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On the thermodynamics of classical spins with isotrop Heisenberg interaction in one-dimensional quasi-periodic structures

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Abstract

An exact expression for the free energy of a system of classical magnetic moments, which occupy sites on a Fibonacci or Thue–Morse quasi-crystal lattice and interact via an isotropic Heisenberg interaction, is obtained. The temperature dependence of the specific heat for certain classes of one-dimensional quasi-crystal lattices is discussed. In the case, when spin rotations are confined in a plane (model of plane rotators), some Fibonacci crystals show an extra peak in the specific heat at low temperatures.

1. Introduction and model

Recently, great attention has been paid to the physical properties of quasi-periodic systems on one-dimensional lattices (1D) [1]. These systems are intermediate between completely periodic, perfect crystals and random, amorphous solids. The 1D quasi-crystal, which is constructed by arranging two different building blocks A and B in a Fibonacci series, has become a standard model for investigations in these systems.

The Fibonacci sequence P_∞ is obtained by the recursion relation $P_{l+1} = \{P_l P_{l-1}\}$ for $l \geqslant 1$ with $P_0 = \{B\}$ and $P_1 = \{A\}$. If F_{l+1} is the total number of elements in the sequence P_{l+1}, we can find F_{l+1} from the recursion relation $F_{l+1} = F_{l-1} + F_l$ for $l \geqslant 1$, with $F_0 = F_1 = 1$.

Generalized Fibonacci lattices are straightforward generalizations of the above, where two building blocks A and B are arranged in the Fibonacci sequence. The generalized Fibonacci sequence $P_\infty^{\alpha,\beta}$ is given by the recursion relation

$$P_{l+1}^{\alpha,\beta} = \{P_l^\alpha P_{l-1}^\beta\}, \tag{1}$$

where $P_0 = \{B\}$ and $P_1 = \{A\}$ for $l \geqslant 1$, and α and β positive integers.

The generalized Fibonacci number $\tilde{F}_{l-1}$ is the total number of building blocks A and B in $P_{l+1}^{\alpha,\beta}$. It has the recurrence relation $\tilde{F}_{l+1} = \alpha\tilde{F}_{l-1} + \beta\tilde{F}_l$, for $l \geqslant 1$ with $\tilde{F}_0 = \tilde{F}_1 = 1$. The relative portion of type A elements is given by

$$P_{\alpha,\beta} = \lim_{l\to\infty} \frac{N_A^{(l)}}{N_A^{(l)} + N_B^{(l)}} = \lim_{l\to\infty} \frac{\tilde{F}_l}{\tilde{F}_l + \tilde{F}_{l-1}}$$

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$$= \frac{\eta_{\alpha,\beta}}{1+\eta_{\alpha,\beta}}, \tag{2}$$

where $N_A^{(l)}$ ($N_B^{(l)}$) is the number of elements of type $A(B)$ and $\eta_{\alpha,\beta} = \tilde{F}_l/\tilde{F}_{l-1}$. In the limit $l \to \infty$, $\eta_{\alpha,\beta}$ goes to $\frac{1}{2}[\beta + (\beta^2 + 4\alpha^2)^{1/2}]$. The Fibonacci sequence with the golden mean is obtained by putting $\alpha = \beta = 1$ and then $\eta_{1,1} = (1+\sqrt{5})/2$.

A Thue–Morse sequence has a quite different kind of aperiodicity than a Fibonacci sequence [2–5]. The Thue–Morse sequence is defined by the recursion relation $M_{l+1} = \{M_l M_l^*\}$ for $l \geqslant 1$ with $M_0 = \{AB\}$ and where M_l^* is the complement of M_l, which can be obtained by interchanging A and B. In each generation of the Thue–Morse sequence the proportion of type A elements to type B elements is $\frac{1}{2}$.

The (electronic, phonon and the plasmons) spectral and transport properties of quasi-periodic Fibonacci and Thue–Morse lattices have been intensively studied in Refs. [2–12]. The thermodynamic properties of a 1D Ising spins on a Finonacci lattice in the absence of a magnetic field have been calculated in the case of equal concentrations of atoms A and B in Refs. [13, 14]. Furthermore, the statistics of a binary alloy has been investigated at low- and high-temperatures taking into account the different concentrations of atoms, or alternatively, a magnetic field [15].

In this paper we concentrate on the thermodynamic proporties of spins in a classical Heisenberg model, where the spins are located at the sites of the generalised Fibonacci lattice or Thue–Morse lattice. We find an exact analytical expression for free energy of the systems, as well in the case when spins are allowed to rotate in a plane (model of plane rotators), as in the case of three dimensional rotation.

