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LETTER TO THE EDITOR

The low-temperature specific heat anomaly of the isotropic one-dimensional Heisenberg antiferromagnet ($S = \frac{1}{2}$) in a magnetic field

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Abstract. The specific heat of the isotropic $S = \frac{1}{2}$ Heisenberg antiferromagnetic chain is proportional to the temperature at low T. The proportionality constant γ is a function of field. We show that the low-field limit is anomalous in the sense that $\lim_{H\to 0} \lim_{T\to 0} \gamma = (1 + \sqrt{e/\pi})/3$ differs from $\lim_{T\to 0} \lim_{H\to 0} \gamma = \frac{2}{3}$. We also obtain an approximate interpolation formula between these two limits for situations in which H and T tend to zero simultaneously.

The magnetic susceptibility of the isotropic antiferromagnetic spin-$\frac{1}{2}$ Heisenberg chain at zero temperature and in a small magnetic field is given by ($J = 1$)

$$\chi = (2/\pi^2)(1 + 1/2|\ln H| - \ln|\ln H|/4 \ln^2 H + \dots). \tag{1}$$

The zero-field constant was evaluated by Griffiths (1964), the first logarithmic correction was anticipated by Yang and Yang (1966) and calculated by Babujian (1983), while the next-to-leading logarithmic contribution was obtained by Lee and Schlottmann (1987).

The zero-field specific heat of the Heisenberg antiferromagnet was found to be proportional to the temperature at low T, the proportionality constant γ being equal to $\frac{2}{3}$. This result has been obtained in two ways: (i) studying the γ of the anisotropic (planar-Heisenberg) chain in the limit of vanishing anisotropy (Yamada 1969 and Takahashi 1973) and (ii) by direct integration of the low-temperature solution of the thermodynamic Bethe *ansatz* equations (Babujian 1983).

The non-analytic field dependence of the susceptibility suggests an anomalous behaviour of the low-temperature specific heat in the presence of a weak magnetic field. The low-temperature specific heat of the anisotropic Heisenberg chain as a function of the anisotropy and the applied magnetic field has been studied by Johnson and McCoy (1972). They noted that the specific heat of the isotropic antiferromagnet in zero field has a singular behaviour. Depending on the way the anisotropy parameter and the magnetic field approach zero the specific heat is either proportional to T or exponentially activated due to the antiferromagnetic Ising–Heisenberg gap. Since this gap vanishes in the isotropic limit, it is expected that $C \propto T$ with the proportionality constant γ being a function of H/T.

It is the purpose of this Letter to investigate the properties of C in the low-T and small-H limit. Our main result is that the zero-field and in-field γ-coefficients differ, i.e.,

$$\lim_{T\to 0}\lim_{H\to 0}\gamma = \tfrac{2}{3} \neq \lim_{H\to 0}\lim_{T\to 0}\gamma = (1+\sqrt{e/\pi})/3. \tag{2}$$

We further provide an interpolation formula between these two values for situations in which H and T tend to zero simultaneously.

To derive our results we use the thermodynamic Bethe *ansatz* equations of the Heisenberg chain (Takahashi 1971, Gaudin 1971). The excited states of the chain consist of magnons and bound states of magnons. A bound state of n magnons is described by the thermodynamic energy potential $\varepsilon_n(\lambda)$ with λ being a real rapidity (related to the momentum). The functions $\varepsilon_n(\lambda)$ satisfy the following non-linearly coupled integral equations (Takahashi 1971)

$$\ln(1+\mathrm{e}^{\varepsilon_n/T}) = 2n\frac{H}{T} - \frac{2J}{T}\frac{n}{n^2+\lambda^2} + \sum_{m=1}^{\infty} A_{nm} * \ln(1+\mathrm{e}^{-\varepsilon_m/T}) \tag{3}$$

where J is the antiferromagnetic coupling constant, the centred asterisk denotes a convolution and the integral kernel is given by

$$A_{nm}(\lambda) = \frac{1}{2\pi}\int \mathrm{d}\omega\, \mathrm{e}^{-\mathrm{i}\omega\lambda}\coth|\omega|(\mathrm{e}^{-|n-m||\omega|} - \mathrm{e}^{-(n+m)|\omega|}).$$

