

Impact of emergent order on energy efficiency in active matter: Insights from a minimal lattice model

Michael W. Jack ^{*}

Department of Physics, *University of Otago*, P.O. Box 56, Dunedin 9054, New Zealand



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We investigate the nonequilibrium steady state of a one-dimensional (i.e., mechanical degree of freedom) run-and-tumble model of left-right oriented Brownian particles with an explicit coupling to a chemical degree of freedom and a macroscopic opposing force. This model enables us to explore the fundamental relationships between the energy process driving individual entities, the emergence of collective behavior, and macroscopic forces in active matter. Sufficiently large alignment interactions can break the right-left symmetry, leading to a macroscopic collective alignment of the particles, or flocking transition. Using a decoupling mean-field approximation, we find that collective alignment requires both sufficiently large alignment interactions and lattice hopping. Further, this collective alignment does not require chemical-to-mechanical coupling and can occur solely through passive mechanical hopping. If chemical-to-mechanical coupling is present, it can lead to a collective drift in the direction of particle alignment even against an opposing mechanical force. Interestingly, in the absence of an opposing force, the particles spontaneously align in a random direction, but in the presence of a force, they tend to align “uphill,” enabling macroscopic work output. The many-body system is formulated in terms of creation and annihilation operators for identical classical particles, which enables us to calculate a range of observables by exploiting techniques from many-body quantum systems.

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I. INTRODUCTION

Active matter is comprised of an assembly of self-driven entities (ranging from birds to synthetic colloidal particles) that operate far from thermal equilibrium by extracting energy from their environment [1–4]. In addition to providing an intriguing nonequilibrium many-body system [2,5], active matter provides a conceptual basis for understanding how the complex structures and behavior of living matter arise from inanimate microscopic particles [6–8].

The focus of much active matter research has been on the large-scale dynamical states and patterns that arise from self-driven entities [1–3,5,7,8]. Researchers have demonstrated that active matter can display a rich phenomenology of collective behaviors, including motility-induced phase separation [9–14], giant number fluctuations [2], and flocking [6]. This collective behavior has been demonstrated experimentally in a wide range of systems, including bacteria [15–18], motile filaments [19,20], cells [21,22], and Janus particles [23–25]. The observed behavior has been quantified using macroscopic field theories through either top-down [3,12] or bottom-up [26–28] approaches. The latter have the advantage that they

connect effective parameters of the field theory to underlying models.

In addition to creating complex structures and exhibiting dynamical collective behavior, living systems can harness energy at the molecular scale to generate macroscopic forces and manipulate their environment. Active matter researchers have also attempted to provide a conceptual basis for understanding this aspect of living matter [8]. One area that has received significant attention is the quantification of the nonequilibrium character of active matter through the entropy production rate [28–31]. This quantification has been made difficult by the fact that the entropy encoded in the observable mechanical degrees of freedom is not equal to the thermodynamic entropy production as it does not contain all the thermodynamically relevant degrees of freedom [28]. Recent progress has been made by the explicit inclusion of the driving degrees of freedom [28,31]. For example, explicit inclusion of the driving Ornstein-Uhlenbeck process results in a thermodynamically consistent entropy production rate for the active Ornstein-Uhlenbeck particle model [31]. Similarly, Ref. [28] arrived at a consistent description of a chemically driven active particle by starting with a microscopic model of chemomechanical coupling and explicitly tracking the thermodynamically relevant degrees of freedom across scales. Thus, explicitly modeling the transfer of microscopic driving forces (usually chemical) to the mechanical degree of freedom is a critical first step in understanding the thermodynamics.

Chemomechanical energy coupling has been extensively studied at the single-particle level in the context of isothermal molecular motors or motor proteins [32–34]. Several researchers have built on this single-particle understanding

^{*}Contact author: michael.jack@otago.ac.nz

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to incorporate microscopic (usually chemical) driving forces into models of active matter [28,35,36]. As a recent example, Ref. [28] uses a systematic bottom-up approach to connect chemical reactions to mechanical motion, leading to a well-studied model of active Brownian particles. As an alternative approach, researchers have explicitly coupled a chemical degree of freedom to the hydrodynamic or collective level through the framework of linear irreversible thermodynamics [37]. However, this is only valid in the linear response regime. To connect their work to commonly used models of active matter, most of these treatments, whether explicitly or implicitly, make a tight-coupling approximation. This limits the ability of these approaches to evaluate potential loss processes and, therefore, understand the complete thermodynamics of active matter.

A second key aspect of the energetics of active matter is understanding how the microscopic processes of active matter can lead to macroscopic forces and the production of work on their environment—crucial for living systems. Examples investigated by researchers include the extraction of work by periodic cycling of the walls confining the active matter [38,39], experiments that use active matter to rotate macroscopic objects [40–42], and the use of active particles to push passive Brownian particles against a load [43,44]. These indirect methods of extracting work from active matter tend to obscure the fundamental mechanisms of energy transfer.

Despite this research into the energetics of active matter, a complete understanding is still lacking. In particular, the fundamental relationship between the emergence of order and the energy conversion process remains unclear. In this paper, we take as a starting point a simple run-and-tumble one-dimensional (1D) lattice model of oriented Brownian particles [26,27]. Simple lattice models have been used in a variety of contexts in active matter, including to demonstrate how collective behavior can arise from microscopic behavior [26,27]. Under coarse graining, the lattice models can resemble the usual hydrodynamic or mean-field equations in certain regimes [26,27,35,45,46]. We add two additional components to this 1D lattice model: (1) an explicit coupling to a chemical degree of freedom beyond the tight-coupling regime and (2) a macroscopic external force so that the system has the possibility of doing work. The resulting thermodynamically consistent model can be used to investigate both energy conversion efficiency and the emergence of order, enabling the relationship between these two fundamental aspects of active matter to be explored. To the best of our knowledge, such a system has not been studied previously.

As an additional novelty, we formulate this many-body system of Brownian particles using creation and annihilation operators for identical classical particles [47–49]. This formalism has been widely used in diffusion-limited chemical reaction research [50], but its application to active-matter systems is rare. It has been used to explore simple lattice models of interacting particles [51] and a path integral formalism has been used to explore active matter systems using a perturbative diagrammatic approach [52,53]. This last work differs from the present study in that it does not explicitly treat the chemical degree of freedom. Here, the use of creation and annihilation operators for identical classical particles enables us to easily incorporate well-known results from single

molecules [33,34] into a many-body system. It also allows us to exploit parallels with quantum many-body systems [54] and calculate number fluctuations.

The remainder of this paper is structured as follows. In Sec. II, we introduce the physical model of the system and discuss general considerations of the steady-state drifts that characterize the nonequilibrium behavior of the system, including energy conversion efficiency. In Sec. III, we introduce the many-body formulation of the system using creation and annihilation operators for classical indistinguishable particles. Sections IV and V explore two limiting cases: noninteracting particles and independent sites without hopping, respectively. Section VI then investigates the full interacting system using two different mean-field techniques: a Bogoliubov-type approach (Sec. VI A) that enables a connection to other mean-field approaches and a decoupling approximation (Sec. VI B) that allows us to explore the weak hopping regime and also calculate on-site number fluctuations in addition to the drift. This last subsection contains the key results of this paper. Finally, Sec. VII concludes the paper and outlines a range of directions for further work.

II. RUN AND TUMBLE ON A LATTICE WITH CHEMOMECHANICAL COUPLING

To treat chemomechanical coupling, we assume that the Brownian particles perform thermally induced hopping on a two-dimensional (2D) lattice [32,55,56], where the up-down degree of freedom (labeled y with lattice coordinate m) is a generalized chemical coordinate and the left-right degree of freedom is mechanical motion (labeled x with lattice coordinate n). Each Brownian particle has an independent right or left orientation (labeled as $d = \rightarrow$ and $d = \leftarrow$) and experiences a chemically induced force in the direction of its orientation. The particles also undergo random orientation flips (i.e., tumbles) and particle-particle interactions that influence the flip rate. Figure 1 provides a schematic of the various transitions in the system. In some respects, this model resembles early work on cooperative molecular motors [34,57]; however, whereas in that work, cooperation or collective behavior was assumed, here it emerges spontaneously.

Some of the key observables in this system are the nonequilibrium steady-state collective drifts in the two dimensions. The per-particle drift in units of inverse time (or directional rates) can, in general, be written as

$$r_x = \frac{1}{2}(r_{x,\rightarrow} + r_{x,\leftarrow}) + \frac{1}{2}(r_{x,\rightarrow} - r_{x,\leftarrow})\phi, \quad (1)$$

$$r_y = \frac{1}{2}(r_{y,\rightarrow} + r_{y,\leftarrow}) + \frac{1}{2}(r_{y,\rightarrow} - r_{y,\leftarrow})\phi, \quad (2)$$

where $r_{x,d}$ and $r_{y,d}$ are the single-particle drifts, $\phi = (N_{\rightarrow} - N_{\leftarrow})/N$ quantifies the relative difference in population of the two orientations N_d , and $N = N_{\rightarrow} + N_{\leftarrow}$ is the total number of particles. Here, we refer to ϕ as the “order parameter” due to the fact that it can only be nonzero due to many-body effects. In subsequent sections, we will show that without particle-particle alignment interactions, random flips lead to equal populations of left- and right-oriented particles in the long-time limit and $\phi = 0$; however, if particle interactions are sufficiently large, then there is a spontaneous alignment of

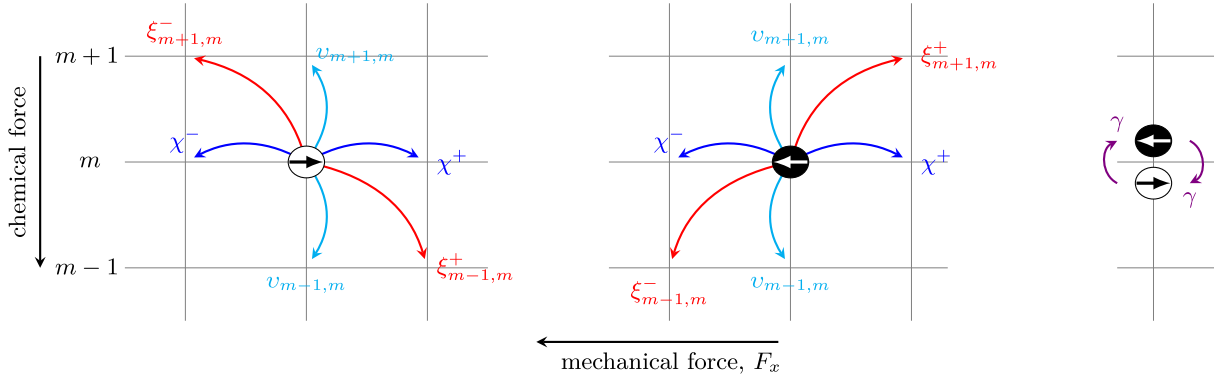


FIG. 1. Schematic of the possible microscopic transitions of the left-right oriented Brownian particles on a lattice. The horizontal axis is the mechanical degree of freedom, and the vertical axis is the chemical degree of freedom, made up of discrete chemical states. $v_{m±1,m}$ (cyan) are the “futile” chemical reaction rates (that bypass the chemomechanical coupling), $\chi^\pm$ (dark blue) are the passive mechanical hopping rates, and $\xi_{m±1,m}^\pm$ (red) couple the chemical and mechanical degrees of freedom. We assume that chemomechanical coupling acts only along the particle orientation. γ (violet) is the rate of flips in orientation or “tumbles.” If $F_x = 0$, this system has a left-right symmetry.

particles that breaks the symmetry between the two orientations, leading to $\phi \neq 0$.