2. The method of calculation

Let us consider the linear chain of magnetic moments in the absence of an external magnetic field with arbitrary interactions between nearest atoms. The partition function of this system is given by

$$Z = \int \cdots \int \exp\left(\sum_{j=1}^{N-1} W_j \boldsymbol{S}_j \boldsymbol{S}_{j+1}\right) \prod_{j=1}^{N} \mathrm{d}\Omega_j, \tag{3}$$

where $W_j \equiv W(j, j+1)$ is, except for a sign, the exchange integral of the nearest moments j and $j+1$, scaled with the statistic temperature kT.

If $W_j < 0$ the ground state is antiferromagnetic and if $W_j > 0$ the ground state is ferromagnetic. The vectors $\boldsymbol{S}_j$ and $\boldsymbol{S}_{j+1}$ characterise the magnetic moments of the sites j and $j+1$ and are of unit length. The vectors $\boldsymbol{S}_j$ are directed into the solid angle $\mathrm{d}\,\Omega_j = \sin\theta_j \,\mathrm{d}\,\theta_j \,\mathrm{d}\varphi_j$ (θ_j, φ_j are the spherical angles of the vector $\boldsymbol{S}_j$). N is a total numbers of sites in the lattice. The integration in Eq. (3) will be carried out over all possible orientations of the moments.

Let us first consider the case, where all dipoles have an arbitrary orientation in the plane. The partition function (3) can then be written in the form

$$Z_{\mathrm{pl}} = \int \cdots \int \exp\left(\sum_{j=1}^{N-1} W_j \cos(\varphi_j - \varphi_{j+1})\right) \times \prod_{j'=1}^{N} \mathrm{d}\varphi_{j'} \tag{4}$$

or equivalently as

$$Z_{\mathrm{pl}} = \int \cdots \int \prod_{j=1}^{N-1} \left[I_0(W_j) + \sum_{n_j=-\infty}^{\infty}{}' I_{n_j}(W_j) \times \exp\{\mathrm{i} n_j(\varphi_j - \varphi_{j+1})\}\right] \prod_{j'=1}^{N} \mathrm{d}\varphi_{j'}. \tag{5}$$

Here, use is made of

$$\exp\{W_j \cos(\varphi_j - \varphi_{j-1})\} = I_0(W_j) + \sum_{n_j=-\infty}^{\infty}{}' I_{n_j}(W_j) \exp\{\mathrm{i} n_j(\varphi_j - \varphi_{j+1})\}, \tag{6}$$

$I_n(x)$ are Bessel functions of nth order with imaginary arguments. The sum $\sum'$ in Eqs. (4) and (5) extend over all n_j excluding $n_j = 0$.

After a final integration over the angles $\varphi_{j'}$ in Eq. (5) one obtains the result

$$Z_{\mathrm{pl}} = (2\pi)^N \prod_{j=1}^{N-1} I_0(W_j). \tag{7}$$

In particular, for a translational invariant lattice: $W_1 = W_2 = \cdots = W_{N-1} = W$ and $N \gg 1$ we have

$$Z_{\mathrm{pl}} = [2\pi I_0(W)]^N. \tag{8}$$

This expression is the same as the one, which was derived by [16] using the transfer-matrix method, for a close system of plane rotators.

The more general case is the one, where the moments have different orientations in three dimensions (model od spherical rotators).

Let us introduce the matrix $\exp(W_j \boldsymbol{S}_j \boldsymbol{S}_{j+1})$. The eigenvalues and eigenoperators of this matrix are determined by the following eigenvalue problem:

$$\int \exp(W_j \boldsymbol{S}_j \boldsymbol{S}_{j+1}) \Phi_\sigma(\boldsymbol{S}_{j+1})\, \mathrm{d}\Omega_{j+1} = \lambda_\sigma \Phi_\sigma(\boldsymbol{S}_j). \tag{9}$$

