Bose–Einstein Condensation in Scalar Active Matter with Diffusivity Edge

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(Dated: January 21, 2019)

Due to their remarkable properties, systems that exhibit self-organization of their components resulting from intrinsic microscopic activity have been extensively studied in the last two decades. In a generic class of active matter, the interactions between the active components are represented via an effective density-dependent diffusivity in a mean-field single-particle description. Here, a new class of scalar active matter is proposed by incorporating a diffusivity edge into the dynamics: when the local density of the system surpasses a critical threshold, the diffusivity vanishes. The effect of the diffusivity edge is studied under the influence of an external potential, which introduces the ability to control the behaviour of the system by changing an effective temperature, which is defined in terms of the single-particle diffusivity and mobility. At a critical effective temperature, a system that is trapped by a harmonic potential is found to undergo a condensation transition, which manifests formal similarities to Bose-Einstein condensation.

Dense active matter provides an enthralling paradigm as its emergent properties are determined by competition between opposing tendencies that originate from both equilibrium and non-equilibrium processes\cite{1,2}. In particular, the proximity of the active agents -- through various non-equilibrium processes such as hydrodynamic interactions\cite{3}, chemical signalling\cite{4–7}, etc. -- might lead to a collective enhancement of activity\cite{8,9} and triggering of instabilities\cite{10–12}, whereas short-ranged physical interactions such as those arising from stickiness and excluded volume effects (and possibly some non-equilibrium processes as well) inhibit the collective activity\cite{13–17}, ultimately leading to formation of globally ordered dense structures\cite{18–20} or dynamic arrest\cite{21,22}. In the absence of long-range orientational ordering, which can be caused by alignment interactions between polar agents in sufficiently dense systems\cite{23,24}, the activity of individual particles can be described by effective enhanced diffusion coefficients beyond the time scale of rotational diffusion\cite{25}. In this regime, the system can be generically described using dynamical equations for the density field at the mean field level. Here, we study such a description of scalar active matter with a generic density dependence in the diffusivity that incorporates a finite threshold: above a critical density the diffusivity vanishes. We demonstrate that the existence of this diffusivity edge leads to a dynamical phase transition that can be categorized as an analogue of Bose-Einstein condensation (BEC) despite the system being classical in nature. The present work builds on the recent surge in the development of generalized thermodynamic descriptions for non-equilibrium active matter\cite{26,27}.

We formulate a mean-field description of the dynamics of the colloidal system described by an effective single-particle density field $\rho(r,t)$ that satisfies a conservation law $\partial_t \rho + \nabla \cdot J = 0$ where the flux is defined as $J = -D(\rho) \nabla \rho + \rho v$ in terms of an effective density-dependent diffusivity $D(\rho)$ and the drift velocity $v$. We assume that the drift originates from an external potential $U(r)$ and involves a density-dependent mobility $\mu(\rho)$, namely $v = \mu(\rho)(-\nabla U)$. Using the single-particle diffusivity $D_s = D(\rho \to 0)$ and the single-particle mobility $\mu_s = \mu(\rho \to 0)$, we define an effective temperature $T_{\text{eff}}$ using the fluctuation–dissipation theorem (FDT), namely, $k_B T_{\text{eff}} \equiv D_s/\mu_s$, and define $\beta \equiv 1/(k_B T_{\text{eff}})$ for simplicity of notation.

We incorporate a generic non-equilibrium character for the system by assuming a breakdown of FDT at finite densities, namely, $D(\rho)/\mu(\rho) \neq D_s/\mu_s$. We assume that this occurs due to density-dependent non-equilibrium effects, which could materialize as a result of collective inhibition as well as collective activation due to motility. Therefore, the diffusivity $D(\rho)$ and the mobility $\mu(\rho)$ will start from their single-particle values for dilute systems and can in general go up or down as the density is increased. To complete the formulation, we define a diffusivity edge at concentration $\rho_c$ as follows: $D(\rho)/\mu(\rho) = 0$ for $\rho \geq \rho_c$. We note that in this work we ignore non-local effects that arise from hydrodynamic interactions when FDT is broken\cite{28} as well as long-range non-equilibrium interactions\cite{12}.

