Critical behaviour in active lattice models of motility-induced phase separation

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Abstract As for the study of equilibrium phase transitions, coarse-grained discrete lattice models feature a computationally more efficient route to investigate the motility-induced phase separation (MIPS) of active particles compared to off-lattice systems. Simulations are less demanding and thus bigger systems with higher accuracy and better statistics can be accessed. Nevertheless, at least in equilibrium the properties of critical points are not affected and fall into the same universality class. Whether this hallmark of statistical physics holds also for active particles is an open challenge. Here, we examine two recently proposed active lattice systems that undergo MIPS with respect to their critical behaviour. We also take a more detailed look on the influence and role of rotational diffusion and active velocity in these systems.

Keywords motility-induced phase separation · active Brownian particles · active lattices · critical behaviour · universality class

1 Introduction

Non-equilibrium active systems composed of self-propelled particles offer a wide range of interesting behaviour and applications [1,2]. A fundamental phenomenon is the so called motility-induced phase separation (MIPS) [4]: At large propulsion speeds and low rotational diffusion, self-propelled particles block each other due to excluded volume and form initial clusters. If the time-scale for the rotational diffusion of the particle orientations at the border of such a cluster is larger than the time it takes to enrich the cluster with additional particles, a dynamical instability leading to non-equilibrium phase separation is induced. Although the phase-separated state resembles passive liquid-gas separation with dense domains surrounded by an active gas, no
explicit attractive interactions are required. Still, the phase behavior is very similar, with the binodal curve of coexisting densities terminated by a critical point below which the system remains homogeneous for all densities. The question whether or not the behavior close to such a non-equilibrium critical point is universal, and if it can be attributed to one of the standard universality classes, is not only of fundamental interest but has also stirred up an ongoing controversy [5,6,7,8].

Numerical studies of active Brownian particles (ABPs) [9,10,11,12,13,14,15,16] are a common approach to investigate MIPS in a simple continuous system. These particles are modelled as disks interacting with each other via a purely repulsive Weeks-Chandler-Anderson potential in the framework of an overdamped Langevin equation. In addition, they are propelled with constant speed along their orientation, which is subject to rotational diffusion. For this system, we have determined the location of the critical point and reported critical exponents, which are incompatible with any of the known universality classes [5]. To gain access to the critical point and the critical exponents, we have proposed a novel method to sample sub boxes that minimizes the influence of interfaces on density fluctuations.

In contrast, investigations of related but different models have come to a different conclusion, supporting Ising universality in off-lattice Active Ornstein-Uhlenbeck particles [8] and in a lattice variant of ABPs [7]. Following generic arguments of renormalization [17], however, all these models should fall into the same universality class and thus exhibit the same critical exponents. Indeed, in a first renormalization study of an active field theory (“active model B+”) [15,19] it was found that the critical behavior is controlled by the Wilson-Fisher fixed point [6]. What, then, is the reason for the reported differences? Regarding geometry and sub boxes, all three numerical works have employed the same method (for details, see Sec. 2.2). One reason could be insufficient statistics, or insufficient range of system sizes leading to a biased estimate of critical exponents. Or, more intriguingly, are there additional features that characterize universality classes in active matter? We stress that MIPS of repulsive particles is a genuine non-equilibrium phenomenon. The effect of self-propulsion on the critical behavior in models that exhibit phase separation already under equilibrium conditions has been studied for Lennard-Jones interactions [20] and a three-dimensional Asakura-Oosawa model [21] driven by a Vicsek-type force [22,23,24] and found to be compatible with the 3d-Ising universality class [25].

In this manuscript, we take another step towards a comprehensive understanding of critical behavior in active matter. To this end, we numerically investigate different variants of two-dimensional active lattice gases with excluded volume and dynamics that break detailed balance. While a range of active lattice gas models has been investigated [26,27,28,29,30,31], we focus on two variants that mimic active Brownian particles. In particular, we study two lattice geometries (the square and hexagonal lattice) and two implementations of the dynamics, either treating rotation and translation serial [7] or concurrently [32]. Our numerical results indicate that details of the dynamics
have an influence on the critical behavior and question the proposition that MIPS falls into Ising universality.

