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LETTER TO THE EDITOR

The low-temperature specific heat anomaly of the SU(2) invariant 1D Heisenberg antiferromagnet of spin S in a small magnetic field

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Abstract. It is expected that the specific heat of the SU(2)-invariant 1D Heisenberg antiferromagnet of spin S is linear to the temperature at low T with the linear coefficient γ_S being a function of field H. Our main result is that $\lim_{H\to 0}\lim_{T\to 0}\gamma_S = \frac{1}{3}[1+\sqrt{S}\Gamma(S)(e/S)^S/\pi] \neq \lim_{T\to 0}\lim_{H\to 0}\gamma_S = 2S/(1+S)$. This extends the previous result for $S=\frac{1}{2}$ to other spin values. We also provide an approximate interpolation formula between these two limits as a function of H/T for very small H and T.

It is well known by the Bethe-ansatz method that the quantum spin chains show much non-trivial behaviour. In particular, the logarithmic singularities appear to be common in the integrable quantum spin chains with SU symmetry. The magnetic susceptibility at zero temperature of the SU(2)-invariant isotropic Heisenberg chain of spin S with an antiferromagnetic coupling J in a small magnetic field is given by ($J=1$)

$$\chi(0,H) = (4S/\pi^2)(1 + S/|\ln H| - S^2 \ln|\ln H|/\ln^2 H + \ldots) \tag{1}$$

which shows logarithmic singularities as $H \to 0$. The constant zero-field χ was obtained by Griffiths (1964), the first logarithmic correction by Babujian (1983) and the second one by Lee and Schlottmann (1987).

The zero-field specific heat of the SU(2)-invariant Heisenberg antiferromagnet of spin S has been studied by Babujian by analysing the thermodynamic Bethe-ansatz equations. He found that the specific heat $C^{H=0} = \gamma_S T$ in the low temperature region with

$$\lim_{T\to 0}\lim_{H\to 0}\gamma_S = \frac{2}{3} - \frac{2}{\pi^2}\sum_{n=1}^{2S-1}\int_0^{x_n} dx\left(\frac{\ln(1-x)}{x} + \frac{\ln x}{1-x}\right) \tag{2}$$

where

$$x_n = \sin^2[\pi/(2S+2)]/\sin^2[\pi(n+1)/(2S+2)].$$

Note that the integral cannot be evaluated exactly except for $\gamma_{1/2} = \frac{2}{3}$ and $\gamma_1 = 1$. However, the numerical calculation shows that the zero-field γ_S converges to the value

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corresponding to that obtained by the prediction of the critical behaviour of 1D quantum spin systems via conformal field theory (Affleck 1986), i.e.,

$$\lim_{T\to 0}\lim_{H\to 0}\gamma_S = 2S/(1+S). \tag{3}$$

For this reason, from now on, we are going to use this expression instead of (2).

In this letter we report the anomalous properties of the specific heat for $T \ll J$ and $2SH \ll J$ by extending the arguments for $S=\frac{1}{2}$ (Lee and Schlottmann 1989) to the higher spins. Our main result is that the linear coefficient of the specific heat, γ_S, depends on the way the singular point $H = T = 0$ is approached, i.e.,

$$\lim_{H\to 0}\lim_{T\to 0}\gamma_S = \tfrac{2}{3}[1+\sqrt{S}\Gamma(S)(e/S)^S/\pi] \neq \lim_{T\to 0}\lim_{H\to 0}\gamma_S = 2S/(1+S) \tag{4}$$

where Γ is the gamma function. We also obtain an approximate interpolation formula between these two limits for situations in which H and T tend to zero simultaneously.

The SU(2) generalization of the $S=\frac{1}{2}$ Heisenberg chain is given by (Kulish *et al* 1981)

$$H_S = J\sum_{i=1}^{N} Q_{2S}(\boldsymbol{S}_i\cdot\boldsymbol{S}_{i+1}) - 2H\sum_{i=1}^{N} S_i^z \tag{5}$$

where J is the antiferromagnetic coupling constant and

$$Q_{2S}(x) = \sum_{j=1}^{2S}(\psi(j+1)-\psi(1))\prod_{l\neq j}^{2S}\frac{x-x_l}{x_j-x_l} \tag{6}$$

with $x_l = \frac{1}{2}[l(l+1)-2S(S+1)]$ and ψ the digamma function.

