

EXACT EXPRESSION FOR THE NUMBER OF ENERGY STATES IN LATTICE MODELS

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We derive a closed-form combinatorial expression for the number of energy states in canonical systems with discrete energy levels. The expression results from the exact low-temperature power series expansion of the partition function. The approach provides interesting insights into basis of statistical mechanics. In particular, it is shown that in some cases the logarithm of the partition function may be considered the generating function for the number of internal states of energy clusters, which characterize system's microscopic configurations. Insights provided by the method allow one to understand the circumstances under which the widespread distributions for the energy, such as the Poisson and exponential distributions, arise. Apart from elementary examples, the framework is validated against the one-dimensional Ising model in zero field.

Keywords: density of states, low temperature series expansion, Bell polynomials, combinatorics, lattice models.

1. Introduction

It has long been recognized that the number of energy states, $g(E)$, with a given value of the energy E , is a key quantity in equilibrium statistical physics. In principle, all energy-related thermodynamic properties of a classical canonical system can be calculated once $g(E)$ is known. In particular, in the case of a system with discrete energy levels, the canonical partition function is $Z(\beta) = \sum_E g(E)e^{-\beta E}$, where the summation is over the allowed energy levels, and quantities such as the Helmholtz free energy, $F(\beta) = -\ln Z(\beta)/\beta$, the ensemble-averaged energy, $\langle E \rangle = -\partial \ln Z(\beta)/\partial \beta$, and the specific heat (which is related to energy fluctuations, $\langle E^2 \rangle - \langle E \rangle^2 = -\partial \langle E \rangle / \partial \beta$) can be simply obtained.

Due to the central role of the energy distribution function, a variety of theoretical and computational studies have addressed the problem of how to obtain $g(E)$, see e.g. [1–7]. On the other hand, relatively little was done to understand how the state-space representation of a considered system relates to its energy distribution and how to recover such information from, for example, the partition function.

In this paper we derive a new and general combinatorial formula for the number of states. The formula results from the exact low-temperature power-series expansion

of the canonical partition function. In our approach $g(E)$ is expressed by the so-called Bell polynomials, which have a very convenient combinatorial interpretation: they describe how equal energy portions can cluster together within the studied system. This, in turn, gives insight into system's microscopic details.

In the low-temperature expansion of the partition function, $Z(\beta) = \sum_{\Omega} e^{-\beta E(\Omega)}$, microstates Ω are counted in order of their importance as the temperature is increased from zero [8, 9]. If the ground state of a system is known and if the successive excitations from this state can be classified in a simple way, one should, at least theoretically, be able to construct such a series, i.e.

$$Z(x) = \sum_{N=0}^{\infty} g(\varepsilon N) x^N, \quad (1)$$

where

$$x = e^{-\beta\varepsilon}, \quad (2)$$

and energy is considered to be discrete

$$E = \varepsilon N, \quad (3)$$

with ε representing a portion of energy and $N = 0, 1, 2, \dots$ (with the ground-state energy equal to zero). In Eq. (1), $g(\varepsilon N)$ represents the number of microscopic configurations in which energy of the system is εN . One should also notice that Eq. (3) states that ε is the smallest portion of energy, such that the considered lattice/discrete model may only have energy levels which are a multiple of ε . For this reason, ε strongly depends on the model, i.e. it is usually somehow built into the initial specification of the model studied. In particular, for the one-dimensional Ising model, the choice of $\varepsilon = 2J$ (where J is the coupling constant between nearest neighbours) is due to the fact that by changing the sign of only one spin the energy of the system changes by the amount of ε .

From Eq. (1) it is apparent that the exact distribution function for the energy, $g(\varepsilon N)$, can be determined from the coefficients of the partition function. As a rule, however, when the order of expansion is increased complexity of contributing terms also increases rapidly. In this context, a *rule of thumb* states that the work involved in *direct* calculating the next term, $g(\varepsilon N)$, is the same as that needed to calculate all the preceding terms, $g(0), g(\varepsilon), \dots, g(\varepsilon N - \varepsilon)$. For this reason, generation of lengthy low-temperature power-series for the partition function is thought to be a highly specialized art. That is why, even in the case of the two-dimensional Ising model on a square lattice, for which the method was primary advanced (see Chapter 6 in [1]), the exact distribution of energies was just obtained in 1996 [2, 10], nearly a half a century after Kaufman's exact solution for the partition function [11].

The aim of this paper is to show that the effort needed to calculate the coefficients of the low-temperature power-series expansion for the canonical partition function is greatly reduced by using the combinatorial scheme described below. The approach is very general and applies to any lattice model. We also argue that

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