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Low-temperature features of thermodynamics of an open isotropic Heisenberg chain

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Low-temperature magnetic susceptibility and specific heat of an antiferromagnetic Heisenberg chain with open boundary conditions are calculated with the help of exact Bethe ansatz method. These characteristics behave with temperature in a different way from the ones of a periodic chain.

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Low-dimensional quantum spin systems, as one of the most interesting phenomena in condensed matter physics, have attracted much interest of theorists and experimentalists during last years. For example, recent experiments on two-dimensional (2D) and 1D antiferromagnetic spin systems reveal very interesting behavior of nonmagnetic impurities [1,2]. In 2D Heisenberg antiferromagnets nonmagnetic impurities may give rise to divergent magnetic susceptibility [3]. In 1D spin chains nonmagnetic impurities cut chains [4]. The behavior of latters is different from the behavior of bulk spins. Exact Bethe ansatz description of open quantum chains was initiated by Gaudin [5]. Thermodynamic characteristics of an essentially anisotropic XXZ spin-1/2 open chain were studied by the Bethe ansatz in [6]. It was shown there that low-temperature characteristics of the XXZ chain may diverge at low temperatures. The ground state magnetic susceptibility of a Heisenberg chain with open boundary conditions was calculated in [7], where it was shown that edge contributions to the susceptibility diverge in the ground state as a function of a homogeneous magnetic field H. On the other hand, it is known that irrelevant boundary operators (in the renormalization group sense) usually give only subleading contributions to any physical quantities.

Very recently two groups studied the low-temperature behavior of characteristics of an open spin-1/2 chain with isotropic Heisenberg antiferromagnetic interactions between nearest spins perturbatively, using bosonization and renormalization group-like approaches [8]. However, there were no exact results for such a characteristics. Motivated by these facts, in this work we study the low-temperature characteristics of a Heisenberg spin-1/2 chain.

Let us study the behavior of the Heisenberg antiferromagnetic spin-1/2 chain of the length L with open boundary conditions with the Hamiltonian $\mathcal{H} = J\sum_{n=1}^{L-1}\mathbf{S}_n\mathbf{S}_{n+1}$, where J is the exchange constant using Bethe's ansatz. The principal difference between Bethe ansatz studies of periodic and open chains consists of reflections at edges of open chain, which produce not only permutations, but also negations of quantum numbers (rapidities) parametrizing eigenfunctions and eigenvalues of the stationary Schrödinger equation [5]. The Bethe ansatz equations (BAE) for the set of rapidities $\{\lambda\}_{j=1}^{M}$, where M is the number of down spins, is [5,7]:

$$\left(\frac{\lambda_j + (i/2)}{\lambda_j - (i/2)}\right)^{2L} \frac{\lambda_j + iS_1}{\lambda_j - iS_1}\frac{\lambda_j + iS_L}{\lambda_j - iS_L} =$$

$$= \prod_{\substack{l=1,\\ l\neq j}}^{M} \frac{\lambda_j - \lambda_l + i}{\lambda_j - \lambda_l - i}\frac{\lambda_j + \lambda_l + i}{\lambda_j + \lambda_l - i}, \qquad (1)$$

$j = 1,\ldots, M$. The energy is

$$E = \frac{1}{4}[-2H(L-2M) + 2h_1 + 2h_2 + (L-1)J] - $$
$$- 2J\sum_{j=1}^{M}(4\lambda_j^2 + 1)^{-1}, \qquad (2)$$

where H is the value of the homogeneous magnetic field and $2S_{1,L} = (J/h_{1,L}) - 1$. Here $h_{1,L}$ are boundary magnetic fields, which act only on the spins at the sites 1 and L, respectively. BAE for an open chain differ from the ones for a closed geometry [9] by the following: (i) there are not only differences but also sums of rapidities on the right-hand sides of BAE for an open case; (ii) the effective length of a chain is doubled; (iii) on the left-hand sides of BAE for an open case there are multipliers connected with nonzero boundary fields. $S_{1,L}$ play the role of effective «boundary spins». These «boundary spins» depend on the values of the boundary fields $h_{1,L}$. For $h_{1,L} = 0$ these boundary spins are infinite, leading to effective twists of π at each edge. At $h_{1,L} = \pm J$ these effective «boundary spins» change their signs. This situation is related to the effective addition or removal of one site to or from the chain, respectively, with finite zero-field magnetic susceptibility. It leads to onsets of complex roots of Bethe ansatz equations Eqs. (1) in the ground state: For $-1/2 < S_{1,L} < 0$ there appear bound states parametrized by complex rapidities $\lambda_j = (i/2)[1 - (J/h_{1,L})]$, localized at edges. Finally, for $h_{1,L} \to \pm\infty$ we have $S_{1,L} \to -1/2$, effectively removing one site, respectively, from the system.