The eigenvalues and the eigenfunctions of this equation have the form

$$\lambda_\sigma(W_j) = \lambda_n = W_j^n \left(\frac{\mathrm{d}}{W_j\, \mathrm{d}W_j}\right)^n \frac{\sinh W_j}{W_j}, \tag{10}$$

$$\Phi_\sigma(\boldsymbol{S}_j) = \Upsilon_{n,m}(\theta_j, \varphi_j) = \left[\frac{2n+1}{4\pi} \frac{(n-|m|)!}{(n+|m|)!}\right]^{1/2} \times P_n^{|m|}(\cos\theta_j) \mathrm{e}^{\mathrm{i}m\varphi_j}, \tag{11}$$

where $\Upsilon_{n,m}(\theta_j, \varphi_j)$ are surface harmonics, $P_n^{|m|}(x)$ are the associated Legender functions, $n = 0, 1, 2, \ldots$, $-n \leqslant m \leqslant n$; $\sigma = \{n, m\}$. From the orthogonality condition of the eigenvectors of the hermitian operators, it follows that

$$\int \Phi_\sigma(\boldsymbol{S}_j) \Phi_{\sigma'}(\boldsymbol{S}_j)\, \mathrm{d}\Omega_j = \delta_{\sigma\sigma'}. \tag{12}$$

Using the standard bilinear representation of a matrix, one can rewrite the matrix

$$\exp(W_j \boldsymbol{S}_j \boldsymbol{S}_{j+1}) = \frac{\sinh W_j}{W_j} + \sum_\sigma{}' \lambda_\sigma(W_j) \Phi_\sigma(\boldsymbol{S}_j) \times \Phi_\sigma(\boldsymbol{S}_{j-1}). \tag{13}$$

In the above expression, the sum runs over the entire spectra except for $\sigma = \{0, 0\}$. Calculating the partition function (3) with Eq. (13) and making use of Eq. (12), gives the following result:

$$Z_{\mathrm{sp}} = (4\pi)^N \prod_{j=1}^{N-1} \frac{\sinh W_j}{W_j}. \tag{14}$$

In the special case of an ideal lattice, the well-known expression

$$Z_{\mathrm{sp}} = \left(4\pi \frac{\sinh W}{W}\right)^N \tag{15}$$

for $N \gg 1$ can be recovered from Eq. (14), which has been obtained by [17] using another method.

3. Free energy of quasi-periodic lattices

The general expressions Eqs. (7) and (14) can be evaluated for the special case of a generalized Fibonacci lattice. The Fibonacci lattice is a special case of a classical 1D Heisenberg model with non-isotropic interactions. The exchange integrals W_j can assume only two possible values W_A or W_B. The sequence of the values W_A and W_B can be derived from the recurrence relation (1).

According to Eqs. (2) and (7), the partition function for the generalized Fibonacci lattice in the case of the plane rotators, will have the following form for $N \to \infty$:

$$Z_{\mathrm{pl}}^{\mathrm{F}} = (2\pi)^N [I_0(W_A)]^{NP_{\alpha,\beta}} [I_0(W_B)]^{N(1-P_{\alpha,\beta})}. \tag{16}$$

Similarly, one deduces for the spherical rotators from Eq. (14),

$$Z_{\mathrm{sp}}^{\mathrm{F}} = (4\pi)^N \left[\frac{\sinh W_A}{W_A}\right]^{NP_{\alpha,\beta}} \left[\frac{\sinh W_B}{W_B}\right]^{N(1-P_{\alpha,\beta})}. \tag{17}$$

The knowledge of an explicit expression for the partition functions, Eqs. (16) and (17), allows us to calculate any physical quantity. Particularly, we are interested in the free energy per site. For the model plane rotators we get

$$N^{-1} F_{\mathrm{pl}}^{\mathrm{F}} = -kT[\ln 2\pi + P_{\alpha,\beta} \ln I_0(W_A) + (1 - P_{\alpha,\beta}) \ln I_0(W_B)] \tag{18}$$

and for the model of spherical rotators one has

$$N^{-1} F_{\mathrm{sp}}^{\mathrm{F}} = -kT \left[\ln 4\pi + P_{\alpha,\beta} \ln \frac{\sinh W_A}{W_A} + (1 - P_{\alpha,\beta}) \ln \frac{\sinh W_B}{W_B}\right]. \tag{19}$$

Here T is the absolute temperature, k is the Boltzmann constant. In order to calculate the free energy of the

