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One-dimensional Ising model with *k*-spin interactions

Yale Fan

Department of Physics, Harvard University, Cambridge, MA 02138, USA

E-mail: yalefan@gmail.com

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Abstract

We examine a generalization of the one-dimensional Ising model involving interactions among neighbourhoods of k adjacent spins. The model is solved by exploiting a connection to an interesting computational problem that we call 'k-SAT on a ring', and is shown to be equivalent to the nearest-neighbour Ising model in the absence of an external magnetic field. The aim of this paper is to explore an interplay of ideas in the context of a toy problem, while introducing a way of thinking about exactly solvable models in terms of 'computational analogues'.

1. Introduction

Statistical mechanics often employs idealized models to understand complex systems, with the goal of predicting macroscopic properties from simplified descriptions of microscopic interactions. Due to the many degrees of freedom involved and the relative scarcity of exactly solvable models, numerical simulations are indispensable tools for gaining insight into such systems [1–3]. In turn, physical reasoning has motivated computational techniques from simulated annealing to probabilistic schemes in coding theory [4], as well as the study of the Ising model from a theoretical computer science perspective [5].

Here, we suggest inverting the relationship between statistical mechanics and computation to arrive at *analytical* solutions to exactly solvable models. The process goes roughly like this: (1) find a correspondence between the Hamiltonian of the model and the parameters of some computational problem, (2) construct an algorithm to solve the problem and (3) deduce the partition function from properties of the algorithm or the solutions. To illustrate this rather unorthodox approach, we consider a generalized 'k-spin Ising model' as a case study that hopefully elucidates what we mean by computational reasoning as applied to exactly solvable models in statistical mechanics. The ideas proposed here, due to their departure from standard methods, may be instructive to both students and general (physics) audiences.

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In the discussion to follow, we will always work in the canonical ensemble. Assuming discrete energy levels, which is the case for the finite lattices that we will consider, the probability p_i that a system will occupy the microstate i with the energy E_i is given by the Boltzmann distribution:

$$p_i = \frac{e^{-\beta E_i}}{Z}, \qquad Z = \sum_i e^{-\beta E_i}, \tag{1}$$

where Z is the partition function and $\beta = 1/k_B T$ is the inverse temperature. When dealing with n spins on a lattice, we will write Z_n to make the system size explicit. Most thermodynamic variables of interest (Helmholtz free energy, heat capacity, mean pressure, entropy, etc), in addition to other observables such as magnetization and magnetic susceptibility, are derivable directly from the partition function. Thus, the partition function encapsulates the description of a system in thermal equilibrium, and we say that a statistical–mechanical model of such a system is 'exactly solvable' if the associated partition function can be evaluated in closed form.

2. The 1D Ising model

To introduce the main example of this paper, we briefly review the solution of the nearest-neighbour Ising model in one dimension. It is the archetype of an exactly solvable model of ferromagnetism, and incorporates the key ingredients of the transfer matrix formalism.

Assuming periodic boundary conditions, the setup consists of n spins on a circle. Let $\sigma_i = \pm 1$ denote the spin at site i, and let $\sigma = (\sigma_1, \ldots, \sigma_n)$ denote a configuration of spins. We use h to denote the external field strength times the dipole moment per spin. The classical Ising Hamiltonian is then

$$H(\sigma) = -J \sum_{i=1}^{n} \sigma_i \sigma_{i+1} - h \sum_{i=1}^{n} \sigma_i.$$

The spin–spin coupling is ferromagnetic if $J > 0$, which encourages mutual alignment to minimize the energy.

