Phase transitions in the multicomponent Widom–Rowlinson model and in hard cubicles on the bcc lattice

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Abstract

We use Monte Carlo techniques and analytical methods to study the phase diagram of the M-component Widom–Rowlinson model on the bcc lattice: there are M species all with the same fugacity y and a nearest-neighbor hard core exclusion between unlike particles. Simulations show that for M ≥ 3 there is a "crystal phase" for z lying between z(M) and z(M) while for z > z(M) there are M demixed phases each consisting of one species. For M = 2 there is a direct second-order transition from the gas phase to the demixed phase while for M ≥ 3 the transition at z(M) appears to be first order putting it in the Potts model universality class. For simple cubic, Firogov–Sinai theory gives z(M) ~ M + 2 + αz(M)^2 + ···. In the crystal phase the particles preferentially occupy one of the cubicles, independent of species, i.e. spatial symmetry but not particle symmetry is broken. For M → ∞ this transition approaches that of the one-component hard cube gas with fugacity y = zM. We find by direct simulations of such a system a transition at y ≈ 0.71 which is consistent with the simulation z(M) for large M. This transition appears to always be of the Ising type.

1. Introduction

The Widom–Rowlinson (WR) model, introduced in 1970 [1] as an ingeniously simple model for the phase study of phase transitions in continuum fluids (for an overview see Ref. [2]), continues to be, like its authors, a rich source of insights and analytical results in many (sometimes quite unexpected) areas [3–6] of statistical mechanics. In this paper, dedicated with great dedication to Ben Widom on the occasion of his 70th
birthday, we continue our study of a variation of the original model from two to \( M \) components on a lattice: hard core exclusion between particles of different species on nearest-neighbor sites.

This model was first considered by Runnels and Lebowitz [7] who proved that when the number of components \( M \) is larger than some minimum \( M_0 \) then the transition from the gas phase at small values of \( z \) to the demixed phase at large values of \( z \) does not take place directly. Instead there is, at intermediate values of \( z \), \( z_c < z < z_d \), an ordered phase in which one of the sublattices (even or odd) is preferentially occupied, i.e., there is a crystalline (antiferromagnetically ordered) phase in which the average particle density on the even and odd sublattices, \( \rho_e \) and \( \rho_o \) are unequal. The average density, \( \rho(I) \), of species \( I = 1, \ldots, M \), on each sublattice is the same for each \( I \), with \( \rho_e(I) = M^{-1} \rho_e \) and \( \rho_o(I) = M^{-1} \rho_o \). The nature of the symmetry-breaking is thus very different from that in the demixed phase at \( z > z_d \) where \( \rho_e = \rho_o = \rho \) but there exists one species, say \( I' \), for which \( \rho(I') > M^{-1} \rho \). The origin of this crystalline phase is purely entropic. For \( z \) fixed and \( M \) large "it pays" for the system "entropy wise" to occupy just one sublattice without any constraint; since there are no interactions between particles on the same sublattice there are \( M \) independent choices at each site if we keep one of the sublattices empty. This more than compensates, at some \( M > M_0 \), for the "loss" of "fugacity energy" occasioned by keeping down the density in one of the sublattices.

A natural question now arises, just how big does \( M_0 \) have to be to see this ordered phase for \( M \geq M_0 \). It was shown in [7] that on the square lattice \( M_0 < 27^2 \), a ridiculously large upper bound. On the other hand, a direct computation on the Bethe lattice [8,9] with \( q \)-neighbors gives \( M_0 = [q/(q - 2)]^2 \), which would suggest \( M_0 \sim 4 \) for the square lattice, \( M_0 \sim 3 \) for the cubic and \( M_0 \sim 2 \) for the bcc lattice. Now it can be shown, using FKG inequalities, that \( M_0 \geq 3 \) on any bipartite lattice [10], but beyond that we have no simple or convincing argument for finding \( M_0 \). We therefore turned to Monte Carlo simulations. This gave on the square lattice \( M_0 = 7 \) [8,9] which is only about twice as large as the Bethe lattice prediction. This wetted our appetite to try the bcc lattice where \( q = 8 \). To our surprise we find here, using Monte Carlo simulations, that \( M_0 \) does indeed equal 3, on the bcc lattice.

