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The residual entropy for a class of one-dimensional classical lattice models

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Abstract. The zero-temperature limit of the characteristic equation of the transfer matrix is derived for one-dimensional classical lattice systems with a finite one-point configuration space and finite-range interactions. In this way, we obtain an explicit polynomial equation for the residual entropy, which only involves the counting of some specific periodic ground-state configurations. We apply the formula to some well known models and compare our method with similar calculations in the literature.

1. Introduction

In statistical mechanics, the notion of residual entropy has been investigated in several contexts. First, a non-vanishing residual entropy violates the third law of thermodynamics and hence this fact alone asks for an explanation. Second, it occurs in the study of the magnetic ordering of certain heavy rare-earth metals (see later). Third, a non-zero residual entropy implies a large degeneracy of the ground state, which is also encountered in spin glasses, the common mechanism being the frustration present in the system. Let us look closer at these points.

The thermodynamical entropy is a state function and can only be measured experimentally up to some additive constant. The third law fixes this constant for a system by making it zero at zero temperature. The corresponding quantity in statistical mechanics is properly defined as a functional on the states which measures their randomness or lack of information content. Roughly, it counts the number of microscopic configurations compatible with some macroscopic constraints, mostly the constant energy. The maximal value $s(T)$ of the entropy density at temperature T determines the equilibrium state and the residual entropy is the limit of $s(T)$ for T tending to zero. Here, the entropy functional is made unique by requiring that, for infinite temperature, it should coincide with the original Boltzmann definition, i.e. if a particle at one lattice point can be in q different states, then the infinite-temperature entropy density equals $\ln q$. Therefore, the zero-temperature entropy density is not necessarily zero, but if it is not it should give information about the ground-state degeneracy. But counting configurations with a fixed energy can be done only for finite volumes, which are taken to infinity afterwards. Hence, a problem may arise about the exchange of thermodynamical and zero-temperature limits. This situation was clarified by Aizenman and Lieb [1] who proved for the kind of systems that we consider (classical lattice models with finite-range interactions) that

$$\lim_{E \to E_0} s(E) = \lim_{\Lambda \uparrow \infty} \sup_{b_\Lambda} \frac{1}{|\Lambda|} \ln N_\Lambda(b_\Lambda) \tag{1}$$

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where $N_\Lambda(b_\Lambda)$ denotes the ground-state degeneracy in the finite volume Λ with boundary condition b_Λ. So the residual effects of the finite-temperature equilibrium states are completely recovered by considering only the finite-volume ground-state degeneracy, but then the largest one for all possible boundary conditions. We remark that, to have a non-vanishing residual entropy, the ground-state degeneracy has to diverge exponentially with the volume.

In this paper, we restrict ourselves furthermore to one-dimensional systems, which enables us to derive more explicit results. Indeed, our main result is that the residual entropy is equal to the logarithm of the largest root of the equation

$$\mu^p + \sum_{k=1}^{p} \mu^{p-k} \sum_{j=1}^{k} (-1)^j c_{j,k} = 0 \tag{2}$$

where $p = q^{n-1}$, q is the number of configurations per lattice point, n is the range of the interaction and $c_{j,k}$ is the number of possible sets consisting of j infinite ground-state configurations which are periodic with periods p_i $(i = 1, \ldots, j)$ that add up to $\Sigma_{i=1}^{j} p_i = k \leqslant p$, and which satisfy an additional constraint (see theorem 4.2). The strength of this result is that only (some of) the periodic configurations with lowest energy have to be considered. If there is only one such configuration, say with period k, then (2) reduces to $\mu^p - \mu^{p-k} = 0$, with largest root $\mu_0 = 1$, so the residual entropy equals $\ln \mu_0 = 0$. If there are two such configurations with periods k_1 and k_2, (2) becomes $\mu^p - \mu^{p-k_1} - \mu^{p-k_2} = 0$, which can have zeros strictly larger than one, and hence a non-vanishing residual entropy.

This situation typically occurs in systems which have different ground states for the coupling constants (or external field) belonging to different regions of the parameter space. For critical values of the parameters, two or more (periodic) ground states have the same energy and they coalesce, generating an infinite multitude of (non-periodic) ground states. Examples are given by some heavy rare-earth metals such as cerium and uranium monopnictides which have complicated phase diagrams with lots of different magnetic phases [2-5]. They all have a very anisotropic periodic layered structure: a strong ferromagnetic interaction within each layer and weaker ferro- and antiferromagnetic couplings between the layers. All spins in one layer are parallel but the direction differs from one layer to another. Their experimental measured phase diagram (for low temperatures) is very similar to the computed phase diagram of the one-dimensional model with Hamiltonian (for one layer, that with index zero):

$$h(\sigma) = -\sum_{k} J_k \sigma_0 \sigma_k - H\sigma_0 \tag{3}$$

with $\sigma_i = \pm 1$, where the J_k may slightly depend on temperature to explain the phase transition from one periodic state to another. All these considerations are heuristic, but the low-temperature behaviour of the simplified model (3) can be treated rigorously. In this paper, we calculate its residual entropy and compare it with results based on formula (1) [6-8] and for the most studied case $h(\sigma) = -\sigma_0\sigma_1 + (1/n)\sigma_0\sigma_n$, we constructed the full equilibrium state in the zero-temperature limit in [9].