We then seek possible stationary states of the system as obtained by setting the net flux

$$ J / D_s = - \left( D(\rho) / D_s \right) \nabla \rho - \left( \mu(\rho) / \mu_s \right) \rho \nabla \beta U, \quad (1) $$

to zero. This yields $d\beta U/d\rho = -\left( \mu_s D(\rho) / D_s \mu(\rho) \right)$, and consequently

$$ \beta U(\rho) = - \int_{\rho_0}^{\rho} \frac{d\rho'}{\beta} \frac{D(\rho')}{D_s} \frac{\mu_s}{\mu(\rho')}, \quad (2) $$

where $\rho_0$ is defined as the density at which energy is at its lowest value of zero, namely, the ground state of the energy spectrum. The stationary distribution $\rho(U)$ can then be obtained by inverting equation (2). Henceforth, we are going to represent $\mu_s D(\rho) / (D_s \mu(\rho))$ as $D(\rho)/D_s$ to keep the presentation simple.

The normalization condition for a total of $N$ particles in $d$-dimensions reads $N = \int d^d r \rho(U(r)) = \int S_d \rho(U(r)) (d-1) dr$ (assuming that the potential is spherically symmetric, where $S_d = 2\pi^{d/2}/\Gamma(d/2)$ is the surface area of the unit sphere embedded in $d$ dimensions. If $U(r)$
can be inverted (to a single-valued function), the normalization condition can be written as

$$N = \int_0^\infty dU g(U) \rho(U)$$

where $g(U) = S_d (r(U))^{d-1} dr$ is the density of states. For example, a harmonic trap in the form of $U = \frac{1}{2} k \rho^2$ yields $g(U) = \left( \frac{2}{\pi} \right)^{d/2} U^{d/2 - 1}$. Since $U$ is a monotonically decaying function of $\rho$, we can rewrite the normalization condition as follows

$$N = \frac{k_B T_{\text{eff}}}{\rho D_s} \int_0^{\rho_0} d\rho D(\rho) g(U(\rho)). \quad (\rho_0 < \rho_c) \quad (3)$$

This condition gives $\rho_0 (T_{\text{eff}})$, which we expect to be a decreasing function of temperature. However, it only applies when $\rho_0 < \rho_c$ as noted. This is because when $\rho_0 \geq \rho_c$, the integrand in equation (3) vanishes identically and no longer contributes, which makes it impossible for the normalization to be satisfied. Therefore, the system develops a condensate with $N_c$ particles at the ground state, and the normalization reads

$$N = N_c + \frac{k_B T_{\text{eff}}}{\rho D_s} \int_0^{\rho_c} d\rho D(\rho) g(U(\rho)). \quad (\rho_0 \geq \rho_c) \quad (4)$$

We can calculate the size of the condensate as a function of temperature below the transition temperature $T_c$, which can be obtained by setting $\rho_0 (T_c) = \rho_c$. When $T_{\text{eff}} \leq T_c$ (corresponding to $\rho_0 \geq \rho_c$), equation (2) tells us that $\beta U(\rho) = u(\rho/\rho_c)$. Noting that $D(\rho) = D_s \gamma(\rho/\rho_c)$ by definition, we can recast equation (4) into the form

$$N = N_c + \frac{k_B T_{\text{eff}}}{\rho D_s} \left( \frac{2}{\pi} \right)^{d/2} \rho_c \int_1^{\rho_c} d\rho \gamma s u(s) \left( \frac{2}{\pi} \right)^{d/2} \rho_c \int_1^{\rho_c} d\rho \gamma s u(s) \left( \frac{2}{\pi} \right)^{d/2}$$

Noting that $T_c$ corresponds to $N_c = 0$, this calculations yields the fraction of particles in the condensate as

$$\frac{N_c}{N} = 1 - \left( \frac{T_{\text{eff}}}{T_c} \right)^{d/2}. \quad (5)$$

This result is plotted in Fig. 1b. Below, we will examine the behaviour of systems that undergo such a condensation transition more concretely, using a number of specific cases.