While we have no clue of how to find rigorously the actual value of \( M_0 \) or of \( z_c(M) \), it was argued in [9] that for a given \( z \) and \( M \) large enough, the typical occupancy pattern on the lattice (ignoring the label \( I \) of the particles) should be like that of a one-component lattice gas with nearest-neighbor hard core exclusion. For the latter system, Dobrushin [11] proved the existence of a crystalline state. This implies that \( z_c(M) \) should behave for large \( M \) as \( y_c/M \), where \( y_c \) is the critical fugacity at which the one-component hard cube gas (occupation at a site \( j \) excludes occupation at all eight neighboring sites) crystallizes. The value of \( y_c \) for the bcc lattice, obtained by Gaunt [12] using series expansion methods, is \( 0.77 \pm 0.05 \). Using MC we obtained \( y_c = 0.71 \pm 0.01 \) which is roughly consistent with Gaunt's value. Our result also agrees well with the values of \( Mz_c(M) \) for large \( M \) being approximately \( 0.72 \pm 0.02 \) for \( M = 50 \) and \( M = 100 \). This provides solid evidence for the existence of a reentry phase
transition in the temperature–magnetic field plane phase diagram of an Ising spin system with nearest-neighbor anti-ferromagnetic interactions on the bcc lattice [13].

We also find, as in [9], that for large $M$, $z_d(M)$ for the crystal-demixed transition can be computed via Pirogov–Sinai theory [14] yielding,

$$ M = z_d + 2 - 2/3z^2 + \cdots \quad (1) $$

which matches up smoothly with our MC results; see Fig. 3. It is easy to show that there is a demixing transition for $M \geq 2$ [3,5,14], the existence of sharp interfaces between coexisting phases, for $M = 2$, on the cubic lattice at large fugacity $z$ was proven in [6].

We next present results of our simulations and refer the reader to [9] for a more detailed description of the model and additional references.

2. Results

Our MC simulations were carried out on a bcc lattice of size $2 \times 2^3 = 2 \times 22^3$ with periodic boundary conditions. On an initially empty lattice, we deposit particles chosen at random from the $M$ components at fugacity $z$ respecting the exclusion of different species occupying neighboring sites. We then sequentially update the lattice using a checkerboard algorithm resulting in a good vectorization. An update of a lattice site $(i_1, i_2, i_3)$ on one of the two simple cubic sublattices $s$, making up the bcc lattice, which is occupied by a particle of type $l$ ($l = 0$ indicating an empty site) is done as follows: We randomly choose a new trial particle of type $I_0$, where $I_0$ can have any integer value between 0 and $M$ with equal probability. $I_0 = 0$ refers to an attempted removal of a particle $I \neq 0$ from the lattice site, which is successful, if a number $X$ randomly chosen with equal probability between 0 and 1 is smaller than the inverse fugacity $1/z$. When this occurs $I$ gets the value 0, otherwise it remains unchanged, $I_0 \neq 0$ refers to an attempted deposition of a particle of type $I_0$. If $I = 0$ then it is successful if each of the four nearest-neighbor sites is either empty or occupied by a particle of the same type ($I_0$) and $X < z$. In this case $I$ gets the value $I_0$, otherwise it remains unchanged. A direct replacement attempt of a particle $I \neq 0$ surrounded by eight empty nearest-neighbor sites is always successful. Typically, in a simulation run after an equilibration of $2 \times 10^5$ Monte Carlo steps (MCS), we update the lattice $10^5$ times, the configuration of every tenth step is taken for the evaluation of the averages.

A typical run with $10^5$ MCS took about 1 CPU h on a CRAY–YMP.

Let $m(i_1, i_2, i_3)$ denote the occupancy of a site, $m(i_1, i_2, i_3) = 0$ if the site $(i_1, i_2, i_3)$ is empty and $m(i_1, i_2, i_3) = 1$ otherwise. As observables we took histograms $P_k(\phi_c)$ of the order parameter $\phi_c$ for the crystal structure and $P_k(\phi_d)$ of the order parameter $\phi_d$ for the demixed phase in subsystems of size $2 \times L^3$,

$$ \phi_c = \frac{1}{2L^3} \sum_{s=1}^2 \sum_{l-1}^{L} \sum_{i_s^{(4)}, i_s^{(5)}, i_s^{(6)}} \left[ 2m(i_1^{(4)}, i_2^{(4)}, i_3^{(4)}) - 1 \right] (-1)^{2x_s - 1} \quad (2) $$

and

$$ \phi_d = \frac{1}{2L^3} \max_{l=1}^{M} N_l \mu/m/M \quad (3) $$

where $N_l \mu$ denotes the number of particles of type $l$ in a subsystem of size $2 \times L^3$ and $m$ is the average overall density.