2 Methods

2.1 Critical behavior

Before embarking on the computational study, let us recall some of the properties close to a critical point. We consider systems that undergo phase separation with two coexisting phases having different densities \( \rho \). The two phases are identified with gas \( \rho_{\text{gas}} \) and liquid \( \rho_{\text{liq}} \). The (average) order parameter is the difference, \( m = \rho_{\text{liq}} - \rho_{\text{gas}} \). As we approach the critical point, the gap \( m \) closes and following a path exactly through the critical point, we would observe

\[
m \sim \tau^\beta,
\]

whereby \( \tau \) measures the distance to the critical point (typically the reduced temperature) and \( \beta \) is the corresponding critical exponent. The transition is continuous, with \( m > 0 \) for \( \tau > 0 \) and \( m = 0 \) in the homogeneous phase for \( \tau < 0 \). In addition, both the susceptibility \( \chi \) and the correlation length \( \xi \) diverge at the critical point,

\[
\begin{align*}
\chi &\sim \tau^{-\gamma}, \\
\xi &\sim \tau^{-\nu},
\end{align*}
\]

defining two more exponents. Of particular importance is Ising universality in systems with short-range interactions and scalar order parameter, for which the exponents can be obtained analytically \[33\]

\[
\beta = \frac{1}{8}, \quad \gamma = \frac{7}{4}, \quad \nu = 1.
\]

Note that the three critical exponents are not independent but obey the hyperscaling relation

\[
\gamma + 2\beta = 2\nu
\]

in two dimensions following from very general arguments \[34\].

The diverging correlation length \( \xi \) implies that the critical behavior is modified in finite systems, where the correlation length is bounded by the system size \( l \). One of the most remarkable successes of computational statistical physics is that the critical behavior can still be extracted from finite simulations \[35,36\]. To locate the critical point, we turn to Binder’s cumulant ratio

\[
Q_l(\tau) = \frac{\langle m_l^2 \rangle^2}{\langle m_l^4 \rangle},
\]

which becomes independent of \( l \) exactly at the critical point. Plotting the ratio \( Q_l \) as a function of some parameter for different \( l \) thus allows—notwithstanding systematic effects as discussed below—to locate the critical point from the intersection of curves. Moreover, the derivative \( dQ_l/d\tau \) at \( \tau = 0 \) yields the
inverse of the critical exponent \(\nu\). Once we have located the critical point, we can extract \(\beta\) from plotting \(\langle m_l \rangle\) as a function of \(\tau\). Finally, we exploit the scaling form \(\chi_l = l^{\gamma/\nu} \tilde{\chi}(l/\xi)\) for the susceptibility with scaling function \(\tilde{\chi}\) that depends on system size through the ratio \(l/\xi\). Plotting the susceptibility (obtained from the fluctuations of the order parameter) as a function of \(l\) allows to extract the ratio \(\gamma/\nu\). We thus have access to the three critical exponents \(\nu, \gamma, \) and \(\beta\).

2.2 Simulations

To access the critical behavior, we need to sample fluctuations of the order parameter \(m_l = (N_l - \langle N_l \rangle)/l^2\) in a finite system with \(N_l\) the number of particles. While the ensemble of choice for these simulations is obviously the grand-canonical ensemble, for driven active systems breaking detailed balance this route is not available due to the absence of a comprehensive framework in which a chemical potential is defined (although attempts have been made \[37, 38\]).

Therefore, we closely follow the method and analysis proposed in Ref. [5]. All simulations were performed in a periodic box with 1:3 geometry. In such elongated boxes, the dense phase nucleates to a slab like structure, cf. Fig. 1. The slab arises along the short side of the box and connects to itself via periodic boundary conditions. Its position inside the simulation box can be easily determined as the center of mass of all particles.