The observation that leads to an exact solution is that the partition function can be written as a sum of terms whose factors involve only adjacent spins:

$$Z_n = \sum_\sigma \exp\left(\beta J \sum_{i=1}^{n} \sigma_i \sigma_{i+1} + \beta h \sum_{i=1}^{n} \sigma_i\right) = \sum_\sigma V(\sigma_1, \sigma_2) V(\sigma_2, \sigma_3) \cdots V(\sigma_n, \sigma_1),$$

where

$$V(\sigma_i, \sigma_{i+1}) = \exp\left[\beta J \sigma_i \sigma_{i+1} + \frac{\beta h}{2}(\sigma_i + \sigma_{i+1})\right].$$

Upon defining the symmetric transfer matrix

$$\mathbf{V} = \begin{pmatrix} V(+,+) & V(+,-) \\ V(-,+) & V(-,-) \end{pmatrix} = \begin{pmatrix} e^{\beta(J+h)} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta(J+h)} \end{pmatrix}, \tag{2}$$

the expression for the partition function can be interpreted as a sequence of matrix multiplications:

$$Z_n = \sum_\sigma \mathbf{V}_{\sigma_1,\sigma_2} \mathbf{V}_{\sigma_2,\sigma_3} \cdots \mathbf{V}_{\sigma_n,\sigma_1} = \sum_{\sigma_1} [\mathbf{V}^n]_{\sigma_1,\sigma_1} = \operatorname{tr} \mathbf{V}^n.$$

Diagonalizing $\mathbf{V}$ gives the eigenvalues

$$\Lambda_\pm = e^{\beta J} \cosh \beta h \pm \sqrt{e^{2\beta J} \sinh^2 \beta h + e^{-2\beta J}},$$

where $|\Lambda_+| > |\Lambda_-|$, whence $Z_n = \Lambda_+^n + \Lambda_-^n \sim \Lambda_+^n$ as $n \to \infty$. In particular, for $h = 0$, we find that

$$Z_n = \lambda_+^n + \lambda_-^n \sim \lambda_+^n, \qquad \text{where} \quad \lambda_\pm = \mathrm{e}^{\beta J} \pm \mathrm{e}^{-\beta J}. \tag{3}$$

The free energy per site is found to be $f(h, T) = -\beta^{-1} \ln \Lambda_+$, from which it follows that the magnetization is

$$M(h, T) = -\frac{\partial f(h, T)}{\partial h} = \mathrm{e}^{\beta J} \sinh \beta h (\mathrm{e}^{2\beta J} \sinh^2 \beta h + \mathrm{e}^{-2\beta J})^{-1/2}.$$

This is an analytic function of h for all finite β, so the model admits no phase transition at any positive temperature. It undergoes a paramagnetic-to-ferromagnetic phase transition only at $T = 0$ ($\beta = \infty$), in which case the spontaneous magnetization is $|M| = 1$.

The Ising model lends itself to many generalizations, whether to higher dimensions, different lattices or modified interactions. Well-studied variations of this model abound even in one dimension [6–11], but models involving products over arbitrary numbers of spins are uncommon (examples of the latter type have been considered in the context of protein folding, where binary variables represent whether contact sites on the protein are open or closed [12, 13]). Here, we study a particularly natural generalization of this sort, which consists of replacing nearest-neighbour coupling with k-neighbourhood coupling, such that the subsets of coupled spins correspond to a sort of k-mer coverage of the spin chain. Putting realism aside, the most interesting aspect of this k-spin model is that while it is so similar in principle to the nearest-neighbour model, similar techniques do not suffice to solve it. Our approach to computing the partition function of this model counts solutions to a related problem and is hence more conceptually similar to the combinatorial approach of Kac and Ward to the two-dimensional Ising model [14] than to conventional algebraic methods, albeit in a much simpler context.

3. The *k*-spin Ising model

We propose the following generalization of the nearest-neighbour Ising model: consider a chain of spins, with periodic boundary conditions, in which neighbourhoods of k adjacent spins interact. Suppose that the interaction energy of each neighbourhood depends on the parity of the number of 'down' spins. Thus, the Hamiltonian takes the form

$$H(\sigma) = -\sum_{i=1}^{n} J_i \sigma_i \sigma_{i+1} \cdots \sigma_{i+k-1} - h \sum_{i=1}^{n} \sigma_i, \tag{4}$$

where $\sigma_{i+n} \equiv \sigma_i$. We assume throughout our discussion that k is even, as this ensures time-reversal symmetry, i.e. invariance of the Hamiltonian under negation of all spins in the absence of an external magnetic field. We show that this model is equivalent to the nearest-neighbour Ising model in zero field by demonstrating the equality of their partition functions when $h = 0$, in the thermodynamic limit $n \to \infty$.