The excited states of the model consist of magnons and bound states of these magnons. Each bound state of n magnons is characterized by the thermodynamic energy potential $\varepsilon_n(\lambda)$, where λ is a real rapidity and related to the momentum. $\varepsilon_n(\lambda)$ where $n=1,\ldots,\infty$, is then determined by the so-called thermodynamic Bethe-ansatz equations (Babujian 1983)

$$\ln(1+e^{\varepsilon_n/T}) = 2n\frac{H}{T} - 2\pi\frac{J}{T}A_{n,2S}*G + \sum_{m=1}^{\infty} A_{n,m}*\ln(1+e^{-\varepsilon_m/T}) \tag{7}$$

where the centre asterisk denotes a convolution, $G(\lambda) = (4\cosh(\lambda\pi/2))^{-1}$ and

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

The free energy per site is given by

$$F(T,H) = F(0,0) - T\int_{-\infty}^{\infty} d\lambda\, G(\lambda)\ln(1+e^{\varepsilon_{2S}/T}) \tag{8}$$

where

$$F(0,0) = \begin{cases} -J\displaystyle\sum_{k=1}^{S}\frac{1}{2k-1} & \text{for integer } S \\ -J\ln 2 - J\displaystyle\sum_{k=1}^{S-1/2}\frac{1}{2k} & \text{for half-integer } S \end{cases}$$

It has been shown that the $\varepsilon_n(\lambda)$ for $n \neq 2S$ are positive for all λ, while $\varepsilon_{2S}(\lambda)$ changes sign when $H \neq 0$. We define a parameter B such that $\varepsilon_{2S}(\pm B) = 0$ since the $\varepsilon_n(\lambda)$ are symmetric and monotonically increasing for $\lambda > 0$. As a consequence of $\varepsilon_{n\neq 2S} > 0$, in the limit $T \to 0$ with finite field we have a contribution of only $m = 2S$ to the integral in equation (7). Hence we can rewrite the integral equation (7) for $n = 2S$ (note that we need only $\varepsilon_{2S}(\lambda)$ to obtain the free energy in equation (8)) as

$$\varepsilon_{2S}(\lambda) = H - 2\pi J G(\lambda) + K * T \ln(1 + \mathrm{e}^{\varepsilon_{2S}/T}) \tag{9}$$

where the integral kernel is given by

$$K(\lambda) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \mathrm{d}\omega\, \mathrm{e}^{-\mathrm{i}\omega\lambda} \frac{\sinh(2S-1)|\omega| + \mathrm{e}^{-|\omega|} \sinh 2S|\omega|}{2\cosh|\omega| \sinh 2S|\omega|}. \tag{10}$$

It is sufficient to expand $\varepsilon_{2S}(\lambda)$ to order T^2 to evaluate the low temperature specific heat coefficient in the field, i.e., $\varepsilon_{2S} \simeq \varepsilon_{2S}^{(0)} + T^2 \varepsilon_{2S}^{(2)}$. We then have the integral equations for $\varepsilon_{2S}^{(0)}$ and $\varepsilon_{2S}^{(2)}$:

$$\varepsilon_{2S}^{(0)}(\lambda) = H - 2\pi J G(\lambda) + 2\int_B^{\infty} \mathrm{d}\lambda'\, K(\lambda - \lambda')\varepsilon_{2S}^{(0)}(\lambda') \tag{11}$$

$$\varepsilon_{2S}^{(2)}(\lambda) = \frac{\pi^2}{6} \left|\frac{\mathrm{d}\varepsilon_{2S}^{(0)}}{\mathrm{d}\lambda}\right|_B^{-1} [K(\lambda + B) + K(\lambda - B)] + 2\int_B^{\infty} \mathrm{d}\lambda'\, K(\lambda - \lambda')\varepsilon_{2S}^{(2)}(\lambda'). \tag{12}$$

Here we have used the Sommerfeld formula to expand $\ln(1 + \mathrm{e}^{\varepsilon_{2S}/T})$ at low T. The free energy is expressed by

$$\begin{aligned} F(T,H) = F(0,0) &- 2\int_B^{\infty} \mathrm{d}\lambda\, G(\lambda)\varepsilon_{2S}^{(0)}(\lambda) \\ &- T^2\left(\frac{\pi^2}{3}\left|\frac{\mathrm{d}\varepsilon_{2S}^{(0)}}{\mathrm{d}\lambda}\right|_B^{-1} G(B) + 2\int_B^{\infty} \mathrm{d}\lambda\, G(\lambda)\varepsilon_{2S}^{(2)}(\lambda)\right). \end{aligned} \tag{13}$$

Equation (11) was solved by Babujian (1983) for very small fields yielding the following useful relations

$$\begin{aligned} &B \sim -(2/\pi)\ln H \\ &\left|\frac{\mathrm{d}\varepsilon_{2S}^{(0)}}{\mathrm{d}\lambda}\right|_B = \frac{\pi H}{4\sqrt{S}}\left(1 + \frac{S}{2|\ln H|} - \frac{S^2 \ln|\ln H|}{2\ln^2 H} + \dots\right). \end{aligned} \tag{14}$$

Note that the parameter B tends to infinity as $H \to 0$.