2.1. Gas-crystal phase transitions

For a given $M$ the transition activity $z_c$ is found by finite size scaling techniques [15,16]. In particular, the $k$th moments of the order parameter distribution $P_k(\phi_c)$,

$$ \langle \phi^k \rangle_L = \int \phi^k P_k(\phi_c) d\phi_c \quad (4) $$

can be evaluated in subsystems of size $2 \times L^3$, and from them the fourth-order cumulant [16] $U_k$,

$$ U_k = 1 - \frac{\langle \phi^4 \rangle_L}{3(\langle \phi^2 \rangle_L)^2} \quad (5) $$

In a one-phase region far away from a critical point the subsystem size typically can be chosen larger than the correlation length $\xi$, $L \gg \xi$ and the order parameter distribution is to a good approximation a Gaussian centered around 0, resulting in $U_k \rightarrow 0$ for $L \rightarrow \infty$. In the two phase coexistence region far away from a critical point we can again assume $L \gg \xi$ and the order parameter distribution is bimodal resulting in $U_k \rightarrow \frac{1}{2}$ for $L \rightarrow \infty$. Near the critical point however we have $L \ll \xi$, and using scaling arguments [16] the cumulant is a function of $L/\xi$, resulting for $\xi \rightarrow \infty$ in the same value of $U_k$ for all different $L$. This method allows the efficient determination of critical points by analyzing the cumulants for different values of $z$ on different length scales $L$. Applied to our model we should see, for low values of $z$, when the system is in the disordered one-phase region, $U_k > U_k$ for $L < L$. Increasing $z$, we obtain, for large enough $M$, a crystal phase with $U_k < U_k$ for $L < L$. Near $z_c$ we expect $U_k \approx U_k$ for $L \neq L$. This method for locating the transition fugacities was used in our previous studies [8,9] on the square lattice as well.

For $M = 3, 4, 5, 10$ we obtain in this way values of $z_c = 0.525 \pm 0.025, 0.3, 0.21, 0.085 \pm 0.01$, respectively, for $M = 15, 17, 19, z_c = 0.055, 0.047, 0.04 \pm 0.001$ and for $M = 100, z_c = 0.000725 \pm 0.000025$. Cumulants for the gas-crystal transition of the hard diamond and the $M=3$-component system are shown in Figs. 1 and 2, respectively. The transition points are presented in Fig. 3 together with the asymptotic expression $\Delta z_c = 0.71$. This corresponds to the value of $\gamma_c$ on the bcc lattice $\gamma_c = 0.71 \pm 0.01$ which we obtained using MC techniques. We also show in Fig. 3 a purely empirical fit of the $1/M^2$-corrections for $z_c, z_c = 0.71/M + C/M^2$, to the MC data, with a value of $C = 2 \pm 0.5$. The minimum number of components required for the existence of the crystal phase on the bcc lattice is $M = 3$. In Fig. 4 we show the approach of the critical fugacity $M\infty$ $z_c$ to the limit of the hard diamond system.
2.2. The demixing transition

For $M = 2$ we obtain a direct transition from the gas phase to the demixed phase at a transition fugacity of $z = 0.55 \pm 0.02$; the transition is second order with Ising exponents as on a simple cubic lattice studied by Dickman et al. [17].

For $M > 2$ we observe a direct first-order transition from the crystal to the demixed phase. This transition was analyzed by studying the order parameter distribution $P_k(\phi_d)$.

In the simulations we find a hysteresis region around $z_d$, going approximately between two values of $z$, say $z_1$ and $z_2$, when increasing and decreasing the fugacity. In cases of a small hysteresis region with extent of less than $|z_1 - z_2| < 0.1$, $z_d$ was taken as
the average of this region, \( z_d = (z_1 + z_2)/2 \). In cases of a larger hysteresis region we located the transition fugacity \( z_d \) by finding the relative stability of one of the two phases during a simulation starting from configurations with both phases present in parallel slices extending over the length of the simulation box, as described in [9]. The resulting phase transition values of \( z_d \) are shown in Fig. 1. We note that with increasing number of components, the transition fugacities approach the exact asymptotic line \( M = z^1 \cdot 2 - 2/3 z^2 + \ldots \).

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