Critical Phenomena in Active Matter

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We investigate the effect of self-propulsion on a mean-field order-disorder transition. Starting from a $\varphi^4$ scalar field theory subject to an exponentially correlated noise, we exploit the Unified Colored Noise Approximation to map the non-equilibrium active dynamics onto an effective equilibrium one. This allows us to follow the evolution of the second-order critical point as a function of the noise parameters: the correlation time $\tau$ and the noise strength $D$. Our results suggest that the universality class of the model remains unchanged. We also estimate the effect of Gaussian fluctuations on the mean-field approximation finding an Ornstein-Zernike like expression for the static structure factor at long wave lengths. Finally, to assess the validity of our predictions, we compare the mean-field theoretical results with numerical simulations of active Lennard-Jones particles in two and three dimensions, finding a good qualitative agreement at small $\tau$ values.

I. INTRODUCTION

Motile cells, living bacteria, synthetic swimmers, flock of birds and school of fish are only a few examples of active systems able to give rise to a plethora of fascinating phenomena that spontaneously arise from their collective behavior [1-3]. In order to reproduce and understand the emergence of cooperative dynamics in active systems, several-minimal models have been put forward, being mostly based on self-propelled agents, hydrodynamics theories but also on rule-base models with alignment interactions [4-7]. In spite of their minimal ingredients, these model systems display a highly collective behavior which results in large-scale pattern formations [8], aggregation [9], swarming [8], off-equilibrium order-disorder transition [7], peculiar rheological properties and disordered arrested states [10,11]. Such a rich phenomenology shares many similarities with collective behavior in condensed matter physics where the emerging of a cooperative dynamics is intimately related to the concept of phase transitions [11]. The analogy between collective behavior in condensed matter and spontaneous aggregation in biological or synthetic systems, suggests that a coarse-grained procedure which neglects the complexity of active agents could reproduce, at least qualitatively, the observed phenomenology [2,7].

Notable attempts in this direction have focused on specific models of isotropic self-propelled particles without aligning interactions [12,15,18]. The fundamental ingredient that defines these non-equilibrium models is that the random force acting on each particle is not of thermal origin, i.e., is not a Brownian noise, but is a self-propulsion force that decorrelates on a time-scale $\tau$. Early theoretical approaches were based on the idea of recasting the non-equilibrium dynamics in an effective equilibrium one with a density dependent diffusion coefficient $D(\phi)$ suggesting a novel phase transition known as “motility induced phase separation”. Following the same idea, some of us have recently shown that the steady state distribution of many active particles driven by Gaussian colored noise can be mapped onto an equilibrium problem where the noise amplitude and its correlation time play the role of control thermodynamic variables [15,19-21]. In that study, the mapping to an effective equilibrium dynamics has been obtained thanks to the “unified colored noise approximation” (UCNA) [22,23]. In addition, the random driving forces have been modeled by an Ornstein-Uhlenbeck process (OUP) which gives rise to a self-propulsion that is Gaussian distributed and exponentially correlated in time. An exponentially correlated propulsion force characterizes also active Brownian [16,21] and “run and tumble” dynamics [25]. The OUP has been shown to model quite well the behavior of passive tracers in active suspensions [26,27]. Recently, many attentions are devoted by several research groups in modeling active particle systems by means of OUP [17,18,28].

Although the Gaussian colored noise model has been analyzed at the level of few particles [15], in the case of a many particles system it presents the same insurmountable difficulties of the equilibrium many-body problem.

From this perspective, it would be desirable to develop a coarse-grained version of the model for studying phase transitions especially to understand the role played by the memory of the noise on phase behavior. To this aim, in this article we propose and investigate a Gaussian colored-noise driven field theory based on the UCNA. In particular, we focus on the effect of colored noise on a second-order phase transition. In this framework, we can compute the shift in the critical temperature due to the finite correlation time of the driving force. The external parameter $\tau$ changes the location of the critical point but not the universality class of the model. We find a reentrant behavior of the critical curve in the activity-noise

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phase diagram showing that, while for small value of \( \tau \), phase transition is enhanced by the correlation time of the noise, at larger \( \tau \) this tendency is inverted. Moreover, we compute the Gaussian fluctuations around the mean-field obtaining an Ornstein-Zernike (OZ) like expression for the static structure factor at low wave lengths. The OZ expression predicts a power-law divergence of the correlation length at the critical point. The analytical mean-field predictions are compared with numerical simulations of a monodisperse active Lennard-Jones fluid in two and three dimensions finding a good agreement at small \( \tau \) values.

