



On the statistics of binary alloys in one-dimensional quasiperiodic lattices

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Abstract

We found the asymptotic solutions at low and high temperatures of the partition function of a general one-dimensional binary alloy. As a particular application, we considered the thermodynamic properties of quasiperiodic Fibonacci lattices. We showed that, at low temperatures, the quasiperiodicity produces an extra peak in the specific heat when plotted versus temperature.

1. Introduction and model

Great attention has been devoted to the study of physical properties of quasiperiodic systems in one-dimensional (1D) lattices in connection with the discovery of icosahedral symmetry in quenched Al–Mn [1] and with experiments in quasiperiodic superstructures [2–4]. The Fibonacci lattice, which is constructed by arranging two different building blocks *A* and *B* in a Fibonacci sequence, has become a standard model in the study of these systems. The Fibonacci sequence S_∞ is obtained by the recursion relation $S_{l+1} = \{S_l S_{l-1}\}$ for $l \geq 1$, with $S_0 = \{B\}$ and $S_1 = \{A\}$. One has $S_2 = \{BA\}$, $S_3 = \{ABA\}$, $S_4 = \{BAABA\}$, $S_5 = \{ABABAAB-A\}$, and so on. The Fibonacci number F_{l+1} is the

total number of elements in S_{l+1} and obeys the recursion relation $F_{l+1} = F_{l-1} + F_l$ for $l \geq 1$, with $F_0 = F_1 = 1$.

The generalized Fibonacci lattices in which the two building blocks *A* and *B* are arranged in the generalized Fibonacci sequence are straightforward generalizations of the Fibonacci lattice. The generalized Fibonacci sequence $S_\infty^{m,n}$ is given recursively by

$$S_{l+1}^{m,n} = \{S_{l-1}^m S_l^n\}, \tag{1}$$

with $S_0 = \{B\}$ and $S_1 = \{A\}$ for $l \geq 1$, and *m* and *n* positive integers.

The generalized Fibonacci number F_{l+1} is the total number of building blocks *A* and *B* in $S_{l+1}^{m,n}$, which obeys the recursion relation

$$F_{l+1} = mF_{l-1} + nF_l, \tag{2}$$

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for $l \geq 1$ with $F_0 = F_1 = 1$. The relative proportion of blocks of type A is given by

$$P_{m,n} = \lim_{l \rightarrow \infty} \frac{N_A^{(l)}}{N_A^{(l)} + N_B^{(l)}} = \lim_{l \rightarrow \infty} \frac{F_l}{F_l + F_{l-1}} = \frac{\tau(m,n)}{1 + \tau(m,n)}, \quad (3)$$

where $N_A^{(l)}$ ($N_B^{(l)}$) is the number of blocks of type A (B) and $\tau(m,n) = F_l/F_{l-1}$ is the l th rational approximant to the “mean”. It is easy to show that in the limit $l \rightarrow \infty$, $\tau(m,n)$ tends to $\frac{1}{2}[n + (n^2 + 4m^2)^{1/2}]$. The Fibonacci sequence with the golden mean is obtained by putting $m = n = 1$ and then $\tau(1,1) = (1 + \sqrt{5})/2$.

The electronic and phonon spectra of quasi-periodic Fibonacci lattices have been studied in Refs. [5–15]. The thermodynamic properties of a bond-diluted Ising model on a Fibonacci lattice at zero magnetic field and equal concentration of atoms 1 and 2 have been investigated by Ghosh [16, 17]. When these concentrations are different, the chemical potential has to be taken into account, which is equivalent to considering an external magnetic field. In this paper, we extend Ghosh's calculations to include different concentrations of atoms or, equivalently, the presence of a magnetic field.