The interesting aspect of the present problem is the approach taken here to estimate the partition function, which looks nothing like the standard techniques of classical statistical mechanics. In particular, the k-spin model is not amenable to a straightforward transfer matrix analysis because when $k > 2$, it does not consist of a sequence of purely adjacently interacting subsystems. However, mapping this model onto a simple computational problem allows us to infer a great deal of information about its structure.

To this end, we introduce the problem of 'k-SAT on a ring'. The nomenclature comes from that of the Boolean satisfiability problem, which asks for an assignment of binary variables $x_i \in \{0, 1\}$ such that the Boolean formula

$$f(x_1, x_2, \ldots, x_n) = C_1 \wedge C_2 \wedge \cdots \wedge C_N \tag{5}$$

evaluates to 1. Here, the C_i are *clauses* (or sub-formulae) that each express a condition on some subset of the bits $\{x_i\}$, while '$\wedge$' denotes the logical conjunction operator, meaning that the formula f is satisfied only when all the clauses are themselves satisfied. An *instance* of k-SAT on a ring consists of n clauses over n bits, so that $N = n$ in formula (5), where the clause C_i is associated with the k adjacent bits $x_i, x_{i+1}, \ldots, x_{i+k-1}$. The first and last bits x_1 and x_n are considered adjacent, hence the 'ring'. The clause C_i is itself described by a bit $a_i \in \{0, 1\}$ and designated as either 'even' ($a_i = 0$) or 'odd' ($a_i = 1$). We say that C_i is satisfied if the *Hamming weight*, or the number of ones, of the bit string $x_i x_{i+1} \cdots x_{i+k-1}$ has parity a_i. For example, the instance of 4-SAT on a ring over 6 bits with clauses $(a_i)_{i=1}^{6} = (1, 0, 1, 0, 0, 0)$ admits the solutions 001011, 011110, 100001, 110100. One sees that the bitwise complement of any solution also corresponds to a solution, as the Hamming weight of a bit string of length k is invariant under negation of all bits.

Solubility of a given instance of k-SAT on a ring requires that the number of odd clauses be even. Indeed, for a variable bit string $x_1 \cdots x_n$, the problem reduces to the system of congruences $x_i + \cdots + x_{i+k-1} \equiv a_i \pmod 2$ for $i = 1, \ldots, n$, taken cyclically. Adding gives $\sum_i a_i \equiv k \sum_i x_i \equiv 0 \pmod 2$, which implies that the number of odd clauses (odd a_i) must also be even. However, a given instance of k-SAT on a ring over n bits need not have any solutions even if this condition is met.

Note that when $h = 0$, one could map a given instance of k-SAT on a ring onto the Hamiltonian (4) by choosing $J_i = (-1)^{a_i} J$. Solutions to the k-SAT problem would then correspond to spin configurations with the ground-state energy, if we identify the spin +1 with the bit 0 and the spin -1 with the bit 1. However, we need not stretch the analogy this far: for simplicity, we consider only ferromagnetic and site-independent interactions with $J_i = J > 0$. The corresponding ($h = 0$) partition function is

$$Z_n = \sum_{\sigma} \exp\left(\beta J \sum_{i=1}^{n} \sigma_i \sigma_{i+1} \cdots \sigma_{i+k-1}\right).$$

It turns out that the correspondence between k-SAT on a ring and the k-spin Ising model allows us to compute this sum over states, as we demonstrate next.