II. THE MODEL

Critical phenomena are a special example of phase transitions and play a pivotal role in Statistical Mechanics [14, 29, 30]. Landau Model is the common starting point to address a phase transition. In order to extend the Landau theory to Active Systems, as a first step we use the LG free energy is

\[
H = \beta \int dx \left( \frac{1}{2} \frac{\delta^2 H}{\delta \varphi^2} |_{SP} + \frac{D}{\tau} \eta(t) \right) ,
\]

where the zero-mean noise \( \eta \) is delta-correlated \( \langle \eta(t) \eta(s) \rangle = 2 \delta(t - s) \), and \( D \) plays the role of (effective) temperature of the model. The Hamiltonian \( H \) is the standard \( \varphi^4 \)

\[
H[\varphi] = \frac{a}{2} \varphi^2 + \frac{b}{4} \varphi^4 ,
\]

where \( a \) depends linearly on \( D \) and changes sign at \( D_0 \).

The \( \varphi \) field model described by a LG free energy subjected to an exponentially correlated noise. The stochastic differential equations (5) can be rewritten as follows

\[
\partial_t \varphi(t) = -\frac{1}{\tau} \varphi(t) + \frac{1}{\tau} \frac{\partial H}{\partial \varphi} + \frac{D^{1/2}}{\tau} \eta(t) ,
\]

\[
\Gamma[\varphi] = 1 + \tau \frac{\partial^2 H}{\partial \varphi^2} .
\]

The Unified Colored Noise Approximation is obtained neglecting \( \partial^2 \varphi \) in Eq. (5) [22, 23]. The corresponding Smoluchowski equation for \( \Gamma[\varphi] \) reads [30]

\[
\partial_t P[\varphi, t] = \partial_\varphi \left\{ \Gamma^{-1}[\varphi] \left( \partial_\varphi \Gamma^{-1}[\varphi] P[\varphi, t] - \partial_\varphi P[\varphi, t] \right) \right\}
\]

and the steady-state distribution is

\[
P_{stag}[\varphi] = N e^{-H_{eff}[\varphi]/D}
\]

\[
H_{eff}[\varphi] \equiv H + \frac{\tau}{2} \left( \frac{\partial H}{\partial \varphi} \right)^2 - D \log \Gamma[\varphi] .
\]

From Eq. (7) follows that \( P_{stag} \) has the structure of an equilibrium distribution in terms of the effective Hamiltonian \( H_{eff} \).

B. Critical line

The critical line \( D_c(\tau) \) is the curve along which the system undergoes a second order phase transition. In a standard \( \varphi^4 \) theory, the location of the critical point is determined by the coefficient of \( \varphi^2 \), i.e., the symmetry is spontaneous broken where \( a \) changes sign. In a mean-field model described by a LG free energy \( F_{LG}(\varphi) = \)

\[
\frac{1}{2} \frac{\delta^2 H}{\delta \varphi^2} |_{SP} + \frac{D}{\tau} \eta(t) .
\]
\( a\varphi^2/2 + B(\varphi) \), the location of the critical point can be computed considering the equation \[ \frac{\partial^2 F_{\text{LG}}}{\partial \varphi^2} \bigg|_{\varphi=0} = a + \frac{\partial^2}{\partial \varphi^2} B \bigg|_{\varphi=0} = 0. \] (8)

In our case, the LG free energy is \( H_{\text{eff}} \), the expression for \( D_c(\tau) \) is given by
\[
\frac{\partial^2 H_{\text{eff}}}{\partial \varphi^2} \bigg|_{\varphi=0} = 0. \tag{9}
\]

Now we write \( a = a_0(D - D_0) \), with \( a_0 \) a positive constant. The critical curve satisfies the equation
\[
a(1 + a\tau) - \frac{6\tau bD}{1 + \tau a} = 0, \tag{10}
\]
and the only real and physical solution is
\[
D_c(\tau) = \frac{1}{\epsilon} \left( \frac{\lambda}{\epsilon} + \gamma - \alpha \right) \tag{11}
\]

The critical curve \( D_c(\tau) \) increases for small \( \tau \), reaches its maximum value \( D^* \) at \( \tau^* \), and decreases to \( D_0 \) for \( \tau \to \infty \). As a consequence the phase diagram in the \((\tau, D)\) plane is reentrant. This is shown in the left inset of Fig. (1) where LG free energy is plotted increasing \( \tau \) for \( D_0 < D < D^* \). The LG free energy develops a double well for \( \tau < \tau < \tau^* \) (magenta and yellow curves), with \( \tau \pm \) the solutions of \( D = D_c(\tau) \). For \( \tau < \tau_- \) or \( \tau > \tau_+ \) the system is in the symmetric phase (blue and red curves, respectively).

