Thermodynamics of integrable chains with alternating spins

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We consider a two-parameter $(\bar{c},\tilde{c})$ family of quantum integrable isotropic Hamiltonians for a chain of alternating spins of spin $s=\frac{1}{2}$ and $s=1$. We determine the thermodynamics for low-temperature T and small external magnetic field H, with $T \ll H$. In the antiferromagnetic $(\bar{c}>0,\tilde{c}>0)$ case, the model has two gapless excitations. In particular, for $\bar{c}=\tilde{c}$, the model is conformally invariant and has central charge $c_{\rm vir}=2$. When one of these parameters is zero, the Bethe ansatz equations admit an infinite number of solutions with lowest energy.

The one-dimensional Heisenberg model, like the hydrogen atom, has served as the guiding example for a very large body of both experimental and theoretical work. Progress has recently been made on closely related models, consisting of chains with *alternating* spins, such as spin-$\frac{1}{2}$ and spin-1. On the experimental side, materials (e.g.,[1] [MnCp$_2^*$] [tetracyanoethylene]) have been synthesized, which, at temperatures above a certain transition temperature T_c, behave as one-dimensional ferromagnets of alternating spins. On the theoretical side, quantum integrable models of chains with alternating spins have recently been constructed.[2] In this paper we investigate the thermodynamics of a two-parameter family of such integrable models. Depending on the values of the parameters, we find both antiferromagnetic and ferromagnetic behavior. When one of these parameters is zero, the Bethe-ansatz equations admit an infinite number of solutions with lowest energy.

We consider a system of N spins $\frac{1}{2}\sigma_2,\frac{1}{2}\sigma_4,\ldots,\frac{1}{2}\sigma_{2N}$ of spin-$\frac{1}{2}$ and N spins $\mathbf{s}_1,\mathbf{s}_3,\ldots,\mathbf{s}_{2N-1}$ of spin-1 in an external magnetic field $H(\geq 0)$ with the Hamiltonian $\mathcal{H}$ given by

$$\mathcal{H}=\bar{c}\bar{\mathcal{H}}+\tilde{c}\tilde{\mathcal{H}}-HS^z\ , \quad (1)$$

where $S^z=\sum_{n=1}^{N}\frac{1}{2}\sigma_{2n}^z+\sum_{n=1}^{N}s_{2n-1}^z$,

$$\bar{\mathcal{H}}=-\tfrac{1}{9}\sum_{n=1}^{N}(2\boldsymbol{\sigma}_{2n}\cdot\mathbf{s}_{2n+1}+1)(2\boldsymbol{\sigma}_{2n+2}\cdot\mathbf{s}_{2n+1}+3)\ , \quad (2)$$

$$\tilde{\mathcal{H}}=-\tfrac{1}{9}\sum_{n=1}^{N}(2\boldsymbol{\sigma}_{2n}\cdot\mathbf{s}_{2n-1}+1)\times[(1+\mathbf{s}_{2n-1}\cdot\mathbf{s}_{2n+1})(2\boldsymbol{\sigma}_{2n}\cdot\mathbf{s}_{2n+1}+1)+2]\ , \quad (3)$$

and $\bar{c}$ and $\tilde{c}$ are real constant parameters. (In this paper, bars and tildes are interchanged with respect to Ref. 2.) Note that the Hamiltonian contains both nearest- and next-to-nearest-neighbor interactions. We assume periodic boundary conditions: $\boldsymbol{\sigma}_{2n}\equiv\boldsymbol{\sigma}_{2n+2N}$ and $\mathbf{s}_{2n+1}\equiv\mathbf{s}_{2n+1+2N}$. Evidently, $\mathcal{H}$ is constructed from scalar products of spin operators, and thus $[\mathcal{H},\mathbf{S}^2]=0$.