To obtain $\lim_{H\to 0}\lim_{T\to 0}\gamma_S$, we can take the limit $B \to \infty$ in equation (13). However we have to be careful in doing this because the integral involving $\varepsilon_{2S}^{(2)}(\lambda)$ contributes to the γ_S values with the same order of $|\mathrm{d}\varepsilon_{2S}^{(0)}/\mathrm{d}\lambda|_B^{-1}\, G(B)$. Hence we cannot simply neglect the integral. For this reason, we have to solve the integral equation (12) to obtain the linear specific heat coefficient γ_S in finite field. For this purpose let us define $\varphi(\lambda) = \varepsilon_{2S}^{(2)}(\lambda + B)$ which satisfies the Wiener–Hopf-type integral equation

$$\begin{aligned} \varphi(\lambda) = \frac{\pi^2}{6}&\left|\frac{\mathrm{d}\varepsilon_{2S}^{(0)}}{\mathrm{d}\lambda}\right|_B^{-1} [K(\lambda) + K(\lambda + B)] \\ &+ \int_0^{\infty} \mathrm{d}\lambda'\, [K(\lambda - \lambda') + K(\lambda + \lambda' + B)]\varphi(\lambda'). \end{aligned}$$

Since we are interested in a small field (i.e., in a large B) and $K(B) \sim 1/B$ for large B, we solve the equation of $\varphi(\lambda)$ iteratively, $\varphi(\lambda) \simeq \varphi_1(\lambda) + \varphi_2(\lambda) + \dots$, with φ_2 being of higher order in $1/B$ than φ_1. Then we have

$$\varphi_1(\lambda) = \frac{\pi^2}{6}\left|\frac{\mathrm{d}\varepsilon_{2S}^{(0)}}{\mathrm{d}\lambda}\right|_B^{-1} K(\lambda) + \int_0^\infty \mathrm{d}\lambda'\, K(\lambda-\lambda')\varphi_1(\lambda)$$

$$\varphi_2(\lambda) = \varphi_1(-\lambda-2B) + \int_0^\infty \mathrm{d}\lambda'\, K(\lambda-\lambda')\varphi_2(\lambda'). \tag{15}$$

After some calculation we obtain $\varphi_1(\lambda \geqslant 0)$

$$\varphi_1(\lambda) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{d}\omega\, \mathrm{e}^{-\mathrm{i}\omega\lambda}\, \frac{\pi^2}{6}\left|\frac{\mathrm{d}\varepsilon_{2S}^{(0)}}{\mathrm{d}\lambda}\right|_B^{-1} (g_S^+(\omega) - 1) \tag{16}$$

where

$$g_S^+(\omega) = \sqrt{(\pi/S)}\,\frac{\Gamma(-\mathrm{i}^{\omega/\pi})(-\mathrm{i}^{2S\omega/e\pi})^{-\mathrm{i}(2S\omega/\pi)}}{\Gamma(\frac{1}{2}-\mathrm{i}^{\omega/\pi})\Gamma(-\mathrm{i}^{2S\omega/\pi})}.$$

It is not difficult to show that φ_2 contributes to order $1/B^2$ (or higher), which is not interesting to us. Inserting (14) and (16) into the free energy (13), we obtain $\lim_{H\to 0}\lim_{T\to 0}\gamma_S = \frac{4}{3}[1 + \sqrt{S}\Gamma(S)(e/S)^S/\pi] \neq \lim_{T\to 0}\lim_{H\to 0}\gamma_S = 2S/(1+S)$. The γ_S in finite field is less than γ_S in zero field as expected since the entropy is reduced in the ordered system. This result also reproduces the one for $S = \frac{1}{2}$ correctly.

Finally let us derive an approximate interpolation formula between the above two values as a function of H/T for very small H and T.