The frustration present in these systems for critical values of the parameters has also been proposed as a basic mechanism in spin glasses [10, 11]. Although there is certainly no spin-glass transition, because the one-dimensional models we consider are deterministic and have finite-range interactions [12], the frustration can be studied on its own and the Parisi spin-glass order parameter can be calculated rigorously [13], using the same transfer-matrix formalism as we do in the following.

We proceed as follows. First we define the transfer matrix and explain what can be done with it. Because this technique has been developed for finite temperatures, we then derive the equation for the finite-temperature entropy density. In the next section, the limit $T \to 0$ is taken and in the last section the resulting formula (2) is applied to some well known models.

2. Transfer matrix

We work immediately in the infinite-volume formalism (see, e.g., [14]). With each site $j \in \mathbb{Z}$ is associated a copy K_j of the set $K = \{0, 1, \ldots, q-1\}$. A state ρ of the system is a probability measure on the set of all infinite configurations $\Omega = \Pi_{j \in \mathbb{Z}} K_j$; it is described by a family of density distributions, i.e. for any finite volume $\Lambda \subset \mathbb{Z}$, there exists a non-negative function ρ_Λ on $K_\Lambda \equiv \Pi_{j \in \Lambda} K_j$ such that $\Sigma_{x \in K_\Lambda} \rho_\Lambda(x) = 1$ and for all $\Lambda' \supseteq \Lambda$, $\rho_\Lambda(x) = \Sigma_{y \in K_{\Lambda' \setminus \Lambda}} \rho_{\Lambda'}(x, y)$.

The entropy of ρ in the finite volume $\Lambda \subset \mathbb{Z}$ is defined as

$$S_\Lambda(\rho) = -\sum_{x \in K_\Lambda} \rho_\Lambda(x) \ln \rho_\Lambda(x)$$

and its entropy density as

$$s(\rho) = \lim_{\Lambda \uparrow \mathbb{Z}} \frac{1}{|\Lambda|} S_\Lambda(\rho).$$

The entropy density always exists for a translation-invariant state ρ, i.e. a state with densities satisfying $\rho_\Lambda \circ \tau_a = \rho_{\tau_a(\Lambda)}$ for all $a \in \mathbb{Z}$, $\Lambda \subseteq \mathbb{Z}$ where τ_a is the space translation $(\tau_a x)_i = x_{i+a}$ for all i, $a \in \mathbb{Z}$, $x \in \Omega$. It can also be proved for any such state ρ that $0 \leq s(\rho) \leq \ln q$.

A translation-invariant interaction of range n is given by a function h on K^n. The local Hamiltonian for an interval $[a, b]$, $b - a > n$, is then defined by

$$H_{[a,b]}(x) = \sum_{a-1 \leq i \leq b-n} h((\tau_i x)_{[1,n]})$$

where $x_{[1,n]}$ denotes the part of length n of the infinite configuration x, starting at site 1.

For any translation-invariant state ρ, the energy density

$$e(\rho) = \lim_{\Lambda \uparrow \mathbb{Z}} \frac{1}{|\Lambda|} \sum_{x \in K_\Lambda} \rho_\Lambda(x) H_\Lambda(x)$$

always exists and its free-energy density at inverse temperature β is defined by

$$f_\beta(\rho) = e(\rho) - \frac{1}{\beta} s(\rho). \tag{4}$$

A state is called an equilibrium state at inverse temperature β if it minimises the functional f_β. It is well known for the kind of systems that we consider that the equilibrium state ρ_β at inverse temperature β is unique and satisfies $\beta f_\beta(\rho_\beta) = -\ln \lambda_\beta$ where λ_β is the largest eigenvalue of the transfer matrix L_β (see, e.g., [14]). The (Ruelle–Araki) transfer matrix L_β for an interaction $h(x_1, \ldots, x_n)$ of range n acts on

functions ϕ on $K_{[1,n-1]}$ as

$$(L_\beta \phi)(x_2, \ldots, x_n) = \sum_{x_1 \in K_1} k_\beta(x_1, \ldots, x_n)\phi(x_1, \ldots, x_{n-1})$$

where $k_\beta(x_1, \ldots, x_n) \equiv \exp[-\beta h(x_1, \ldots, x_n)]$. Also the equilibrium state itself can be obtained from the transfer matrix [15]. If ϕ_β and ψ_β denote the positive eigenfunctions of L_β, respectively L_β^* belonging to λ_β, then the density distributions $\rho_{[a,b]}$ with $b-a>n$ are given by

$$\rho_{[a,b]}(x_{[a,b]}) = \frac{\phi_\beta(x_a, \ldots, x_{a+n-2})\psi_\beta(x_{b-n+2}, \ldots, x_b)\exp[-\beta H_{[a,b]}(x_{[a,b]})]}{\lambda_\beta^{b-a-n+2} \sum_{x_1 \ldots x_{n-1}} \phi_\beta(x_1, \ldots, x_{n-1})\psi_\beta(x_1, \ldots, x_{n-1})}.$$

We remark that L_β is the $(n-1)$th root of the usual (Kramers-Wannier) transfer matrix $\mathscr{L}_\beta$ which is defined by

$$\mathscr{L}_\beta \phi(x_1, \ldots, x_n) = \sum_{(y_1, \ldots, y_n) \in K_{[1,n]}} \exp[-\beta H_{[1,2n]}(x_1, \ldots, x_n, y_1, \ldots, y_n)]\phi(y_1, \ldots, y_n).$$

The choice to work with L_β looks rather innocent but 'it should be observed that the calculation of the residual entropy as the zero-temperature limit of the first derivative of the corresponding free energy for $n>2$ is practically futile, for such a calculation requires analysis of an eigenvalue problem of order 2^{n}' for the transfer matrix $\mathscr{L}_\beta$ (quoted from [8]) whereas this is exactly what we do for L_β. This is possible because the matrix of L_β contains so many zeros in contrast with that of $\mathscr{L}_\beta$.