Consider a situation where inhibition causes the effective diffusivity in this mean-field description to monotonically decrease as a function of density, until it vanishes at $\rho = \rho_c$. Figure 1a shows the density-dependent diffusivity, and the resulting stationary distribution $\rho(U)$ is presented in Fig. 1c. For $\rho_0 < \rho_c$, the distribution approaches a Boltzmann weight $\rho_0 e^{-\beta U}$ while increasing $\rho_0$ with respect to $\rho_c$ leads to progressively faster-than-exponential decay, until the slope of the distribution diverges at $U = 0$ for $\rho_1 = \rho_c$, which is the onset of condensation. For $\rho_0 > \rho_c$, the slope at $U = 0$ continues to diverge, while the asymptotic value $\rho(0^+) = \rho_c$ will be systematically smaller than $\rho_0$. This signals the presence of a condensate at $U = 0$, which populates $N_c$ particles as determined by equations (4) and (5).

To better illustrate the properties of the condensation transition let us consider a step function profile for diffusivity, namely, $D(\rho < \rho_c) = D_a$ and $D(\rho \geq \rho_c) = 0$. Then, for the stationary distribution $\rho$ we find $\rho_0 e^{-\beta U}$ for $\rho_0 < \rho_c$ and $\rho_0 e^{-\beta U}$ for $\rho_0 > \rho_c$. Using this explicit form, we can use the normalization condition equation (3) to obtain the value of $\rho_0$, which for the harmonic potential yields

$$\rho_0 = N (2 \pi k_B T_{\text{eff}}/k)^{-d/2}. \quad (6)$$

Using this, we can find the transition temperature as $T_c = \frac{k_B}{2 \pi k_B} (N/\rho_c)^{2/d}$ by setting

![Figure 1](image-url)
$\rho_0(T_c) = \rho_c$. We can also calculate the average energy of the system as $\langle U \rangle = \int_0^\infty dU g(U) U \rho(U)$. This yields

$$\langle U \rangle = \begin{cases} \frac{d}{2}Nk_BT_{\text{eff}}, & \text{for } \rho_0 < \rho_c, \\ \frac{d}{2} \left( \frac{2\pi}{T_e} \right)^{d/2} \rho_c (k_BT_{\text{eff}})^{d/2+1}, & \text{for } \rho_0 \geq \rho_c, \end{cases}$$

which can be rewritten as

$$\langle U \rangle = \frac{d}{2}Nk_BT_{\text{eff}} \begin{cases} \left( \frac{T_{\text{eff}}}{T_e} \right)^{d/2}, & \text{for } T_{\text{eff}} \leq T_c, \\ 1, & \text{for } T_{\text{eff}} > T_c. \end{cases}$$

This result is plotted in Fig. 1d. Consequently, we obtain the following expression for the heat capacity of the system

$$C = \frac{d}{dT_{\text{eff}}} \langle U \rangle = \frac{d}{2}Nk_B \begin{cases} \frac{d}{2} + 1 \left( \frac{T_{\text{eff}}}{T_e} \right)^{d/2}, & \text{for } T_{\text{eff}} \leq T_c, \\ 1, & \text{for } T_{\text{eff}} > T_c, \end{cases}$$

which is plotted in Fig. 1e. Equations (6) and (8) highlight a strong analogy to Bose–Einstein condensation[29, 30].

We next consider a $D(\rho)$ profile that contains collective activation at intermediate densities before the inhibition at higher level of crowding gives rise to a diffusivity edge, as shown in Fig. 2a. In this case, the stationary distribution that is shown in Fig. 2b shows a tendency for the particles to occupy higher energy states more than the equilibrium case, while the formation of the Bose condensate happens by following the same stages as in the inhibited case, namely, divergence of the slope of $\rho(U)$ at $U = 0$ when $\rho_0 = \rho_c$ and the subsequent depletion that is accompanied by the formation of the condensate at the ground state.

