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High and Low Ternperature Analytic Expressions for the Classical One-Dimensional Anysotropic Planar Model

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Using the transfer matrix method for the one-dimensional classical anisotropic planar model, we present analytic expressions for the two-spins correlation functions in the limits of high and low temperatures. An alignment of spins along the easy direction i— found at low temperatures, leading the system to an Ising-like beheviour.

Usando o método da matrix transferência para o modelo planar anisotrópico clássico unidimensional, apresentamos expressões analíticas para as funções correlação de dois spins nos limites de altas e baixas temperaturas. Um alinhamento de spins ao longo do eixo de mais fácil magnetização é encontrado em baixas temperaturas, levando o sistema a se comportar como no modelo de Ising.

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1. INTRODUCTION

There is a vast literature on one-dimensional magnetic sistems[1]. Particularly, for the one-dimensional planar model we can mention some important works, namely: Lieb, Schultz and Mattis[2] studied the model with spin 1/2; Niemeijer[3] developed some calculations for the spin 1/2 planar. systern in presence of an applied field; Joyce[4] obtained closed-form expressions for the termodynamic functions in the classical isotropic case, while Stanley[5] solved the general case of n-dimensional classical vector spins for arbitrary *n*. Recently, Loveluck[6] obtained numerical results for the classical planar model in the presence of an applied field and Satija[7] derived explicit formulas for the Heisenberg-Ising, Heisenberg-xy, and xy-Ising crossovers at low temperatures, using a quantum Hamiltonian forrnalism.

Anisotropy effects on one-dimensional classical systems have been studied in some extent since the introduction of the transfer matrix method in the study of these systems by Joyce[8]. For instance, this method has been applied to the Heisenberg model with single-site anisotropy by Loveluck et *al.*[9] and to the Heisenberg model with dipolar anisotropy by Hone and Pires[10] and Faria and Pires[11].

In this paper we will consider the one-dimensional classical anisotropic planar system with nearest-neighbours interactions for a ferromagnet, represented by the Hamiltonian

$$H = - \sum_{i=1}^{N} (as_i^x s_{i+1}^x + bs_i^y s_{i+1}^y) \tag{1.1}$$

where $s_i^x = \cos\theta_i$ and $s_i^y = \sin\theta_i$ are the components of the classical spin unit vector s_i, a and b are positive constants and we will take $a \geq b$, and use cyclic boundary conditions: $s_{N+1} \equiv s_1$. The system represented by the Hamiltonian (1.1) is interesting because at low temperatures it crosses-over from planar to Ising-like behaviour: at low temperature, for $a > b$, it is energetically more favorable forthe system to align along the x direction.

2. PARTITION FUNCTION

As pointed out by Joyce[8], the partition function as well as the zero-field correlation function can be calculated in terms of Mathieu functions. To see it, we will write the Hamiltonian (1.1) in the form $H = \sum_i H_{i,i+1}$ where

$$-\beta H_{i,i+1} = \beta a(\cos\theta_i \cos\theta_{i+1} + \tanh\mu \sin\theta_i \sin\theta_{i+1}) = f_{i,i+1} \tag{2.1}$$

and

$$\beta = 1/k_B T \quad , \tag{2.2}$$

$$\tanh\mu = b/a \tag{2.3}$$

The partition function

$$Z = \prod_i \int \frac{d\theta_i}{2\pi} \exp(f_{i,i+1}) \tag{2.4}$$

can be expressed in terms of the eingenfunctions $\psi_m(\theta)$ and eingenvalues λ_m of the transfer matrix $\exp(f_{i,i+1})$. They are solutions of the integral equation

$$(1/2\pi) \int d\theta_{i+1} \exp(f_{i,i+1}) \psi_m(\theta_{i+1}) = \lambda_m \psi_m(\theta_i) \tag{2.5}$$