Consider how these differences affect thermodynamic characteristics in the limit of large L and M (with M/L fixed). In the framework of the string hypothesis [10] we look for the solution of Eqs. (1) in the form of strings $\lambda_j = \lambda_{j,m} + i[(m+1)/2 - \nu]$ with $\nu = 1,\ldots, m$, valid with the accuracy $O(\exp(-L))$; taking then the logarithm we get for BAE:

$$\theta_{m,1}(\lambda_j^m) + \frac{1}{2L}[\theta_{m,2S_1}(\lambda_j^m) + \theta_{m,2S_2}(\lambda_j^m)] = \frac{\pi}{L} I_{j,m} +$$
$$+ \frac{1}{2L}\sum_{\substack{n=1\\ n\neq m}}^{\infty}\sum_{l=1}^{M_n}[\Theta_{mn}(\lambda_j^m - \lambda_l^n) + \Theta_{mn}(\lambda_j^m + \lambda_l^n)], \qquad (3)$$

where $\theta_n(x) = 2\tan^{-1}(x/n)$,

$$\theta_{m,n}(x) = \sum_{l=1}^{\min([m],[n])} \theta_{m+1+n-2l}(x), \qquad (4)$$

$[x]$ denotes the integer part of x,

$$\Theta_{mn}(x) = (1-\delta_{m,n})\theta_{|m-n|}(x) + 2\theta_{|m-n|+2}(x) + \ldots +$$
$$+ 2\theta_{m+n-2}(x) + \theta_{m+n}(x), \qquad (5)$$

and integers

$$1 \le I_{j,m} \le [L + M_m - 2\sum_{n=1}^{\infty}\min(m,n)M_n]$$

appear because the logarithm is the multi-valued function. We look for solutions to thermodynamic BAE for large L, keeping corrections of order of L^{-1}, too. In this limit we introduce distribution functions (densities) for particles, $\rho_m(x)$, and holes, $\rho_{mh}(x)$, corresponding to strings of length m:

$$\rho_{mh}(\lambda) + \frac{1}{2}\sum_{n=1}^{\infty}[A_{m,n}(\lambda - \lambda') + A_{m,n}(\lambda + \lambda')] *$$
$$* [\rho_n(\lambda') - p(\lambda')\delta_{m,1}] = \frac{1}{2L}\sum_{n=1}^{\infty}[A_{m,n}(\lambda - \lambda') +$$
$$+ A_{m,n}(\lambda + \lambda')] * p(\lambda')(\delta_{m,[2S_1]} + \delta_{m,[2S_2]}), \quad (6)$$

where $p(\lambda) = 1/[4\cosh(\pi\lambda/2)]$, $*$ denotes the convolution,

$$A_{m,n}(x) = a_{|m-n|}(x) + a_{m+n}(x) +$$
$$+ 2\sum_{l=1}^{\min(n,m)-1} a_{m+n-2l}(x), \qquad (7)$$

and $a_m(x) = 2m/[\pi(4x^2 + m^2)]$. The internal energy E and the total magnetic moment M^z are given as

$$E = E_0 - \frac{1}{2}\sum_{m=1}^{\infty} m\int_0^{\infty} d\lambda\, \theta'_{m,1}(\lambda)\rho_m(\lambda),$$

$$M^z = \frac{L}{2} - L\sum_{m=1}^{\infty} m\int_0^{\infty} d\lambda\, \rho_m(\lambda), \qquad (8)$$