We assume that the chemical reaction driving the particles is maintained out of equilibrium such that $\Delta\mu < 0$ is the (constant) chemical potential or chemical driving force in the negative y direction (i.e., $r_{y,d} < 0$) [36]. We also consider the possibility of a mechanical force, $F_x \geq 0$, opposing the motion in the positive x direction such that $\Delta W = F_x \ell \geq 0$ is the work done by the system against the force, where ℓ is the lattice spacing.

Let us first consider the case where there is no opposing force and $\Delta W = 0$, and there is a left-right symmetry. In this case, it is possible to show that $r_{y,\rightarrow} = r_{y,\leftarrow}$ and $r_{x,\rightarrow} = -r_{x,\leftarrow}$. From Eq. (1) we see that, in this case, nonzero collective flow in the mechanical coordinate $r_x \neq 0$ requires $\phi \neq 0$. When $\Delta W = 0$, an energy efficiency cannot be defined, but it is useful to define the *efficacy* at which the chemical process is converted into directed motion [58]:

$$\Lambda = -\frac{|r_x|}{r_y}. \quad (3)$$

This definition satisfies $0 \leq \Lambda \leq 1$. With the above results, this reduces to

$$\Lambda = \frac{-|r_{x,\rightarrow}\phi|}{r_{y,\rightarrow}} \quad (4)$$

showing that nonzero efficacy requires spontaneous alignment of particles.

In the case where $\Delta W \neq 0$, we can define the efficiency of chemomechanical energy conversion as

$$\eta = \frac{\Delta W r_x}{\Delta \mu r_y}, \quad (5)$$

where $\Delta W r_x$ is the per particle rate of mechanical work done (or power output) by the system and $\Delta \mu r_y$ is the rate of consumption of chemical energy. As we will show, the per particle entropy generation rate is given by

$$T\sigma = \Delta \mu r_y - \Delta W r_x \geq 0, \quad (6)$$

where T is the temperature. The inequality in Eq. (6) ensures that the efficiency is constrained such that $0 \leq \eta \leq 1$, with

the equality occurring at equilibrium when $\sigma = 0$. As r_x and r_y depend on ϕ , the entropy generation rate also depends on the collective behavior.

As $\Delta\mu < 0$, $r_y < 0$, and energy conversion occurs when $r_x > 0$ (i.e., the mechanical drift is against the opposing force). From Eqs. (1) and (2), we can write

$$\eta = \frac{\Delta W[(r_{x,\rightarrow} + r_{x,\leftarrow}) + (r_{x,\rightarrow} - r_{x,\leftarrow})\phi]}{\Delta \mu[(r_{y,\rightarrow} + r_{y,\leftarrow}) + (r_{y,\rightarrow} - r_{y,\leftarrow})\phi]}. \quad (7)$$

Conversion to mechanical work (positive numerator) requires both sufficient coupling to the chemical degree of freedom for the right-oriented particles to propagate uphill against the opposing force ($r_{x,\rightarrow} > 0$) and the right-oriented population to be dominant ($\phi > 0$). These general considerations already show that efficacy, efficiency, and entropy generation rate have complex relationships with both the single-particle energy conversion process and collective behavior.

III. MANY-BODY FORMULATION

The order parameter, ϕ , is determined by particle-particle interactions and requires a many-body treatment. We choose to formulate this many-body system using creation and annihilation operators for indistinguishable classical particles [47–49]. Unlike quantum particles, Brownian particles can, in principle, be distinguished; however, if we are interested in collective effects, then treating them as indistinguishable represents a significant simplification. In this formalism, the state of the system, $|P(t)\rangle$, evolves in time via

$$\frac{d|P(t)\rangle}{dt} = \hat{\mathcal{L}}|P(t)\rangle, \quad (8)$$

where $\hat{\mathcal{L}}$ is the evolution operator. The evolution operator is written in terms of bosonic creation ($\hat{a}_{n,m,d}^\dagger$) and annihilation ($\hat{a}_{n,m,d}$) operators [59] for indistinguishable Brownian particles. Similar to quantum mechanics, these operators describe the creation and annihilation of a Brownian particle in a particular microscopic state and satisfy the usual bosonic commutation relations $[\hat{a}_{n,m,d}, \hat{a}_{n',m',d'}^\dagger] = \delta_{nn'}\delta_{mm'}\delta_{dd'}$.

The evolution operator describing the current system is given by

$$\hat{\mathcal{L}} = \sum_{n,m} \left[\sum_d (\hat{L}_{n,m,d}^v + \hat{L}_{n,m,d}^\chi + \hat{L}_{n,m,d}^\zeta) + \hat{L}_{n,m}^\gamma \right], \quad (9)$$

where

$$\begin{aligned} \hat{L}_{n,m,d}^v &= (\hat{a}_{n,m+1,d}^\dagger - \hat{a}_{n,m,d}^\dagger) v_{m+1,m} \hat{a}_{n,m,d} \\ &+ (\hat{a}_{n,m-1,d}^\dagger - \hat{a}_{n,m,d}^\dagger) v_{m-1,m} \hat{a}_{n,m,d}, \end{aligned} \quad (10)$$

$$\begin{aligned} \hat{L}_{n,m,d}^\chi &= (\hat{a}_{n+1,m,d}^\dagger - \hat{a}_{n,m,d}^\dagger) \chi^+ \hat{a}_{n,m,d} \\ &+ (\hat{a}_{n-1,m,d}^\dagger - \hat{a}_{n,m,d}^\dagger) \chi^- \hat{a}_{n,m,d}, \end{aligned} \quad (11)$$

$$\begin{aligned} \hat{L}_{n,m,\pm}^\zeta &= (\hat{a}_{n\pm 1,m-1,\pm}^\dagger - \hat{a}_{n,m,\pm}^\dagger) \zeta_{m-1,m}^\pm \hat{a}_{n,m,\pm} \\ &+ (\hat{a}_{n\mp 1,m+1,\pm}^\dagger - \hat{a}_{n,m,\pm}^\dagger) \zeta_{m+1,m}^\mp \hat{a}_{n,m,\pm}, \end{aligned} \quad (12)$$

$$\hat{L}_{n,m}^\gamma = (\hat{a}_{n,m,\leftarrow}^\dagger - \hat{a}_{n,m,\rightarrow}^\dagger) (\hat{\gamma}_{n,\leftarrow} \hat{a}_{n,m,\rightarrow} - \hat{\gamma}_{n,\rightarrow} \hat{a}_{n,m,\leftarrow}). \quad (13)$$

The negative diagonal terms ensure that the system evolution is stable (i.e., the real part of the eigenvalues of $\hat{\mathcal{L}}$ is negative) and a zeroth eigenvalue of $\hat{\mathcal{L}}$ exists, $\hat{\mathcal{L}}|P_0\rangle = 0$, such that the system has a steady state given by $|P_0\rangle$.

$v_{m\pm 1,m}$ are the chemical coupling rates and satisfy the local detailed balance condition [33]

$$\frac{v_{m-1,m}}{v_{m,m-1}} = e^{-\Delta\bar{\mu}}, \quad (14)$$

where $\Delta\bar{\mu} = \Delta\mu/k_B T < 0$ is the chemical potential or chemical driving force (in units of $k_B T$) driving the system out of equilibrium. The $v_{m\pm 1,m}$ rates are “futile chemical reaction rates” in that they do not couple to the mechanical degree of freedom.

$\chi^\pm$ are the rates for the passive mechanical hopping, and $\zeta_{m\pm 1,m}^\pm$ are the hopping rates that couple the chemical and mechanical degrees of freedom. They satisfy the detailed balance conditions

$$\frac{\chi^+}{\chi^-} = e^{-\Delta\bar{W}}, \quad (15)$$

$$\frac{\zeta_{m-1,m}^+}{\zeta_{m,m-1}^-} = e^{-\Delta\bar{W} - \Delta\bar{\mu}}, \quad (16)$$

$$\frac{\zeta_{m-1,m}^-}{\zeta_{m,m-1}^+} = e^{\Delta\bar{W} - \Delta\bar{\mu}}, \quad (17)$$

where $\Delta\bar{W} = \Delta W/k_B T$. We assume that when $\Delta W = 0$, $\zeta_{m\pm 1,m}^+ = \zeta_{m\pm 1,m}^-$, such that the full evolution operator $\hat{\mathcal{L}}$ has a symmetry between right and left orientations in this case. In subsequent sections, we will see how this symmetry can be broken by the interactions between the particles. For simplicity, here we take $\chi^\pm = \chi_0 e^{\mp \frac{1}{2} \Delta\bar{W}}$, $\zeta_{m\mp 1,m}^+ = \zeta_{m-1,m}^0 e^{-\frac{1}{2} \Delta\bar{W} \mp \frac{1}{2} \Delta\bar{\mu}}$, $\zeta_{m\mp 1,m}^- = \zeta_{m-1,m}^0 e^{\frac{1}{2} \Delta\bar{W} \mp \frac{1}{2} \Delta\bar{\mu}}$, and $v_{m\mp 1,m} = v_{m-1,m}^0 e^{\mp \frac{1}{2} \Delta\bar{\mu}}$, which satisfy Eqs. (14)–(17).

$\hat{\gamma}_{n,d}$ are the rates at which the particles flip orientations and, due to particle-particle interactions, depend on the population

in the n th site. We assume the form [59]

$$\hat{\gamma}_{n,d} = \gamma \exp \left\{ \beta_\gamma \sum_m \hat{n}_{n,m,d} \right\}, \quad (18)$$

where $\hat{n}_{n,m,d} = \hat{a}_{n,m,d}^\dagger \hat{a}_{n,m,d}$ is the number operator, γ is the single-particle orientation flip rate, and $\beta_\gamma \geq 0$ is a unitless parameter representing the strength of the particle interactions. This form arises from a consideration of short-range particle-particle interactions in the discrete limit [59]. In the case $\beta_\gamma > 0$, the flip rate from right to left (left to right) is exponentially enhanced by the presence of other left-oriented (right-oriented) particles in the n th site. We can thus consider $\beta_\gamma \geq 0$ as quantifying the strength of the attractive interaction between aligned particles. It is useful to write $\hat{\gamma}$ in normally ordered form (with the creation operators to the left and annihilation operators to the right):

$$\hat{\gamma}_{n,d} = \gamma : \exp \left\{ \beta'_\gamma \sum_m \hat{n}_{n,m,d} \right\} :, \quad (19)$$

where $\beta'_\gamma = e^{\beta_\gamma} - 1$ and the double colons denote that the quantity between the colons is normally ordered [54].

