3/2}\lambda), \quad (6.5a)$$

$$\lambda = \exp\left(\frac{-2\mu_0 H + J(1+A)}{T}\right), \quad (6.5b)$$

therefore

$$f(T, H) = -\mu_0 H - \frac{T^{3/2}}{\pi} \sqrt{\frac{2}{J}} \int_0^\infty \ln(1 + \lambda \exp(-x^2)) dx + O(\lambda T^2). \quad (6.5c)$$

In the case $J < 0, A > 1$ and $\mu_0 H \gg T$ one has

$$\varepsilon_f(x) = \frac{J \operatorname{sh} \emptyset \operatorname{sh} j\emptyset}{\operatorname{ch} j\emptyset - \cos \emptyset x} + 2j\mu_0 H + O(T^{-3/2}\lambda), \quad (6.6a)$$

$$\lambda = \exp\left(\frac{-2\mu_0 H - J(1-A)}{T}\right), \quad (6.6b)$$

$$f(T, H) = -\mu_0 H - T^{3/2} \frac{1}{\sqrt{2\pi|J|}} \exp\left(\frac{-2\mu_0 H - J(1-A)}{T}\right). \quad (6.6c)$$

As $f(T, H)$ is invariant under the transformation $(J, A) \rightarrow (-J, -A)$, one has

$$f(T, H) = -\mu_0 H - T^{3/2} \frac{1}{\sqrt{2\pi J}} \exp\left(\frac{-2\mu_0 H + J(1+A)}{T}\right), \quad (6.7)$$

for $J > 0, A \leq -1$ and $\mu_0 H \gg T$. The results, (6.5c) and (6.7), analytically continue as functions of A to those of § 3 b) at $A = \pm 1$.

The results for the Heisenberg-Ising ring are summarized in Fig. 2. In the shaded region and on the segment d , the system shows T -linear low-temperature specific heat. On the line a , C_H is proportional to $T^{1/2}$. In the region $2\mu_0 H > (1+A)$, specific heat is proportional to $T^{-3/2} \exp(-\alpha/T)$.

Putting $l=1$ in Eq. (5.2a), one can derive the low-temperature free energy

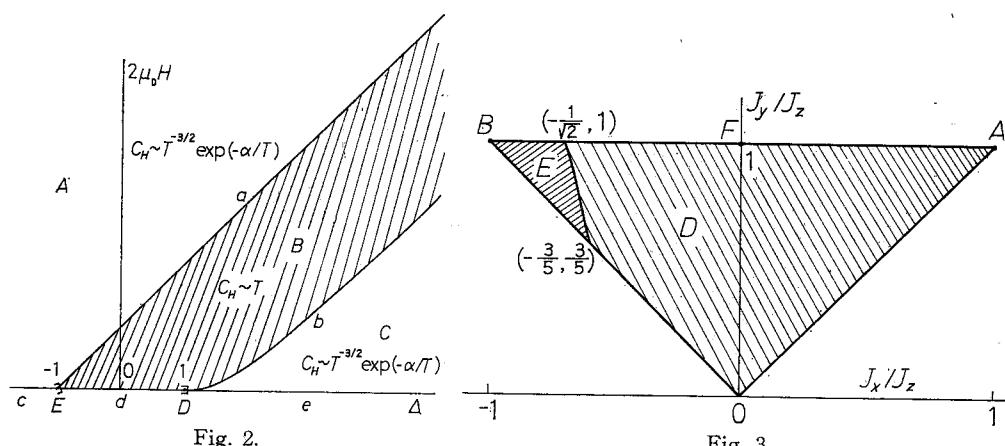


Fig. 2. Properties of the low-temperature specific heat of the Heisenberg-Ising model at $J=+1$. Regions A , B , C contain neither lines a , b , c , d , e nor end points D , E . Point D is contained in line d and point E is contained in line c .

Fig. 3. Properties of the low-temperature specific heat of the X - Y - Z model in zero field.

of Heisenberg-Ising model in zero field. This coincides with (6.2b) at $H=0$. We summarize the results for the X - Y - Z model in zero field in Fig. 3. On the line AFB except B , the specific heat (C) is proportional to T . In the shaded region and on lines AO except points A and O , C to $T^{-3/2} \exp(-\alpha/T)$. On the point O (Ising case), C to $T^{-2} \exp(-\alpha/T)$. In the regions D and E , the energy gap α is given by (5.11a) and (5.11b) respectively. One should note that the gap cannot be analytically continued from region D to E .

b) Unsolved problems

We can obtain neither low-temperature specific heat of H-I ring at $H=0$, $A \leq -1$, $J>0$ nor that of X - Y - Z ring at $J_z \geq J_y = -J_z > 0$.

If the magnetic susceptibility is invariant in reversing the order of the limits $T \rightarrow 0$, $H \rightarrow 0$, i.e.

$$\lim_{T \rightarrow 0} \lim_{H \rightarrow 0} \chi = \lim_{H \rightarrow 0} \lim_{T \rightarrow 0} \chi,$$

it is required

$$C''(0) = \frac{1}{2(\pi - \theta)} \quad \text{for (4.1)},$$

and

$$C''(0) = \frac{1}{2\theta} \quad \text{for (4.2).}$$

But we can prove neither its validity nor $C(0) = \pi/6$ from Eqs. (4.1) or Eqs. (4.2).