Before we start with the calculation of the residual entropy, we give the strategy that we follow. For any real number α, we can rewrite (4) for the equilibrium state ρ_β as

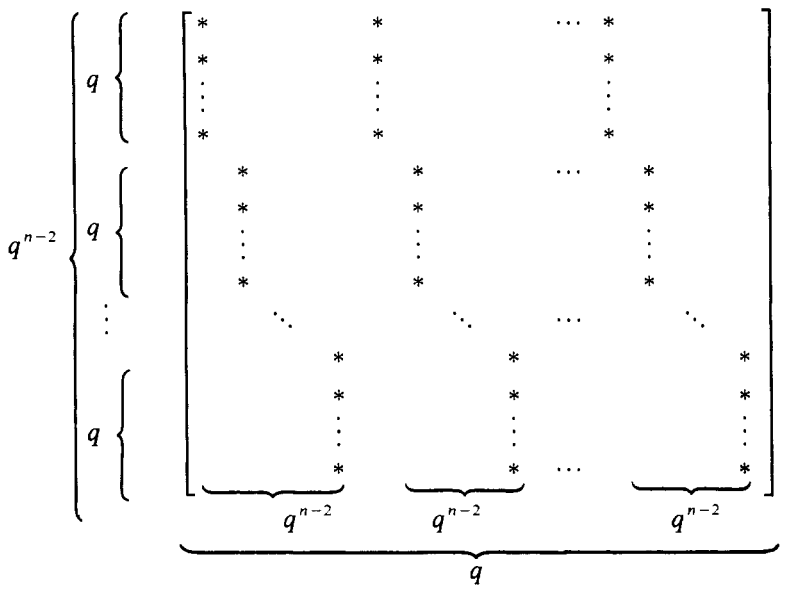
$$s(\rho_\beta) = \beta(e(\rho_\beta) - \alpha) + \alpha\beta + \ln \lambda_\beta. \tag{5}$$

First, we show that there exists an α_0 such that $\ln \mu_\beta \equiv \alpha_0\beta + \ln \lambda_\beta$ has a finite limit for $\beta \to \infty$ and we will write down explicitly the polynomial for which $\mu_0 \equiv \lim_{\beta\to\infty} \mu_\beta$ is the largest root. Since $s(\rho_\beta)$ is uniformly bounded in β, it follows from (5) that $\lim_{\beta\to\infty} e(\rho_\beta) = \alpha_0$. Hence α_0 is the ground-state energy density. As a by-product of the proof, we find that there exists at least one periodic configuration in which the ground-state energy density α_0 is attained. Finally, we will argue that $e(\rho_\beta)$ converges exponentially fast to α_0 such that $\lim_{\beta\to\infty} \beta(e(\rho_\beta) - \alpha_0) = 0$ and we can conclude that the residual entropy $\lim_{\beta\to\infty} s(\rho_\beta)$ exists and equals $\ln \mu_0$.

3. The equation for the finite-temperature entropy

If $K = \{0, 1, \ldots, q-1\}$ is the configuration space per point, the function $\phi(x_1, \ldots, x_{n-1})$ with $x_i \in K$, $i = 1, \ldots, n-1$, can be represented by a p-component column vector, where $p = q^{n-1}$. We order the components from top to bottom according to the numerical value represented by their variables in the numerical system with base q (therefore we count from 0 to $q-1$ instead of from 1 to q): the first component starting from the top is $\phi(0, 0, \ldots, 0)$, the second $\phi(0, 0, \ldots, 0, 1)$, etc, with the last one $\phi(q-1, q-1, \ldots, q-1)$. This fixes a basis in which L_β is represented by a $p \times p$ matrix M_β which

can be easily seen to be of the following form:



The stars stand for the non-vanishing elements $k_\beta(x_1, \ldots, x_n)$ and each row and column contains q such elements. Their ordering is again according to the numerical value of their arguments in the system with base q: in ascending order from the left top downwards and if one arrives at the bottom line, continuing with the element in the top line one column to the right, etc. So the first element is $k_\beta(0, \ldots, 0)$ and, in general, one can easily check that the element $k_\beta(x_1, \ldots, x_n)$ is situated on the crossing of the $(x_1 x_2 \ldots x_{n-1})$th column with the $(x_2 x_3 \ldots x_n)$th row.

The idea of how to calculate $\det(M_\beta - \lambda \mathbb{1})$ is simple but requires some new notions. We start from the definition. The determinant of a $r \times r$ matrix $A = (a_{ij})$ is given by

$$\det A = \sum_{\pi \in S_r} \operatorname{sgn}(\pi) a_{1,\pi(1)} a_{2,\pi(2)} \ldots a_{r,\pi(r)} \tag{6}$$

with S_r the group of permutations of $\{1, 2, \ldots, r\}$ and $\operatorname{sgn}(\pi)$ the sign of π. To compute $\det A$, one has to choose one element from each row and each column and multiply them. An example will clarify the procedure.

