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THE CORRELATION FUNCTION AND THE THERMODYNAMIC QUANTITIES OF THE MIXED SYSTEM

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The thermodynamics of an inhomogeneous 1D Heisenberg chain with alternating classical and quantum spins is studied. The explicit expressions for the free energy, specific heat, thermal spin correlations, and linear susceptibility are found.

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The Heisenberg spin lattices have been extensively studied throughout many years as the simplest models for magnetic phenomena. Motivated by the famous Bethe solution in 1D [1], a number of theoretical and experimental investigations of quantum spin chains with the nearest-neighbor interaction has been performed in the last thirty years by using exact Bethe ansatz [2, 3], high- and low-temperature expansions [4], and renormalization group calculations [5, 6]. In the meantime, attention has been paid also to the classical version of the model in which spins are represented by unit vectors located on the sites of 1D lattice for both cases of periodic [7, 8] and open boundary conditions [9]. In comparison to the overcomplicated form of the solution to the quantum systems, the classical results look rather simple and allow one to read the expressions for thermodynamic quantities explicitly in the absence of a magnetic field [7–9].

In various situations which now can be realized in magnetic substances, the arrangement of spins might be quite different either from classical or pure quantum situation. The lattice structure of chemical compounds can comprise magnetic ions with spins of different magnitudes arranged periodically [10] in a family of quasi-one-dimensional chains. In the limit of weak interchain coupling, one can approximate the system by noninteracting 1D chains with the nearest-neighbor interaction of different spins (say, spins 1/2 on even sites and spin 5/2 on odd ones). These two interacting sublattices are very different, and the resulting quantum chain is not integrable. However, one could introduce *classical* spins instead of the spins of higher magnitude which makes the chain more tractable.

In this case, taking the trace with respect to quantum and classical degrees of freedom can be performed separately, which leads to analytic result in the absence of magnetic field.

The aim of this note is to find explicit expression for the thermodynamic quantities of these mixed classical-quantum chains in 1D, and to calculate its linear susceptibility.

The starting point is the Hamiltonian of the finite lattice of the form

$$H_N = \frac{J}{2}\sum_{j=1}^{N}(\mathbf{n}_{2j-1}\boldsymbol{\sigma}_{2j} + \boldsymbol{\sigma}_{2j}\mathbf{n}_{2j+1}), \tag{1}$$

where $\mathbf{n}_{2j-1}$ ($\mathbf{n}_{2j-1}^2 = 1$) are the vectors of classical spins located on odd sites of the lattice and $\boldsymbol{\sigma}_{2j}$ are Pauli matrices representing quantum $s = 1/2$ spins located on even sites. We will consider the lattices of $2N+1$ sites under open boundary conditions. In the thermodynamic limit, the results become independent of the type of boundaries, and one expects that the correct behavior of the specific heat, spin correlations in the bulk and linear susceptibility will be achieved starting from this simplest choice of the boundaries.

The calculation of the trace in the partition function of the chain

$$Z_N = \mathrm{Tr}\left[\exp\left(-\frac{H_N}{T}\right)\right]$$

becomes more easy if one notices that the quantum spins are not coupled to each other but only to their neighboring classical spins. Then one can apply the formula

$$\exp\left(\frac{\mathbf{a}}{2}\boldsymbol{\sigma}_{2j}\right) = \cosh a/2 + \sinh a/2\frac{\mathbf{a}\boldsymbol{\sigma}_{2j}}{a}, \quad a = |\mathbf{a}|.$$

The partition function can be written as

$$Z_N = \mathrm{tr}_{\{\sigma_{2j}\}}\mathrm{tr}_{\{\mathbf{n}_{2j-1}\}}\prod_{j=1}^{N}\left(\cosh\frac{J}{2T}N_j + \sinh\frac{J}{2T}N_j\frac{\mathbf{N}_j\boldsymbol{\sigma}_{2j}}{N_j}\right), \tag{2}$$

where

$$\mathbf{N}_j = \mathbf{n}_{2j-1} + \mathbf{n}_{2j+1}.$$

The summation over quantum spins is now performed easily and one finds:

$$Z_N = 2^N\prod_{j=1}^{N+1}\int_{\Omega_j}\frac{d\Omega_j}{4\pi}\prod_{j=1}^{N}\cosh\frac{J}{T}\sqrt{\frac{1+\mathbf{n}_j\mathbf{n}_{j+1}}{2}}.$$

