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Ising low-temperature polynomials and hard-sphere gases on cubic lattices of general dimension

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HIGHLIGHTS

- We compute the Ising low-T series through 13th order in general dimension.
- From the Ising data we get the virial series for a hard sphere lattice gas.
- We get the critical parameters of the hard sphere gas in general dimension.

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ABSTRACT

We derive and analyze the low-activity and low-density expansions of the pressure for the model of a hard-sphere gas on cubic lattices of general dimension d, through the 13th order. These calculations are based on our recent extension to dimension d of the low-temperature expansions for the specific free-energy of the spin-1/2 Ising models subject to a uniform magnetic field on the (hyper-)simple-cubic lattices. Estimates of the model parameters are given also for some other lattices.

1. Introduction

A simpler and mathematically more tractable discretization of the long-studied hard-sphere fluid in continuum space is called "hard-sphere lattice gas" (HSLG) with nearest-neighbor exclusion [1–5]. In this model the sites of a regular lattice are the only allowed positions of the constituents. The pair interaction potential is $+\infty$ for constituents centered on nearest-neighbor sites and vanishes otherwise. Double occupancy of sites is forbidden. In particular in 2d, on a square (sq) lattice, the spheres of the model can be viewed as "hard-squares" oriented at $\pi/4$ with respect to the lattice axes and whose diagonals equal two lattice spacings. In 3d the spheres are effectively "hard octaedra" and analogously for higher-dimensional lattices, they are polytopes (i.e. convex hyper-polyhedra) whose vertices are the nearest neighbors of the sites on which they are centered.

If the properties of the HSLG on a finite lattice are described by the statistical mechanics formalism of the grand partition function, it turns out that the nth coefficient of the low-activity (LA) series-expansion of the grand-potential has the same combinatorial definition [3–5] as the coefficient of the highest power of the temperature-like variable u in the nth low-temperature (LT) polynomial of a ferromagnetic Ising model with spin $S = 1/2$ on the same lattice. This relationship remains valid when the thermodynamic limit is taken. When this fact was recognized, it became trivial to write down the

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LA expansions of the pressure once the LT expansion of the Ising model on the same lattice, in presence of a magnetic field, is known.

Thus, for the one-dimensional lattice, one can write a LA expansion valid to all orders. For the *sq* lattice, initially the LA expansion could be obtained [3–5] in this way only through the 12th order. The derivation was later extended [6] through the 21st order. Finally, by a more powerful approach based on the corner-transfer-matrix method [7], the LA series was pushed through the 42nd order and more recently [8] through the 92nd order.

For the triangular lattice ("*hard-hexagon*" model), an exact solution [9,10] of the HSLG model was devised. It is expected [11] that also the honeycomb (*hc*) lattice case (called the "*hard-triangle*" model) is soluble, however, presently we know only a 25th order LA expansion derived from the LT Ising expansion [12,13] for the *hc* lattice. For lattices of dimension $d > 2$, the transfer-matrix techniques are not efficient, so that one has to rely only on the LT Ising expansions and no LA data of extension comparable with that of the *sq* lattice can be derived. In the case of the three-dimensional hydrogen-peroxide (*hpo*) lattice, a bipartite cubic lattice of coordination number 3, the known Ising LT series [14] yields a 23rd order LA series for the HSLG model. For the three-dimensional bipartite *diamond* lattice, with coordination number 4, the first 17 LA coefficients can be obtained [15]. Only the first 15 Ising LT polynomials are presently known [6,16] for the simple-cubic (*sc*) lattice in 3*d* and the hyper-simple-cubic (*hsc*) in 4*d*, while the first 11 polynomials [17] are known in the case of the body-centered-cubic (*bcc*) lattice. No LT data at all existed up to now for the *hsc* and the hyper-body-centered-cubic (*hbcc*) lattices of dimension $d > 4$.

We have recently calculated [18] the Ising LT polynomials for all *hsc* lattices in general dimension *d* through the 13th order. As a result, in this paper we can present the LA and low-density (LD) expansions for the HSLG through the same order, having observed that the LD expansion coefficients $v_k(d)$ of the pressure are polynomials of degree $[\frac{k}{2}]$ in *d*. It is worth noticing that also the LD expansion coefficients of the pressure for the dimer model on the *hsc* lattices share a similar (slow) polynomial dependence on *d*, making it possible to determine [19] the LD expansions through the 20th order.

We shall analyze the LA expansions for the HSLG to extract information about the properties of the model for $d > 4$, which, up to now, have been the subject of a single accurate MonteCarlo(MC) study [20]. To support some of the indications suggested from our study for the higher-dimensional lattices, we shall also perform an analysis of the LA and the LD series for the *hc*, the *hpo* and the *diamond* lattices, to which little attention was devoted in the literature.

It is also well known that, using the standard correspondence [2] between the lattice gas and the spin-1/2 Ising model, one can relate the HSLG with an LT anti-ferromagnetic Ising spin system subject to a magnetic field [3,21,22] on the same lattice and thus further insight can come also from this standpoint. In particular, in analogy with the LA series, the high-activity (HA) expansions coefficients (in powers of $1/z$) for the pressure can be directly read [4] from the Ising LT anti-ferromagnetic polynomials. Unfortunately, the LT anti-ferromagnetic data are scarce and therefore direct methods [4,5] have been necessary to compute the HA series [7], presently known only through order 23 for the *sq* lattice, and through the 16th or the 19th orders, respectively for the simple-cubic (*sc*) and the body-centered-cubic (*bcc*) lattices. No such series exist for the lattices with $d > 4$, with which we shall be mainly concerned in this paper.

For the HSLG model one is mainly interested into

(a) the leading *nonphysical* singularity [23] of the pressure located at a small negative value of the activity. Its exponent is known to be simply related to that of the universal [1,24,25] Yang-Lee edge-singularity for spin systems of the same dimension, as well as to the exponents of several other systems [26], such as the directed branched polymers, the undirected site or bond animals, etc.

(b) The parameters of the expected *physical* phase-transition which takes place as the density increases and changes the LD disordered phase into an HD ordered one. In this transition, associated with the nearest singularity of the pressure on the positive activity (or density) axis and accurately checked [20,27,28] to be Ising-like for the bipartite lattices to which we shall restrict this study, one of the two equivalent sublattices becomes preferentially occupied at HD, while at LD (or equivalently at LA), the constituents are uniformly distributed all over the lattice sites. We may also remark [29] that the transition is "entropy-driven", because the internal energy vanishes for the allowed configurations of the system and the temperature turns out to be an irrelevant constant, so that the free energy coincides up to a sign with the entropy.

The paper is organized as follows. In Section 2, we recall the structure of the LT expansion for a ferromagnetic spin 1/2 Ising model and write down the corresponding LA and LD expansions of the pressure for the HSLG. The analysis of these expansions for lattices of various dimensions, leads to a conjecture on the nature of the nearest singularity in the complex density plane for $d \geq 3$, and is presented in Section 3. Simple estimates of the entropy constants for lattices of not too high *d* are discussed in Section 4. The last Section contains a summary of our results.

Appendix A reviews in some detail our derivation of the LT polynomials of the spin 1/2 Ising model subject to a magnetic field, from the corresponding HT expansion.

In Appendix B, we argue that the virial expansion coefficients $v_k(d)$ can be expressed as polynomials in *d* of degree $[\frac{k}{2}]$ and present handy expressions of the LA and the LD expansions of the pressure valid for *hsc* lattices of general dimension.