The corresponding energy eigenvalues are given by[2]

$$E=\bar{c}\bar{E}+\tilde{c}\tilde{E}-H(\tfrac{3}{2}N-M)\ , \quad (4)$$

where

$$\bar{E}=\tfrac{5}{3}N-i\sum_{j=1}^{M}\frac{d}{d\lambda_j}\ln\left[\frac{\lambda_j+(i/2)}{\lambda_j-(i/2)}\right]\ ,$$
$$\tilde{E}=-\tfrac{1}{2}N-i\sum_{j=1}^{M}\frac{d}{d\lambda_j}\ln\left[\frac{\lambda_j+i}{\lambda_j-i}\right]\ , \quad (5)$$

where the variables λ_j satisfy the Bethe-ansatz (BA) equations

$$\left[\frac{\lambda_j+(i/2)}{\lambda_j-(i/2)}\frac{\lambda_j+i}{\lambda_j-i}\right]^N=-\prod_{k=1}^{M}\frac{\lambda_j-\lambda_k+i}{\lambda_j-\lambda_k-i}\ ,\qquad j=1,\ldots,M\ . \quad (6)$$

We consider here a strictly alternating arrangement of spins, with spins-$\frac{1}{2}$ at even sites and spins-1 at odd sites. For any other ordering of the spins, one can construct a corresponding Hamiltonian, which has the same energy eigenvalues and BA equations. Similar systems of equations, with either $\bar{c}$ or $\tilde{c}$ equal to zero, arise for spin chains with impurities.[3]

This system of equations admits the same string solutions that are found for the Heisenberg model. In the thermodynamic limit, the model is characterized by particle densities $\rho_n(\lambda)$ and hole densities $\tilde{\rho}_n(\lambda)$. Following the standard procedure (see, e.g., Refs. 4 and 5), we find that these densities obey the constraints

$$\tilde{\rho}_n+\sum_{m=1}^{\infty}A_{nm}*\rho_m=a_n+\sum_{l=1}^{\min(n,2)}a_{n+3-2l}\ , \quad (7)$$

where

$$a_n(\lambda)=\frac{1}{2\pi}\frac{n}{\lambda^2+(n^2/4)}\ , \tag{8}$$

$$A_{nm}(\lambda)=\delta_{nm}\delta(\lambda)+(1-\delta_{nm})a_{|n-m|}(\lambda)+a_{n+m}(\lambda)+2\sum_{l=1}^{\min(n,m)-1}a_{|n-m|+2l}(\lambda)\ , \tag{9}$$

and $*$ denotes the convolution $(f*g)(\lambda)=\int_{-\infty}^{\infty}d\lambda' f(\lambda-\lambda')g(\lambda')$.

The thermodynamic Bethe-ansatz (TBA) equations describing the equilibrium system at temperature T are

$$T\ln(1+e^{\epsilon_n/T})=\sum_{m=1}^{\infty}A_{nm}*T\ln(1+e^{-\epsilon_m/T})-2\pi\left[\bar{c}a_n+\tilde{c}\sum_{l=1}^{\min(n,2)}a_{n+3-2l}\right]+nH\ , \tag{10}$$

where

$$\epsilon_n(\lambda)=T\ln[\tilde{\rho}_n(\lambda)/\rho_n(\lambda)]\ . \tag{11}$$

(The particle and hole densities are understood to be those at equilibrium.) The equilibrium free energy is given by

$$F=2Ne_0-NT\int_{-\infty}^{\infty}d\lambda\, s(\lambda)\ln[(1+e^{\epsilon_1(\lambda)/T})\times(1+e^{\epsilon_2(\lambda)/T})]\ , \tag{12}$$

where $s(\lambda)=1/(2ch\,\pi\lambda)$, and

$$2e_0=\bar{c}[\tfrac{5}{3}-(2\ln2+4-\pi)]+\tilde{c}[-\tfrac{1}{2}-(6-\pi)]\ .$$

In the high-temperature limit with zero field, these equations give the expected value for the entropy, namely, $S=N\ln6$. We now consider small values of T and H, with $T\ll H$. We define $\varepsilon_n(\lambda)=\lim_{T\to0}\epsilon_n(\lambda)$. Keeping in mind that $\epsilon_n>0$ for $H>0$ and $n\geq3$, we obtain from the TBA equations the following system of linear integral equations for ε_1 and ε_2:

$$\varepsilon_1=-2\pi\bar{c}s+s*\varepsilon_2^+\ ,\qquad \varepsilon_2=\tfrac{1}{2}H-2\pi\tilde{c}s+h*\varepsilon_2^++s*\varepsilon_1^+\ , \tag{13}$$

where $h=s*a_1$, and the superscript $+$ on a function denotes the positive part of that function; i.e., $\varepsilon^+\equiv\frac{1}{2}(\varepsilon+|\varepsilon|)$.