On the other hand, the transfer matrix $\exp(f_{i,i+1})$ can be expanded in terms of the Mathieu functions[12], giving

$$\exp(f_{i,i+1}) = \sqrt{8\pi} \sum_m \Big[(1/M_m^e)\, ce_m(\theta_i,-h^2)\, ce_m(\theta_{i+1},-h^2)$$

$$\times Mc_m(\cosh\mu,-ih) + (1/M_m^0)\, se_m(\theta_i,-h^2)\, se_m(\theta_{i+1},-h^2)$$

$$\times Ms_m(\cosh\mu,-ih)\Big] = g(\theta_i,\theta_{i+1}) \tag{2.6}$$

with

$$h = a/k_B T \cosh\mu = \beta(a^2 - b^2)^{1/2} \ . \tag{2.7}$$

M_m^e and M_m^0 are normalization constants given by

$$M_m^e = \int_0^{2\pi} |ce_m(\theta,-h^2)|^2 \, d\theta = \pi \tag{2.8}$$

and

$$M_m^0 = \int_0^{2\pi} [se_m(\theta,-h^2)]^2 \, d\theta = \pi \tag{2.9}$$

Hence, the normalization eingenfunctions of (2.5) are the Mathieu functions $ce_m(\theta,-h^2)$ (even) and $se_m(0,-h^2)$ (odd), and the corresponding eingenvalues are the radial functions $i^m\, Mc_m(\cosh\mu,\ -ih)$ and $i^m\,\mathrm{Ms}_m(\cosh\mu,\ -ih)$.

In the limit $N\to\infty$ the largest eingenvalue of (2.5) will be dominant in the calculation of the partition function:

$$\lim_{N\to\infty} \left(\frac{1}{N} \ln Z_N\right) \approx \sqrt{2/\pi}\, Mc_0(\cosh\mu,-ih) \ . \tag{2.10}$$

3. SPIN CORRELATION FUNCTIONS AND MAGNETIC SUSCEPTIBILITY

The spin-spin correlation functions are defined by

$$\langle s_j^\alpha\, s_{j+r}^\alpha \rangle = \prod_i \int \frac{d\theta_{i+1}}{2\pi} \exp\, (f_{i,i+1}) s_j^\alpha\, s_{j+r}^\alpha \tag{3.1}$$

For large N, **Eq.** (3.1) gives

$$\langle s_i^x\, s_j^x \rangle = \sum_{m=1}^{\infty} (\lambda_m^e/\lambda_0^e)^{|j-i|} D_m(h) \tag{3.2}$$

$$\langle s_i^y\, s_j^y \rangle = \sum_{m=1}^{\infty} (\lambda_m^0/\lambda_0^e)^{|j-i|} E_m(h) \tag{3.3}$$

where

$$D_m(h) = (1/M_m^e\, M_0^e) \left[\int_0^{2\pi} ce_0(\theta,-h^2)\, ce_m(\theta,-h^2)\, \cos\theta\, d\theta\right]^2 \tag{3.4}$$

$$E_m(h) = (1/M_0^e\, M_m^0) \left[\int_0^{2\pi} ce_0(\theta,-h^2)\, se_m(\theta,-h^2)\, \sin\theta\, d\theta\right]^2 \tag{3.5}$$

and $\lambda_m^e(\lambda_m^0)$ is an even (odd) eingenvalue of (2.5).

High - and low-temperature behaviour of correlationfunctions and zero-field susceptibility can be obtained frcm (3.2) and (3.3) using appropriate expansions of the Mathieu functions in power series as follows.