It is worth noting that a reentrant behavior of the Boyle’s line has been observed in the virial series of many mutually interacting particles in the presence of correlated noise \[ 19 \]. The small \( \tau \) behavior indicates that memory effects in the dynamics raise the critical effective temperature, suggesting that the activity promotes criticality.

In order to compare the analytical expression for \( D_c(\tau) \) with the true order parameter dynamics, we have solved numerically the non-equilibrium dynamics. Eqs. (3) have been numerically integrated for \( N_t = 10^6 \) steps with \( \Delta t = 10^{-3} \). The parameters of the model are \( a_0 = 4, D_0 = 1,2 \) and \( b = 1 \). From the trajectories \( \varphi(t) \) we have computed \( P[\varphi] = \delta(\varphi(t) - \varphi)|_{t=t^0} \), where the angular bracket indicates both the averages, over the trajectories and over the initial condition. The critical point has been obtained by fitting the histogram of \( P[\varphi] \) to \( f(x) = A \exp (-\tilde{a}\varphi^2 - b\varphi^4) \). We have considered average over \( 5 \cdot 10^2 \) initial conditions. The resulting \( P_{st}[\varphi] \) for \( \tau = 0.1 \) is shown in Fig. (1), right inset. As one can see in the main panel of the same figure, the theoretical curve \( \Delta D_c/D_0 \), with \( \Delta D_c = D_c(\tau) - D_c(0) \), reproduces very well the numerical data in a wide range of \( \tau \).

For small \( \tau \) we can approximate \( \log \Gamma(\varphi) \sim D\tau \tilde{a}^2 \varphi H \) obtaining an effective \( \varphi^6 \) theory. It is well known in literature that \( \varphi^6 \) theory admits a tricritical point where the second order phase transition changes in a first order phase transition \[ 20 \]. However, in our model the tricritical point is located in an unphysical region. The effective hamiltonian reads
\[
H_{\text{eff}}^{\text{small}}[\varphi] = \frac{\tilde{a}}{2} \varphi^2 + \frac{\tilde{b}}{4} \varphi^4 + \frac{\tilde{c}}{6} \varphi^6 \tag{12}
\]
\[
\tilde{a} = a(1 + a\tau) - 6Db\tau \\
\tilde{b} = b + 4ab\tau \\
\tilde{c} = 3b^2\tau.
\]

In this case, the critical line \( D_c^{\text{small}} \) is given by \( \tilde{a} = 0 \) and satisfies
\[
a(1 + a\tau) - 6Db\tau = 0. \tag{13}
\]

Along \( D_c^{\text{small}}, \) \( \varphi_0 \) behaves like \( \varphi_0 \sim (D - D_c)^{\beta} \) with \( \beta = 1/2 \), i.e., the classical mean-field value for the \( \beta \) exponent \[ 14 \].

### III. Numerical Simulations

Now we compare the mean-field picture with its finite-dimensional counterpart. With this aim, we have performed numerical simulations of \( N \) spherical particles interacting through \( \phi(r) = 4e_0[(r/\sigma)^{-12} - (r/\sigma)^{-6}] \) in two \((d = 2)\) and three \((d = 3)\) dimensional boxes of side \( L \)
with periodic boundary conditions. The density of the system is $\rho_m = N/L^d$. The energy is measured in unit $e_0$ and the density in unit $\sigma^{-d}$. The microscopical model undergoes a gas-liquid (GL) phase separation that is described by a conserved scalar order parameter $\rho\Delta - \rho_c$. The nature of the order parameter implies Model B dynamics along the phase separation \[37\]. However, the location of the critical point, i.e., the endpoint of the phase separation, is a static property of the system. As mentioned earlier, Model A and Model B show the same static properties: we will adopt the mean field scenario emerging from Model A to capture qualitatively the behaviour of the critical line in finite dimension.