The qualitative behavior of the solutions depends on the sign of the parameters $\bar{c}$ and $\tilde{c}$, and the various cases must be studied individually. Let us first consider the antiferromagnetic case $\bar{c}>0$, $\tilde{c}>0$. In this case, for $H=0$ the solutions $\varepsilon_1(\lambda)$ and $\varepsilon_2(\lambda)$ are readily found, and are seen to be negative for all λ. Hence, for the ground state, $\rho_1(\lambda)=\rho_2(\lambda)=s(\lambda)$, and all other particle and hole densities are equal to zero.[6] Thus, the ground state is a "sea" of strings of length 1 and a "sea" of strings of length 2, in agreement with the alternative analysis of Ref. 2.[7] This corresponds to the antiferromagnetic ground states of integrable chains[5] of spin $s=\frac{1}{2}$ and 1.

For H small but nonzero, we can solve for ε_1 and ε_2 by generating from (13) a system of Wiener-Hopf equations. To this end, we define α_n to be the zeros of $\varepsilon_n(\lambda)$, i.e., $\varepsilon_n(\alpha_n)=0$, for $n=1,2$. We assume

$$\alpha_n=-\frac{1}{\pi}\left[\ln H+\ln\kappa_n+O\left[\frac{1}{\ln H}\right]\right]\ , \tag{14}$$

where the constants κ_n (which are independent of H) have still to be determined. Introducing the functions

$$S_n(\lambda)=\begin{cases}e^{\pi\alpha_n}\kappa_n\varepsilon_n(\lambda+\alpha_n), & \lambda>0\\ 0, & \lambda<0\ ,\end{cases} \tag{15}$$

we obtain (for $H\to0$) the following system of Wiener-Hopf equations

$$S_1(\lambda)=-2\pi\bar{c}\kappa_1e^{-\pi\lambda}+\int_0^{\infty}d\lambda'\, s(\lambda-\lambda'+\alpha_1-\alpha_2)S_2(\lambda')\ ,$$
$$S_2(\lambda)=\tfrac{1}{2}-2\pi\tilde{c}\kappa_2e^{-\pi\lambda}+\int_0^{\infty}d\lambda'\,[s(\lambda-\lambda'+\alpha_2-\alpha_1)S_1(\lambda')+h(\lambda-\lambda')S_2(\lambda')],\quad \lambda\geq0\ . \tag{16}$$

In order to find the leading-order temperature dependence of the free energy, we must compute the leading correction to the solutions $\epsilon_n=\varepsilon_n$ of the linearized Eqs. (13). Hence, we set $\epsilon_n(\lambda)=\varepsilon_n(\lambda)+\eta_n(\lambda)$ in the TBA equations and expand to leading order in η_n, as is explained in Refs. 8 and 9. In terms of the functions

$$T_n(\lambda)=\begin{cases}\dfrac{6e^{-\pi\alpha_n}}{\pi^2T^2\kappa_n}\eta_n(\lambda+\alpha_n), & \lambda>0\\ 0, & \lambda<0\ ,\end{cases} \tag{17}$$

we obtain (for $H\to0$) a second system of Wiener-Hopf equations:

$$T_1(\lambda)=\frac{s(\lambda+\alpha_1-\alpha_2)}{S_2'(0)}+\int_0^{\infty}d\lambda'\, s(\lambda-\lambda'+\alpha_1-\alpha_2)T_2(\lambda')\ ,$$
$$T_2(\lambda)=\frac{h(\lambda)}{S_2'(0)}+\frac{s(\lambda+\alpha_2-\alpha_1)}{S_1'(0)}+\int_0^{\infty}d\lambda'[s(\lambda-\lambda'+\alpha_2-\alpha_1)T_1(\lambda')+h(\lambda-\lambda')T_2(\lambda')],\quad \lambda\geq0\ , \tag{18}$$

where $S_n'(0)=dS_n/d\lambda|_{\lambda=0^+}$.