To further examine the effect of activity, we consider a piecewise diffusivity profile

$$D(\rho) = \begin{cases} D_a, & \text{for } 0 \leq \rho < \rho_a, \\ D_a, & \text{for } \rho_a \leq \rho < \rho_c, \\ 0, & \text{for } \rho_c \leq \rho, \end{cases}$$

where $D_a$ is the diffusivity in the activated region. Let us define $\alpha \equiv D_a/D_s$ as the measure of activation. The behaviour of the system will depend on how the ground-state density $\rho_0$ compares with the density scales $\rho_a$ and $\rho_c$. The different categories are discussed below.
The stationary solution in this regime is found as the Boltzmann weight \( \rho_0 e^{-\beta U} \) with \( \rho_0 = N(2\pi k_B T_{\text{eff}}/k)^{-d/2} \) and the average energy given as \( \langle U \rangle = \frac{d}{2} N k_B T_{\text{eff}} \), which yields \( C = \frac{d}{2} N k_B \). Setting \( \rho_0 = \rho_a \), we find the transition temperature \( T_a = \frac{\beta}{k_B N} (N/\rho_a)^{2/d} \) below which the system will start to be influenced by the activation. The dilute regime corresponds to \( T_{\text{eff}} > T_a \).

**Intermediate density regime** \( \rho_a \leq \rho < \rho_c \). In this range of densities, which corresponds to \( T_{\text{eff}} \leq T_a \), the stationary solution is found as follows
\[
\rho(U) = \begin{cases} 
\rho_a (\rho_a/\rho)^\alpha e^{-\beta U}, & \text{for } \rho < \rho_a, \\
\rho_0 e^{-\beta U/\alpha}, & \text{for } \rho_a \leq \rho < \rho_0,
\end{cases} \tag{10}
\]
which resembles a distribution with two different temperatures for different ranges of energy. In this regime, we obtain the particle number normalization condition as
\[
N = \frac{\rho_a (2\pi/k)^{d/2}}{\Gamma(d/2)} (k_B T_{\text{eff}})^{d/2} \Gamma \left( \frac{d}{2} \right) H_{\frac{d}{2}} \left( \alpha, \ln \frac{\rho_0}{\rho_a} \right), \tag{11}
\]
and the average internal energy content as
\[
\langle U \rangle = \frac{\rho_a (2\pi/k)^{d/2}}{\Gamma(d/2)} (k_B T_{\text{eff}})^{d/2} \Gamma \left( \frac{d}{2} + 1 \right) H_{\frac{d}{2}+1} \left( \alpha, \ln \frac{\rho_0}{\rho_a} \right), \tag{12}
\]
in terms of the following function
\[
H_\alpha(x) \equiv e^x \left( \frac{x}{\Gamma(x)} - \Gamma(x) \right) + e^{\alpha x} \Gamma(x, \alpha x), \tag{13}
\]
where \( \Gamma(x, \alpha x) = \int_0^\infty dx x^{x-1} e^{-x} \) is the upper incomplete gamma function. From the expression for average energy, we can calculate the heat capacity as follows
\[
C = \frac{N k_B}{d/2} + \frac{d}{2} \frac{H_{\frac{d}{2}+1} \left( \alpha, \ln \frac{\rho_0}{\rho_a} \right)}{H_{\frac{d}{2}} \left( \alpha, \ln \frac{\rho_0}{\rho_a} \right)} \tag{14}
\]
\[
- \frac{d}{2} \frac{H_{\frac{d}{2}} \left( \alpha, \ln \frac{\rho_0}{\rho_a} \right)}{H_{\frac{d}{2}} \left( \alpha, \ln \frac{\rho_0}{\rho_a} \right)} \left( \ln \frac{\rho_0}{\rho_a} \right)^\alpha \Gamma \left( \frac{d}{2} + 1, \alpha \ln \frac{\rho_0}{\rho_a} \right).
\]
The average internal energy (shown in Fig. 2c) starts with a negative curvature for activated particles (\( \alpha > 1 \)) and a positive curvature for inhibited particles (\( \alpha < 1 \)). The slope of this curve corresponds to the heat capacity, which is shown in Fig. 2d. It starts from \( \alpha d/2 \) (in units of \( N k_B \)) at small effective temperatures and goes through a ripple before asymptotically approaching \( d/2 \) at sufficiently large effective temperatures. These results are valid at all effective temperatures (or densities) when \( \rho_c \to \infty \).