As $\Delta\mu \neq 0$, this system is out of equilibrium and as a result $\hat{\mathcal{L}}$ is nonself-adjoint: $\hat{\mathcal{L}} \neq \hat{\mathcal{L}}^\dagger$. For nonself-adjoint matrices, the left and right eigenstates do not have a simple relationship [47]. The left eigenstate of the evolution operator corresponding to the zeroth eigenvalue is given by $\langle Q_0 | \hat{\mathcal{L}} = 0$ and needs to be found independently of $|P_0\rangle$. Using $\langle Q_0 |$, we can define the state normalization condition $\langle Q_0 | P(t) \rangle = 1$, and the average of an operator $\hat{O}$ as [47]

$$\langle \hat{O} \rangle(t) \equiv \langle Q_0 | \hat{O} | P(t) \rangle. \quad (20)$$

Here, we are most interested in the nonequilibrium steady-state $\langle \hat{O} \rangle_{ss} \equiv \langle Q_0 | \hat{O} | P_0 \rangle$. The non-self-adjoint nature of the evolution operator and the definition of the average via Eq. (20) are the key mathematical differences between this formalism and quantum mechanics [47].

Here, we consider N particles in a 2D periodic system with M_y chemical and M_x mechanical states, where we are interested in the nonequilibrium steady-state drift and on-site number fluctuations. In this case, it suffices to use the reduced evolution operator for a single period given by [59]

$$\hat{\mathcal{L}}_R = \sum_{n=1, m=1}^{M_x, M_y} \left[\sum_d (\hat{L}_{n,m,d}^\chi + \hat{L}_{n,m,d}^v + \hat{L}_{n,m,d}^\zeta) + \hat{L}_{n,m}^\gamma \right], \quad (21)$$

with the periodic boundary conditions: $n = 0 \rightarrow n = M_x$, $n = M_x + 1 \rightarrow n = 1$, $m = 0 \rightarrow m = M_y$, and $m = M_y + 1 \rightarrow m = 1$. The simplest system that can perform a chemical cycle is $M_y = 3$, and this will be the focus of this paper.

The single particle drifts are given by [59]

$$r_{x,\pm} = \frac{1}{N} \sum_{n=1, m=1}^{M_x, M_y} \langle \hat{j}_{n,m,\pm}^\chi \rangle_{ss} + \langle \hat{j}_{n,m,\pm}^\zeta \rangle_{ss}, \quad (22)$$

$$r_{y,\pm} = \frac{1}{N} \sum_{n=1, m=1}^{M_x, M_y} \langle \hat{j}_{n,m,\pm}^v \rangle_{ss} \mp \langle \hat{j}_{n,m,\pm}^\zeta \rangle_{ss}, \quad (23)$$

where

$$\begin{aligned}\hat{J}_{n,m,\rightleftharpoons}^{\chi} &= \hat{a}_{n+1,m,\rightleftharpoons}^{\dagger} \chi^+ \hat{a}_{n,m,\rightleftharpoons} - \hat{a}_{n,m,\rightleftharpoons}^{\dagger} \chi^- \hat{a}_{n+1,m,\rightleftharpoons} \\ \hat{J}_{n,m,\rightleftharpoons}^{\zeta} &= \hat{a}_{n+1,m,\rightleftharpoons}^{\dagger} \zeta_{m,\rightleftharpoons}^+ \hat{a}_{n,m,\rightleftharpoons} \\ &\quad - \hat{a}_{n,m,\rightleftharpoons}^{\dagger} \zeta_{m,\rightleftharpoons}^- \hat{a}_{n+1,m,\rightleftharpoons},\end{aligned}\quad (24)$$

$$\begin{aligned}\hat{J}_{n,m,\rightleftharpoons}^{\nu} &= \hat{a}_{n,m+1,\rightleftharpoons}^{\dagger} \nu_{m+1,m} \hat{a}_{n,m,\rightleftharpoons} \\ &\quad - \hat{a}_{n,m,\rightleftharpoons}^{\dagger} \nu_{m,m+1} \hat{a}_{n,m+1,\rightleftharpoons}\end{aligned}\quad (25)$$

are the current operators in the mechanical and chemical degrees of freedom, respectively. The single-particle drifts, Eqs. (22) and (23), can be derived from considering the “Heisenberg equations” of motion for the number operators (see Appendix E) [59]. When $\Delta W = 0$, $\langle \hat{J}_{n,m,\rightleftharpoons}^{\chi} \rangle_{ss} = 0$ and it is clear that the $0 \leq \Lambda \leq 1$ as claimed in Sec. II.

The steady-state entropy production rate can be determined from its standard definition [33,60]

$$\begin{aligned}N\sigma/k_B &\equiv \sum_{n,m,d} \langle \hat{J}_{n,m,d}^{\chi} \rangle_{ss} \ln \left(\frac{\chi^+}{\chi^-} \right) \\ &\quad + \sum_{n,m,d} \langle \hat{J}_{n,m,d}^{\nu} \rangle_{ss} \ln \left(\frac{\nu_{m,m-1}}{\nu_{m-1,m}} \right) \\ &\quad + \sum_{n,m} \langle \hat{J}_{n,m,\rightarrow}^{\zeta} \rangle_{ss} \ln \left(\frac{\zeta_{m-1,m}^+}{\zeta_{m,m-1}^-} \right) \\ &\quad + \sum_{n,m} \langle \hat{J}_{n,m,\leftarrow}^{\zeta} \rangle_{ss} \ln \left(\frac{\zeta_{m+1,m}^+}{\zeta_{m,m+1}^-} \right).\end{aligned}\quad (26)$$

Using the detailed balance conditions (14)–(17) and the definitions (22) and (23), we can derive Eq. (6). As we are explicitly treating the chemical degree of freedom, this entropy generation rate contains all relevant degrees of freedom, and we have not carried out any coarse graining [28].

Other observables of interest are the on-site number fluctuations. Defining $\hat{n}_{n,d} = \sum_m \hat{n}_{n,m,d}$, the normalized two-body correlation functions for each lattice site are defined by

$$g_{dd} \equiv \frac{\langle : \hat{n}_{n,d} \hat{n}_{n,d} : \rangle_{ss}}{\bar{n}_d^2} \quad (27)$$

$$= 1 + \frac{V(n_d) - \bar{n}_d}{\bar{n}_d^2}, \quad (28)$$

$$g_{\rightarrow\leftarrow} \equiv \frac{\langle \hat{n}_{n,\rightarrow} \hat{n}_{n,\leftarrow} \rangle_{ss}}{\bar{n}_{\rightarrow} \bar{n}_{\leftarrow}}, \quad (29)$$

where $V(n_d) = \langle \hat{n}_{n,d}^2 \rangle_{ss} - \bar{n}_d^2$ is the variance in number and $\bar{n}_d = \langle \hat{n}_{n,d} \rangle_{ss}$. In these definitions, we have dropped the site index n as we assume that each lattice site is identical. $g_{jj} = 1$ represents Poissonian number fluctuations and $g_{ij} = 1$ for $i \neq j$ means that the particles in each direction are uncorrelated. $g_{ii} > 1$ represents super-Poissonian number fluctuations (or particle “bunching”) and $g_{ij} > 1$ ($g_{ij} < 1$) for $i \neq j$ shows that particles of different orientations are (anti)correlated. A final quantity of interest is the variance in the population difference

given by

$$V(n_{\rightarrow} - n_{\leftarrow}) = \langle (\hat{n}_{n,\rightarrow} - \hat{n}_{n,\leftarrow})^2 \rangle_{ss} - (\bar{n}_{\rightarrow} - \bar{n}_{\leftarrow})^2 \quad (30)$$

$$\begin{aligned}&= V(n_{\rightarrow}) + V(n_{\leftarrow}) \\ &\quad - 2[\langle \hat{n}_{n,\rightarrow} \hat{n}_{n,\leftarrow} \rangle_{ss} - \bar{n}_{\rightarrow} \bar{n}_{\leftarrow}].\end{aligned}\quad (31)$$

IV. NONINTERACTING PARTICLES

Let us first consider the noninteracting case where $\beta_{\gamma} = 0$. In this case, the evolution operator is quadratic in the annihilation and creation operators and can be diagonalized exactly. Performing this diagonalization (initially for $\gamma = 0$), Eq. (21) becomes

$$\begin{aligned}\hat{\mathcal{L}}_R &= \sum_{k,l} \left[\sum_d (\lambda_{k,l,d} - \gamma) \hat{b}_{k,l,d}^{\dagger} \hat{b}_{k,l,d} \right. \\ &\quad \left. + \gamma (\hat{b}_{k,l,\rightarrow}^{\dagger} \hat{b}_{k,l,\leftarrow} + \hat{b}_{k,l,\leftarrow}^{\dagger} \hat{b}_{k,l,\rightarrow}) \right],\end{aligned}\quad (32)$$

where $k = 0, 2\pi/M_x, 4\pi/M_x, \dots, 2\pi$, and we have introduced the k modes

$$\hat{b}_{k,l,d} = \frac{1}{\sqrt{M_x}} \sum_{n,m} (U_{k,d}^{-1})_{m,l} e^{-ikn} \hat{a}_{n,m,d}, \quad (33)$$

$$\hat{b}_{k,l,d}^{\dagger} = \frac{1}{\sqrt{M_x}} \sum_{n,m} (U_{k,d})_{l,m} e^{+ikn} \hat{a}_{n,m,d}^{\dagger}. \quad (34)$$

The inverse transformation is

$$\hat{a}_{n,m,d} = \frac{1}{\sqrt{M_x}} \sum_{k,l} (U_{k,d})_{l,m} e^{+ikn} \hat{b}_{k,l,d}, \quad (35)$$

$$\hat{a}_{n,m,d}^{\dagger} = \frac{1}{\sqrt{M_x}} \sum_{k,l} (U_{k,d}^{-1})_{m,l} e^{-ikn} \hat{b}_{k,l,d}^{\dagger}. \quad (36)$$

Focusing on the $M_y = 3$ case, $\lambda_{k,l,d}$ (with negative real part) are the eigenvalues of the matrix

$$L_{k,d} = [(e^{-ik} - 1)\chi^+ + (e^{+ik} - 1)\chi^-] \mathbb{1} + Y + Z_{k,d}, \quad (37)$$

where

$$Y = \begin{bmatrix} -\nu_{2,1} - \nu_{3,1} & \nu_{1,2} & \nu_{1,3} \\ \nu_{2,1} & -\nu_{1,2} - \nu_{3,2} & \nu_{2,3} \\ \nu_{3,1} & \nu_{3,2} & -\nu_{1,3} - \nu_{2,3} \end{bmatrix}, \quad (38)$$

$$Z_{k,\rightleftharpoons} = \begin{bmatrix} -\zeta_{2,1}^{\mp} - \zeta_{3,1}^{\pm} & \zeta_{1,2}^{\pm} e^{\mp ik} & \zeta_{1,3}^{\mp} e^{\pm ik} \\ \zeta_{2,1}^{\mp} e^{\pm ik} & -\zeta_{1,2}^{\pm} - \zeta_{3,2}^{\mp} & \zeta_{2,3}^{\pm} e^{\mp ik} \\ \zeta_{3,1}^{\pm} e^{\mp ik} & \zeta_{3,2}^{\mp} e^{\pm ik} & -\zeta_{1,3}^{\mp} - \zeta_{2,3}^{\pm} \end{bmatrix}. \quad (39)$$

The matrices $U_{k,d}$ satisfy

$$U_{k,d}^{-1} L_{k,d} U_{k,d} = D_{k,d}, \quad (40)$$

$$U_{k,d}^{-1} U_{k,d} = U_{k,d} U_{k,d}^{-1} = \mathbb{1}, \quad (41)$$

where $D_{k,d}$ is a diagonal matrix of eigenvalues $\lambda_{k,l,d}$. The eigenvalues are ordered such that $\text{Re}\{\lambda_{k,1,d}\} \geq \text{Re}\{\lambda_{k,2,d}\} \geq \text{Re}\{\lambda_{k,3,d}\}$. If $\Delta W = 0$, then $Z_{k,\rightarrow} = Z_{k,\leftarrow}^*$ and the eigenvalues satisfy $\lambda_{k,l,\rightarrow} = \lambda_{k,l,\leftarrow}^*$.