The integration over elements of solid angles can now be done as follows [9]. Let us start from integration over $d\Omega_1$ and fix $\mathbf{n}_2$ in the positive direction of z axis. One finds

$$\int \frac{d\Omega_1}{4\pi} f(\mathbf{n}_1\mathbf{n}_2) = \frac{1}{2}\int_{-1}^{1} f(x)\,dx.$$

Continuing this procedure with $\mathbf{n}_2, \mathbf{n}_3, \ldots$, one arrives at

$$Z_N = \left[\int_{-1}^{1} dx \cosh \frac{J}{T}\sqrt{\frac{1+x}{2}}\right]^N = \\ = \left[4\left(\frac{T\sinh\, J/T}{J} - \frac{T^2(\cosh\, J/T - 1)}{J^2}\right)\right]^N. \quad (3)$$

In the thermodynamic limit, the free energy per site reads

$$f = -2T\left(\frac{T\sinh\, J/T}{J} - \frac{T^2(\cosh\, J/T - 1)}{J^2}\right). \quad (4)$$

The specific heat of the chain is now calculated as

$$C_{H=0} = 2\sinh\frac{J}{T}\left(\frac{6T}{J} + \frac{J}{T}\right) - 6\cosh\frac{J}{T}\left(1 + \frac{2T^2}{J^2}\right) + \frac{12T^2}{J^2}. \quad (5)$$

Next, let us calculate the correlation function $\langle \mathbf{s}_j\mathbf{s}_k\rangle$ of the mixed system. Consider at first the case in which both j and k are odd, i.e., the spins $\mathbf{s}_j$ and $\mathbf{s}_k$ are classical. Then one can write

$$\langle \mathbf{s}_{2j-1}\mathbf{s}_{2k-1}\rangle = Z_N^{-1}\mathrm{tr}_{\{\mathbf{n}_{2l-1}\}}\prod_{l=1}^{N}\cosh\frac{J}{2T}N_l\mathbf{n}_{2j-1}\mathbf{n}_{2k-1}.$$

Notice that the integrations over $\mathbf{n}_{2l-1}$, $l = 1, \ldots, j-1$ and $l = k+1, \ldots, N+1$ give the same result as in the integrations in the calculation of the partition function. Thus, the integral can be recast as

$$\langle \mathbf{s}_{2j-1}\mathbf{s}_{2k-1}\rangle = u\left(\frac{J}{T}\right)^{-|k-j|}\prod_{l=j}^{k}\int_{\Omega_l}\frac{d\Omega_l}{4\pi}\cosh\frac{J}{2T}N_l\mathbf{n}_j\mathbf{n}_k,$$

where

$$u(x) = 2\left(\frac{\sinh\, x}{x} - \frac{\cosh\, x - 1}{x^2}\right). \quad (6)$$

To simplify this expression further, consider the integral

$$I_{\mathbf{m},\mathbf{n}_{j+1}} = \int\limits_{\Omega_j} \frac{d\Omega_j}{4\pi}(\mathbf{n}_j\mathbf{m})f(\mathbf{n}_j\mathbf{n}_{j+1}).$$

Taking the direction of $\mathbf{n}_{j+1}$ as a polar axis and denoting the polar angles of $\mathbf{m}$ as (λ,ν), one can write

$$I_{\mathbf{m},\mathbf{n}_{j+1}} = \frac{1}{4\pi}\int\limits_0^{2\pi} d\phi \int\limits_0^{\pi} \sin\theta\, d\theta\, m(\cos\theta\cos\lambda + \sin\theta\sin\lambda\cos(\phi-\nu))f(\cos\theta) =$$

$$= \frac{1}{2}m\int\limits_{-1}^{1} x\,dx\,\cos\lambda f(x) = \frac{1}{2}\mathbf{m}\mathbf{n}_{j+1}\int\limits_{-1}^{1} x\,dx\,f(x).$$