Both systems (16) and (18) involve the same 2×2 matrix kernel, which in Fourier space is given by

$$\hat{K}(\omega)=\begin{bmatrix} 0 & e^{-i\omega(\alpha_1-\alpha_2)}\hat{s}(\omega) \\ e^{i\omega(\alpha_1-\alpha_2)}\hat{s}(\omega) & \hat{h}(\omega) \end{bmatrix} . \quad (19)$$

[Our convention for Fourier transforms is that $\hat{f}(\omega)=\int_{-\infty}^{\infty}d\lambda\, e^{i\lambda\omega}f(\lambda)$.] Results from Ref. 10 imply that the following factorization exists:

$$[1-\hat{K}(\omega)]^{-1}=G_+(\omega)G_-(\omega), \quad -\infty<\omega<\infty , \quad (20)$$

where $G_+(\omega)$ and $G_+^{-1}(\omega)$ are analytic in the upper-half complex ω plane with $G_+(+\infty)=1$, and (for ω in the lower-half plane) $G_-(\omega)=G_+(-\omega)^T$.

Using standard Wiener-Hopf methods, we conclude that the solutions of Eqs. (16) and (18) are given (in matrix notation) by

$$\hat{S}(\omega)=\frac{i}{2}\left[\frac{1}{\omega+i0}-\frac{1}{\omega+i\pi}\right]G_+(\omega)G_-(0)\begin{bmatrix}0\\1\end{bmatrix} \quad (21)$$

and

$$\hat{T}(\omega)=(G_+(\omega)-1)\begin{bmatrix}1/S_1'(0)\\1/S_2'(0)\end{bmatrix} , \quad (22)$$

where

$$S'(0)=-\lim_{|\omega|\to\infty}\omega^2\hat{S}(\omega)=\frac{\pi}{2}G_-(0)\begin{bmatrix}0\\1\end{bmatrix} . \quad (23)$$

Moreover, the parameters κ_n introduced in Eq. (14) are given by

$$\kappa=\begin{bmatrix}\kappa_1\\\kappa_2\end{bmatrix}=\frac{1}{4\pi}\begin{bmatrix}1/\bar{c} & 0\\ 0 & 1/\tilde{c}\end{bmatrix}G_-(-i\pi)^{-1}G_-(0)\begin{bmatrix}0\\1\end{bmatrix} . \quad (24)$$

In order to calculate the free energy per site $f=F/2N$, we substitute $\epsilon_n=\varepsilon_n+\eta_n$ into the expression (12) for the free energy, as is explained in Refs. 8 and 9. We obtain

$$f=e_0-H^2A-\frac{\pi^2T^2}{6}B , \quad (25)$$

with

$$A=\kappa^T\hat{S}(i\pi), \quad B=\kappa^T\left[\hat{T}(i\pi)+\begin{bmatrix}1/S_1'(0)\\1/S_2'(0)\end{bmatrix}\right] . \quad (26)$$

For $\bar{c}\neq\tilde{c}$, the quantities A and B cannot be explicitly evaluated without having explicit expressions for the factors $G_+(\omega)$ and $G_-(\omega)$, which we have not yet found.

For the special case $\bar{c}=\tilde{c}\equiv c$, the quantities A and B can be readily evaluated, and we conclude (for $T\ll H$)

$$f=e_0-\frac{1}{4\pi^2c}H^2-\frac{1}{6c}T^2 . \quad (27)$$

It follows that the magnetic susceptibility and specific heat, to lowest order, are given by

$$\chi=-\left.\frac{\partial^2 f}{\partial H^2}\right|_T=\frac{1}{2\pi^2c}, \quad C_H=-T\left.\frac{\partial^2 f}{\partial T^2}\right|_H=\frac{1}{3c}T , \quad (28)$$

respectively.