In general, the eigensystem is complicated; however, for $k = 0$, we can see from Eqs. (37)–(39) that the matrix $L_{0,d}$ satisfies

$$(L_{0,d})_{l,l} = -\sum_{m \neq l} (L_{0,d})_{m,l}, \quad \text{for all } l. \quad (42)$$

As a consequence, $\lambda_{0,1,d} = 0$ and $(U_{0,d}^{-1})_{m,1} = \text{const.}$ We choose the normalization $(U_{0,d}^{-1})_{m,1} = 1$, for all m and $\sum_{m=1}^3 (U_{0,d})_{1,m} = 1$, such that $(U_{0,\leftarrow})_{1,m}$ gives the relative population of the m th chemical state in the chemical ground state $l = 1$.

When $\gamma = 0$, $\hat{\mathcal{L}}_R$ reduces to

$$\hat{\mathcal{L}}_R = \sum_{k,l,d} \lambda_{k,l,d} \hat{b}_{k,l,d}^\dagger \hat{b}_{k,l,d} \quad (43)$$

and the particles with different orientations are completely independent. The nonequilibrium steady state is given by the “condensation” of all bosons into their respective slowest modes, i.e., $|P_0\rangle = \frac{1}{\sqrt{N_{\rightarrow} N_{\leftarrow}}} \hat{b}_{0,1,\rightarrow}^{\dagger N_{\rightarrow}} \hat{b}_{0,1,\leftarrow}^{\dagger N_{\leftarrow}} |0\rangle$. We also have $\langle Q_0 | = \frac{1}{\sqrt{N_{\rightarrow} N_{\leftarrow}}} \langle 0 | \hat{b}_{0,1,\rightarrow}^{N_{\rightarrow}} \hat{b}_{0,1,\leftarrow}^{N_{\leftarrow}}$. We can calculate the nonequilibrium steady-state drift by writing $\hat{j}_{n,m,d}^x$ in terms of the k modes and using the fact that all particles have condensed into the zeroth modes. The drift is given by Eq. (1) with

$$\phi = \frac{1}{N} [\langle \hat{b}_{0,1,\rightarrow}^\dagger \hat{b}_{0,1,\rightarrow} \rangle_{ss} - \langle \hat{b}_{0,1,\leftarrow}^\dagger \hat{b}_{0,1,\leftarrow} \rangle_{ss}], \quad (44)$$

$$r_{x,d} = \Xi_d^+ - \Xi_d^- + \chi^+ - \chi^-, \quad (45)$$

where

$$\Xi_{\rightarrow}^\pm = \sum_m \zeta_{m \mp 1,m}^\pm (U_{0,\rightarrow})_{1,m}, \quad (46)$$

$$\Xi_{\leftarrow}^\pm = \sum_m \zeta_{m \pm 1,m}^\pm (U_{0,\leftarrow})_{1,m}, \quad (47)$$

which represent the chemomechanical forward and backward transitions, weighted by the ground-state chemical populations. Note that in the case where the hopping rates are independent of the chemical state m (i.e., $v_{m,m \pm 1} = v_{(\pm)}$, $\zeta_{m,m \pm 1}^+ = \zeta_{(\pm)}^+$, and $\zeta_{m,m \pm 1}^- = \zeta_{(\pm)}^-$), it is possible to solve the eigensystem analytically and also derive analytical expressions for the drift in terms of the forces [56]. However, since this is almost never the case in motor proteins [34], here we retain the more general chemical state dependence of these rates.

If $\Delta W = 0$, then $\chi^+ = \chi^-$, $U_{0,\rightarrow} = U_{0,\leftarrow}$, and $\Xi_{\rightarrow}^\pm = \Xi_{\leftarrow}^\pm$ and $r_{x,\rightarrow} = -r_{x,\leftarrow}$ and we have

$$r_x = (\Xi_{\rightarrow}^+ - \Xi_{\rightarrow}^-) \phi \quad (48)$$

showing that both $\phi \neq 0$ and chemomechanical coupling are required for net mechanical drift. This drift is driven by the difference in forward and backward chemical coupling strengths: $\zeta_{m-1,m}^\pm - \zeta_{m+1,m}^\pm$.

For $\Delta W \neq 0$, $U_{0,\rightarrow} \neq U_{0,\leftarrow}$, and $r_{x,\rightarrow} \neq r_{x,\leftarrow}$. The dependence of $r_{x,d}$ on ΔW is shown in Fig. 2. $r_{x,d}$ decreases monotonically with increasing opposing force $\Delta W > 0$. $r_{x,\leftarrow} < 0$, whereas for small opposing mechanical forces, $r_{x,\rightarrow}$ is positive. If in addition, $\phi > 0$, then $r_x > 0$, representing chemical energy being converted into mechanical work

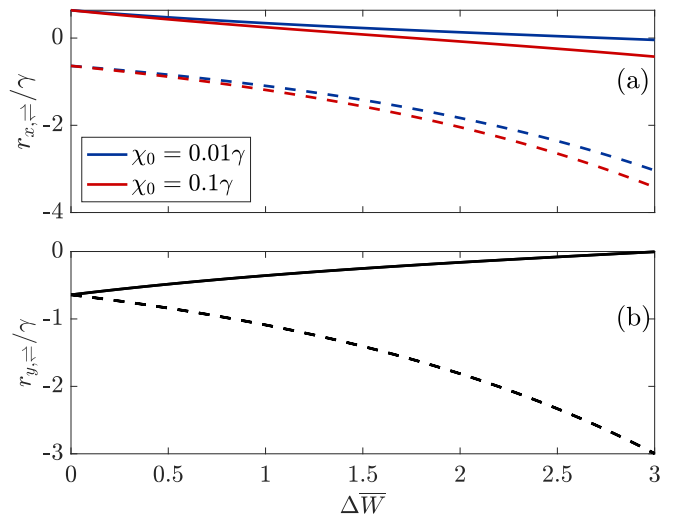


FIG. 2. Mechanical [panel (a)] and chemical [panel (b)] drift as a function of opposing force. The solid lines show $r_{x/y,\rightarrow}$ and the dashed lines $r_{x/y,\leftarrow}$ for different values of χ_0 . (Note χ_0 does not affect $r_{y,d}$.) Other parameters are $\Delta\mu = -3k_B T$, $v_{1,2}^0 = v_{2,3}^0 = v_{3,1}^0 = 0.001\gamma$, $\zeta_{1,2}^0 = 10\gamma$, and $\zeta_{2,3}^0 = \zeta_{3,1}^0 = 0.1\gamma$.

against an opposing force. In these cases, the efficiency is given by Eq. (5).

Similarly, writing $\hat{j}_{n,m,d}^y$ in terms of the k modes, we can show that the drift is given by Eq. (2) with Eq. (44) and

$$r_{y,\leftarrow} = \mp \Xi_{\leftarrow}^\pm \pm \Xi_{\leftarrow}^\mp - \Upsilon_{\leftarrow}^s + \Upsilon_{\leftarrow}^{ns}, \quad (49)$$

where

$$\Upsilon_d^s = \sum_m Y_{m-1,m} (U_{0,d})_{1,m}, \quad (50)$$

$$\Upsilon_d^{ns} = \sum_m Y_{m+1,m} (U_{0,d})_{1,m} \quad (51)$$

are the spontaneous and nonspontaneous transitions weighted by the ground-state chemical states.

If $\Delta W = 0$, then $\Upsilon_{\rightarrow}^s = \Upsilon_{\leftarrow}^s$ and $\Upsilon_{\rightarrow}^{ns} = \Upsilon_{\leftarrow}^{ns}$ and $r_y = r_{y,\rightarrow} = r_{y,\leftarrow}$. From Eq. (2) we can see that, in this case, the value of ϕ has no impact on the chemical drift and a finite chemical drift arises from the difference in forward and backward chemical coupling strengths alone. We can write the efficacy as

$$\Lambda = \frac{|(\Xi_{\rightarrow}^+ - \Xi_{\rightarrow}^-) \phi|}{\Upsilon_{\rightarrow}^s - \Upsilon_{\rightarrow}^{ns} + \Xi_{\rightarrow}^+ - \Xi_{\rightarrow}^-}. \quad (52)$$

This shows that large efficacy requires small futile chemical reactions and $\phi \neq 0$.

The dependence of $r_{y,d}$ on ΔW is shown in Fig. 2. $r_{y,\rightarrow}$ ($r_{y,\leftarrow}$) increases (decreases) monotonically with increasing opposing force $\Delta W > 0$. For $\Delta W > 0$, $r_{y,\rightarrow} > r_{y,\leftarrow}$ (both are negative for $\Delta\bar{W} \leq |\Delta\bar{\mu}|$, which we assume to be the case in this paper) and from Eq. (2) the overall chemical energy consumption rate $|r_y|$ reduces (increases) if particles are aligned uphill ($\phi > 0$) (downhill ($\phi < 0$)).

When $\gamma \neq 0$, the modes of the evolution operators are mixtures of the particles in the two orientations, and we can

write

$$\hat{\mathcal{L}}_R = \sum_{k,l} \omega_{k,l,+} \hat{d}_{k,l,+}^\dagger \hat{d}_{k,l,+} + \omega_{k,l,-} \hat{d}_{k,l,-}^\dagger \hat{d}_{k,l,-}, \quad (53)$$

where

$$\hat{d}_{k,l,\pm} \propto \gamma \hat{b}_{k,l,\leftarrow} + (\lambda_{k,l,\rightarrow} - \omega_{k,l,\mp} - \gamma) \hat{b}_{k,l,\rightarrow} \quad (54)$$

and

$$\omega_{k,l,\pm} = \frac{1}{2}(\lambda_{k,l,\rightarrow} + \lambda_{k,l,\leftarrow}) - \gamma \pm \sqrt{\frac{1}{4}(\lambda_{k,l,\rightarrow} - \lambda_{k,l,\leftarrow})^2 + \gamma^2}. \quad (55)$$

The zeroth mode $\omega_{0,1,+} = 0$ is given by an equal superposition of the two orientations $\hat{d}_{0,1,+} = \frac{1}{\sqrt{2}}(\hat{b}_{0,1,\rightarrow} + \hat{b}_{0,1,\leftarrow})$. In the steady state, all particles condense into this mode and $\phi = 0$. Physically, this arises because of the redistribution of particles across the two orientations for long times when $\gamma \neq 0$ and $\beta_\gamma = 0$.