Let us consider an alloy consisting of two types of atoms, 1 and 2, lying on a 1D chain in any order and with an arbitrary interaction between nearest atoms. We denote by $V_{\alpha\beta}(i)$ the interaction energy between atom α (which can be either 1 or 2) on site i and atom β ($= 1, 2$) on site $i + 1$. By symmetry, these interaction energies verify $V_{\alpha\beta}(i) = V_{\beta\alpha}(i)$. The Hamiltonian of the system is given by

$$H = \frac{1}{2} \sum_i^N \{ V_{11}(i)c_i c_{i+1} + V_{12}(i)c_i(1 - c_{i+1}) + V_{21}(i)(1 - c_i)c_{i+1} + V_{22}(i)(1 - c_i)(1 - c_{i+1}) \}, \quad (4)$$

where c_i is equal to 1 if site i is occupied with an atom of type 1 and equal to 0 if the atom is of type 2; see, e.g. Ref. [18]. It is convenient to replace c_i by $c_i = (\sigma_i + 1)/2$, where σ_i takes the values ± 1 .

With this transformation the Hamiltonian becomes

$$H = H_0 - \sum_{j=1}^N \Phi_j \sigma_j - \sum_{j=1}^N W_j \sigma_j \sigma_{j+1}, \quad (5)$$

where H_0 is a constant, independent of the atomic configuration, and does not enter into calculations; $4W_j = -V_{11}(j) - V_{22}(j) + 2V_{12}(j)$ is the exchange energy between nearest atoms (when $V_{12} < (V_{11} + V_{22})/2$, atoms 1 and 2 tend to be situated alternately) and $4\Phi_j = V_{22}(j) - V_{11}(j)$. Note that the appearance of the local field Φ_j in Eq. (5) is produced by the breaking of the translational symmetry in the inhomogeneous model.

The conservation of the atoms of the system is defined by the following conditions:

$$\sum_{j=1}^N \sigma_j = (2C_0 - 1)N, \quad (6)$$

where $C_0 = N_1/N$ is the concentration of atoms of type 1, and N is the total number of atoms.

2. Method of solution

The partition function of the system is given by

$$Z = \sum_{\sigma_1 = \pm 1} \cdots \sum_{\sigma_N = \pm 1} \exp \left\{ \beta \sum_{j=1}^N (\mu + \Phi_j) \sigma_j + \beta \sum_{j=1}^N W_j \sigma_j \sigma_{j+1} \right\}, \quad (7)$$

where $\beta = 1/kT$ is the inverse temperature, and μ is the chemical potential, which we will find from Eq. (6).

In the case of a translational invariant lattice ($W_1 = W_2 = \cdots = W_N = W$, $\Phi_j = \text{constant}$) the partition function Z can be obtained by means of the transfer matrix technique [19]. Following this method, the exponential in Eq. (7) can be factored into terms each involving only two neighbouring atoms and the partition function Z corresponding to a closed sequence of N atoms ($\sigma_1 = \sigma_{N+1}$) can be written in the following form:

$$Z = \sum_{\sigma_1 = \pm 1} \cdots \sum_{\sigma_N = \pm 1} P_1(\sigma_1, \sigma_2) P_2(\sigma_2, \sigma_3) \cdots P_N(\sigma_N, \sigma_1) = \text{Tr } P_1 P_2 \cdots P_N = \text{Tr } P. \quad (8)$$

In this expression $P_j(\sigma_j, \sigma_{j+1}) = \exp(\tilde{\mu}_j \sigma_j + \tilde{W}_j \sigma_j \sigma_{j+1})$ are the elements of a two-by-two transfer matrix

$$P_j = \begin{pmatrix} P_j(1, 1) & P_j(1, -1) \\ P_j(-1, 1) & P_j(-1, -1) \end{pmatrix} = \begin{pmatrix} e^{\tilde{\mu}_j + \tilde{W}_j} & e^{\tilde{\mu}_j - \tilde{W}_j} \\ e^{-\tilde{\mu}_j - \tilde{W}_j} & e^{-\tilde{\mu}_j + \tilde{W}_j} \end{pmatrix}, \tag{9}$$

where $\tilde{\mu}_j = \beta(\mu + \Phi_j)$ and $\tilde{W}_j = \beta W_j$.

In the homogeneous case, all the transfer matrices P_j are equal and so $P = P_j^N$. Thus, the calculation of the trace of the matrix P is equivalent to finding the maximum eigenvalue of the matrix P_j . Unfortunately, for alloys with inhomogeneous interactions the transfer matrices P_j do not commute and we have to calculate the product of all the transfer matrices. This is the main difficulty of this problem.