The free energy is given by

$$F(T,H) = -J\ln 2 - T\int_{-\infty}^{\infty}\mathrm{d}\lambda\, G_0(\lambda)\ln(1+\mathrm{e}^{\varepsilon_1(\lambda)/T}) \tag{4}$$

where $G_n(\lambda)$ is defined by

$$G_n(\lambda) = \frac{1}{2\pi}\int \mathrm{d}\omega\, \mathrm{e}^{-\mathrm{i}\omega\lambda}\frac{\mathrm{e}^{-n|\omega|}}{2\cosh|\omega|}. \tag{5}$$

The functions ε_n are symmetric, $\varepsilon_n(-\lambda) = \varepsilon_n(\lambda)$ and are monotonically increasing for $\lambda > 0$. Takahashi (1971) has shown that for $n \neq 1$, the potentials $\varepsilon_n(\lambda)$ are positive for all λ, while $\varepsilon_1(\lambda)$ changes sign if $H \neq 0$. We define a parameter B such that $\varepsilon_1(\pm B) = 0$. This implies that in the limit $T \to 0$ with field, the contributions of $m \geqslant 2$ to the integrals in equation (3) are exponentially small and negligible. Hence, we can rewrite the integral equation (3) for $n = 1$ as

$$\varepsilon_1 = H - 2\pi J G_0 + G_1 * T\ln(1+\mathrm{e}^{\varepsilon_1/T}). \tag{6}$$

To obtain the low-temperature coefficient γ of the free energy, we expand $\varepsilon_1(\lambda)$ to order T^2, $\varepsilon_1 \simeq \varepsilon_1^{(0)} + T^2\varepsilon_1^{(2)}$. Using the Sommerfeld formula, the integral equations for $\varepsilon_1^{(0)}$ and $\varepsilon_1^{(2)}$ become

$$\varepsilon_1^{(0)}(\lambda) = H - 2\pi J G_0(\lambda) + 2\int_B^{\infty}\mathrm{d}\lambda'\, G_1(\lambda-\lambda')\varepsilon_1^{(0)}(\lambda') \tag{7}$$

$$\varepsilon_1^{(2)}(\lambda) = \frac{\pi^2}{6}\left|\frac{\mathrm{d}\varepsilon_1^{(0)}}{\mathrm{d}\lambda}\right|_B^{-1}(G_1(\lambda+B) + G_1(\lambda-B)) + 2\int_B^{\infty}\mathrm{d}\lambda'\, G_1(\lambda-\lambda')\varepsilon_1^{(2)}(\lambda'). \tag{8}$$

The free energy is then given by

$$F = -J\ln 2 - 2\int_B^\infty \mathrm{d}\lambda\, G_0(\lambda)\varepsilon_1^{(0)}(\lambda) - T^2\left(\frac{\pi^2}{3}\left|\frac{\mathrm{d}\varepsilon_1^{(0)}}{\mathrm{d}\lambda}\right|_B^{-1} G_0(B) + 2\int_B^\infty \mathrm{d}\lambda\, G_0(\lambda)\varepsilon_1^{(2)}(\lambda)\right). \tag{9}$$

Equation (7) is the ground-state integral equation solved for a small field ($0 < H \ll J$) by Babujian (1983). The parameter B increases monotonically with decreasing field and tends to infinity as $H \to 0$, approximately like $B \sim -(\pi/2)\ln H$.