For this state, we find

$$g_{dd} = 1 - 1/N, \quad (56)$$

$$g_{\rightarrow\leftarrow} = 1, \quad (57)$$

$$V(n_{\rightarrow} - n_{\leftarrow}) = \rho(1 - 1/2M_x), \quad (58)$$

where $\rho = N/M_x$ and we have used the identities $[\hat{a}_{n,m,d}, \hat{d}_{0,1,+}^\dagger] = N(U_{0,d})_{1,m} \hat{d}_{0,1,+}^{N-1}/\sqrt{2M_x}$ and $[\hat{d}_{0,1,+}^\dagger, \hat{a}_{n,m,d}^\dagger] = N(U_{0,d}^{-1})_{m,1} \hat{d}_{0,1,+}^{N-1}/\sqrt{2M_x}$. These results imply that for large N , the on-site number fluctuations are well approximated by a Poissonian distribution for each orientation, and there is no correlation between the two orientations.

V. NO HOPPING

Let us consider another special case where there is no hopping between sites $\chi^\pm = \zeta_{m\pm 1,m}^\pm = 0$, but we have interactions between particles $\gamma \neq 0$ and $\beta_\gamma \neq 0$. In this case, the sites decouple, and we can write

$$\sum_{m,d} \hat{L}_{n,m,d}^\nu = \sum_{l,d} \lambda_{0,l,d} \hat{c}_{l,d}^\dagger \hat{c}_{l,d}, \quad (59)$$

where

$$\hat{c}_{l,d} = \sum_m (U_{0,d}^{-1})_{m,l} \hat{a}_{n,m,d}, \quad (60)$$

$$\hat{c}_{l,d}^\dagger = \sum_m (U_{0,d})_{l,m} \hat{a}_{n,m,d}^\dagger, \quad (61)$$

and $\lambda_{0,l,d}$ and $U_{0,d}$ are the eigenvalues and eigenstates of $L_{0,d}$ [see Eq. (37)] with $\zeta_{m\pm 1,m}^\pm = 0$. Expanding $\hat{L}_{n,m}^\gamma$ in the $\hat{c}_{l,d}$ modes, we have

$$\sum_m \hat{L}_{n,m}^\gamma = \sum_l \gamma (\hat{c}_{l,\leftarrow}^\dagger - \hat{c}_{l,\rightarrow}^\dagger) (\hat{c}_{l,\rightarrow} e^{\beta_\gamma \hat{n}_{\leftarrow}} - \hat{c}_{l,\leftarrow} e^{\beta_\gamma \hat{n}_{\rightarrow}}), \quad (62)$$

where $\hat{n}_d = \sum_l \hat{c}_{l,d}^\dagger \hat{c}_{l,d}$ and we have used $U_{0,\rightarrow} = U_{0,\leftarrow}$. As Eq. (59) can only be zero if all the population is in the $l = 1$ mode (as $\lambda_{0,1,d} = 0$), the evolution operator governing the

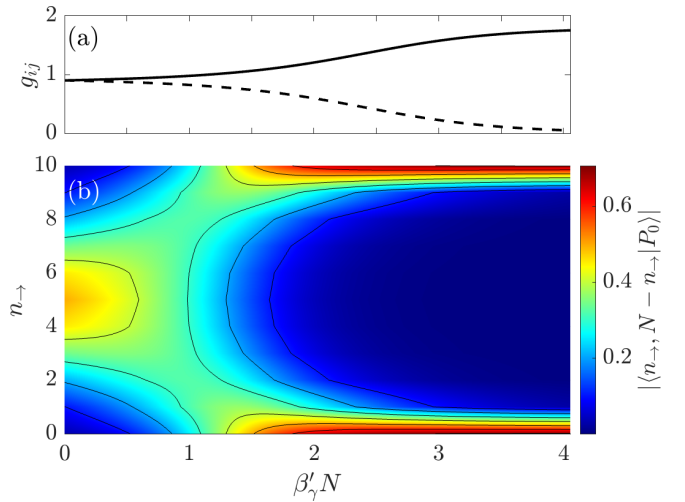


FIG. 3. Panel (a) shows the ground state $|P_0\rangle$ in the no-hopping case as a function of $\beta_\gamma' N$. Panel (b) shows $g_{\rightarrow\rightarrow}$ (solid line) and $g_{\rightarrow\leftarrow}$ (dashed line). Parameters are $N = 10$.

long-time behavior is

$$\hat{\mathcal{L}}_{LT} = \gamma (\hat{A}_{\leftarrow}^\dagger - \hat{A}_{\rightarrow}^\dagger) (\hat{A}_{\rightarrow} e^{\beta_\gamma \hat{n}_{\leftarrow}} - \hat{A}_{\leftarrow} e^{\beta_\gamma \hat{n}_{\rightarrow}}), \quad (63)$$

where $\hat{A}_d = \hat{c}_{1,d}$, $\hat{A}_d^\dagger = \hat{c}_{1,d}^\dagger$, and $\hat{n}_d = \hat{A}_d^\dagger \hat{A}_d$.

The total number of particles $N = \hat{n}_{\rightarrow} + \hat{n}_{\leftarrow}$ is conserved and the states $|n_{\rightarrow}, N - n_{\rightarrow}\rangle = \hat{A}_{\leftarrow}^{\dagger(N-n_{\rightarrow})} |\{0\}\rangle / \sqrt{n_{\rightarrow}!(N-n_{\rightarrow})!}$ form a complete set. It is possible to show (see Appendix A) that the left and right ground states are given by

$$\langle Q_0 | = (N!)^{1/2} \langle \{0\} | \left[\frac{1}{\sqrt{2}} (\hat{A}_{\rightarrow} + \hat{A}_{\leftarrow}) \right]^N \quad (64)$$

$$= \frac{1}{2^{N/2}} \sum_{n_{\rightarrow}=0}^N \binom{N}{n_{\rightarrow}}^{1/2} \langle n_{\rightarrow}, N - n_{\rightarrow} |, \quad (65)$$

$$|P_0\rangle \propto e^{\frac{\beta_\gamma}{4} (\hat{n}_{\rightarrow} - \hat{n}_{\leftarrow})^2} |Q_0\rangle, \quad (66)$$

where the normalization is fixed by $\langle Q_0 | P_0 \rangle = 1$. Both $|P_0\rangle$ and $\langle Q_0 |$ preserve the symmetry between the two orientations and $\phi = 0$.

When $\beta_\gamma N$ is small, the ground state $|P_0\rangle$ is similar to $|Q_0\rangle$ and is distributed across the number states and peaked about $|N/2, N/2\rangle$. However, for $\beta_\gamma N \gg 1$, the number fluctuations increase dramatically until the system is driven into a superposition of the extreme states $|N, 0\rangle$ and $|0, N\rangle$. This behavior is illustrated in Fig. 3(b). In this case, g_{ij} reduces to the two-mode two-body correlation functions

$$g_{dd} \equiv \frac{\langle \hat{A}_d^\dagger \hat{A}_d^\dagger \hat{A}_d \hat{A}_d \rangle_{ss}}{\bar{n}_d^2}, \quad (67)$$

$$g_{\rightarrow\leftarrow} \equiv \frac{\langle \hat{A}_{\rightarrow}^\dagger \hat{A}_{\leftarrow}^\dagger \hat{A}_{\leftarrow} \hat{A}_{\rightarrow} \rangle_{ss}}{\bar{n}_{\rightarrow} \bar{n}_{\leftarrow}}. \quad (68)$$

Figure 3(a) shows that when $\beta_\gamma' N = 0$, the number fluctuations are Poissonian, representing a coherent state. As $\beta_\gamma' N$ increases, number fluctuations of both orientations become super-Poissonian (here $g_{\rightarrow\rightarrow} = g_{\leftarrow\leftarrow}$) and the orientations become strongly anticorrelated $g_{\rightarrow\leftarrow} < 1$. The number

difference fluctuations $V(n_{\rightarrow} - n_{\leftarrow})$ vary from N to $\sim N^2$ across these values of $\beta'_y N$. Thus, for large $\beta'_y N$ in the steady state, particles of one orientation bunch together in each site to the exclusion of the other orientation while maintaining overall macroscopic balance between the particles such that $\phi = 0$. This contrasts markedly with the behavior discussed in Sec. IV, suggesting that intersite hopping and the nonlinear particle-particle interactions compete with each other.

VI. INTERACTING CASE: MEAN-FIELD APPROACHES

In the noninteracting case, the ground state of the system has a macroscopic occupation of N particles in the slowest modes. This suggests that a mean-field approach will be useful. We consider two different mean-field approaches: a Bogoliubov-type approach (Sec. VI A) that linearizes around a large occupation in the ground state, and a decoupling mean-field that assumes the system state can be factorized by site.

A. Bogoliubov-type approach

A Bogoliubov-type approach assumes that we can write

$$\hat{a}_{n,m,\equiv} = \sqrt{\rho} \alpha_{m,\equiv} + \delta \hat{a}_{n,m,\equiv}, \quad (69)$$

$$\hat{a}_{n,m,\equiv}^\dagger = \sqrt{\rho} \alpha_{m,\equiv}^\dagger + \delta \hat{a}_{n,m,\equiv}^\dagger, \quad (70)$$

where $\rho = N/M_x$ and $\alpha_{m,\equiv}$ and $\alpha_{m,\equiv}^\dagger$ are complex numbers of the order $1/\sqrt{M_y}$ and the δ terms are of order $1/\sqrt{M_x M_y}$. In contrast to the usual quantum Bogoliubov approach, here we need to consider the left and right sides of the evolution operator and, in addition, $\alpha_{m,\equiv}^\dagger$ is not necessarily the complex conjugate of $\alpha_{m,\equiv}$ [59].