We can avoid this difficulty in two limiting cases. These two cases correspond to very low and very high temperatures. We can transform the partition function Eq. (7) and write it in the form (see appendix)

$$Z = K(\mu, T) \prod_{j=1}^N \cosh \tilde{W}_j. \tag{10}$$

Here

$$K(\mu, T) = \sum_{\{s_j\}=1}^2 a_1(s_1, s_2) a_2(s_2, s_3) \cdots a_N(s_N, s_1) \times \exp \left\{ \sum_{j=1}^N \sigma_j \tilde{\mu}_j \right\}, \tag{11}$$

where $a_j(s_j, s_{j+1}) = 1 + \varepsilon_j \exp i\pi(s_j + s_{j+1})$ and $\varepsilon_j = \tanh \tilde{W}_j$.

When the number of atoms of type 1 and 2 is the same we have $\mu = \Phi_j = 0$, and when $N \rightarrow \infty$ we recover the well-known result for the inhomogeneous Ising model at zero magnetic field [20]:

$$Z_0 = 2^N \prod_{j=1}^N \cosh \tilde{W}_j. \tag{12}$$

At very low temperatures, $\tilde{W}_j \gg 1$ and $\varepsilon_j \approx 1$. We can rotate the matrix $a_j(s_j, s_{j+1})$ and obtain a new

commuting set of transfer matrices \bar{a}_j of the form

$$\bar{a}_j = \begin{pmatrix} 2 \exp[-\frac{1}{2}(\tilde{\mu}_j + \tilde{\mu}_{j+1})] & 0 \\ 0 & 2 \exp[\frac{1}{2}(\tilde{\mu}_j + \tilde{\mu}_{j+1})] \end{pmatrix}. \tag{13}$$

So, for large N , we find that the partition function Z is given by

$$Z_1 = Z_0 \exp \beta(N\mu + \sum_{j=1}^N \Phi_j). \tag{14}$$

At high temperatures, we have $\tilde{W}_j \ll 1$, $\varepsilon_j \approx 0$ and $a_j(s_j, s_{j+1}) \approx 1$, thus $K(\mu, T) = 2^N \prod_{j=1}^N \cosh \tilde{\mu}_j$ and

$$Z_h = Z_0 \sum_{j=1}^N \cosh \tilde{\mu}_j. \tag{15}$$

Let us consider now the case of the generalized Fibonacci lattice. We assume that each function $V_{\alpha\alpha'}(j)$ can take one of the two values $V_{\alpha\alpha'}(A)$ or $V_{\alpha\alpha'}(B)$. Consequently, W_j and Φ_j will also take two possible values W_A, W_B and Φ_A, Φ_B . The sequence of these quantities can be obtained from the defining recursive relation, Eq. (1). Then, Eq. (14), which gives us the partition function at low temperatures, becomes, for the Fibonacci lattice,

$$Z_1^F = Z_0^F \exp \{ N\beta[\mu + P_{m,n}\Phi_A + (1 - P_{m,n})\Phi_B] \}, \tag{16}$$

where

$$Z_0^F = 2^N (\cosh \tilde{W}_A)^{P_{m,n}N} (\cosh \tilde{W}_B)^{(1 - P_{m,n})N}. \tag{17}$$

Analogously, at high temperatures, Eq. (15) becomes

$$Z_h^F = Z_0^F [\cosh \beta(\mu + \Phi_A)]^{P_{m,n}N} \times [\cosh \beta(\mu + \Phi_B)]^{(1 - P_{m,n})N}. \tag{18}$$

These partition functions depend on the chemical potential μ and can be calculated through the formula

$$N(2C_0 - 1) = \partial \ln Z / \partial (\beta\mu), \tag{19}$$

which follows from Eq. (6) and which ensures conservation of the two types of atoms of the system.