Our procedure to solve the integral equation (8) is similar to the one used by Babujian to obtain $\varepsilon_1^{(0)}$. Defining $\varphi(\lambda) = \varepsilon_1^{(2)}(\lambda + B)$, we have that $\varphi(\lambda)$ satisfies the equation

$$\varphi(\lambda) = \frac{\pi^2}{6}\left|\frac{\mathrm{d}\varepsilon_1^{(0)}}{\mathrm{d}\lambda}\right|_B^{-1}(G_1(\lambda) + G_1(\lambda + 2B)) + \int_0^\infty \mathrm{d}\lambda'\,(G_1(\lambda - \lambda') + G_1(\lambda + \lambda' + 2B))\varphi(\lambda'). \tag{10}$$

We solve this equation iteratively, $\varphi(\lambda) \simeq \varphi_1(\lambda) + \varphi_2(\lambda) + \ldots$, where φ_2 is of higher order in $1/B$ than φ_1. Since $G_1(B) \sim 1/B$ for large B, we separate the integral equations for $\varphi_1(\lambda)$ and $\varphi_2(\lambda)$ as follows:

$$\begin{aligned}\varphi_1(\lambda) &= \frac{\pi^2}{6}\left|\frac{\mathrm{d}\varepsilon_1^{(0)}}{\mathrm{d}\lambda}\right|_B^{-1} G_1(\lambda) + \int_0^\infty \mathrm{d}\lambda'\, G_1(\lambda - \lambda')\varphi_1(\lambda') \\ \varphi_2(\lambda) &= \varphi_1(-\lambda - 2B) + \int_0^\infty \mathrm{d}\lambda'\, G_1(\lambda - \lambda')\varphi_2(\lambda')\end{aligned} \tag{11}$$

etc. The equations (11) are of the Wiener-Hopf type and the solution $\varphi_1(\lambda)$ for $\lambda \geqslant 0$ is given by

$$\varphi_1(\lambda) = \frac{1}{2\pi}\int \mathrm{d}\omega\, \mathrm{e}^{-\mathrm{i}\omega\lambda}\frac{\pi^2}{6}\left|\frac{\mathrm{d}\varepsilon_1^{(0)}}{\mathrm{d}\lambda}\right|_B^{-1}(g^+(\omega) - 1) \tag{12}$$

where

$$g^+(\omega) = \sqrt{2\pi}(-\mathrm{i}\omega/e\pi)^{-\mathrm{i}\omega/\pi}/\Gamma(\tfrac{1}{2} - \mathrm{i}\omega/\pi).$$

Inserting φ_1 into the free energy expression (9), we obtain that $\gamma = (1 + \sqrt{e/\pi})/3$ in a small field. This result differs from the zero-field γ-value, $\gamma = \frac{2}{3}$, but does not show logarithmic corrections as found for the susceptibility, equation (1). (Note that φ_2 can only contribute to order $1/B^2$ or higher, i.e., not to the logarithmic order of the two leading terms in (1).) The in-field γ-value is less than $\frac{2}{3}$, the zero-field γ, as expected, since the magnetic field polarises the spins of the system so that the entropy and specific heat are reduced.

So far we have shown that the specific heat coefficient γ in the presence of a magnetic field is different from the zero-field value, i.e., $\lim_{H\to 0}\lim_{T\to 0}\gamma = (1 + \sqrt{e/\pi})/3 \neq \lim_{T\to 0}\lim_{H\to 0}\gamma = \frac{2}{3}$. Hence γ depends on the way the point $H = T = 0$ is approached. In the following we derive an approximate interpolation formula between the above two limits, valid for very small H and T.