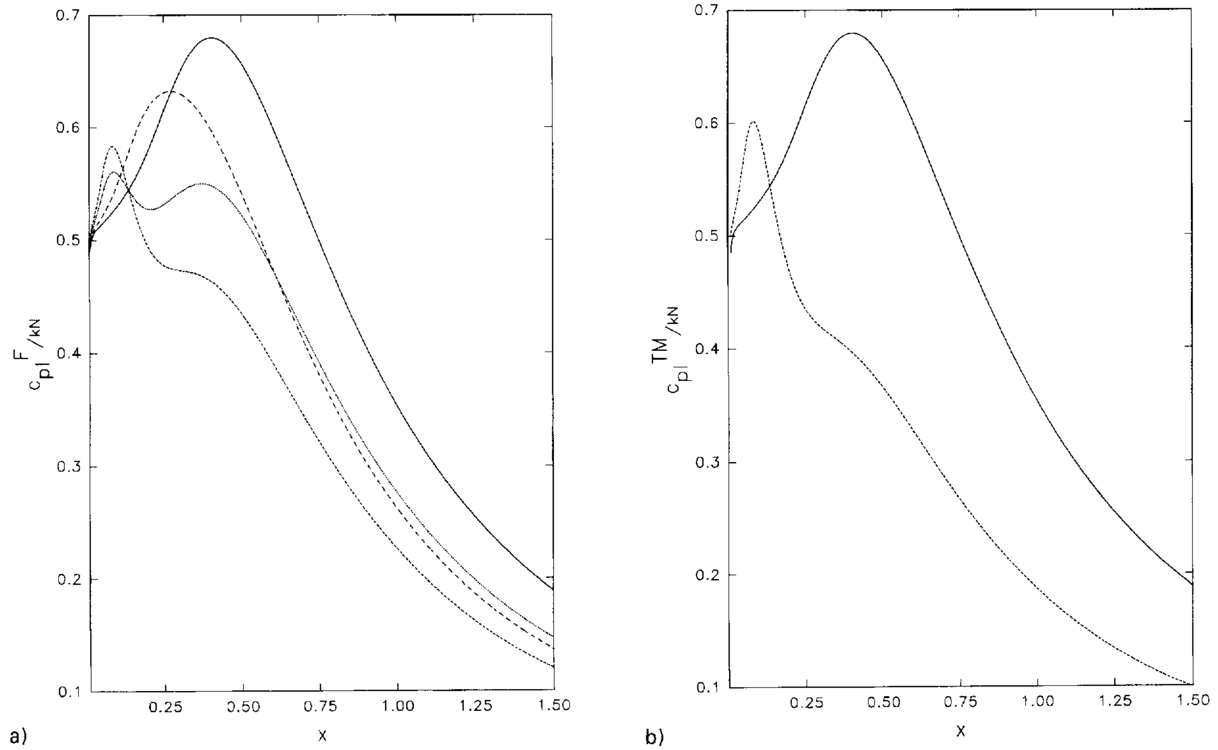

Fig. 1. Specific heat is shown as a function of temperature, $x = kT/W_A$, for the linear chain of plane rotators: (a) Fibonacci lattice with parameters $v = 0.5$, $\alpha = \beta = 1$ (long-dashed line); $v = 0.2$, $\alpha = \beta = 1$ (dashed line); $v = 0.2$, $\alpha = 1$, $\beta = 3$ (dotted line) and $v = 1$ for a regular lattice (full line); (b) Thue–Morse lattice with parameters $v = 0.5$, (full line); $v = 0.2$, (dashed line).

Thue–Morse lattice, one has to replace $P_{\alpha,\beta}$ by $\frac{1}{2}$ in expressions (18) and (19).

4. Discussion

To illustrate the influence of the lattice's quasi-periodicity on the thermodynamic properties, we consider the specific heats of the Heisenberg model on the one-dimensional generalized Fibonacci and on the Thue–Morse lattice using Eqs. (18) and (19). For the plane rotator model, we get

$$C^{\mathrm{F}}_{\mathrm{pl}}/kN = P_{\alpha,\beta} W_A^2 [1 - W_A^{-1} f(W_A) - f^2(W_A)] + (1 - P_{\alpha,\beta}) W_B^2 [1 - W_B^{-1} f(W_B) - f^2(W_B)], \quad (20)$$

where $f(x) = I_1(x)/I_0(x)$.