In order to measure dense and dilute phase as well as to avoid interface regions between the two phases, we place two quadratic sub boxes of size \(l\) above each other right in the center of mass to sample the dense phase (see Fig. 1). Another set of two sub boxes is placed shifted away by one half of the simulation box’s width from the center of mass to sample the dilute phase. In total, we sample the number of particles \(N_l\) within the 4 sub boxes of size \(l\) in a simulation box of size \(2l \times 6l\). By adjusting the size of the simulation box to the sub-box size, we couple the maximum correlation length to \(l\) and achieve a clear crossing point of \(Q_l\) for different \(l\). The susceptibility is evaluated as \(\chi_l = \langle (N_l - \langle N_l \rangle)^2 \rangle / \langle N_l \rangle\). Coexistence densities of dense and dilute phase (\(\rho_{\text{liq}}\)
and \( \rho_{\text{gas}} \) are obtained as plateau values of density profiles generated from a simulation box of size \( 252 \times 84 \) (corresponding to \( l = 42 \)) at activities slightly above the tentative critical point.

3 Model I: Serial rotation/translation

3.1 Model description

We first turn to the model studied in Ref. [7] employing a hexagonal lattice, which we will refer to as model I. On a hexagonal lattice each particle has six neighbouring sites and six discrete directions it can be orientated towards (Fig. 2). Specifically, each Monte Carlo (MC) step works as follows:

1. A particle is picked at random.
2. A Gaussian distributed random number (with standard deviation \( \sigma \) and zero mean) is drawn and rounded to the nearest integer \( n \). The current orientation of the particle is adjusted by that integer (\( n = 1 \) means one step clockwise, \( n = -1 \) means one step counterclockwise, \( n = 2 \) means two steps clockwise, and so on), cf. Fig. 2(a).
3. A movement along the new orientation of the particle is chosen with probability \( w_+ = 25/30 \), other directions are chosen with probability \( w_t = 1/30 \) each mimicking translational diffusion, cf. Fig. 2(b).
4. If the target lattice site is empty the move is accepted, otherwise the move is rejected. This ensures that each lattice site is either unoccupied or occupied by exactly one particle.

Note that the adjustment of orientation in step 2 is always accepted and a translation does not change the orientation of the particle. Since \( w_+ \) and \( w_t \) are fixed, the “activity” of the system is solely adjusted via the rotational diffusion, which is defined by the width \( \sigma \) of the Gaussian distribution. A low value for \( \sigma \) corresponds to low rotational diffusion and therefore highly persistent motion.

![Fig. 2 Sketch to illustrate serial model I on a hexagonal lattice. (a) First, the orientation (arrow) of the particle is updated drawing a random number from a Gaussian distribution. (b) Then, a move along the particle’s orientation is attempted with rate \( w_+ \), diffusion along another direction is attempted with rate \( w_t \) each. (c) Probability to keep the current orientation as a function of \( \sigma \) (as given by the integral over the Gaussian distribution from \(-0.5\) to \(0.5\)). Dashed and dotted lines correspond to critical values for model I on the hexagonal (\( \sigma_c \approx 0.3048 \)) and square lattice (\( \sigma_c \approx 0.2415 \)).](image)
3.2 Analysis and results

By closely following the analysis described in Sec. 2.2, we determine the critical point $\sigma_{cr,I} \simeq 0.3048$ as the average of the cumulant ratio crossings (Fig. 3) for the four largest system sizes under consideration ($l = 24, 30, 36, 42$). This value is in agreement with the results published in Ref. [7], which has analyzed systems of comparable system sizes.