where $E_0 = -[2(HL + h_1 + h_2) - (L-1)J]/4$ is the energy of the ferromagnetic state. The (complimentary) set of thermodynamic equations for dressed energies $\varepsilon_n(\lambda) = T\ln[\rho_{nh}(\lambda)/\rho_n(\lambda)] = \eta_n(\lambda)$ is

$$Hm - J\theta'_{m,1}(\lambda) = T\ln[1 + \eta_m(\lambda)] -$$
$$-\sum_n \frac{T}{2}[A_{n,m}(\lambda - \lambda') + A_{n,m}(\lambda + \lambda')] * \ln[1 + \eta_n^{-1}(\lambda')]. \qquad (9)$$

Thermodynamic BAE for densities are linear integral equations. There are two kinds of driving terms (not dependent on ρ_m and ρ_{mh}: the ones of order of 1, and the ones of order of L^{-1}). Hence, we can divide densities as $\rho_n(\lambda) = \rho_n^{(0)}(\lambda) + L^{-1}\rho_n^{(1)}(\lambda)$ (and the same for densities of holes). Then one can separate BAE for densities into two sets: one of the scale 1 for the main (of order of L) contribution and the other one of the scale L^{-1} for the finite contribution (of order of 1). The former describes thermodynamics of bulk spins, which is equivalent to the ones for the chain with periodic boundary conditions [7]. The latter reveals the contribution from edges. In what follows we shall concentrate namely on that contribution only. Since $\varepsilon_m(\lambda)$, $\rho_m(\lambda)$ and $\rho_{mh}(\lambda)$ are even functions, one can rewrite the thermodynamic BAE following [11] as (we drop the superscript (1) in what follows)

$$Hm - J\theta'_{m,1}(\lambda) = T \ln [1 + \eta_m(\lambda)] - \\ - T\sum_n A_{n,m}(\lambda - \lambda') * \ln [1 + \eta_n^{-1}(\lambda')], \quad (10)$$

and

$$\rho_{mh}(\lambda) = -\sum_{n=1}^{\infty} A_{mn}(\lambda - \lambda') * [\rho_n(\lambda') - \\ - p(\lambda')(\delta_{m,1} + \delta_{m,2} + \delta_{m,[2S_1]} + \delta_{m,[2S_2]})], \quad (11)$$

where we introduced additional terms to avoid double counting due to the symmetrization of functions (with $\lambda = 0$) and to take into account the term with $\lambda_\alpha = \lambda_\beta$ in the right-hand side of Eqs. (1).

In what follows we shall concentrate on the low temperature, $T << J$, dependencies of the magnetic susceptibility and specific heat caused by free edges themselves (i.e., for $h_{1,L} = 0$ and even L). Equations (10) and (11) are very similar in structure to the ones, which describe thermodynamics of the Kondo impurity in a metal [12]. The principal difference, however, is that the contributions to the magnetization and the energy of order of 1 of the open spin-1/2 Heisenberg chain, see Eq. (8), have no terms, which do not depend on dressed densities, while such terms are present for the Bethe ansatz description of the Kondo problem [12]. Following known methods of consideration of the low temperature corrections, we find the contribution to the free energy of the Heisenberg chain for $H << T$, caused by free edges:

$$F_{\text{edges}} = -\frac{H}{8} \tanh [H/2T] \times \\ \times \left(\frac{1}{|\ln T_0 / T|} - \frac{\ln |\ln T_0/T|}{2 \ln^2 T_0/T} \right) - \frac{\pi^2 T}{32|\ln T_0/T|^3} + \ldots , \quad (12)$$

where $T_0 = a\pi\sqrt{\pi/e}J$ (a is a constant). This implies the expressions for the low-temperature magnetic susceptibility of an open Heisenberg chain, caused by free edges

$$\chi_{\text{edges}} = \frac{1}{8T|\ln T_0/T|}\left(1 - \frac{\ln |\ln T_0/T|}{2\,|\ln T_0/T|}\right) + \ldots \quad (13)$$

One can see that the magnetic susceptibility of open edges of the chain diverges as $T \to 0$. However, this divergency is different from the usually presumed Curie-like $1/T$ behavior. Logarithmic terms appear due to the interaction in the SU(2)-symmetric spin-1/2 system. This is different from the constant behavior of the magnetic susceptibility of bulk spins (and the ones of a periodic chain) at low temperatures.