For $q = 2$(spin $\frac{1}{2}$) and an interaction of range four, we have to calculate the determinant of

$$A - \lambda \mathbb{1} = \begin{bmatrix} a_0 - \lambda & 0 & 0 & 0 & a_8 & 0 & 0 & 0 \\ a_1 & -\lambda & 0 & 0 & a_9 & 0 & 0 & 0 \\ 0 & a_2 & -\lambda & 0 & 0 & a_{10} & 0 & 0 \\ 0 & a_3 & 0 & -\lambda & 0 & a_{11} & 0 & 0 \\ 0 & 0 & a_4 & 0 & -\lambda & 0 & a_{12} & 0 \\ 0 & 0 & a_5 & 0 & 0 & -\lambda & a_{13} & 0 \\ 0 & 0 & 0 & a_6 & 0 & 0 & -\lambda & a_{14} \\ 0 & 0 & 0 & a_7 & 0 & 0 & 0 & a_{15} - \lambda \end{bmatrix}.$$

Writing $\det(A - \lambda \mathbb{1}) = \sum_{i=0}^{8} c_i \lambda^i$, we already know that $c_8 = 1$, $c_7 = a_0 + a_{15}$ and $c_0 = \det A$. To determine c_6, we look for two a_i to combine with six factors $-\lambda$. Suppose we

choose a_1, then we cannot take $-\lambda$ any longer in the second row; this $-\lambda$, however also belongs to the second column, such that there a_2 (or a_3) has to be taken; but then the $-\lambda$ in the third (or fourth) row and column is forbidden and we are forced to choose between a_4 and a_5 (or a_6 and a_7). In any case, a_1 will not appear in the coefficient c_6 since every coefficient that contains a_1, necessarily contains two other a_i and so does not have enough space left for six times $-\lambda$. We try the next possibility: take a_2, so a_4 (or a_5) and hence also a_8 or a_9 (or a_{10} or a_{11}). Again we obtain too many a_i. It also becomes clear that we can better invert our search. If we have to check all a_i, we can do it systematically as well. In this way we get several loops traversing the matrix. If this loop closes after visiting r different elements, we found a coefficient of λ^{8-r}. A possible loop starting from a_1, is, e.g.,

$$a_1 \to a_3 \to a_6 \to a_{12} \to a_8 \to a_1. \tag{7}$$

This loop has length five, such that $\det(A-\lambda\mathbb{1})$ contains the term $\pm a_1 a_3 a_6 a_{12} a_8 \lambda^3$.

Can we deduce a rule from this about what is special about the elements (7)? A closer look shows that the structure of the matrix allows only two types of transitions:

$$\begin{aligned} &a_k \to a_{(2k)\mathrm{mod}16} \\ &a_k \to a_{(2k+1)\mathrm{mod}16}. \end{aligned} \tag{8}$$

If we write this in the binary system, the underlying rule becomes clear. One has $a_k = a(x_1x_2x_3x_4)$ with $x_i = 0,\ 1$. The operation $k \to 2k$ corresponds to $x_1x_2x_3x_4 \to x_1x_2x_3x_40$, and modulo 16 means deleting the first digit $(x_1x_2x_3x_40)\mathrm{mod}16 = x_2x_3x_40$. The second possible transition is $x_1x_2x_3x_4 \to x_2x_3x_41$. Summing up, (8) corresponds to the operation

$$a(x_1x_2x_3x_4) \to a(x_2x_3x_4x_5). \tag{9}$$

Repeating this k times, we obtain a contribution

$$\prod_{i=1}^{k} a(x_i x_{i+1} x_{i+2} x_{i+3}). \tag{10}$$

To be a coefficient of λ^{p-k}, it has to satisfy extra conditions. To formulate these, we put all x_i, occuring in (10), in one configuration of length $k+3$:

$$(x_1, x_2, x_3, x_4, x_5, \ldots, x_{k-1}, x_k, x_{k+1}, x_{k+2}, x_{k+3}). \tag{11}$$

Four successive x_i from this configuration will be called a 4-window (or window if no confusion is possible). Each window determines one factor of the product (10). The operating (7) corresponds to moving the window over the configuration (11).

A first condition on (11) is that the loop is only closed if the next element to be added in (10) equals the first one, i.e. $(x_{k+1}, x_{k+2}, x_{k+3}, x_{k+4}) = (x_1, x_2, x_3, x_4)$. Second, we want the loop to close after applying (9) k times, no more but no less; we cannot visit an element more than once. This implies that (11) should not contain two identical windows.

Since $a(x_1x_2x_3x_4) = k_\beta(x_1, x_2, x_3, x_4) = \exp[-\beta h(x_1, x_2, x_3, x_4)]$, the product (10) is nothing other than

$$\begin{aligned} \prod_{i=1}^{k} k_\beta(x_i, x_{i+1}, x_{i+2}, x_{i+3}) &= \exp\left(-\beta \sum_{i=1}^{k} h(x_i, x_{i+1}, x_{i+2}, x_{i+3})\right) \\ &= \exp[-\beta H_{[1,k+3]}(x_1, \ldots, x_{k+3})]. \end{aligned} \tag{12}$$

If we define the infinite periodic configuration with period k

$$x = (\ldots x_{k-2}, x_{k-1}, x_k, x_1, x_2, \ldots, x_k, x_1, x_2 \ldots)$$

then its energy density is equal to

$$\hat{h}(x) \equiv \lim_{N\to\infty} \frac{1}{2N+1} H_{[-N,N]}(x_{[-N,N]})$$

$$= \frac{1}{k}[h(x_1, x_2, x_3, x_4) + h(x_2, x_3, x_4, x_5) + \ldots + h(x_k, x_1, x_2, x_3)]$$

which means that the exponent of (12) is $k\hat{h}(x)$. The two above-mentioned conditions, stated in terms of x, require x to be a k-periodic configuration that contains k different windows. Summarising, we have shown that, given such a configuration, $\det(A - \lambda \mathbb{1})$ contains a term of the form $\pm\exp(-\beta k\hat{h}(x))\lambda^{p-k}$. Are all terms of this form? Do we not overcount some terms? What sign do they have?