**High density regime** \( \rho_c \leq \rho \). For finite \( \rho_c \), there exists a regime at which the condensation happens when the density surpasses \( \rho_c \). The stationary distribution in this case, which corresponds to \( T_{\text{eff}} \leq T_c < T_a \), is given as
\[
\rho(U) = \begin{cases} 
\rho_a (\rho_c/\rho_a)^\alpha e^{-\beta U}, & \text{for } \rho < \rho_a, \\
\rho_c e^{-\beta U/\alpha}, & \text{for } \rho_a \leq \rho < \rho_c, \\
\text{condensate}, & \text{for } \rho_c \leq \rho < \rho_0,
\end{cases} \tag{15}
\]
using which we can calculate the average internal energy as
\[
\langle U \rangle = \frac{\rho_a (2\pi/k)^{d/2}}{\Gamma(d/2)} (k_B T_{\text{eff}})^{d/2} \Gamma \left( \frac{d}{2} + 1 \right) \left( \frac{\rho}{\rho_a} \right)^\alpha \frac{H_{\frac{d}{2}} \left( \alpha, \ln \frac{\rho_0}{\rho_a} \right)}{H_{\frac{d}{2}} \left( \alpha, \ln \frac{\rho_0}{\rho_a} \right)} \left( T_{\text{eff}} \right)^{d/2} k_B T_{\text{eff}}, \tag{16}
\]
and the heat capacity of the system as
\[
C = \frac{N k_B}{d/2} + \frac{d}{2} \frac{H_{\frac{d}{2}+1} \left( \alpha, \ln \frac{\rho_0}{\rho_a} \right)}{H_{\frac{d}{2}} \left( \alpha, \ln \frac{\rho_0}{\rho_a} \right)} \left( T_{\text{eff}} \right)^{d/2} k_B T_{\text{eff}}. \tag{17}
\]

The corresponding plots of energy and heat capacity in this case are given in Fig. 2e and Fig. 2f, respectively, where the system develops the condensate at \( T_{\text{eff}} \leq T_c \), with the resulting characteristic discontinuity in the heat capacity.

We have thus shown that the existence of a diffusivity edge leads to the formation of a condensate, through a transition that is formally equivalent to Bose-Einstein condensation. Trapping scalar active matter allows us to manipulate it using the effective temperature that can be extracted from the ratio between the asymptotic values of the diffusivity and the mobility at the dilute limit, to observe the variety of signatures that exist in the generalized thermodynamic quantities as described above, and in particular, the heat capacity.

Our work has similarities with the formulation that is used to describe motility-induced phase separation (MIPS), with the key difference that the instability in MIPS is triggered by the effective diffusivity changing sign thereby promoting the formation of a dense cluster beyond a threshold density[13]. Enforcing the diffusivity edge preempts that instability and gives rise to a new universality class that is formally equivalent to a BEC. We also note that in quantum mechanics we are limited to very specific forms of BEC, as the kinetic energy of bosonic particles can adopt only a limited number of forms; e.g. \( p^2/2m \) for non-relativistic massive bosons in dilute gases. Our formulation allows us to explore countless new classes of BEC by designing appropriate forms of external trapping potential, say by using holographic optical traps[2]. Such generalizations will have a remarkable prospect, as they might unravel new non-equilibrium physics – of the type that generalized quantum correlated systems might some day be able to reproduce – using synthetic active matter.

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