Fig. 4(a-c) shows results for the order parameter, the susceptibility, and the derivative of the cumulant ratio. Fitting power laws yields the following exponents

$$\beta \simeq 0.157, \quad \gamma/\nu \simeq 1.68, \quad 1/\nu \simeq 1.03$$

and thus $\nu \simeq 0.97$ and $\gamma \simeq 1.63$. While the agreement with the corresponding 2d-Ising values is reasonable for $\nu$ ($\nu_{\text{Ising}} = 1.0$) and $\gamma$ ($\gamma_{\text{Ising}} = 1.75$), the exponent $\beta$ differs by more than 25% from $\beta_{\text{Ising}} = 0.125$. This disagreement is also clearly visible in Fig. 4(a).

To test the influence of the underlying lattice geometry, we have also performed an analogous investigation of the model on a square lattice with $w_x = 17/20$ for movements along the particles current orientation and $w_t = 1/20$ for the three remaining directions. The results are shown in Fig. 4(d-f) with exponents

$$\beta \simeq 0.153, \quad \gamma/\nu \simeq 1.69, \quad 1/\nu \simeq 1.02$$

and thus $\nu \simeq 0.98$ and $\gamma \simeq 1.66$. These critical exponents are very similar to the hexagonal case and within numerical uncertainties, indicating that the influence of the underlying lattice is negligible as one would expect.

![Fig. 3 Cumulant ratios $Q_l$ for model I on the hexagonal lattice. The dotted line indicates the estimated critical value $\sigma_c \simeq 0.3048$ as the mean crossing point for $l = 24, 30, 36, 42$. Note that each tick on the x-axis corresponds to one simulation point.](image-url)
Fig. 4 (a-c) Estimating the critical exponents for model I. Plotted are (a) the order parameter $\rho_{\text{liq}} - \rho_{\text{gas}}$, (b) the susceptibility $\chi$, and (c) the slope of the cumulant ratio at the critical point. (d-f) Corresponding determination for model I but on a square lattice with $\sigma_c \approx 0.2415$. Grey dots in (a) and (d) were excluded from the analysis. The black dashed lines show the slopes with the critical exponents for the 2d Ising system.

4 Model II: Concurrent rotation/translation

4.1 Model description

The second model is based on a square lattice and has been proposed in Ref. [32]. As illustrated in Fig. 5, there are now six possible moves: either rotation of the particle orientation clockwise or counterclockwise by 90° with weight $w_1$ [Fig. 5(a)], or translation along the orientation with weight $w_+$ or any of the three other directions with weight $w_t$ [Fig. 5(b)]. In contrast to Model I, the weight $w_1 = 0.1$ for rotation is now kept constant and we vary $w_+$ with $w_t = 1$. Moreover, in each MC step one of the moves is selected according to its weight. Hence, the particle can either rotate or move in one time step, which we term concurrent.

Fig. 5 Sketch to illustrate model II on a square lattice. (a) The particle orientation is turned clockwise or counterclockwise by 90° with rate $w_1$. (b) A move along the orientation is attempted with rate $w_+$, diffusion into any other direction with rate $w_t$ each. Note that only one of these moves is attempted in each time step. The probability for each move is given by the respective rate divided by the sum of all rates.
Fig. 6 Cumulant crossing for Model II yielding a critical point at \( w_{+,c}\simeq 4.76 \) as determined by the mean crossing point for \( l = 24,30,36,42 \) (dotted line). Note that each tick on the x-axis represents a \( w_+ \) at which simulations for the various system sizes took place.