4. Zero-field partition function

Every n-bit instance of k-SAT on a ring can be represented as an n-tuple $\alpha = (a_1, \ldots, a_n)$ that specifies the parity of each clause. Hence $\alpha \in \{0, 1\}^n$, in contrast to the spin configuration $\sigma = (\sigma_1, \ldots, \sigma_n)$, which takes values in $\{+1, -1\}^n$. Let $w(\alpha)$ denote the Hamming weight of a 'clause configuration' α, so that α encodes the conditions in a problem instance with $n - w(\alpha)$ even clauses and $w(\alpha)$ odd clauses. Then, the partition function in zero field can be written as

$$Z_n = \sum_{\alpha} N(\alpha) \exp\left[\beta J (n - 2w(\alpha))\right], \tag{6}$$

where $N(\alpha)$ denotes the number of solutions to the problem instance represented by α. Here, we have made the obvious identification of solutions with spin configurations.

We immediately observe several facts regarding the function $N(\alpha)$. First, the 'average' value of $N(\alpha)$ is 1. Indeed, each of the 2^n bit strings of length n gives rise to exactly one solution to an instance of k-SAT on a ring, so that

$$\sum_{\alpha} N(\alpha) = 2^n. \tag{7}$$

Second, $N(\alpha)$ takes only two possible values, 0 or a power of 2, and depends on α only insofar as which value it takes. This is because $N(\alpha)$ counts the number of solutions to a system of linear equations over the finite field $\mathbb{Z}/2\mathbb{Z}$, as mentioned in the previous section. This linear system can be written in the form $\mathbf{Mx} = \boldsymbol{\alpha}$ where $\mathbf{M}$ is a circulant matrix and $\boldsymbol{\alpha}$ is a column vector whose entries are those of the n-tuple α. The rank r of the matrix $\mathbf{M}$ depends only on k and n—hence the number of solutions to the linear system is 2^{n-r} if a particular solution $\mathbf{x}$ to the equation $\mathbf{Mx} = \boldsymbol{\alpha}$ exists and 0 otherwise. Third, we have that

$$N(\alpha) \leqslant 2^{\gcd(k,n)}, \tag{8}$$

where $\gcd(a, b)$ denotes the greatest common divisor of the integers a and b. To see this, consider the following algorithm for solving an instance of k-SAT on a ring over n bits. Assigning an arbitrary value to one of the n bits in an attempt to guess a solution uniquely determines $n/\gcd(k, n)$ of the bits in a manner consistent with the given clauses. For example, choose a value for bit 1. From the first clause, the Hamming weight of bits 2 through k is determined. From the second clause and the Hamming weight of bits 2 through k, the value of bit $k + 1$ is determined. Continue in this manner to determine bits $2k + 1$, $3k + 1$, etc. Clearly, assigning arbitrary values to the first $\gcd(k, n)$ undetermined bits will determine the values of all n bits. To exhaustively determine all solutions to an instance of k-SAT on a ring using this method will require $\gcd(k, n)$ passes for each of the $2^{\gcd(k,n)}$ possible choices for the first few bits. Because there are $2^{\gcd(k,n)}$ choices for these first $\gcd(k, n)$ undetermined bits, there exist at most $2^{\gcd(k,n)}$ solutions to an instance of k-SAT on a ring over n bits. By considering simple examples (such as that of the previous section), one can show that this bound is tight and that equality is not always attained.

The last of these observations yields a trivial upper bound on the partition function: we have from (6) that

$$Z_n \leqslant 2^{\gcd(k,n)} \mathrm{e}^{\beta J n} \sum_{\alpha} \mathrm{e}^{-2\beta J w(\alpha)} \leqslant 2^k \mathrm{e}^{\beta J n} \sum_{w=0}^{n} \binom{n}{w} \mathrm{e}^{-2\beta J w} = 2^k \mathrm{e}^{\beta J n} (1 + \mathrm{e}^{-2\beta J})^n = 2^k \lambda_+^n,$$

with λ_+ defined in (3). In the thermodynamic limit, this upper bound equals the standard Ising partition function up to a factor independent of n.