Theorem 3.1. The characteristic equation for the transfer matrix L_β of the models as described in § 2 is given by

$$\lambda^p + \sum_{k=1}^{p} \lambda^{p-k} \sum_{j=1}^{k} (-1)^j \sum_{x(k_1)\ldots x(k_j)}' \exp\left(-\beta \sum_{i=1}^{j} k_i \hat{h}(x(k_i))\right) = 0 \qquad (13)$$

where $\Sigma'_{x(k_1)\ldots x(k_j)}$ runs over all possible sets of j k_i-periodic configurations $x(k_i)$, $i = 1, \ldots, j$, modulo translations, which together contain $k = \Sigma_{i=1}^{j} k_i$, different n-windows.

This statement means the following: let $x(k)$ be a configuration with period k containing k different n-windows (this is the maximal number of different n-windows a k-periodic configuration can have). Then the characteristic equation of L_β necessarily contains the term $-\exp[-\beta k\hat{h}(x(k))]\lambda^{p-k}$. Furthermore, two periodic configurations $x(k_1)$ and $x(k_2)$ with periods k_1 and k_2 can also be combined into a term of the characteristic equation, at least if they together have $k_1 + k_2$ different n-windows (again the maximal number that a k_1- and k_2-periodic configuration can have together). This corresponds to drawing two loops in the matrix that do not interfere. The contribution from these two configurations is $\exp\{-\beta[k_1\hat{h}(x(k_1)) + k_2\hat{h}(x(k_2))]\}$. One can continue this procedure with more configurations by requiring that the total number of different n-windows should always equal the sum of their periods. To avoid double counting, we impose the condition 'modulo translation': if a configuration x is the translation of x', then only one of them may be taken into account. In fact, the sum Σ' runs over sets of j classes $[x(k_i)]$ where the class $[x(k_i)]$ contains the configuration $x(k_i)$ and its k_i translates.

Proof. We have to show, first, that any term in the characteristic equation of L_β is of the form as in (13), and second, that it can be written in a unique way in this form.

(*a*) We remark that any permutation may be broken up into a product of cycles, the sign of the permutation being equal to the product of the signs of the cycles. The sign of a cycle is $+1$ (-1) if it has odd (even) length. So, each term in (6) splits up into a number of factors of the form

$$\operatorname{sgn}(\tilde{\pi}) a_{i_1,\tilde{\pi}(i_1)} a_{i_2,\tilde{\pi}(i_2)} \ldots a_{i_s,\tilde{\pi}(i_s)}$$

where $\tilde{\pi}$ is a cycle of length s. Let an arbitrary term in the coefficient of λ^{p-k} be given which is different from zero. Formula (6) implies it to be a product of k elements

$k_\beta(x_1, \ldots, x_n)$, the remaining $p-k$ elements being equal to $-\lambda$. The permutation corresponding to this choice contains at least $p-k$ cycles with one element: every $-\lambda$ is located on the diagonal. Let us call π the restriction of the permutation to the remaining k elements of the form $k_\beta(x_1, \ldots, x_n)$ and consider one cycle of length s in the decomposition of π.

We use the two properties deduced from the structure of L_β: if $k_\beta(x_1, \ldots, x_n)$ occurs in the coefficient, then also an element of the form $k_\beta(x_2, x_3, \ldots, x_n, x_{n+1})$ occurs (the argument for general q and n is the same as in the example for $q=2$ and $n=4$), and secondly, the element $k_\beta(x_1, \ldots, x_n)$ is situated in the $(x_2x_3 \ldots x_n)$th row and the $(x_1x_2 \ldots x_{n-1})$th column.

The first fact implies that the s factors $k_\beta(x_1, \ldots, x_n)$ give a contribution

$$\pm \prod_{i=1}^{s} k_\beta(x_i, x_{i+1}, \ldots, x_{i+n-1}) = \pm \exp\left(-\beta \sum_{i=1}^{s} h(x_i, x_{i+1}, \ldots, x_{i+n-1})\right)$$

where $x_{k+i} = x_i$ for $i = 1, \ldots, n-1$. The sum in the exponent is s times the energy density of the infinite s-periodic configuration:

$$x \equiv (\ldots x_{s-2}, x_{s-1}, x_s, x_1, x_2, \ldots, x_s, x_1, x_2 \ldots).$$

To be sure that no element is visited more than once, the condition is imposed that $x(s)$ has precisely s different n-windows.

If the column numbers of the s elements in the matrix L_β are given by

$$x_1x_2 \ldots x_{n-1}, x_2x_3 \ldots x_n, \ldots, x_kx_{k+1} \ldots x_{n+k-2}$$

then, according to the second rule, the corresponding row numbers are, respectively,

$$x_2x_3 \ldots x_n, x_3 \ldots x_{n+1}, \ldots, x_k \ldots x_{n+k-2}, x_{k+1} \ldots x_{n+k-1} \equiv x_1x_2 \ldots x_{n-1}$$

since $x_{k+i} = x_i$ for $i = 1, \ldots, n-1$. But this is nothing other than a cyclic permutation with sign $(-1)^{s+1}$.