Substituting Eq. (17), for low temperatures, and Eq. (18), for high temperatures, in Eq. (19), we find μ as a function of C_0 . At the high temperature, for example, μ is implicitly given by

$$P_{m,n} \tanh \beta(\mu + \Phi_A) + (1 - P_{m,n}) \tanh \beta(\mu + \Phi_B) = 2C_0 - 1. \quad (20)$$

The knowledge of an explicit expression for the partition function, Eqs. (16) and (18), allows us to calculate any other physical quantities. We are interested in the free energy per site F , which is given by

$$N^{-1}F_1^F = \phi_0 - [\mu + P_{m,n}\Phi_A + (1 - P_{m,n})\Phi_B], \quad (21)$$

at low temperatures, and by

$$N^{-1}F_h^F = \phi_0 - \beta^{-1} \{ P_{m,n} \ln[\cosh \beta(\mu + \Phi_A)] + (1 - P_{m,n}) \ln[\cosh \beta(\mu + \Phi_B)] \}, \quad (22)$$

at high temperatures, where ϕ_0 is defined as

$$\phi_0 = -\beta^{-1} \{ P_{m,n} \ln[2 \cosh \tilde{W}_A] + (1 - P_{m,n}) \ln[2 \cosh \tilde{W}_B] \}. \quad (23)$$

The influence of the quasiperiodic lattice on the thermodynamic properties produces a peak in the specific heat at low temperatures, never reported before. This peak appears even in the $C_0 = 0.5$ case, where we can consider the exactly solvable Ising model. In this case, the specific heat C can be calculated by deriving Eq. (23), with $\mu = 0$ and $C_0 = 0.5$, twice with respect to temperature. We obtain

$$\frac{C}{k_B N} = P_{m,n} \tilde{W}_A^2 \cosh^{-2} \tilde{W}_A + (1 - P_{m,n}) \tilde{W}_B^2 \cosh^{-2} \tilde{W}_B. \quad (24)$$

3. Numerical results and conclusions

In Fig. 1, we plot the specific heat C at the zero field, given by Eq. (24), as a function of normalized temperature, $x = kT/W_A$, for four values of the parameters $\nu = W_B/W_A$ and m, n . The dashed line corresponds to $\nu = 0.5$, $m = 1$ and $n = 1$; the full

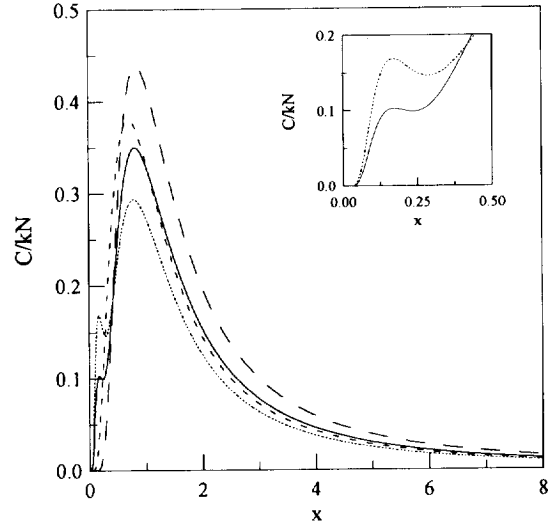


Fig. 1. Specific heat as a function of temperature, $x = kT/W_A$, for a Fibonacci lattice with parameters $\nu = 0.5$, $m = 1$, $n = 1$ (dashed line); $\nu = 0.2$, $m = 1$, $n = 1$ (full line); $\nu = 0.2$, $m = 1$, $n = 3$ (dotted line), and for a regular lattice (long-dashed line).

line to $\nu = 0.2$, $m = 1$ and $n = 1$; and the dotted line to $\nu = 0.2$, $m = 1$ and $n = 3$. The long-dashed line is for $\nu = W_B/W_A = 1$ and so corresponds to a regular lattice.

Note that the main peak in the specific heat for the Fibonacci lattice is smaller and nearer lower temperatures than the peak corresponding to the ordinary Ising model [19]. However, the main difference between both models is the extra peak that appears at very low temperatures for the Fibonacci lattice. This extra peak vanishes when n increases (or, to be more precise, when $P_{m,n}$ decreases). So, the quasiperiodicity of the lattice produces a small, but fairly atypical and interesting behaviour of the specific heat at low temperatures.