High Temperatures

At high temperatures the parameter h is small and we can use the asymptotic expressions for ce_m and se_m [13]

$$ce_0(\theta, -h^2) \approx (1/\sqrt{2})(1 + \frac{h^2}{2} \cos 2\theta) + o(h^4) \qquad (3.6)$$

$$ce_1(e, -h^2) \approx \text{cose} \ t \ \frac{h^2}{8} \cos 3a + o(h^4) \qquad (3.7)$$

$$se_1(\theta, -h^2) \approx \sin\theta + \frac{h^2}{8} \sin 3\theta + o(h^4) \qquad (3.8)$$

Substituting (3.6), (3.7) and (3.8) into equations (3.4) and (3.5), we easily obtain

$$D_1(h) \approx (1/2)\ (1 + h^2/2) + o(h^4) \qquad (3.9)$$

$$E_1(h) = (1/2)\ (1 - h^2/2) + o(h^4)\ . \qquad (3.10)$$

We can note that to this order of approxímation, we already obtain the sum rule $<(s_\ell^x)^2> + <(s_R^y)^2> = <(s_{9,})^2> = \sum_R [D_\ell(h) + E_\ell(h)] = 1$, taking into account only the first term of (3.2) and (3.3). Also, the ratios $D_\ell(h)/D_1(h)$ and $E_\ell(h)/E_1(h)$ decrease with R. Then, we can neglect D_ℓ and E_ℓ for $\ell > 1$.

From (2.5), with the choice $\theta_i = 0$, for simplicity, and taking the appropriate Mathieu functions ψ_m for each case, we have

$$\lambda_0^e = [1/ce_0(0,-h^2)] \int_0^{2\pi} g(0,\theta)\ ce_0(\theta,-h^2)(d\theta/2\pi) \qquad (3.11)$$

$$\lambda_1^e = [1/ce_1(0,-h^2)] \int_0^{2\pi} g(0,\theta)\ ce_1(\theta,-h^2)(d\theta/2\pi) \qquad (3.12)$$

The above integrals can be solved with help of the equations (2.6), (3.6) and (3.7). The results are given in terms of modified Bessel functions

$$\lambda_0^e \simeq (1 + h^2/2)^{-1} \left[I_0(-k) + \frac{h^2}{2} I_2(-k)\right] \qquad (3.13)$$

$$\lambda_1^e \simeq -(1 + h^2/8)^{-1}\left[I_1(-k) + \frac{h^2}{8} I_3(-k)\right] , \qquad (3.14)$$

with $k = \beta a$.

Since $se_1(\theta_i, -h^2) = 0$ at $\theta_i = 0$, we set-up $\theta_i = \pi/2$ into (2.5) and in a similar way we obtain

$$\lambda_1^0 \approx -(1 - h^2/8)\left[I_1(-p) - \frac{h^2}{8} I_3(-p)\right] , \qquad (3.15)$$

with $p = \beta b$.

Hence, the two-spins correlation functions $<s_0^a s_\ell^a>$ are given, at high temperatures, by

$$<s_0^x\ s_\ell^x> \simeq (1/2)(1 + 3h^2/8)^\ell \left[\frac{I_1(k) + (h^2/8)I_3(k)}{I_0(k) + (h^2/8)I_2(k)}\right]^\ell (1 + h^2/2) \qquad (3.16)$$

$$<s_0^y\ s_\ell^y> \approx (1/2)(1 + 5h^2/8)^\ell \left[\frac{I_1(p) - (h^2/8)I_3(p)}{I_0(k) + (h^2/2)I_2(k)}\right]^\ell (1 - h^2/2) \qquad (3.17)$$

where we have used the property

$$I_n(-x) = (-1)^n I_n(x) \qquad (3.18)$$

The zero-field susceptibility[14] may be calculated from (3.16) and (3.17) in the limit for large N, giving

$$\lim_{N\to\infty} (2\ k_B T/Ng^2\mu_B^2)\ \chi_T^x \approx$$

$$\frac{I_0(k) + I_1(k) + (h^2/8)\left[I_3(k) + 4I_2(k) + 7I_1(k) + 4I_0(k)\right]}{I_0(k) - I_1(k) - (h^2/8)\left[I_3(k) + 3I_1(k) - 4I_2(k)\right]} , \qquad (3.19)$$

$$\lim_{N\to\infty} (2\ k_B T/Ng^2\mu_B^2)\ \chi_T^y \approx$$

$$\frac{I_0(k) + I_1(p) - (h^2/8)\left[I_3(p) - 4I_2(p) - I_1(p) + 4I_0(k)\right]}{I_0(k) - I_1(p) + (h^2/8)\left[I_3(p) - 5I_1(p) + 4I_2(k)\right]} \qquad (3.20)$$