The self-propulsion is modeled by means of a random driving force exponentially correlated in time. The equation of motion of the particle $i$, with $i = 1, ..., N$, is

$$\dot{r}_i = f_i - \mu \sum_{j \neq i} \phi'(r_{ij})r_{ij}/r_{ij},$$

where $\mu = 1$ is the mobility and $r_{ij} \equiv |r_i - r_j|$. The random force satisfies $\langle f_i^\alpha \rangle = 0$ and $\langle f_i^\alpha(t)f_j^\beta(s) \rangle = 2D\delta_{ij}\delta_{\alpha\beta}e^{-|t-s|/\tau}/\tau$, where the Greek symbols indicate the cartesian components. In this picture the external parameters $D$ and $\tau$ can be independently varied as well as in the Landau model previously considered. For $\tau = 0$ one recovers the Lennard-Jones fluid in the Brownian regime. We study the system close to the LJ critical density $\rho_c \sim 0.4$ ($N = 2500$ in 2d and $N = 8000$ in 3d). Moreover, performing simulations at different values of $\rho_m$ \[47\], we have checked that the value $\rho_c$ does not vary with $\tau$. The critical values $D_c(\tau)$ have been evaluated looking at the intersection points of the Binder cumulant $U_\ell = 1 - \langle \delta \rho^4 \rangle/3\langle \delta \rho^2 \rangle^2$ \[58\] at different $\ell$, with $\delta \rho = \rho - \langle \rho \rangle$, where the average is defined.

The resulting phase diagram is shown in Fig. 2-a with snapshots of the 2d simulations (bottom left inset in the same panel). The full lines are obtained by fitting the data with Eq. \[11\] leaving both $a_0$ and $b$ as free parameters. As one can see for small $\tau$ the theory reproduces quite well the numerical data. However with the model simulated we cannot probe the regime at larger $\tau$ values since crystallization occurs at $\tau > 0.3$ (the gray area in Fig. 2-a). In order to prevent crystallization, one can introduce frustration in the microscopical model considering, for instance, a binary mixture \[41\]. Hence, the existence of the reentrance in the activity-noise phase diagram remains an open question that we aim at answering in a future work. It is worth noting that our starting point is a $\varphi^4$ theory. In such a case we can not describe a phase diagram that shows both gas/liquid and gas/crystal phase transition. Nevertheless, it is possible to generalize our mean-field model considering a different field theory in order to take into account other kind of phase transitions \[14\].

In the crystal regime, the nucleated liquid droplets rearrange into small crystal clusters. The presence of the crystal clusters is evident in the snapshot shown in Fig. 2-a, right.
IV. GAUSSIAN FLUCTUATIONS

Let us discuss the effect of the correlated noise on the Gaussian fluctuations around the mean field \[ \phi(x) \]. The Hamiltonian in \( d \)-dimensions is

\[
H_G[\phi(x,t)] = \frac{1}{2} \int d^d x \left[ (\nabla \phi(x,t))^2 + a \phi(x,t)^2 \right].
\]

We will consider both Model A/B dynamics with exponentially correlated noise. We can rewrite Eqs. (3) including the spatial dependency in a compact way as follows

\[
\partial_t \phi(x,t) = - (i \nabla)^2 \phi + (-\nabla)^2 \theta(x,t)
\]
\[
\partial_t \theta(x,t) = - \frac{\theta(x,t)}{\tau} + \frac{D^{1/2}}{\tau} \eta(x,t).
\]

The exponent \( \psi \) is 0 (Model A) or 1 (Model B). The noise is white \( \langle \eta(x,t) \rangle = 0 \), and delta-correlated, \( \langle \eta(x,t)\eta(y,s) \rangle = 2\delta(x-y)\delta(t-s) \).

Now we introduce the spatial Fourier transform of a field \( \phi(x) \) as

\[
\phi_k = \frac{1}{(2\pi)^d} \int d^d x \ e^{-i\mathbf{k} \cdot \mathbf{x}} \phi(x).
\]

We can perform the spatial Fourier transform of \( \varphi(x,t) \) and \( \theta(x,t) \) obtaining the time evolution of the \( k \)-th Fourier component of \( \varphi \) in UCNA, i.e., considering \( \partial_t^2 \varphi_k = 0 \), that is governed by the following equation

\[
\partial_t \varphi_k = - \Gamma_k \varphi_k + D_k \eta_k
\]
\[
\Gamma_k \equiv \frac{k^2 + a}{1 + \tau(k^2 + a)}
\]
\[
D_k \equiv \frac{(ik)^2}{1 + \tau(k^2 + a)},
\]