Calculation of the last integral yields

$$\langle \mathbf{s}_{2j-1}\mathbf{s}_{2k-1}\rangle = u\left(\frac{J}{T}\right)^{-|k-j|} v\left(\frac{J}{T}\right)^{|k-j|}, \tag{7}$$

where

$$v(x) = 2\left(\left(1+\frac{12}{x^2}\right)\frac{\sinh x}{x} + \frac{\cosh x - 1}{x^2}\left(1-\frac{12}{x^2}\right) - \frac{6}{x^2}\cosh x\right). \tag{8}$$

Consider now the situation in which one spin is classical, i.e., it is located on an odd site, and another one is quantum and located on an even site. One can write

$$\langle \mathbf{s}_{2j-1}\mathbf{s}_{2k}\rangle = \frac{1}{2}Z_N^{-1}\mathrm{tr}_{\{\mathbf{n}_{2l-1}\}}\mathrm{tr}_{\{\sigma_{2l}\}}\times$$

$$\times\prod_{l=1}^{N}\left[\cosh\frac{J}{2T}N_l + \sinh\frac{J}{2T}N_l\frac{\mathbf{N}_l\boldsymbol{\sigma}_{2l}}{N_l}\right]\mathbf{n}_{2j-1}\boldsymbol{\sigma}_{2k} =$$

$$= 2^{N-1}Z_N^{-1}\mathrm{tr}_{\{\mathbf{n}_{2l-1}\}}\left(\prod_{j\neq k}^{N}\cosh\frac{J}{2T}N_j\right)\frac{\sinh\frac{J}{2T}N_k}{N_k}\mathbf{n}_{2j-1}\mathbf{N}_k.$$

As in the calculation of the partition function, the integration over $\mathbf{n}_1,\ldots,\mathbf{n}_{2j-3}$, $\mathbf{n}_{2k+1},\ldots,\mathbf{n}_{2N+1}$ results in factors $u(J/T)$ which cancel the corresponding factors in Z_N. The integrations over $\mathbf{n}_{2j-1},\ldots,\mathbf{n}_{2k-3}$ are similar to those of the calculations of $\langle \mathbf{s}_{2j-1}\mathbf{s}_{2k-1}\rangle$. Each of them produces factor $v(J/T)$. The last integral can be written as

$$I_k = \int \frac{d\Omega_{2k-1}}{4\pi} \frac{\sinh \frac{J}{2T} N_k}{N_k} (\mathbf{n}_{2k-1} + \mathbf{n}_{2k+1})\, \mathbf{n}_{2k-1}.$$

By choosing the direction of the vector $\mathbf{n}_{2k+1}$ as a polar axis, the integrand can be transformed and the result can be presented in the form

$$I_k = \frac{1}{4} \int_{-1}^{1} dx \sqrt{\frac{1+x}{2}} \sinh \frac{J}{T} \sqrt{\frac{1+x}{2}} = w\left(\frac{J}{T}\right),$$

where

$$w(x) = x^{-1} \left(\cosh x - \frac{2 \sinh x}{x} + \frac{2(\cosh x - 1)}{x^2} \right). \tag{9}$$

Taking (9) into account, one can write the correlation function of one classical and one quantum spin as

$$\begin{aligned} \langle \mathbf{s}_{2j-1}\mathbf{s}_{2k}\rangle &= \left[\frac{v\left(\frac{J}{T}\right)}{u\left(\frac{J}{T}\right)}\right]^{|j-k|} \frac{w\left(\frac{J}{T}\right)}{u\left(\frac{J}{T}\right)}, \quad j \leqslant k, \\ \langle \mathbf{s}_{2j-1}\mathbf{s}_{2k}\rangle &= \left[\frac{v\left(\frac{J}{T}\right)}{u\left(\frac{J}{T}\right)}\right]^{|j-k|-1} \frac{w\left(\frac{J}{T}\right)}{u\left(\frac{J}{T}\right)}, \quad j > k. \end{aligned} \tag{10}$$