We substitute Eqs. (69) and (70) into Eqs. (10)–(13) and expand in orders of the δ terms. Following standard Bogoliubov theory [54], we use the normally ordered form Eq. (19) before the substitution. To zeroth order, we have $1 = \sum_{m,d} \alpha_{m,d}^\dagger \alpha_{m,d}$ and Eqs. (10)–(12) can be made to equal zero by putting $\alpha_{m,\equiv}^\dagger = 1$. Independently, they can also be made to equal zero by putting $\alpha_{m,\equiv} \propto (U_{0,\equiv})_{1,m}$ but leaving the population difference ϕ unspecified. See Appendix B for details. Inserting these solutions into the final equation (13) and requiring the right-hand factor to equal zero, we have

$$\exp\left[\frac{1}{2}\beta'_y \rho(1+\phi)\right] \alpha_{m,\leftarrow} = \exp\left[\frac{1}{2}\beta'_y \rho(1-\phi)\right] \alpha_{m,\rightarrow}, \quad (71)$$

where $\phi = \sum_m \alpha_{m,\rightarrow} - \sum_m \alpha_{m,\leftarrow}$. Summing over m and rearranging, we find

$$\tanh\left[\frac{1}{2}\beta'_y \rho \phi\right] - \phi = 0. \quad (72)$$

If $\beta'_y \rho < 2$, the only solution to Eq. (72) is $\phi = 0$ and the particles are evenly distributed between the two orientations. However, if $\beta'_y \rho > 2$, we have two additional $\phi \neq 0$ solutions (symmetric about $\phi = 0$) given by the implicit equation

$$\beta'_y \rho = \frac{1}{\phi} \ln\left(\frac{1+\phi}{1-\phi}\right). \quad (73)$$

It is possible to show by expanding to quadratic order in the δ terms that only the $\phi \neq 0$ solutions are stable above the $\beta'_y \rho > 2$ threshold (see Appendix B). The relation between $\beta'_y \rho \geq 2$ and $\phi \neq 0$ is shown in Fig. 4. From Eq. (1), we

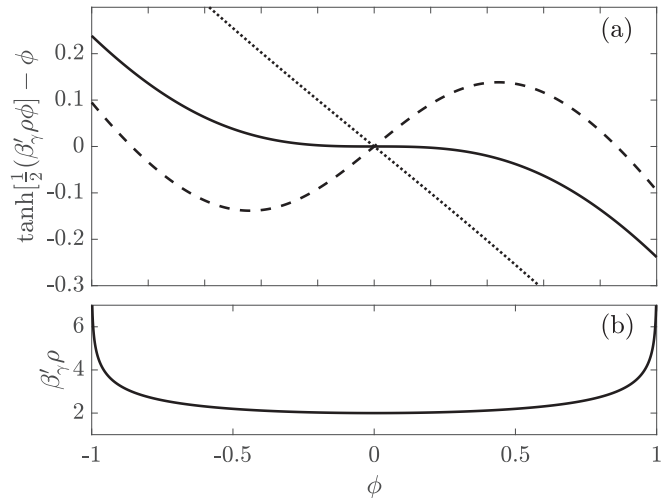


FIG. 4. Panel (a) shows $\tanh[\frac{1}{2}\beta'_y \rho \phi] - \phi$, which has nonzero solutions only when $\beta'_y \rho > 2$. The lines correspond to $\beta'_y \rho = 1$ (dotted line), $\beta'_y \rho = 2$ (solid), and $\beta'_y \rho = 3$ (dashed). Panel (b) shows $\beta'_y \rho$ as a function of ϕ .

conclude that in the symmetric case where $\Delta W = 0$ a net drift in the mechanical coordinate is a possibility above the threshold $\beta'_y \rho > 2$.

We are now in a position to link this lattice model to continuous macroscopic field theories or hydrodynamic treatments of active matter by coarse graining [26]. Let us assume that we are close to the steady state and that the system is confined to the ground chemical state, yet still exhibits some long-range ($x \gg \ell$) spatial variation. Based on the above mean-field treatment, we can make the substitution $\hat{a}_{n,m,d}^\dagger(t) \rightarrow 1$ and $\hat{a}_{n,m,d}(t) \rightarrow (U_{0,d})_{1,m} p_{n,d}(t)$ in the “Heisenberg equations” for $\hat{n}_{n,m,d}$ (see Appendix E), where $p_{n,d}(t)$ is the n th site population. Then, putting $x = \ell n$ and making the coarse-grain approximation $\ell \rightarrow 0$ such that $p_{n,d}(t) \rightarrow \rho_d(t, x)$ become continuous functions of x , we can write

$$\begin{aligned} \frac{\partial \rho}{\partial t} &= -v_+^x \frac{\partial \rho}{\partial x} - v_-^x \frac{\partial m}{\partial x} + D_+ \frac{\partial^2 \rho}{\partial x^2} + D_- \frac{\partial^2 m}{\partial x^2}, \\ \frac{\partial m}{\partial t} &= -v_-^x \frac{\partial \rho}{\partial x} - v_+^x \frac{\partial m}{\partial x} + D_- \frac{\partial^2 \rho}{\partial x^2} + D_+ \frac{\partial^2 m}{\partial x^2} \\ &\quad + 2\gamma e^{\frac{1}{2}\beta'_y \rho} \left\{ \rho \sinh\left[\frac{1}{2}\beta'_y m\right] - m \cosh\left[\frac{1}{2}\beta'_y m\right] \right\}, \end{aligned} \quad (74)$$

where $\rho(x, t) \equiv \rho_{\rightarrow}(x, t) + \rho_{\leftarrow}(x, t)$ and $m(x, t) \equiv \rho_{\rightarrow}(x, t) - \rho_{\leftarrow}(x, t) = \rho(x, t)\phi(x, t)$. In Eqs. (74) and (75), we have defined the variables $v_{\pm}^x = \frac{\ell}{2}(r_{\rightarrow}^x \pm r_{\leftarrow}^x)$, $D_{\pm} = \frac{\ell^2}{4}[\kappa_{\rightarrow} \pm \kappa_{\leftarrow}]$, where

$$\kappa_d = \chi^+ + \chi^- + \Xi_d^+ + \Xi_d^- \quad (76)$$

in terms of the underlying microscopic system parameters.

If $\Delta W = 0$, then $v_+^x = 0$ and $D_- = 0$ and Eqs. (74) and (75) become very similar to the mean-field equations used previously to describe the flocking transition of active spins [26]. In the present case, the parameters of the mean-field model are determined by the underlying chemomechanical model. Thus, we can explore efficiency, entropy production, and collective

behavior in our system. The mean-field equation for the “magnetism” $m(x, t)$ in Eq. (2) of Ref. [26] differs from Eq. (75) in that the argument of sinh and cosh functions in Ref. [26] is $m(x, t)/\rho(x, t)$ rather than just $m(x, t)$ —which in our case arises from the assumed form of the alignment interactions [Eq. (18)]. Interestingly, in contrast to the results here and in the next section, via numerical solutions of their mean-field equations, Ref. [26] found that large fluctuations prevent spontaneous symmetry breaking in the thermodynamic limit in 1D. We do not solve the mean-field equations (74) and (75) here but instead consider an alternative mean-field approach that enables us to investigate the transition and local number fluctuations in more detail.

B. Decoupling mean-field approach

The Bogoliubov treatment contrasts markedly with the no-hopping case, suggesting that it only holds in the limit of large hopping. To treat the more general case, we consider a decoupling mean-field [61–63] or Gutzwiller wave function approach for classical identical particles [64]. In this approach, the steady state is approximated as the product of single-site states

$$|P_0\rangle = \prod_{n=1}^{M_x} |p_0\rangle_n, \quad \langle Q_0| = \prod_{n=1}^{M_x} \langle q_0|_n. \quad (77)$$

An effective single-site evolution operator is found by averaging over the operators acting on neighboring sites

$$\hat{\mathcal{L}}_n^{\text{eff}} = \prod_{n \neq j} \langle q_0|_j \hat{\mathcal{L}}_R \prod_{n \neq j'} |p_0\rangle_{j'}. \quad (78)$$

In the steady state, each site is in an identical state and we can drop the n index and also write $\alpha_{m,d} = \langle \hat{a}_{m,d} \rangle / \sqrt{\rho}$ and $\alpha_{m,d}^\dagger = \langle \hat{a}_{m,d}^\dagger \rangle / \sqrt{\rho}$ and the effective evolution operator becomes

$$\begin{aligned} \hat{\mathcal{L}}_{\text{eff}} = & \sum_d \hat{a}_d^\dagger K_d \hat{a}_d + \langle \hat{a}_d^\dagger K_d \hat{a}_d \rangle + \sqrt{\rho} (\hat{a}_d^\dagger O_d \alpha_d + \alpha_d^\dagger O_d \hat{a}_d) \\ & + \gamma (\hat{a}_{\leftarrow}^\dagger - \hat{a}_{\rightarrow}^\dagger) (e^{\beta_\gamma \hat{n}_{\leftarrow}} \hat{a}_{\rightarrow} - e^{\beta_\gamma \hat{n}_{\rightarrow}} \hat{a}_{\leftarrow}), \end{aligned} \quad (79)$$

where $\hat{a}_d = [\hat{a}_{1,d}, \hat{a}_{2,d}, \hat{a}_{1,d}]^T$ and $\alpha_d = [\alpha_{1,d}, \alpha_{2,d}, \alpha_{1,d}]^T$. The matrices are given by

$$(K_d)_{i,j} = Y_{i,j} - (\chi^+ + \chi^-) \delta_{i,j} + (Z_{0,d})_{i,i} \delta_{i,j}, \quad (80)$$

$$(O_d)_{i,j} = \begin{cases} (Z_{0,d})_{i,j}, & i \neq j, \\ \chi^+ + \chi^-, & i = j, \end{cases} \quad (81)$$

such that $O_d + K_d = L_{0,d}$. There is some arbitrariness in defining the effective evolution operator because of the constant terms arising from the other sites. Here, we have included enough constant terms to ensure that $\hat{\mathcal{L}}_{\text{eff}}$ leads to stable evolution and has a steady state.

Using the decoupling approximation, it follows that the steady-state average of an operator of the form $\hat{O} = \prod_n \hat{o}_n$ is

$$\langle \hat{O} \rangle_{\text{ss}} = \langle Q_0 | \hat{O} | P_0 \rangle = \prod_{n=1}^{M_x} \langle q_0 |_n \hat{o}_n | p_0 \rangle_n, \quad (82)$$

where (dropping the n index) the left and right ground states of a single site are given by

$$\langle q_0 | \hat{\mathcal{L}}^{\text{eff}} = 0, \quad (83)$$

$$\hat{\mathcal{L}}^{\text{eff}} | p_0 \rangle = 0. \quad (84)$$

As $\hat{\mathcal{L}}^{\text{eff}}$ also depends on $\langle q_0 |$ and $| p_0 \rangle$ via the parameters α_d and $\alpha_d^\dagger$, Eqs. (83) and (84) need to be solved self-consistently.

The single-site evolution operator $\hat{\mathcal{L}}^{\text{eff}}$ does not conserve particle number. Based on this and the results from the Bogoliubov treatment in Sec. VIA, we make the ansatz that the left eigenstate, $\langle q_0 |$, is given by the (unnormalized) coherent state

$$\langle q_0 | = \langle \{0\} | \exp \left[\sqrt{\rho} \sum_{d,m} \alpha_{m,d}^\dagger \hat{a}_{m,d} \right], \quad (85)$$

such that $\langle q_0 | \hat{a}_{m,d}^\dagger = \sqrt{\rho} \langle q_0 | \alpha_{m,d}^\dagger$. If this is true, then $\langle \hat{a}_d^\dagger K_d \hat{a}_d \rangle = \rho \alpha_d^\dagger K_d \alpha_d$ and we can write

$$\begin{aligned} \langle q_0 | \hat{\mathcal{L}}_{\text{eff}} = & \sqrt{\rho} \sum_d \langle q_0 | \alpha_d^\dagger L_{0,d} (\hat{a}_d + \alpha_d) \\ & + \gamma \langle q_0 | (\alpha_{\leftarrow}^\dagger - \alpha_{\rightarrow}^\dagger) (e^{\beta_\gamma \hat{n}_{\leftarrow}} \hat{a}_{\rightarrow} - e^{\beta_\gamma \hat{n}_{\rightarrow}} \hat{a}_{\leftarrow}), \end{aligned} \quad (86)$$

where we have used Eqs. (80) and (81). Since the elements of the zeroth left eigenstate of $L_{0,d}$ are $(U_{0,d}^{-1})_{1,m}$, we can confirm that Eq. (85) is the left-hand steady state if $\alpha_{m,d}^\dagger \propto (U_{0,d}^{-1})_{1,m} = 1$ and $\alpha_{m,\rightarrow}^\dagger = \alpha_{m,\leftarrow}^\dagger$.