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Appendix

In this appendix we show how to calculate Eq. (8) by an iteration procedure. Let us start from $Z^{(2)} = \text{Tr } P_1 P_2$. We can directly check that

$$Z^{(2)} = \text{Tr } P_1 P_2 = \text{Tr } L_1 G_1 L_2 G_2, \tag{A.1}$$

where

$$L_j = \begin{pmatrix} \cosh \tilde{\mu}_j & -\sinh \tilde{\mu}_j \\ -\sinh \tilde{\mu}_j & \cosh \tilde{\mu}_j \end{pmatrix}, \tag{A.2}$$

$$G_j = \begin{pmatrix} 2 \cosh \tilde{W}_j & 0 \\ 0 & 2 \sinh \tilde{W}_j \end{pmatrix}. \tag{A.3}$$

We can write Eq. (A.1) in the form

$$Z^{(2)} = \sum_{kqmt} (L_1)_{kq} (G_1)_{qm} (L_2)_{mt} (G_2)_{tk}, \tag{A.4}$$

where $(L_j)_{kq}$ is the matrix element of L_j . Let us write this matrix elements of the operator L_j in the bi-linear form

$$(L_j)_{kq} = \sum_{i=1}^2 \lambda_i^{(j)} V_i^k V_i^q, \tag{A.5}$$

where V_j^k is the j th eigenvector of the operator L_j , and $\lambda_i^{(j)}$ its corresponding eigenvalue. From Eq. (A.5), we obtain that the transfer matrix L_j has the following eigenvalues and eigenvectors:

$$\lambda_1^{(j)} = \exp(-\tilde{\mu}_j), \quad \lambda_2^{(j)} = \exp(\tilde{\mu}_j), \tag{A.6}$$

$$V_1^k = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad V_2^k = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}. \tag{A.7}$$

Analogously,

$$(G_j)_{qm} = \sum_{i=1}^2 \gamma_i^{(j)} U_i^q U_i^m, \tag{A.8}$$

where $\gamma_i^{(j)}$ are the eigenvectors and U_i^q the eigenvalues of the operator G_j :

$$\gamma_1^{(j)} = 2 \cosh \tilde{W}_j, \quad \gamma_2^{(j)} = 2 \sinh \tilde{W}_j, \tag{A.9}$$

$$U_1^q = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad U_2^q = \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \tag{A.10}$$

Substituting Eqs. (A.5) and (A.9) in Eq. (A.4), we obtain

$$Z^{(2)} = \sum_{s_1 s_2 l_1 l_2} \lambda_{s_1}^{(1)} \lambda_{s_2}^{(2)} \gamma_{l_1}^{(1)} \gamma_{l_2}^{(2)} Q_{s_1 l_1} Q_{l_1 s_2} Q_{s_2 l_2} Q_{l_2 s_1}, \tag{A.11}$$

where $Q_{l_i, s_i} = \sum_{k=1}^2 U_{l_i}^k V_{s_i}^k$. Using Eqs. (A.6), (A.7), (A.9) and (A.10), we find

$$Q_{l_i, s_i} = \frac{1}{\sqrt{2}} (\delta_{l_i, 1} - \delta_{l_i, 2} \exp i\pi s_i), \tag{A.12}$$

where $\delta_{l, k}$ is the delta of Kronecker. We can finally arrive at the following expression:

$$Z^{(2)} = \cosh \tilde{W}_1 \cosh \tilde{W}_2 \sum_{s_1 s_2} \lambda_{s_1}^{(1)} \lambda_{s_2}^{(2)} a_1(s_1, s_2) a_2(s_2, s_1), \tag{A.13}$$

where $a_j(s_j, s_j') = 1 + \varepsilon_j \exp i\pi(s_j + s_j')$ and $\varepsilon_j = \gamma_2^{(j)} / \gamma_1^{(j)}$. The formula (A.13) can be immediately generalized to the case $Z = Z^{(N)}$.

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