4.2 Analysis and results

Fig. 6 shows the crossings of the cumulant ratios \( Q_l \) for different box lengths \( l \). The crossings start to converge for the bigger boxes with \( l \geq 24 \). Hence, we only take these system sizes into account and determine the critical point to be at \( w_{+,c}\simeq 4.76 \). Corresponding results for the critical exponents are displayed in Fig. 7, for which we find

\[
\beta \simeq 0.221, \quad \gamma/\nu \simeq 1.65, \quad 1/\nu \simeq 1.02. \quad (8)
\]

While \( \gamma \simeq 1.68 \) and \( \nu \simeq 0.98 \) again exhibit reasonable agreement with 2d-Ising values (1.75 and 1, respectively), \( \beta = 0.221 \) exceeds the corresponding value (0.125) by almost a factor of two. Note that \( \beta \) needs to be measured further from the critical point than in model I because the density profiles lose their stability faster. This indicates that fluctuations are stronger and the slab in the 1:3 simulation box stays less stable in the vicinity of the critical point for model II.

5 Discussion and Conclusions

Our results for the critical exponents are summarized in Table I. We have also added the corresponding values for active Brownian particles as determined
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| model          | β     | γ/ν   | 1/ν   | ν     | γ/ν + 2β/ν |
|----------------|-------|-------|-------|-------|------------|
| 2D Ising       | 0.125 | 1.75  | 1     | 1     | 1.75       |
| ABPs [5]       | 0.45  | 1.47  | 0.67  | 1.5   | 2.2        |
| model I (hex.) | 0.157 | 1.68  | 1.03  | 0.97  | 1.63       |
| model I (sq.)  | 0.153 | 1.69  | 1.02  | 0.98  | 1.66       |
| model II (sq.) | 0.221 | 1.65  | 1.02  | 0.98  | 1.68       |

Table 1: Comparison of critical exponents. The last column is the hyperscaling relation Eq. (4), which is approximately obeyed by all models.

in Ref. [5]. For all lattice models studied here, we find values for ν that are in very good agreement with Ising universality (< 3% smaller) and values for γ/ν that are in good agreement (< 5% smaller). These values are in agreement with plots shown in Ref. [7], which concludes that Ising universality holds. This conclusion seems questionable when taking the exponent β into account, which deviates substantially. Indeed, the determination of β is technically the most challenging. However, note that the hyperscaling relation Eq. (4) places a strong constraint on the exponents. From γ/ν ≃ 1.68 and ν ≃ 0.98 we can obtain an estimate for β ≃ 0.157 that is in excellent agreement with the numerically estimated values for Model I on both lattice geometries, supporting that reduction of γ (and ν) is not a statistical effect but systematic.

The value for β estimated for Model II is even larger. However, in this case the hyperscaling relation is only fulfilled approximately, which might indicate that β is too large. We have observed that obtaining “good” crossings of the cumulant ratio in this model is more challenging, which might be because the speed is changed in contrast to the rotational diffusion in model I. Moreover, the distance to the critical point is larger since the determination of ρ_{liq} − ρ_{gas} requires stable slabs. We notice that the ratio γ/ν has become even smaller, moving away from the Ising value. While this seems to indicate an influence of the different dynamic rules on the critical behavior, we cannot rule out that the scaling closer to the critical point changes (but note the value of γ/ν).

Even further from Ising universality are off-lattice active Brownian particles, where also the exponent ν now changes substantially from ν = 1 to ν ≃ 1.5. Still, the hyperscaling relation is again approximately fulfilled, indicating that the exponents are consistent.

Based on our numerical results, we find the general conclusion from Ref. [7] that MIPS belongs to the 2d Ising universality class to be somewhat premature. Our results even cast some serious doubts on the weaker claim that model I exhibits 2d Ising behaviour. At this point we would like to emphasize that the numerical evidence presented in Ref. [7] is based on figures similar to our Figs. 4(b) and (c) in which the slopes for the 2d Ising values were drawn on top of the simulation values suggesting excellent agreement. However, the authors neither provide values for γ or ν, nor did they mention the discrepancy for the exponent β.

Instead, we see mounting evidence that the critical behaviour for models exhibiting MIPS is at least to some degree model-dependent. Whether or not
there is an underlying Ising universality or any universality at all, and to which extent deviations occur and why still remains an interesting and challenging question for simulations and theory alike.

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