We can now also write the effective evolution operator as

$$\begin{aligned} \hat{\mathcal{L}}_{\text{eff}} = & \sum_d \hat{a}_d^\dagger L_d \hat{a}_d + \rho L_d \alpha_d - (\hat{a}_d^\dagger - \sqrt{\rho}) O_d (\hat{a}_d - \sqrt{\rho} \alpha_d) \\ & + \gamma (\hat{a}_{\leftarrow}^\dagger - \hat{a}_{\rightarrow}^\dagger) (e^{\beta_\gamma \hat{n}_{\leftarrow}} \hat{a}_{\rightarrow} - e^{\beta_\gamma \hat{n}_{\rightarrow}} \hat{a}_{\leftarrow}). \end{aligned} \quad (87)$$

Diagonalizing L_d by the transformation Eqs. (60) and (61) and operating to the right on $| p_0 \rangle$, we see that the first term will be zero only if all the population is in the $l = 1$ mode for each orientation. Then, similar to Sec. V, we drop all other modes ($l \neq 1$) and make the replacement $\hat{a}_{m,d} \rightarrow (U_{0,d})_{1,m} \hat{A}_d$ and $\hat{a}_{m,d}^\dagger \rightarrow (U_{0,d}^{-1})_{m,1} \hat{A}_d^\dagger = \hat{A}_d^\dagger$. We can now write the left-hand ground state as

$$\langle q_0 | = \langle \{0\} | e^{\sqrt{\rho}(\hat{A}_{\leftarrow} + \hat{A}_{\rightarrow})} \quad (88)$$

and the long-time evolution operator as

$$\begin{aligned} \hat{\mathcal{L}}_{\text{LT}}^{\text{eff}} = & -\kappa_{\rightarrow} (\hat{A}_{\rightarrow}^\dagger - \sqrt{\rho}) (\hat{A}_{\rightarrow} - \frac{1}{2} \sqrt{\rho} [1 + \phi]) \\ & - \kappa_{\leftarrow} (\hat{A}_{\leftarrow}^\dagger - \sqrt{\rho}) (\hat{A}_{\leftarrow} - \frac{1}{2} \sqrt{\rho} [1 - \phi]) \\ & + \gamma (\hat{A}_{\leftarrow}^\dagger - \hat{A}_{\rightarrow}^\dagger) (e^{\beta_\gamma \hat{n}_{\leftarrow}} \hat{A}_{\rightarrow} - e^{\beta_\gamma \hat{n}_{\rightarrow}} \hat{A}_{\leftarrow}), \end{aligned} \quad (89)$$

where the effective hopping rates κ_d are given by Eq. (76). In Eq. (89), we have used the fact that $\langle \hat{A}_{\leftarrow}^\dagger \hat{A}_{\leftarrow} \rangle = \sqrt{\rho} \langle \hat{A}_{\leftarrow} \rangle = \frac{1}{2} \sqrt{\rho} (1 \pm \phi)$ to write the evolution operator in terms of the relative population difference ϕ . Note that in contrast to the no-hopping case in Sec. V, Eq. (88) implies that the symmetric mode $\frac{1}{\sqrt{2}} (\hat{A}_{\rightarrow} + \hat{A}_{\leftarrow})$ has nonzero number fluctuations. Nonzero number fluctuations naturally arise for $\kappa_d > 0$ (see Appendix D). This does mean, however, that the Gutzwiller approximation is not valid in the $\kappa_d \rightarrow 0$ limit.

Evaluating the steady-state current $\langle j_{n,m,\rightarrow}^x \rangle_{ss}$, using Eq. (82) it is straightforward to show (see Appendix C) that the drift per particle in the mechanical and chemical degrees of freedom has the same form as Eqs. (1) and (2) with $\phi = (\langle \hat{A}_{\rightarrow} \rangle - \langle \hat{A}_{\leftarrow} \rangle) / \sqrt{\rho}$. Other interesting observables are the steady-state two-body correlation functions defined by Eqs. (67) and (68).

In the case where $\beta_\gamma = 0$, it is straightforward to show that

$$|p_0\rangle \propto e^{\sqrt{\rho}(\hat{A}_{\rightarrow}^\dagger + \hat{A}_{\leftarrow}^\dagger)} | \{0\} \rangle \quad (90)$$

such that $\langle \hat{A}_{\rightarrow} \rangle = \langle \hat{A}_{\leftarrow} \rangle = \sqrt{\rho}$. Thus, in the $\beta_\gamma = 0$ case, $\phi = 0$ as we found previously in Sec. IV.

If $\beta_\gamma \neq 0$, then $|p_0\rangle$ needs to be determined numerically. We present a numerical method to solve for $|p_0\rangle$ below. First, the state for a single site is expanded in terms of the number states of the modes $\hat{A}_d$ for each orientation, as

$$|p_0\rangle = \sum_{n_{\rightarrow}, n_{\leftarrow}} c^{n_{\rightarrow}, n_{\leftarrow}} |n_{\rightarrow}, n_{\leftarrow}\rangle. \quad (91)$$

The unknown coefficients $c^{n_{\rightarrow}, n_{\leftarrow}}$ can be determined by the following numerical procedure. We consider the effective evolution operator to be a function of the parameter ϕ . We define $|\tilde{p}_0(\phi)\rangle$ by

$$\hat{\mathcal{L}}_{\text{eff}}^{\text{LT}}(\phi) |\tilde{p}_0(\phi)\rangle = \lambda_1(\phi) |\tilde{p}_0(\phi)\rangle, \quad (92)$$

$$\langle q_0 | \tilde{p}_0(\phi) \rangle = 1, \quad (93)$$

where $\text{Re}\{\lambda_1(\phi)\} \leq 0$ is the lowest magnitude eigenvalue. We then need to find the ϕ that minimizes

$$\delta_f = |\sqrt{\rho}(1 + \phi)/2 - \langle q_0 | \hat{A}_{\rightarrow} | \tilde{p}_0(\phi) \rangle|. \quad (94)$$

The result of this minimization gives us $|p_0\rangle$ and the corresponding ϕ . This one-variable minimization process can be solved by standard methods. To avoid the optimization getting stuck in a local minimum, we seed the minimization with both a positive and a negative initial value and take the result that yields the eigenvalue with the smallest magnitude. This algorithm yields a solution in a few minutes on a desktop workstation for medium values of the β'_γ parameter and number states truncated at $n_d < 24$.

Let us first consider the case where $\Delta W = 0$ and there is no preferred particle orientation ($\kappa_{\rightarrow} = \kappa_{\leftarrow}$). In Fig. 5, we show ϕ and the normalized correlation functions g_{ij} [see Eqs. (67) and (68)] in the ground state as a function of increasing $\beta'_\gamma \rho$ in the case $\kappa_d/\gamma \gg 1$ where we expect the Bogoliubov approximation to hold. Similar to the Bogoliubov results, we see ϕ develops a finite value once $\beta'_\gamma \rho \gtrsim 2$. Note that for $\kappa_{\rightarrow} = \kappa_{\leftarrow}$ the sign of ϕ is random as there is no preferred direction of alignment. $g_{ij} \approx 1$ for all i and j until the transition—which is the regime where the Bogoliubov treatment is expected to hold. As $\beta'_\gamma \rho$ increases beyond the transition, $g_{\rightarrow\rightarrow}$ tends to 1 similar to a coherent state, while $g_{\leftarrow\leftarrow} > 1$ grows large. Strong anticorrelations between the two orientations are also observed.

In Fig. 6, we show $|\phi|$ as a function of both $\beta'_\gamma \rho$ and $\kappa_{\rightarrow} = \kappa_{\leftarrow}$. This figure shows that as hopping between sites decreases relative to the flip interaction, there is a region where $\phi = 0$ far above the threshold $\beta'_\gamma \rho \gtrsim 2$. This dependence of the collective alignment (i.e., flock transition) on

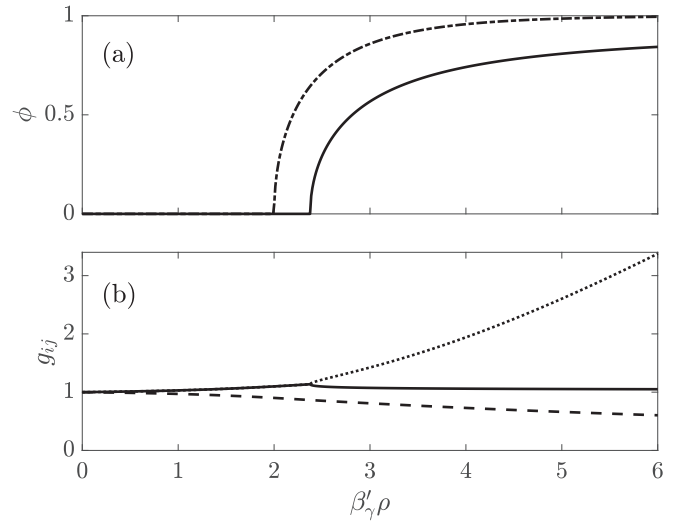


FIG. 5. Panel (a) shows ϕ as a function of increasing $\beta'_\gamma \rho$ in the large $\kappa_{\rightarrow} = \kappa_{\leftarrow}$ limit. In this figure, we only show the $\phi > 0$ case. The Bogoliubov result is shown by a dash-dotted line for comparison. Panel (b) shows $g_{\rightarrow\rightarrow}$ (solid line), $g_{\leftarrow\leftarrow}$ (dotted line), and $g_{\rightarrow\leftarrow}$ (dashed line). In this plot, $\rho = 2$ and $\kappa_{\rightarrow} = \kappa_{\leftarrow} = 30\gamma$.

hopping between sites is one of the key results of this paper and is not predicted by the usual Bogoliubov-type mean-field treatment [26,27,46]. The reason for this is that the Bogoliubov treatment assumes that hopping creates correlations between the sites and number fluctuations are small; however, as seen in Sec. V, the alignment interactions compete with the hopping. In fact, in the small hopping regime, the number fluctuations become large [e.g., $g_{dd} \gg 1$], and the Bogoliubov approximation becomes invalid. For example, in Fig. 7 we see that for large hopping $V(n_{\rightarrow} - n_{\leftarrow}) \approx \rho$ and the Bogoliubov treatment is a reasonable approximation, whereas for small hopping, $V(n_{\rightarrow} - n_{\leftarrow}) \gg \rho$. In this region, $V(n_{\rightarrow} - n_{\leftarrow})$ resembles the no-hopping case of Sec. V.