Hence, $x(s)$ yields a contribution $(-1)^{s+1} \exp[-\beta s \hat{h}(x(s))]$. If the permutation π consists of j cycles π_i with, respectively, length k_i, then the total contribution to the coefficient of $(-\lambda)^{p-k}$ is equal to

$$(-1)^{\sum_{i=1}^{j}(k_i+1)} \exp\left(-\beta \sum_{i=1}^{j} k_i \hat{h}(x(k_i))\right) = (-1)^{k+j} \exp\left(-\beta \sum_{i=1}^{j} k_i \hat{h}(x(k_i))\right)$$

where the $x(k_i)$ are k_i-periodic configurations with together $k = \sum_{i=1}^{j} k_i$ different n-windows. We obtain (13) after divividing the whole term by $(-1)^p$.

(*b*) Given a set of j k_i-periodic configurations $x(k_i)$ with $k \equiv \sum_{i=1}^{j} k_i$ different n-windows. If $W_n(x) \equiv \{(\tau_a x)_{[1,n]} | a \in \mathbb{Z}\}$ denotes the set of all n-windows of the configuration x, then we define $W = \bigcup_{i=1}^{j} W_n(x(k_i))$. This W determines a set of k elements $k_\beta(x)$, $x \in W$. The question is whether these k elements (and hence the set W) can be obtained from another set of j' k_i'-periodic configurations $x(k_i')$ with $\sum_{i=1}^{j'} k_i' = k$ and $\bigcup_{i=1}^{j'} W_n(x(k_i')) = W$. But this is clearly not possible—to represent a non-vanishing term in the determinant, the set W has to define a permutation π as follows: if $(x_1, \ldots, x_n) \in W$, then $x_1, \ldots x_{n-1} = \pi(x_2 \ldots x_n)$. If this permutation can be found, it is unique. Moreover, the decomposition of a permutation into cycles is unique and a cycle determines a unique infinite periodic configuration up to translations. Hence, the sum over all non-zero terms is a sum over permutations or over sets of cycles or over sets of periodic configurations modulo translations.

4. The residual entropy

We will analyse formula (13) in the limit as $\beta \to \infty$. Let X denote the set of all periodic configurations with period k smaller than p and containing k different n-windows, it is clearly a finite set. Put $\alpha_0 = \min\{\hat{h}(x) | x \in X\}$. To study the behaviour of (13) for large β, we substitute $\lambda = \mu \exp(-\alpha_0 \beta)$ and divide (13) by $\exp(-p\alpha_0\beta)$. Then we obtain

$$P_\beta(\mu) \equiv \mu^p + \sum_{k=1}^{p} \mu^{p-k} \sum_{j=1}^{k} (-1)^j \sum_{x(k_1)\ldots x(k_j)} \exp\left(-\beta \sum_{i=1}^{j} k_i[\hat{h}(x(k_i)) - \alpha_0]\right) = 0.$$

This equation splits up into two parts: $P_\beta(\mu) = P_0(\mu) + P_{\beta-}(\mu)$ where

$$P_0(\mu) = \mu^p + \sum_{k=1}^{p} \mu^{p-k} \sum_{j=1}^{k} (-1)^j \sum_{x(k_1)\ldots x(k_j)}' 1 \tag{14}$$

is a polynomial in μ independent of β and $P_{\beta-}(\mu)$ is a polynomial in μ of degree strictly less than that of $P_0(\mu)$ and with coefficients which are all strictly exponentially decreasing in β.

Lemma 4.1. If μ_β denotes the largest root of $P_\beta(\mu)$ and μ_0 that of $P_0(\mu)$, then $\lim_{\beta\to\infty}\mu_\beta$ exists and is equal to μ_0, the convergence going exponentially fast.

Proof. First, we show that μ_β is uniformly bounded in β. Indeed, suppose that there is a sequence β_k, $k = 1, 2, \ldots$, such that $\lim_{k\to\infty}\mu_{\beta_k} = \infty$. Then, dividing the equality $P_0(\mu_{\beta_k}) + P_{\beta_k-}(\mu_{\beta_k}) = 0$ by $\mu_{\beta_k}^p$ and taking the limit $k \to \infty$ would certainly lead to a contradiction since the degree of $P_{\beta-}$ is strictly less than that of P_0. Now, the same equality with μ_β uniformly bounded implies that there exist constants K and $c > 0$ such that $|P_0(\mu_\beta)| \leqslant K\exp(-c\beta)$. Together with the fact that μ_β is continuous in β for β finite (see, e.g., [16]), this means that for all β large enough, μ_β is arbitrarily close to one of the zeros of P_0, say $\bar{\mu}$. In fact, taking smaller and smaller neighbourhoods around $\bar{\mu}$, one sees that $\lim_{\beta\to\infty}\mu_\beta$ exists and equals $\bar{\mu}$. Moreover, for any $a > 0$, there exists a constant K' such that $|P_\beta(\mu) - P_0(\mu)| < K'\exp(-c\beta)$ for all μ, $|\mu| < \mu_0 + a$. Hence, P_β must have a zero closer and closer to μ_0 as $\beta \to \infty$. This is only possible if $\mu_0 = \bar{\mu} = \lim_{\beta\to\infty}\mu_\beta$. Finally, from the inequality $|P_0(\mu_0) - P_0(\mu_\beta)| < K\exp(-c\beta)$, the exponential convergence of μ_β can be deduced.