where \( k \equiv |\mathbf{k}| \). Again, the noise \( \eta_k \) is white \( \langle \eta_k \rangle = 0 \), and delta-correlated \( \langle \eta_k(t)\eta_k(s) \rangle = 2\delta_{ks}\delta(t-s) \). We can estimate the critical slowing down exponent by averaging Eq. (15) over the noise. It follows that \( \langle \varphi_k(t) \rangle \propto \exp(-t/\tau_k) \), with \( \tau_k = \Gamma_k^{-1} \). Introducing \( \xi^2 = \psi^{-1} \), we can write the relaxation time of the mode \( k \) as \( \tau_k = \xi^2 f(k\xi,\tau\xi^{-2}) \). The value of the dynamical critical exponent \( z = 2(1 + \psi) \) turns out to be the same as in the case of equilibrium dynamics [37].

From Eq. (18) we can compute the stationary fluctuations \( \langle |\varphi_k|^2 \rangle = \xi^2 g(k\xi,\tau) \) with

\[
g(k\xi,\tau) = \frac{D}{(k^2\xi^2 + 1) \left[ 1 + \tau(k\xi)^2 \xi^{-2(1+\psi)}(k^2\xi^2 + 1) \right]}.
\]

When \( k \to 0 \), \( \langle |\varphi_k|^2 \rangle \) diverges as \( \xi = a^{-\nu} \), with the classical value \( \nu = 1/2 \). From Eq. (19) follows that, above the transition, the static structure factor \( S(k) \) for small \( k \) is well described by the usual OZ expression \( S(k) \sim (k^2\xi^2 + 1)^{-1} \). In Fig. 2-b we show the rescaled \( S(k) \) in 2d for \( \tau = 10^{-3} \), \( 10^{-2} \), \( 10^{-1} \) and \( D > D_c(\tau) \). According to OZ, the rescaled \( S(k) \) overlaps on the same master curve. Moreover, as it is shown in the inset of Fig. 2-b, \( \xi \) follows a power law \( (D - D_c)^{-\nu} \) with \( \nu_N = 0.73 \) for \( N = 2500 \). The value of the exponent does not depend on \( \tau \), i.e., as predicted by the mean-field picture. Since we are in finite dimension, it is different from the classical value 1/2 [14]. It is worth noting that \( \nu \) has been evaluated for \( N = 2500 \). In order to estimate the critical exponent \( \nu \) in the thermodynamic limit, we should take into account the finite-size correction to \( D_c \), i.e., \( D_c(L) = D_c + aL^{-b} \) [42]. This aspect will be investigated in a future work.

V. CONCLUSIONS

In this article, we have posed a fundamental question about the influence of self-propulsion on the order-disorder transitions. By means of UCNA, we have recast the non-equilibrium dynamics of the model A/B in the presence of correlated noise onto an effective equilibrium theory. In this way we have extended the static picture of the Landau theory of critical phenomena to order-disorder transitions in the presence of exponentially correlated noise. The location of the critical point is a non-universal quantity because depends on the correlation time of the noise \( \tau \). Through the effective equilibrium theory, we have computed analytically the critical line \( D_c(\tau) \), i.e., the shift in critical temperature due to the activity. Considering the numerical solution of the non-equilibrium dynamics of the order parameter in zero dimension, we have observed a good agreement between \( D_c(\tau) \) and the critical points obtained numerically. Moreover, the effective theory suggests that the out-of-equilibrium dynamics does not change the universality class. This finding is in agreement with previous studies on Ising-like nonequilibrium models [43–45] where it has been observed that the absence of detailed balance on the microscopic scale does not change the universality class of the Ising model.

By performing numerical simulations in 2d and 3d of active LJ fluid driven by OUP, we have obtained that the mean-field scenario can be used to describe the behavior of the critical line in the small \( \tau \) regime. However, the reentrant behaviour predicted by the mean-field scenario does not occur in the considered microscopical model. In particular, the numerical simulations show a gas/crystal phase transition at larger \( \tau \) that can not be captured by the theory.

With the numerical data presented in this paper we can conclude that, for small \( \tau \) and independently on density, the out-of-equilibrium dynamics gives rise to a second order phase transition that shares the same properties with its equilibrium counterpart, i.e., \( \tau = 0 \).

Finally, we have evaluated the Gaussian fluctuations approaching the critical point from the disordered phase.
According to the theory, we have demonstrated that the static structure factor at low $k$ is well described by OZ expression. Here, we have considered a $\varphi^4$ scalar field theory, however our approach can be generalized to other field theories in order to study the properties of different universality classes under the effect of self propulsion.

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