We can compare these results with the pure isotropic systern setting $h = 0$ in the above expressions to find

$$\langle \vec{s}_0 \cdot \vec{s}_\ell \rangle = \left[I_1(k)/I_0(k)\right]^\ell , \qquad (3.21)$$

$$\lim_{N\to\infty} (2\, k_B T/Ng^2\mu_B^2)\, \chi_T = \left[\frac{I_0(k) + I_1(k)}{I_0(k) - I_1(k)}\right] , \qquad (3.22)$$

which are in accordance with the expressions fonded out by Joyce[4] and Stanley[5] for the isotropic Hamiltonian.

Low Teniperatures

For small T, we can use expansions of Mathieu functions given by Sips[15] for large values of h [13].

Let $y = \sqrt{h}\cos\theta$. Then, we have

$$ce_0(\theta,h^2) \approx c_0\, e^{-y^2/2} \{H_0(y) - (1/16h)\left[H_2(y) + H_4(y)\right] +$$

$$+ (1/128h^2)\left[-9H_2(y) - H_4(y) + H_6(y)/16 + H_8(y)/256\right]\} + o(h^{-3}) \qquad (3.23)$$

$$ce_1(\theta,h^2) \approx (1/\sqrt{2})\, c_1\, e^{-y^2/2} \{H_1(y) - (1/16h)\left[H_3(y) + H_5(y)/8\right] +$$

$$+ (1/128h^2)\left[-15H_3(y) - 3H_5(y)/2 + H_7(y)/16 + H_9(y)/256\right]\} + o(h^{-3})$$

$$(3.24)$$

$$se_1(\theta,h^2) \approx s_0\, e^{-y^2/2} \{H_0(y) + (1/16h)\left[H_2(y) - H_4(y)/8\right] +$$

$$+ (1/128h^2)\left[9H_2(y) - H_4(y) - H_6(y)/16 + H_8(y)/256\right]\} \sin\theta + o(h^{-3}) ,$$

$$(3.25)$$

where

$$c_0 \approx (\pi h/4)^{1/4} \left[1 + 1/4h + 27/128h^2 + o(h^{-3})\right]^{-1/2} \quad (3.26)$$

$$c_1 \approx (\pi h/4)^{1/4} \left[1 + 3/4h + 159/128h^2 + o(h^{-3})\right]^{-1/2} \quad (3.27)$$

$$c_2 \approx (\pi h/4)^{1/4} \left[1 - 1/4h - 21/128h^2 + o(h^{-3})\right]^{-1/2} , \quad (3.28)$$

and $H_n(y)$ is a Hermite polinomial of n^{-th} order.

From (3.5), setting the change of variable $\theta \to \pi/2 - \theta$ and with help of the relations between Mathieu functions of different arguments[13], we find

$$E_1(h) = \frac{1}{\pi^2}\left[-\int_{\pi/2}^{-3\pi/2} ce_0(\theta,h^2)ce_1(\theta,h^2)\cos\theta\, d\theta\right]^2 \quad (3.29)$$

We note that from (3.23) and (3.24) the integral in (3.29) will depend on a term exp $(-y^2)$ which will be predominant for h large, except when $y \sim 0$. Then, this integral will take considerable values only if $\theta \approx \pi/2, -\pi/2, -3\pi/2$. Setting the change of variable $\theta \to y$, we can write for large h

$$\int_{\pi/2}^{-3\pi/2} d\theta \to 4 \int_0^{\infty} dy. \quad (3.30)$$

Now, it is a simple matter to show that to first order in h

$$E_1(h) = 1/2h . \quad (3.31)$$

And in a similar way, we find

$$D_1(h) \approx 1 - 1/2h . \quad (3.32)$$

The same arguments that we used for taking only the first term of (3.4) and (3.5) for high temperatures can be used here.