The next step consists in the calculation of the correlation function of two quantum spins,

$$\langle \mathbf{s}_{2j}\mathbf{s}_{2k}\rangle = \frac{1}{4} Z_N^{-1} \mathrm{tr}_{\{\mathbf{n}_{2l-1}\}} \mathrm{tr}_{\{\sigma_{2l}\}} \prod_{l=1}^{N} \left[\cosh \frac{J}{2T} N_l + \sinh \frac{J}{2T} N_l \frac{\mathbf{N}_l \boldsymbol{\sigma}_{2l}}{N_l} \right] \boldsymbol{\sigma}_{2j} \boldsymbol{\sigma}_{2k}. \tag{11}$$

Taking the trace over quantum spins now yields

$$\langle \mathbf{s}_{2j}\mathbf{s}_{2k}\rangle = Z_N^{-1} 2^{N-2} \mathrm{tr}_{\{n_{2l-1}\}} \sinh \frac{J}{2T} N_j \sinh \frac{J}{2T} N_k \frac{\mathbf{N}_j \mathbf{N}_k}{N_j N_k} \prod_{l \neq j,k} \cosh \frac{J}{2T} N_l. \tag{12}$$

The calculation of the last trace can be done now as follows. Note at first that the integrations over $\mathbf{n}_1, \ldots, \mathbf{n}_{2j-3}$ give the factors $u(J/T)$ which cancel corresponding factors in the partition function. The first nontrivial integration is over n_{2j-1} and the integral reads

$$\int \frac{d\Omega_{2j-1}}{4\pi} \sinh \frac{J}{T} \sqrt{\frac{1 + \mathbf{n}_{2j-1}\mathbf{n}_{2j+1}}{2}} \frac{(\mathbf{n}_{2j-1} + \mathbf{n}_{2j+1})\mathbf{N}_k}{2(1 + \mathbf{n}_{2j-1}\mathbf{n}_{2j+1})N_k}.$$

Let us now choose $\mathbf{n}_{2j+1}$ as a polar axis and take reference plane as a plane of the vectors $\mathbf{n}_{2j+1}, \mathbf{N}_k$, so the last vector would have the polar angles $(\lambda, 0)$. Then the integral can be written as

$$\frac{1}{4\pi}\int_0^{2\pi} d\phi \int_0^{\pi} \sin\theta\, d\theta\, \sinh\frac{J}{T}\sqrt{\frac{(1+\cos\theta)}{2}}\times$$

$$\times\frac{\cos\lambda+\cos\theta\cos\lambda+\sin\theta\sin\lambda\cos\phi}{2(1+\cos\theta)} = \frac{1}{4}\int_{-1}^{1} dx\, \sinh\frac{J}{T}\sqrt{\frac{1+x}{2}}\,\frac{\mathbf{n}_{2j+1}\mathbf{N}_k}{N_k} =$$

$$= \frac{\mathbf{n}_{2j+1}\mathbf{N}_k}{N_k}\int_0^1 x\, dx \sinh\frac{J}{T}x = \frac{\mathbf{n}_{2j+1}\mathbf{N}_k}{N_k} t\left(\frac{J}{T}\right),$$

where

$$t(x) = x^{-1}\left(\cosh x - \frac{\sinh x}{x}\right). \tag{13}$$

Now, continuing with the integrations over $\mathbf{n}_{2j+1}, \ldots, \mathbf{n}_{2k-3}$, one is left with the factors $v(J/T)/u(J/T)$. The integration over $\mathbf{n}_{2k-1}$ is of the type considered before in the calculations of the correlation between one classical and one quantum spin, and results in the factor $w(J/T)/u(J/T)$. Putting all the parts together, one finds

$$\langle \mathbf{s}_{2j}\mathbf{s}_{2k}\rangle = \frac{t(J/T)w(J/T)}{u(J/T)^2}\,\frac{v(J/T)}{u(J/T)}^{|j-k|-1} \quad \text{if} \quad |j-k| \geqslant 1. \tag{14}$$