We can say more, however. Assuming the existence of the thermodynamic limit

$$\lim_{n\to\infty} n^{-1} \ln Z_n,$$

which is proportional to the free energy per site, the partition function must approach an analytic—in fact, exponential—function of n as $n \to \infty$. This is a purely physical requirement, and expresses the fact that the free energy of a large system should scale proportionally with its size [1]. Thus, the partition function should not depend on the coarse number-theoretic properties of n, asymptotically, and we may assume for convenience that $\gcd(k, n) = 1$. Physically, one can imagine building up the system of n spins by adding spins in blocks of k, starting with a single spin: the resulting values of n, namely 1, $k + 1$, $2k + 1$, and so on, are all coprime to k. The manner in which we construct the system is irrelevant when taking the thermodynamic limit, which justifies the assumption that $\gcd(k, n) = 1$. Under this assumption, $N(\alpha) = 2$ if $w(\alpha)$ is even and $N(\alpha) = 0$ otherwise. This is because there

are 2^{n-1} tuples α such that $w(\alpha)$ is even and an equal number such that $w(\alpha)$ is odd, and we observed in the previous section that $N(\alpha) = 0$ if $w(\alpha)$ is odd. Therefore, it follows from (7) and (8) that $N(\alpha) = 2^n/2^{n-1} = 2$ if $w(\alpha)$ is even. This observation allows us to extract the exponential dependence of the partition function:

$$Z_n = \sum_{w(\alpha)\text{ even}} 2\mathrm{e}^{\beta J(n-2w(\alpha))} = 2\mathrm{e}^{\beta Jn} \sum_{w\text{ even}} \binom{n}{w} \mathrm{e}^{-2\beta Jw} = \mathrm{e}^{\beta Jn} \sum_{w=0}^{n} \binom{n}{w} [1 + (-1)^w] \mathrm{e}^{-2\beta Jw}$$

$$= \mathrm{e}^{\beta Jn}(1 + \mathrm{e}^{-2\beta J})^n + \mathrm{e}^{\beta Jn}(1 - \mathrm{e}^{-2\beta J})^n = \lambda_+^n + \lambda_-^n \sim \lambda_+^n.$$

This partition function exactly matches that of the nearest-neighbour Ising model in zero field (3), as we wished to show.

As a final observation, it is interesting to note the similarity between this system and one in which only spins *separated* by some number of sites interact. Indeed, any 'separated' interaction of fixed range is also equivalent to the nearest-neighbour interaction in the thermodynamic limit. To show this, let ℓ be a positive integer, and consider an Ising-like spin system with Hamiltonian

$$H(\sigma) = -J \sum_{i=1}^{n} \sigma_i \sigma_{i+\ell}.$$

Define the transfer matrix $\mathbf{T}$ obtained by substituting $h = 0$ into expression (2) for $\mathbf{V}$:

$$\mathbf{T} = \begin{pmatrix} \mathbf{T}_{++} & \mathbf{T}_{+-} \\ \mathbf{T}_{-+} & \mathbf{T}_{--} \end{pmatrix} = \begin{pmatrix} \mathrm{e}^{\beta J} & \mathrm{e}^{-\beta J} \\ \mathrm{e}^{-\beta J} & \mathrm{e}^{\beta J} \end{pmatrix}.$$

Effecting the matrix multiplications gives

$$Z_n = \sum_{\sigma} \prod_{i=1}^{n} \mathbf{T}_{\sigma_i,\sigma_{\ell+i}} = \sum_{\sigma} \prod_{i=1}^{\gcd(\ell,n)} \mathbf{T}_{\sigma_i,\sigma_{\ell+i}} \mathbf{T}_{\sigma_{\ell+i},\sigma_{2\ell+i}} \mathbf{T}_{\sigma_{2\ell+i},\sigma_{3\ell+i}} \cdots \mathbf{T}_{\sigma_{n-\ell+i},\sigma_i}$$

$$= \sum_{\sigma_1} \sum_{\sigma_2} \cdots \sum_{\sigma_{\gcd(\ell,n)}} \prod_{i=1}^{\gcd(\ell,n)} \left[\mathbf{T}^{n/\gcd(\ell,n)}\right]_{\sigma_i,\sigma_i} = \left[\mathrm{tr}\left(\mathbf{T}^{n/\gcd(\ell,n)}\right)\right]^{\gcd(\ell,n)}.$$