Theorem 4.2. Let h be a Hamiltonian as described in § 2 with range n and q configurations per point. Let G denote the set of all periodic configurations which have a period smaller than $p = q^{n-1}$, the number of different n-windows equal to their period and which have minimal energy density. Then the residual entropy of this model is equal to the logarithm of the largest root of the equation

$$\mu^p + \sum_{k=1}^{p} \mu^{p-k} \sum_{j=1}^{k} (-1)^j c^{j,k} = 0 \tag{15}$$

where $c_{j,k}$ is the number of all possible sets of j configurations $x(1), \ldots, x(j) \in G$ modulo translations such that the sum of their periods is k and such that they together have k different n-windows.

Proof. The proof proceeds as indicated at the end of § 2. We have already found a number α_0 such that $\ln \mu_\beta = \alpha_0\beta + \ln \lambda_\beta$ has a finite limit for $\beta \to \infty$ and because of lemma 4.1, the polynomial for which $\mu_0 = \lim_{\beta\to\infty}\mu_\beta$ is the largest root is given by (14)

or equivalently by (15). Hence, the only thing that remains to be proved is the exponential convergence of the energy density to the ground-state energy density. This follows from the facts that $\lambda_\beta = \exp(-\alpha_0\beta)\mu_\beta$, with μ_β converging exponentially fast in β, and that M_β contains only exponentials in β. Indeed, they imply that the solutions ϕ_β and ψ_β of $(M_\beta - \lambda_\beta)\phi_\beta = 0$ and $(M_\beta^* - \lambda_\beta)\psi_\beta = 0$ and hence also ρ_β and $e(\beta) = \Sigma_x \rho_\beta(x)h(x)$ are fractions of linear combinations of exponentials in β and powers of μ_β. But we already know that $\lim_{\beta\to\infty} e(\beta) = \alpha_0$, so one necessarily has $e(\beta) = (\alpha_0 + P_1(\beta))/(1 + P_2(\beta))$ with $P_1(\beta)$ and $P_2(\beta)$ exponentially decreasing functions in β. This completes the proof since $e(\beta) - \alpha_0 = (P_1(\beta) - \alpha_0 P_2(\beta))/(1 + P_2(\beta))$ converges exponentially fast to zero.

Corollary 4.3. (i) If there is only one periodic configuration with the lowest energy density, say with period k, then (15) reduces to $\mu^p - \mu^{p-k} = 0$ with largest root $\mu_0 = 1$. So the residual entropy in this case is zero.

(ii) All models with the same interaction range and configuration space per point which have the same periodic ground-state configurations also have the same residual entropy.

(iii) It follows from the proof, whether the residual entropy is zero or not, that there always exists at least one periodic configuration with period p' smaller than p and with p' different n-windows, whose energy density is equal to the ground-state energy density.

(iv) If $\mathcal{T}$ denotes the set of all translation-invariant states, then the number α_0 equals

$$\alpha_0 = \min\{e(\rho) | \rho \in \mathcal{T}\}.$$

Indeed, since the equilibrium state ρ_β satisfies the variational principle (see, e.g., [14, 15]), i.e.

$$f_\beta(\rho_\beta) \leqslant f_\beta(\rho) \qquad \forall \rho \in \mathcal{T}$$

we get, rewriting (4), that

$$e(\rho_\beta) \leqslant e(\rho) + \frac{1}{\beta}(s(\rho_\beta) - s(\rho)) \qquad \forall \rho \in \mathcal{T}.$$

But the entropy density is uniformly bounded in β, such that we obtain

$$\alpha_0 = \lim_{\beta\to\infty} e(\rho_\beta) \leqslant e(\rho) \qquad \forall \rho \in \mathcal{T}.$$

On the other hand, given a k-periodic configuration z with energy density $\hat{h}(z) = \alpha_0$, one can easily construct a translation-invariant state ρ with the same energy density by taking for its density distributions

$$\rho_\Lambda(x_\Lambda) = \frac{1}{k}\sum_{a=1}^{k} \delta_{x_\Lambda, (\tau_a z)_\Lambda}.$$

Remark 4.4. All configurations in the set G of theorem 4.2 are ground-state configurations. A ground-state configuration is, by definition, a configuration $x \in K^{\mathbb{Z}}$, which is stable under local perturbations [1], i.e. $\forall \Lambda \subseteq \mathbb{Z}$, $\forall y \in K^{\mathbb{Z}}$ with $y_{\Lambda^c} = x_{\Lambda^c}$,

$$\lim_{\Lambda\uparrow\mathbb{Z}} (H_\Lambda(y_\Lambda) - H_\Lambda(x_\Lambda)) \geqslant 0.$$

We prove the statement by contradiction. Let $x \in G$ and assume there exists a $\Lambda \subseteq \mathbb{Z}$ and a $y \in K^{\mathbb{Z}}$ such that $x_{\Lambda'} = y_{\Lambda'}$ and $H_{\Lambda'}(y_{\Lambda'}) < H_{\Lambda'}(x_{\Lambda'})$, $\forall \Lambda' \supseteq \Lambda_0$ for some Λ_0 large enough. Now, define the configuration $\bar{x} \in K^{\mathbb{Z}}$ which is the periodic continuation of y_{Λ_0}, i.e. for which $\bar{x}_{\Lambda_0} = y_{\Lambda_0}$ is one period. Then the translation-invariant state constructed from $\bar{x}$ has the same energy density as $\bar{x}$ which is strictly smaller than α_0, in contradiction with corollary 4.3.