We have obtained all possible correlations between spins which are given by the formulas (7), (10), (14). To get the linear susceptibility of the chain $\chi_1(T, N)$, one needs to calculate three sums,

$$3\chi_1(T,N) = \frac{1}{T(2N+1)}(S_1+S_2+S_3), \tag{15}$$

$$S_1 = \sum_{j,k}^{N+1} \langle \mathbf{s}_{2j-1}\mathbf{s}_{2k-1}\rangle, \tag{16}$$

$$S_2 = \sum_{j=1}^{N+1}\sum_{k=1}^{N} \langle \mathbf{s}_{2j-1}\mathbf{s}_{2k}\rangle, \tag{17}$$

$$S_3 = \sum_{j,k=1}^{N} \langle \mathbf{s}_{2j}\mathbf{s}_{2k}\rangle. \tag{18}$$

It follows from (7) that the first sum (16) can be cast into the form

$$S_1 = N + 1 + 2\sum_{k=2}^{N+1}\sum_{s=1}^{k-1}(v/u)^s = N + 1 + 2\sum_{k=2}^{N+1}\frac{v/u-(v/u)^k}{1-v/u} =$$

$$= N + 1 + \frac{2Nv/u}{1-v/u} - 2\left(\frac{v/u}{1-v/u}\right)^2(1-(v/u)^N). \quad (19)$$

The equations (10) and (17) give

$$S_2 = \frac{2w}{u}\sum_{k=1}^{N}\sum_{j=1}^{k}(v/u)^{k-j} = \frac{2w}{u}\sum_{k=1}^{N}\frac{1-(v/u)^k}{1-v/u} =$$

$$= \frac{2w}{u}\left(\frac{N}{1-v/u} - \frac{v/u-(v/u)^{N+1}}{(1-v/u)^2}\right). \quad (20)$$

Finally, the third sum can be rewritten as

$$S_1 = N + \frac{2tw}{u^2}\sum_{k=2}^{N}\sum_{s=1}^{k-1}(v/u)^{s-1} = N + \frac{2tw}{u^2}\sum_{k=2}^{N}\frac{1-(v/u)^{k-1}}{1-v/u} =$$

$$= N + \frac{2(N-1)tw/u^2}{1-v/u} - \frac{2tw}{u^2}\frac{v/u}{(1-v/u)^2}(1-(v/u)^{N-1}). \quad (21)$$

Summing up the terms (19)–(21), one finds

$$3T\chi_1(T,N) = 1 + \frac{2}{(2N+1)(1-v/u)}[N(v+w)/u + (N-1)tw/u^2] -$$

$$- \frac{2v/u}{(1-v/u)^2}[v/u + w/u + tw/u^2 - (v/u)^{N-1}(v^2+vw+tw)/u^2)], \quad (22)$$

where $u\left(\frac{J}{T}\right), v(J/T), w(J/T)$, and $t(J/T)$ are given by the formulas (6), (8)–(9), (13). In the thermodynamic limit $N \to \infty$, one can use the fact that $v(J/T)/u(J/T) < 1$. Explicit calculation of the limit yields

$$3T\chi_1(T) = 1 + \frac{v(J/T) + w(J/T)(1 + t(J/T)/u(J/T))}{u(J/T) - v(J/T)}. \quad (23)$$

To conclude, we have calculated thermodynamic quantities at zero magnetic field and linear susceptibility of the mixed classical-quantum chain. At low temperatures, one finds $\chi_1(T) \propto T^{-2}$ as in the homogeneous classical and quantum systems. As in pure classical case, we did not succeed in the calculation of the equation of state for $H \neq 0$ since it needs knowledge of correlations of arbitrary number of spins. The estimation of linear susceptibilty shows, however, that the difference between pure and mixed chains might be only quantitative.

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