The integral equation (7) yields asymptotically free spin solutions for $\varepsilon_n(\lambda)$ whenever either $|\lambda|$ is large or the string index n is sufficiently away from $2S$. The free spin solution is given by

$$\varepsilon_n = T \ln \sinh^2(n+1)x_0/\sinh^2 x_0 \tag{17}$$

where $x_0 = H/T$. Since at low T the free spin solution gives $\varepsilon_n \simeq 2nH$, we approximate the integral equation (7) for $n = 2S$ by assuming the free solutions for $m \neq 2S$. We then have an integral equation for $n = 2S$ decoupled from all others, i.e.,

$$\varepsilon_{2S}(\lambda) = \tilde{H}_S(T) - 2\pi J G(\lambda) + K * T \ln(1 + \mathrm{e}^{\varepsilon_{2S}/T}) \tag{18}$$

where $\tilde{H}_S$, the effective field induced by the contributions of $\varepsilon_{n\neq 2S}$ at low T, is given by

$$\tilde{H}_S(T) = T \ln \frac{\sinh 2Sx_0[\sinh(2S+1)x_0]^{-1+1/2S}}{\sinh x_0} + T \ln \frac{\sinh(2S+2)x_0}{\sinh(2S+1)x_0}.$$

The first term represents the contributions of $\varepsilon_{n<2S}$ and vanishes for $S = \frac{1}{2}$ as expected, while the second term is obtained by the approximation for $\varepsilon_{n>2S}$. $\tilde{H}_S$ yields a correct zero-T limit, i.e., $\lim_{T\to 0}\tilde{H}_S(T) = \lim_{x_0\to 0}\tilde{H}_S = H$. However, our approximation does not take into account the zero-H limit appropriately. The simplest way to fix this limit is to introduce a parameter α_S to $\tilde{H}_S$ such that

$$\tilde{H}_S(T) = T \ln \frac{\sinh 2Sx_0[\sinh(2S+1)x_0]^{-1+1/2S}}{\sinh x_0} + T \ln \frac{\sinh(\alpha_S+1)x_0}{\sinh \alpha_S x_0}. \tag{19}$$

α_S will be determined later using the zero-field γ_S values. Since equation (18) is just the integral equation (9) with H being replaced by $\tilde{H}_S(T)$, using the same procedure as before we obtain the linear specific heat coefficient ($J = 1$)

$$\gamma_S(T, H) = \tfrac{1}{3}[1 + \sqrt{S}\Gamma(S)(e/S)^S/\pi] + (4S/\pi^2)(\partial\tilde{H}_S/\partial T)^2(1 + S/|\ln\tilde{H}_S| - S^2\ln|\ln\tilde{H}_S|/\ln^2\tilde{H}_S + \ldots). \tag{20}$$

This expression recovers the γ_S values in the zero-temperature limit as expected, i.e., $\tfrac{1}{3}[1 + \sqrt{S}\Gamma(S)(e/S)^S/\pi]$. While in the zero-field limit, i.e., $x_0 \to 0$, it yields

$$\lim_{T\to 0}\lim_{H\to 0}\gamma_S = \tfrac{1}{3}[1 + \sqrt{S}\Gamma(S)(e/S)^S/\pi] + (4S/\pi^2)\ln^2[2S(2S+1)^{-1+1/2S}(1 + 1/\alpha_S)]. \tag{21}$$

Now we evaluate the parameter α_S by equating the equation (21) to the expected zero-field $\gamma_S = 2S/(1+S)$. α_S is then given by

$$\alpha_S^{-1} = \exp\{[(\pi^2/4S)(\gamma_S^{\text{zero field}} - \gamma_S^{\text{in field}})]^{1/2} + \ln(2S+1)^{1-1/2S}/2S\} - 1$$

where $\gamma_S^{\text{zero field}} = 2S/(1+S)$ and $\gamma_S^{\text{in field}} = \tfrac{1}{3}[1 + \sqrt{S}\Gamma(S)(e/S)^S/\pi]$. Note that our interpolation formula (20) is valid only for $T \ll J$ and $2SH \ll J$. Hence it follows that the linear specific heat coefficient γ_S is monotonically decreasing from the $\gamma_S^{\text{zero field}}$ value as x_0 is increased, and is rapidly saturated to the $\gamma_S^{\text{in field}}$ value.

We expect that the above arguments for the SU(2)-invariant Heisenberg antiferromagnet of arbitrary spin S can be extended to the SU(N)-invariant spin chains with N being $2S + 1$ (Sutherland 1975).

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