The low-temperature entropy of the Heisenberg chain caused by free edges is calculated as

$$\mathcal{S}_{\text{edges}} = \frac{\pi^2}{32|\ln T_0/T|^3} + \ldots , \quad (14)$$

which implies the low-temperature specific heat

$$c_{\text{edges}} = \frac{3\pi^2}{32 \ln^4 T_0 / T} + \ldots \quad (15)$$

The last equation implies that the low-temperature Sommerfeld coefficient is divergent as

$$\gamma_{\text{edges}} = \frac{3\pi^2}{32T \ln^4 T_0/T} + \ldots \quad (16)$$

It is again, very different from the behavior of the specific heat of bulk spins (and the ones of a periodic chain) at low temperatures. While the Sommerfeld coefficient of free edges is divergent at low temperatures, the edges's entropy and specific heat are finite, as it must be. It turns out that the Wilson ratio of the contributions from free edges is divergent, in a drastic contrast with the finite value of such a coefficient for bulk spins. It is important to emphasize that while Eq. (13) agrees with the expressions, obtained in the approximate calculations [8], the expressions for the low-temperature entropy and specific heat are different from the ones, obtained using approximate bosonization method. We point out, that namely cubic in $1/|\ln T_0/T|$ terms for $H = 0$ appear in the low-temperature corrections of the behavior of the free energy of the Kondo impurity [12] and the bulk free energy of a Heisenberg spin-1/2 chain [13], while there are no linear terms in those dependencies.

In conclusion, using the exact Bethe ansatz method we calculated the low-temperature characteristics of free edges of an open Heisenberg antiferromagnetic spin-1/2 chain. We have shown that the magnetic susceptibility and low-temperature Sommerfeld coefficient of the specific heat of free edges of an open chain are divergent, unlike similar characteristics for bulk spins of the chain. Notice, that similar behavior of low-temperature magnetic susceptibility of quasi-one-dimensional compounds of Cu was observed [2].

1. A.V. Mahajan, H. Alloul, G. Collin, and J.F. Marucco, *Phys. Rev. Lett.* **72**, 3100 (1994).
2. G. Xu, G. Aeppli, M.E. Fisher, C. Broholm, J.F. DiTusa, C.D. Frost, T. Ito, K. Oka, R.L. Paul, H. Takagi, and M.M.J. Treacy, *Science* **289**, 419 (2000).
3. K.H. Höglund and A.W. Sandvik, *Phys. Rev. Lett.* **91**, 077204 (2003); S. Sachdev, C. Buragohain, and M. Voita, *Science* **286**, 2479 (1999).
4. S. Eggert, I. Affleck, and M.D.P. Horton, *Phys. Rev. Lett.* **89**, 047202 (2002); A.A. Zvyagin, *Phys. Rev. Lett.* **90**, 089701 (2003).
5. M. Gaudin, *Phys. Rev.* **A4**, 386 (1971); *La Fonction d'Onde de Bethe*, Paris, Masson (1983).
6. P.A. de Sa and A.M. Tsvelik, *Phys. Rev.* **B52**, 3067 (1995).
7. H. Frahm and A.A. Zvyagin, *J. Phys.: Condensed Matter* **9**, 9939 (1997).
8. S. Fujimoto and S. Eggert, *preprint cond-mat/0310230*; A. Furusaki and T. Hikihara, *preprint cond-mat/0310517*.
9. H. Bethe, *Z. Phys.* **71**, 205 (1931).
10. M. Takahashi, *Thermodynamics of One-Dimensional Solvable Models*, Cambridge, Cambridge University Press (1999).
11. F.C. Alcaraz, M.N. Barber, M.T. Batchelor, R.J. Baxter, and G.R.W. Quispel, *J. Phys. A: Math. Gen.* **20**, 6397 (1987).
12. A.M. Tsvelick and P.B. Wiegmann, *Adv. Phys.* **32**, 453 (1983).
13. A. Klümper, *Europ. Phys. J.* **B5**, 677 (1998).