Acknowledgment

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Appendix A

—Calculation of the third term of high-temperature expansion—

Here we continue the calculation of Appendix C of Ref. 1). From Eqs. (C.3) of Ref. 1) we have

$$\sum_{l=1}^{\infty} [\delta_{jl}(1 + (\eta_j^{(0)})^{-1}) - D_{jl}^*] c_l^{(2)} = \frac{1}{2} ((\eta_j^{(0)})^{-1} + (\eta_j^{(0)})^{-2}) (c_j^{(1)})^2. \quad (\text{A.1})$$

Then we have

$$\widehat{c_j^{(2)}}(\omega) = \sum_{l=1}^{\infty} \widehat{B}_{jl}(\omega) \frac{(\eta_l^{(0)})^{-1} + (\eta_l^{(0)})^{-2}}{2} \widehat{(c_l^{(1)})^2}(\omega),$$

where $\widehat{B}_{jl}(\omega)$ is the jl element of inverse matrix of $\{\delta_{jl}(1 + (\eta_j^{(0)})^{-1}) - D_{jl}^*(\omega)\}$. One can show

$$\widehat{B}_{1l}(\omega) = -2 \operatorname{ch} \omega \widehat{c}_l^{(1)}(\omega) (-1)^{r(l)+1},$$

where $r(j)$ is defined by $m_{r(j)} \leq j < m_{r(j)+1}$, therefore

$$\widehat{c_1^{(2)}} = \frac{1}{2} \sum_{l=1}^{\infty} (-1)^{r(l)} \{(\eta_l^{(0)})^{-1} + (\eta_l^{(0)})^{-2}\} 2 \operatorname{ch} \omega \widehat{c}_l^{(1)}(\omega) \widehat{(c_l^{(1)})^2}(\omega). \quad (\text{A.2})$$

Then the third term of $1/T$ expansion of f is

$$\begin{aligned} -A^2 \int_{-\infty}^{\infty} s_1(x) c_1^{(2)}(x) dx &= -\frac{A^2}{2} \sum_{l=1}^{\infty} (-1)^{r(l)} \{(\eta_l^{(0)})^{-1} + (\eta_l^{(0)})^{-2}\} \int_{-\infty}^{\infty} \{c_l^{(1)}(x)\}^3 dx \\ &= -\frac{A^2}{2} \left[\sum_{i=0}^{\infty} (-1)^i \left(\sum_{l=m_i+1}^{m_{i+1}-1} U_l \right) + \sum_{i=1}^{\infty} (-1)^i U_{m_i} \right], \end{aligned} \quad (\text{A.3})$$

where

$$U_i = [(\eta_i^{(0)})^{-1} + (\eta_i^{(0)})^{-2}] \int_{-\infty}^{\infty} \{c_i^{(1)}(x)\}^3 dx.$$

Substituting (C.2) and (C.6) of Ref. 1) into the above equation and carrying out integration, we obtain

$$\begin{aligned} U_i &= \frac{1}{8\pi p_0^2 f_{m_{i+1}} \{f(1)\}^3} \left[\frac{1}{f_i f_{i+1}} \{h_{m_{i+1}}^{(3)} - h_{i+1}^{(3)} - 6 \cot \psi_{m_{i+1}} (h_i^{(2)} - h_{i+1}^{(2)}) + 2(\psi_i + \psi_{i+1})\} \right. \\ &\quad + \frac{1}{f_{i+1} f_{i+2}} \{h_{m_{i+1}}^{(3)} + h_{i+1}^{(3)} + 6 \cot \psi_{m_{i+1}} (h_{i+1}^{(2)} - h_{i+2}^{(2)}) + 2(\psi_{i+1} + \psi_{i+2})\} \\ &\quad \left. + \frac{f_{i+2}}{f_i^2 f_{i+1}} h_i^{(3)} - \frac{f_i}{f_{i+1} f_{i+2}^2} h_{i+2}^{(3)} \right] \quad \text{for } m_i \leq l < m_{i+1}, \end{aligned}$$

where

$$\begin{aligned}\psi_i &= q_i \pi / p_0, \quad \psi_{i+1} = \pi (q_i + (-1)^{i+1} p_{i+1}) / p_0, \\ \psi_{i+2} &= (q_i + 2(-1)^{i+1} p_{i+1}) / p_0, \quad \psi_{m_{i+1}} = q_{m_{i+1}} \pi / p_0, \\ h_j^{(3)} &= -3 \cot \psi_j + (1 + 3 \cot^2 \psi_j) \psi_j, \\ h_j^{(2)} &= 1 - \cot \psi_j \cdot \psi_j, \\ f_i &= f(n_i - 1), \quad f_{i+1} = f(n_i + y_i - 1), \\ f_{i+2} &= f(n_i + 2y_i - 1), \quad f_{m_{i+1}} = f(m_{i+1} - 1).\end{aligned}$$

Using

$$\begin{aligned}\frac{f_{i+2}}{f_i^2 f_{i+1}} &= -\frac{1}{f_i f_{i+1}} + \frac{2 \operatorname{ch} y_i \mu_0 H}{f_i^2}, \\ \frac{f_i}{f_{i+1} f_{i+2}^2} &= -\frac{1}{f_{i+1} f_{i+2}} + \frac{2 \operatorname{ch} y_i \mu_0 H}{f_{i+2}^2}\end{aligned}$$

and

$$\frac{1}{f_i f_{i+1}} = \frac{1}{f_{m_{i+1}}} \left(\frac{e^{-n_i \mu_0 H}}{f_i} - \frac{e^{-n_{i+1} \mu_0 H}}{f_{i+1}} \right),$$

one finds that almost all the terms in (A.3) cancel out except a few terms, and obtains finally

$$(A \cdot 3) = -\frac{J^2}{4} \left\{ \frac{1 + 2\Delta^2}{(2 \operatorname{ch} \mu_0 H)^2} - \frac{6\Delta^2}{(2 \operatorname{ch} \mu_0 H)^4} \right\}. \quad (A \cdot 4)$$

This coincides with the third term of (1.2).

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