This model has[2,11] two gapless excitations, with corresponding speeds of sound $\bar{v}=2\pi\bar{c}$ and $\tilde{v}=2\pi\tilde{c}$. Evidently, the case $\bar{c}=\tilde{c}$ is the unique case for which the two speeds of sound coincide, and the model is conformally invariant. For a critical chain, the low-temperature free energy per site is given by[12,13]

$$f=e_0-\frac{\pi c_{\rm vir}}{6v_s}T^2+\cdots , \quad (29)$$

where $c_{\rm vir}$ is the central charge of the Virasoro algebra and v_s is the speed of sound. Therefore, from (27) we see that $c_{\rm vir}=2$. Presumably it is no coincidence that precisely for the conformally invariant case, explicit expressions for $G_+(\omega)$ and $G_-(\omega)$ are not needed to evaluate the free energy.

We now consider the case $\bar{c}=0$, $\tilde{c}>0$. For this case, there is a one-parameter (α) family of lowest-energy states. Indeed, consider the following one-parameter family of densities:

$$\begin{aligned}&\rho_1=\alpha s, \quad \tilde{\rho}_1=(1-\alpha)s ,\\ &\rho_2=s+(1-\alpha)s*s, \quad 0\le\alpha\le 1 ,\end{aligned} \quad (30)$$

and all other particle and hole densities are equal to zero. These densities obey the constraints (7), and give (independently of the value of α) the same lowest value for the energy. Moreover, to leading order in N, the spin is $S^z=0$, and the entropy is

$$S=-\frac{N}{2}[\alpha\ln\alpha+(1-\alpha)\ln(1-\alpha)] .$$

In particular, for $\alpha\neq 0,1$, the entropy is nonzero and is proportional to N, implying an infinite degeneracy of states. This degeneracy is consistent with the fact that, above the $\alpha=1$ vacuum, there are excitations (namely, holes in the sea of real roots), which have *zero energy* and nonzero momentum.[2] We are not aware of any other model with such properties.[14]

We speculate that the system can be brought to these various states by first preparing the system at finite T and H, and then approaching the origin ($T=0$, $H=0$) of the (T,H) plane from appropriate directions. The ground state of the system is the state, which is reached by approaching the origin along the line $H=0$. Unfortunately, we cannot determine the particular value of α corresponding to this state, since this would entail computing $\lim_{T\to 0}\lim_{H\to 0}\epsilon_1/T$, while we know how to calculate only for $T\ll H$.[15] By approaching the origin of the (T,H) plane along the line $T=0$, the state with $\alpha=0$ is reached.

We have calculated the free energy for small values of T and H, with $T\ll H$. The calculation is similar to the one above, except that now one must take into account that $\varepsilon_1(\lambda)$ does not have a zero. We find that, to leading order, the free energy per site is given by

$$f = e_0 + \frac{1}{4\pi^3 \tilde{c}} H^2 \ln H + \frac{1}{12\pi \tilde{c}} T^2 \ln H \ . \qquad (31)$$

Contrary to appearance, this result does *not* imply that f diverges for $H \to 0$, since in the region where the calculation is valid ($T \ll H$), the last term is finite. This result is nevertheless unusual, since it implies that C_H/T is a function of H. It would be interesting to find a Fermi-liquid-type explanation[16] for the $\ln H$ factors.

Similar results are obtained for the case $\bar{c}=0$, $\tilde{c}>0$. For the case $\bar{c}<0$, $\tilde{c}>0$ and $\bar{c}>0$, $\tilde{c}<0$, the model either has a ferromagnetic ground state and a finite gap, or it has no gap, depending on the precise values of $\bar{c}$, $\tilde{c}$, and H. For the cases $\bar{c}$, $\tilde{c} \le 0$, the model is ferromagnetic.