We can calculate approximate expressionç for λ_m^e and λ_m^0 using (2.5) and asymptotic expansions for the Mathieu functions. For instance, taking $\theta_i = 0$ in (2.5), we have

$$\lambda_0^e \approx [2c_0/\pi\sqrt{h}\; ce_0(\pi/2,h^2)] \int_0^\infty e^{-y^2/2}\, e^{\beta a(1-y^2/h)^{1/2}}\, (1 - y^2/h)$$

$$\times \{H_0(y) - (1/16h)[H_2(y) + H_4(y)/8] + (1/128h^2)[-9H_2(y) - H_4(y) +$$

$$+ H_6(y)/6 + H_8(y)/256]\}\, dy\ . \tag{3.33}$$

Expanding $(1 - y^2/h)^{-1/2}$ and $e^{\beta a(1-y^2/h)^{1/2}}$ in powers of $h^{-1}\, y^2$ we can solve the integral (3.33) using the Gamma function. We find

$$\lambda_0^e \approx \sqrt{2/\pi h}\; e^{\beta a}\, [1 - (1/16h)(8\beta a - 9/2) +$$

$$+ (1/128h^2)(545/16 - 50\,\beta a + 48\,\beta^2 a^2)]\, (1 + 1/32h + 81/2048h^2)^{-1}\ . \tag{3.34}$$

In a similar way, we have

$$\lambda_1^e \approx \sqrt{2/\pi h}\;\; e^{\beta a}\, [1 + (1/16h)(1/2 - 8\beta a) +$$

$$+ (1/128h^2)(81/16 - 34\beta a + 48\,\beta^2 a^2)](1 - 7/32h - 255/2048h^2)^{-1}\ . \tag{3.35}$$

For λ_1^0 we cannot use the above procedure because $se_1(0,-h^2) = 0$, so we take the θ_i derivative of (2.5) and following similar sceps we obtain

$$\lambda_1^0 \approx (\sqrt{2}\;\beta b\;\; e^{\beta a}/\sqrt{\pi}\; h^{3/2})\;\; [1 - (1/32h)(48\beta a\; - 21)]\; \times\; (1 - 3/32h)^{-1}\ . \tag{3.36}$$

Hence

$$\lambda_1^e/\lambda_0^e \approx 1 + o(h^{-3}) \tag{3.37}$$

$$\lambda_1^0/\lambda_0^e \approx (\beta b/h)\left[1 + (1/2h)(1 - 2\beta a) + o(h^{-2}) + \ldots\right] . \quad (3.38)$$

Putting all results together we can write

$$<s_0^x\ s_\ell^x> \approx (1 - 1/2h)\ \left[1 + o(h^{-3}) + \ldots\right]^\ell , \quad (3.39)$$

$$<s_0^y\ s_\ell^y> \approx (1/2h)\{\left[1+(1/2h)(1 - 2\beta a)\right](\beta b/h)\}^\ell . \quad (3.40)$$

From the above expressions we can see that when T gets close to zero the correlation function $<s_0^y\ s_\ell^y>$ vanishes with T and $<s_0^x\ s_\ell^x> \to 1$, thus the system behaves like an Ising system. The spins align along the x - direction.

Using the transfer rnatrix technique we can solve the anysotropic model numerically for all values of T [16] even in the presence of an external magnetic field[17] and such procedure is more convenient than using the expansions in terms of Mathieu functions. However, the approach presented in this paper is usefull because it allows ustoget high and low temperature analytic expressions for the termodynamic functions.

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