If either $|\lambda|$ or the string length n are sufficiently large, the driving terms of the integral equations become small and the solution for $\varepsilon_n(\lambda)$ is asymptotically the free spin one, i.e.

$$\varepsilon_n = T\ln\{[\sinh^2(n+1)x_0]/(\sinh^2 x_0)\} \tag{13}$$

where $x_0 = H/T$. We now approximate equation (3) for $n = 1$ by inserting the free spin ε_n for all $n \geqslant 2$ and obtain

$$\varepsilon_1 = \tilde{H}(T) - 2\pi J G_0 + G_1 * T\ln(1 + e^{\varepsilon_1/T}). \tag{14}$$

In this way we decoupled the integral equation for $n = 1$ from all others. Here $\tilde{H}(T)$ is the effective field induced by the contributions of ε_n for $n \geqslant 2$ at low T and is given by

$$\tilde{H}(T) = T\ln[(\sinh 3x_0)/(\sinh 2x_0)]. \tag{15}$$

Note that $\tilde{H}(T)$ reduces to H as $T \to 0$, since $x_0 \to \infty$. Because of our approximation, however, the low-field behaviour is not taken into account appropriately. In order to recover the correct zero-field γ we incorporate a parameter α into $\tilde{H}(T)$ (to be determined later), so that

$$\tilde{H}(T) = T\ln\{[\sinh(2\alpha+1)x_0]/(\sinh 2\alpha x_0)\}. \tag{15a}$$

Note that equation (14) is just the integral equation (6) except for the replacement of the field H by the effective field $\tilde{H}(T)$, so we can use the same procedure to solve the integral equation as before. In this way the free energy ($J = 1$) is given by

$$F = -\ln 2 - (T^2/6)(1 + \sqrt{e/\pi}) - (\tilde{H}^2(T)/\pi^2)(1 + 1/2\,|\ln \tilde{H}|$$
$$- \ln|\ln \tilde{H}|/4\ln^2 \tilde{H} + \ldots). \tag{16}$$

Note that at $T = 0$ this expression yields the correct low-field susceptibility given by equation (1). By differentiating with respect to T we obtain the entropy of the system

$$S/T = (1+\sqrt{e/\pi})/3 + (2/\pi^2)(\tilde{H}(T)/T)[\tilde{H}(T)/T + 2\alpha x_0 \coth 2\alpha x_0 / -(2\alpha+1)x_0$$
$$\times \coth(2\alpha+1)x_0](1 + 1/2|\ln\tilde{H}| - \ln|\ln\tilde{H}|/4\ln^2\tilde{H} + \ldots). \tag{17}$$

In the limit $T \to 0$ with H finite (i.e., $x_0 \to \infty$), we recover the γ-value, $(1+\sqrt{e/\pi})/3$. On the other hand, the γ-value in the zero-field limit (i.e. $x_0 \to 0$) is

$$\lim_{T\to 0}\lim_{H\to 0} \gamma = (1+\sqrt{e/\pi})/3 + (2/\pi^2)\ln^2[(2\alpha+1)/2\alpha]. \tag{18}$$

We determine the parameter α by equating (18) to the expected zero-field $\gamma = \frac{2}{3}$, $\alpha \simeq 1.24$. According to our interpolation formula, equation (17), the low-temperature specific heat coefficient γ is monotonically decreasing from $\frac{2}{3}$ to $(1+\sqrt{e/\pi})/3$ as x_0 is increased from zero to infinity. Note that equation (17) is valid only for fields and temperatures much smaller than the antiferromagnetic coupling. As a consequence the γ-value is quite rapidly saturated to its value in the limit $x_0 \to \infty$.

The above arguments for the isotropic one-dimensional spin-$\frac{1}{2}$ Heisenberg antiferromagnet can straightforwardly be extended to chains with higher spin and SU(2) invariance (Babujian (1983) model).

Finally we would like to discuss our results in the context of the Kondo problem. The thermodynamic Bethe *ansatz* equations of the Heisenberg chain and the Kondo problem have a very similar structure and the analogy between the two models has frequently been invoked (Andrei *et al* 1983, Tsvelick and Wiegmann 1983). For the Kondo problem, a constant Wilson ratio, i.e. $\lim \gamma/\chi = 2\pi^2/3$, independent of the strength of the magnetic field, has been obtained. For the Heisenberg chain, on the other hand, our results prove that γ/χ is not universal, imposing in this way some limitations in the correspondence between the physical properties of the two models.

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