Note added. After this work was completed, we received a copy of Ref. 17, which discusses chains of alternating spin-$\frac{1}{2}$ and spin s. However, that paper considers neither the effect of an external magnetic field, nor the behavior of the models away from the conformally invariant point (i.e., for $\bar{c} \neq \tilde{c}$).

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[1]G. T. Yee, J. M. Manriquez, D. A. Dixon, R. S. McLean, D. M. Groski, R. B. Flippen, K. S. Narayan, A. J. Epstein, and J. S. Miller, Adv. Mater. **3**, 309 (1991).

[2]H. J. de Vega and F. Woynarovich, J. Phys. A **25**, 4499 (1992).

[3]N. Andrei and H. Johannesson, Phys. Lett. **100A**, 108 (1984); K. Lee and P. Schlottmann, Phys. Rev. B **37**, 379 (1988); P. Schlottmann, J. Phys. Condens. Matter **3**, 6617 (1991).

[4]A. M. Tsvelick and P. B. Wiegmann, Adv. Phys. **32**, 453 (1983).

[5]H. M. Babujian, Nucl. Phys. **B215**, 317 (1983); L. A. Takhtajan, Phys. Lett. **87A**, 479 (1982).

[6]By definition, the set of ground-state densities should be determined through Eq. (11) by computing $\lim_{T\to 0}\lim_{H\to 0}\epsilon_n/T$, and then imposing the constraints (7). Here, we compute instead $\lim_{H\to 0}\lim_{T\to 0}\epsilon_n/T$, and we assume that the two limits commute. If the limits did not commute, there would be another set of densities, which would also satisfy the constraints (7) and give the same value for the energy. We believe that for the case $\bar{c}>0$, $\tilde{c}>0$ such an additional set of densities does not exist.

[7]The Bethe-ansatz states are highest weight vectors of SU(2); i.e., these states have spin quantum numbers $s=s^z \ge 0$. [See, e.g., L. D. Faddeev and L. A. Takhtajan, J. Sov. Math. **24**, 241 (1984).] Hence, the ground state is indeed a spin singlet $s=s^z=0$.

[8]J. D. Johnson and B. M. McCoy, Phys. Rev. A **6**, 1613 (1972). See also C. N. Yang and C. P. Yang, Phys. Rev. **150**, 327 (1966).

[9]L. Mezincescu and R. I. Nepomechie, in *Quantum Groups, Integrable Models and Statistical Systems*, edited by J. Le Tourneux and L. Vinet (World Scientific, Singapore, 1993), p. 168.

[10]I. C. Gohberg and M. G. Krein, in *American Mathematical Society Translations, Series 2* (American Mathematical Society, Providence, 1960), Vol. 14, p. 217.

[11]We define the momentum here as one-half the log of the two-site shift operator. This yields the stated values for the speeds of sound, and a system of length $2N$ [see Eq. (25)]. In Ref. 2, the log of the two-site shift operator is used, which leads to half these values for the speeds and length. We thank M. Martins for a discussion on this point.

[12]H. W. J. Blöte, J. L. Cardy, and M. P. Nightingale, Phys. Rev. Lett. **56**, 742 (1986).

[13]I. Affleck, Phys. Rev. Lett. **56**, 746 (1986).

[14]Implicit in this discussion is the conventional assumption that a set of densities, which satisfies the constraints (7) and has lowest-energy, corresponds to an eigenstate of the Hamiltonian.

[15]In contrast to the case $\bar{c}>0$, $\tilde{c}>0$, here we expect that $\lim_{T\to 0}\lim_{H\to 0}\epsilon_1/T \neq \lim_{H\to 0}\lim_{T\to 0}\epsilon_1/T$.

[16]For the isotropic antiferromagnetic spin-$\frac{1}{2}$ Heisenberg chain, such an analysis is given by T. Yamada, Prog. Theor. Phys. **41**, 880 (1969). See also Johnson and McCoy, Ref. 8.

[17]S. R. Aladim and M. J. Martins (unpublished).