5. Application

One of the simplest models with non-vanishing residual entropy is that with Hamiltonian

$$h_n(x_1, x_2, \ldots, x_n) = -x_1x_2 + \frac{1}{n-1} x_1x_n \qquad x_i \in \{-1, 1\}. \tag{16}$$

The case $n = 3$ was solved by Stephenson [6] and has residual entropy $\ln[(1+\sqrt{5})/2]$. Redner [7] proves, using (1) for free boundary conditions, that the residual entropy for the general case is equal to $\ln \mu_0$ where μ_0 is the largest root of $\mu_0^{n-1} = \mu_0^{n-2} + 1$. According to (1), this is a lower bound, but it turns out to be exact. In fact (16) is a special case of the more general class of models with a critical field

$$h_n^J(x_1, x_2, \ldots, x_n) = -x_1x_2 + Jx_1x_n - Hx_1$$

with $H = 2[J - 1/(n-1)] > 0$. Again, counting ground-state configurations with periodic boundary conditions, Hajduković and Milošević [8] find for h_n^J the same residual entropy as Redner did for the model h_{2n}.

These models illustrate very nicely how a large frustration may be caused by competition between several interactions. To determine the ground-state configurations, we follow the discussion of [8].

If $J < 1/(n-1)$, the antiferromagnetic interaction (second term) is too weak to compensate the ferromagnetic one (first term), so there will be a ferromagnetic ground state in the direction of the field.

If $J > 1/(n-1)$, the antiferromagnetic tendency wins and we can use the field H to control the ground state. If the field is weak, i.e. $H < 2[J - 1/(n-1)]$, it cannot compensate the antiferromagnetic interaction and there will be an $(n-1)$-fold degenerate ground state with configurations consisting of domains of $n-1$ parallel spins which are alternately aligned up and down. If $H > 2[J - 1/(n-1)]$, the field is too strong: the ground state is ferromagnetic in the direction of the field. Only if $H = 2[J - 1/(n-1)]$, both types of ground states (ferromagnetic and antiferromagnetic) have the same energy density together with all configurations consisting of domains of parallel spins which point alternately up and down; the domains of spins pointing down still have length $n-1$, but the domains of spins aligned up may have any length greater than or equal to $n-1$.

Finally, if $J = 1/(n-1)$, no field is needed to balance both tendencies. Here, there are two ferromagnetic and $n-1$ antiferromagnetic configurations with the lowest energy density and with them all being configurations consisting of domains of at least $n-1$ parallel spins.

Now, the strength of our result is clear: we only have to consider the periodic configurations (up to translations) and moreover only those with different n-windows.

For the models with non-vanishing field, there are only three of them: the ferromagnetic one x_f with period 1 (all spins up), a first antiferromagnetic one x_{a_1} with period $2(n-1)$ ($n-1$ spins up followed by $n-1$ spins down, etc) and a second one x_{a_2} with period $2n-1$ (n spins up followed by $n-1$ spins down, etc). More than n neighbouring spins pointing up would give rise to equal n-windows. For the same reason, x_f and x_{a_2} cannot be combined in the equation for the residual entropy: only x_f and x_{a_1} can. This gives

$$\mu^p + (-1)^1\mu^{p-1} + (-1)^1\mu^{p-2(n-1)} + [(-1)^1 + (-1)^2]\mu^{p-2n+1}$$
$$= \mu^{p-2n+2}(\mu^{2(n-1)} - \mu^{2(n-1)-1} - 1) = 0.$$

In the special case $J = 1/(n-1)$, the spin-flip symmetry is restored and there are two ferromagnetic configurations x_{f_1} (all spins up) and x_{f_2} (all spins down) and four antiferromagnetic ones.

x_{a_1} with period $2(n-1)$: $n-1$ spins up, $n-1$ spins down, etc.
x_{a_2} with period $2n-1$: n spins up, $n-1$ spins down, etc.
x_{a_3} with period $2n-1$: $n-1$ spins up, n spins down, etc.
x_{a_4} with period $2n$: n spins up, n spins down, etc.

To have different n-windows, the following combinations are allowed:

$$x_{f_1} + x_{f_2},\ x_{f_1} + x_{a_1},\ x_{f_2} + x_{a_1},\ x_{f_1} + x_{a_3},\ x_{f_2} + x_{a_2},\ x_{f_1} + x_{f_2} + x_{a_1}.$$

This gives, for the residual-entropy equation

$$\mu^p - 2\mu^{p-1} + \mu^{p-2} - \mu^{p-2(n-1)} + (-2+2)\mu^{p-2n+1} + (-1+2-1)\mu^{p-2n}$$
$$= \mu^{p-2(n-1)}[\mu^{2(n-1)-2}(\mu-1)^2 - 1]$$
$$= \mu^{p-2(n-1)}(\mu^{n-1} - \mu^{n-2} + 1)(\mu^{n-1} - \mu^{n-2} - 1) = 0.$$

The largest root is that of $\mu^{n-1} - \mu^{n-2} - 1 = 0$ as found in [7, 9].

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