For the spherical rotators, the specific heat is given by

$$C^{\mathrm{F}}/kN = P_{\alpha,\beta}\left[1 - \frac{W_A^2}{\sinh^2 W_A}\right] + (1 - P_{\alpha,\beta})\left[1 - \frac{W_B^2}{\sinh^2 W_B}\right]. \quad (21)$$

Using Eqs. (20) and (21), we plot the temperature dependence of $C(T)$ in $x = kT/W_A$ (see Eq. (3)) for the different parameters $v = W_B/W_A$, α and β (see Figs. 1 and 2). It can be seen, that in the case of the spherical rotators (Fig. 2(a) and 2(b)) the quasi-periodicity of the lattice does not cause any qualitative change in the temperature dependence of the specific heat, when compared with the ordinary Heisenberg model. In the case of the model of plane rotators (see Fig. 1(a) and 1(b)), the maximum of the specific heat $C^{\mathrm{F}}_{\mathrm{pl}}(T)$ is smaller than in the case of the ordinary Heisenberg model, and it shifts to lower temperatures. However,

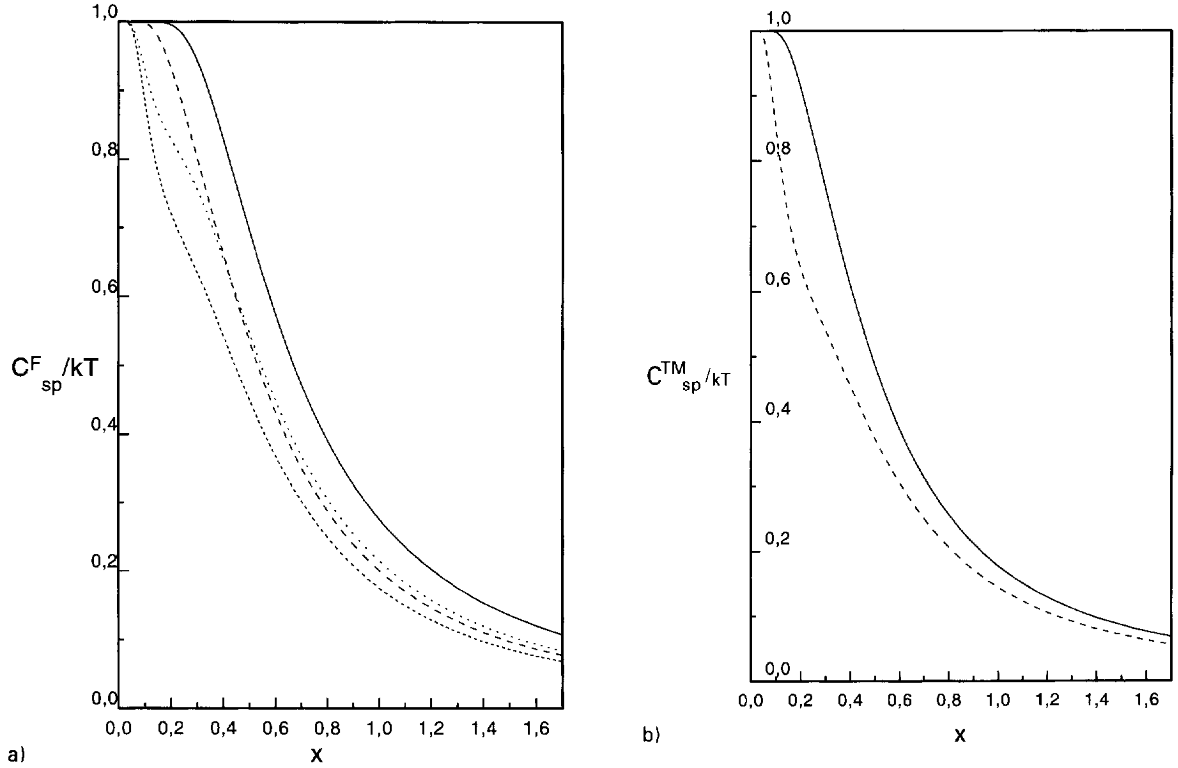

Fig. 2. Specific heat is plotted as a function of temperature, $x = kT/W_A$, for the linear chain of three-dimensional rotators: (a) Fibonacci lattice with parameters $v = 0.5$, $\alpha = \beta = 1$ (long dashed line); $v = 0.2$, $\alpha = \beta = 1$ (dashed line); $v = 0.2$, $\alpha = 1$, $\beta = 3$ and $v = 1$ for a regular lattice (full line); (b) Thue–Morse lattice with parameters $v = 0.5$, (full line); $v = 0.2$, (dashed line).

there is a striking difference between the two models. The Fibonacci lattice shows an additional peak for small values of v at low temperatures (dotted line in Fig. 1). This peak flattens, when $P_{\alpha,\beta}$ decreases. Since the heat capacity contains information about the ordering of the system, Fig. 1 indicates near ordering in the quasi-periodic Fibonacci lattice for plane rotators. Analogous behaviour for the heat capacity in the bond-diluted Ising model on a Fibonacci lattice with different concentrations of atoms was obtained by Badalian et al. [15].

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