The thermodynamic limit is well defined because

$$Z_n = \left[\lambda_+^{n/\gcd(\ell,n)} + \lambda_-^{n/\gcd(\ell,n)}\right]^{\gcd(\ell,n)}, \tag{9}$$

and since $\gcd(\ell, n) = O(1)$, the term $\lambda_+^{n/\gcd(\ell,n)}$ dominates as $n \to \infty$, whence $Z_n \sim \lambda_+^n$. Letting $\ell = k/2$ in formula (9) gives a surprisingly good numerical approximation to the partition function of the k-spin Ising model. It is an even better approximation than the nearest-neighbour Ising partition function, which makes sense because the k-spin Ising model can be viewed as a 'smeared-out' version of the model in which sites i and $i + k/2$ interact (see table 1).

5. Discussion

We have introduced a method of solving the k-spin Ising model in zero field by mapping its Hamiltonian onto a computational problem. The method may be applicable to other models for computing partition functions and correlation functions, or simply for didactic purposes. Given the increasing interconnectedness of statistical physics and computation, it seems fruitful to explore ways of thinking about exactly solvable models from a fundamentally algorithmic point of view.

Table 1. Comparison of the nearest-neighbour ('N–N') and $(k/2)$th-neighbour ('$k/2$-N') Ising models with the k-spin model for $k = 4, \ldots, 30$. The entries of the middle (right) column are the numbers d such that the nearest-neighbour ($(k/2)$th-neighbour) partition function disagrees with the k-spin partition function whenever n is a multiple of d. Values were determined numerically for n up to 30 and then extrapolated. As can be seen, the $(k/2)$th-neighbour partition function consistently matches the k-spin partition function more often than does the nearest-neighbour partition function. Interesting numerical patterns emerge, which suggest that the exact k-spin partition function depends on both the number of distinct primes dividing k and their multiplicities; a full analysis is beyond the scope of this paper.

k	N–N	$k/2$-N
4	2	4
6	3	6
8	2	8
10	5	10
12	2, 3	4
14	7	14
16	2	16
18	3	6
20	2, 5	4
22	11	22
24	2, 3	8
26	13	26
28	2, 7	4
30	3, 5	6, 10

The k-spin Ising model further illustrates that replacing nearest-neighbour interactions with similar short-range interactions may hardly have any effect in the thermodynamic limit. In this way, slightly different small-scale assumptions reproduce the same large-scale properties. We have yet to study the $h > 0$ case of the k-spin Ising model, but numerical calculations for small n indicate that the free energy function does differ from that of the nearest-neighbour Ising model in an external field.

We conclude with a note on the motivation behind the model considered in this paper. The k-spin Ising model, in the guise of k-SAT on a ring, arises as a generalization of the problem of '2-SAT on a ring', which appears as a pedagogical example in the very first paper on adiabatic quantum computation [17]. In this paper, Farhi *et al* encode the 2-SAT problem in a (quantum) Hamiltonian H_P and verify it to be solvable in polynomial time on an adiabatic quantum computer. Incidentally, their techniques can be extended to show that k-SAT on a ring is solvable in polynomial time on an adiabatic quantum computer (it is trivially solvable in polynomial time on a classical computer). The proof of this fact provides further justification for why k must be even: a crucial step relies on restricting analysis to an invariant subspace of a judiciously chosen unitary operator whose existence assumes the time-reversal (or bit-negation) symmetry of H_P, which in turn exists only when k is even.

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