In Fig. 8, we plot $\phi > 0$ and g_{ij} as a function of $\kappa_{\rightarrow} = \kappa_{\leftarrow}$ keeping $\beta'_\gamma \rho = 4$ constant. This shows that for small κ_d the

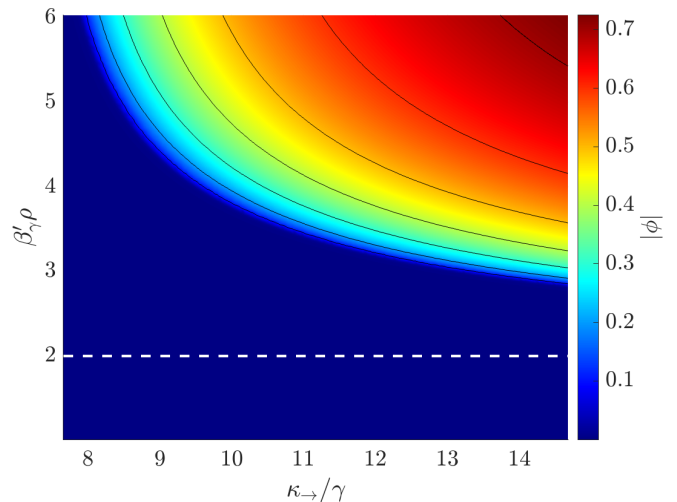


FIG. 6. $|\phi|$ as a function of $\beta'_\gamma \rho$ and $\kappa_{\rightarrow} = \kappa_{\leftarrow}$. In this plot, $\rho = 2$ and the white dotted line is the Bogoliubov threshold.

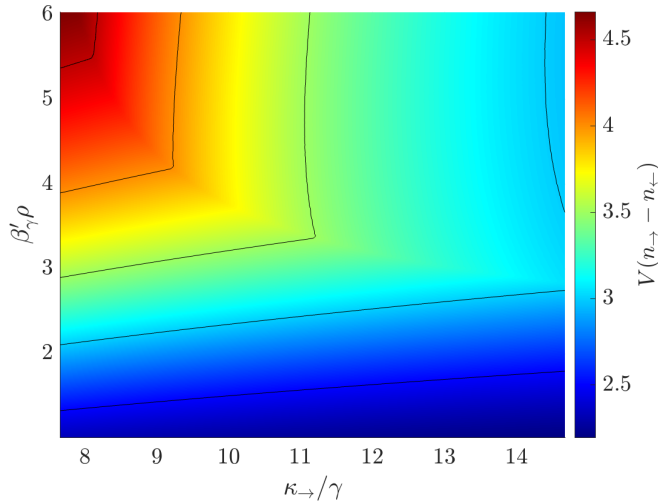


FIG. 7. $V(n_{\rightarrow} - n_{\leftarrow})$ as a function of $\beta'_\gamma \rho$ and $\kappa_{\rightarrow}$. In this plot, $\rho = 2$ and we have only shown the $\phi > 0$ case.

state of the system is similar to the no-hopping case studied in Sec. V: $\phi = 0$, large number fluctuations ($g_{dd} > 1$), and anticorrelated orientations ($g_{\rightarrow\leftarrow} < 1$). As $\kappa_{\rightarrow} = \kappa_{\leftarrow}$ increases, the system gains an asymmetry due to spontaneous particle alignment until it fully localizes in one of the orientations for large κ_d . The number fluctuations of the $\rightarrow$ mode then tend back toward those of a coherent state.

Both the passive mechanical hopping and chemomechanical coupling rates contribute to κ_d [see Eq. (76)]. Thus, collective alignment behavior (i.e., $\phi \neq 0$) is not reliant on chemomechanical coupling. It will arise as long as κ_d/γ is sufficiently large. This is one of the key findings of this paper and follows directly from the fact that both alignment interactions and a sufficiently high hopping rate are required for the transition. By explicitly separating passive mechanical and chemomechanical hopping, as we have done here, we can see

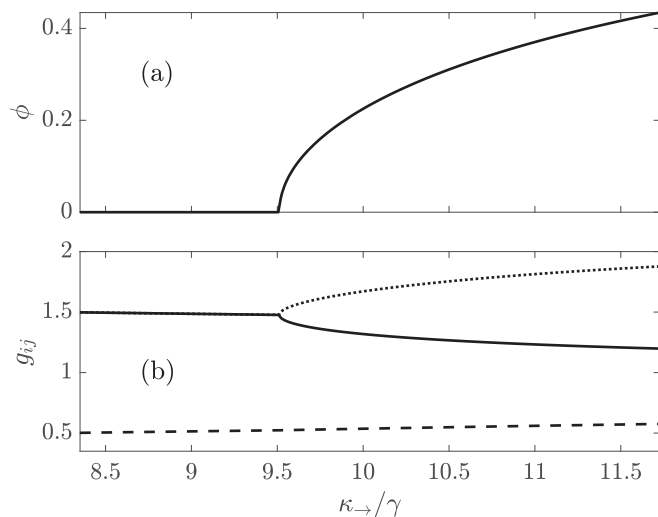


FIG. 8. Panel (a) shows ϕ as a function of $\kappa_{\rightarrow} = \kappa_{\leftarrow}$. In this figure, we only show the $\phi > 0$ case. Panel (b) shows $g_{\rightarrow\rightarrow}$ (solid line), $g_{\leftarrow\leftarrow}$ (dotted line), and $g_{\rightarrow\leftarrow}$ (dashed line). In this plot, $\rho = 2$ and $\beta'_\gamma \rho = 4$.

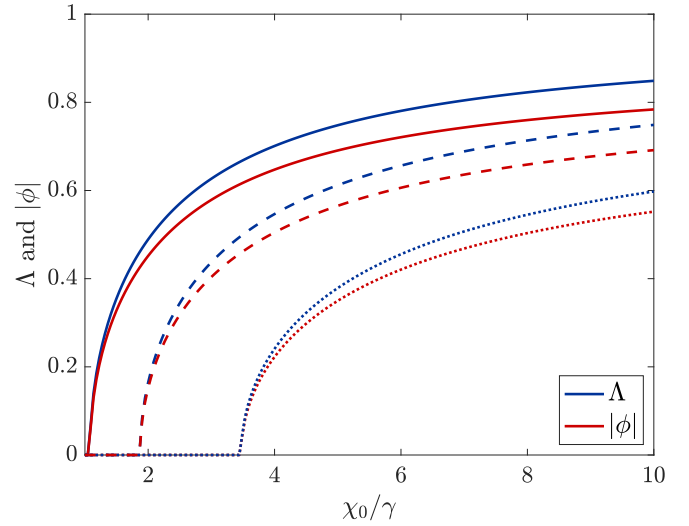


FIG. 9. Efficacy Λ (blue lines) and $|\phi|$ (red lines) as a function of χ_0/γ for $\beta'_\gamma \rho = 6$ (solid lines), $\beta'_\gamma \rho = 4$ (dashed lines), and $\beta'_\gamma \rho = 3$ (dotted lines). Other parameters are $\zeta_{12}^0 = 2\gamma$, $\zeta_{2,3}^0 = \zeta_{3,1}^0 = \gamma$, $v_{1,2}^0 = v_{2,3}^0 = v_{1,2}^0 = 0.1\gamma$, $\Delta\mu = -3k_bT$, $\Delta W = 0$, and $\rho = 2$. For these parameters, $\kappa_{\rightarrow} = \kappa_{\leftarrow}$ varies linearly from $\sim 7.8\gamma$ to $\sim 25\gamma$.

that chemomechanical coupling transitions are not necessary for collective alignment.

This result has an interesting impact on the efficacy of conversion of the chemical process into mechanical motion, Λ . From Eq. (52), it is obvious that futile chemical reactions lower the efficacy. The impact of passive mechanical coupling is less obvious as Λ is also determined by the alignment of particles. In fact, as the alignment is determined by both the chemomechanical coupling and the passive hopping, it is possible to increase Λ by increasing the passive hopping. In Fig. 9, we show the efficacy as a function of χ_0 keeping the other rates constant. For χ_0 small, the chemomechanical coupling rates, while much larger than the futile chemical rates, are not sufficient to result in alignment of particles; however, as χ_0 increases, κ_d increases and the efficacy is largely dictated by the value of ϕ .

When $\Delta W \neq 0$, $\kappa_{\rightarrow} \neq \kappa_{\leftarrow}$ and the left-right symmetry between is broken. In this case, the system will have a preferred orientation. Due to the complex interactions between hopping and particle-particle interactions, the relationship between the preferred orientation and κ_d is not obvious. In Fig. 10, we show the result of numerical solutions for the steady state. For small $\kappa_{\rightarrow} \approx \kappa_{\leftarrow}$, similar to the no-hopping case in Sec. V, $\phi = 0$ and the particles in the two orientations are highly anticorrelated and have large number fluctuations. For larger κ_d , there are three regimes. If $\kappa_{\rightarrow} \approx \kappa_{\leftarrow}$ is sufficiently large, then, as there is no preferred direction, the system randomly chooses $\phi > 0$ or $\phi < 0$ as discussed previously. For $\kappa_{\leftarrow} \gg \kappa_{\rightarrow}$, the system chooses $\phi > 0$, and $\kappa_{\leftarrow} \ll \kappa_{\rightarrow}$ results in $\phi < 0$.

As $\Delta W > 0$ implies $\kappa_{\leftarrow} \gg \kappa_{\rightarrow}$ where $\phi > 0$, we have the interesting outcome that the particles prefer to align uphill (i.e., in the direction of the smaller κ_d). This is another key result of this paper that has not been previously reported in the literature. In the absence of nonlinearity, we would expect the opposite. A possible physical mechanism for this result

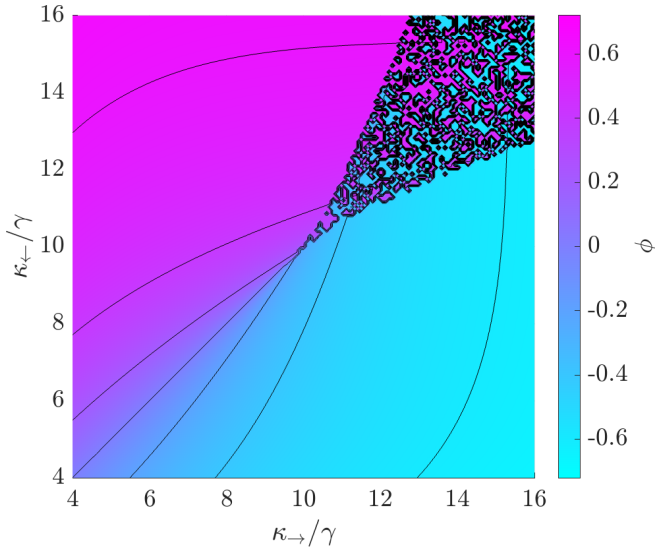


FIG. 10. Order parameter ϕ as a function of $\kappa_{\rightarrow}$ and $\kappa_{\leftarrow}$, $\beta'_\gamma \rho = 4$.

is as follows. Hopping of left-oriented particles between sites due to a large $\kappa_{\leftarrow}$ tends to give rise to number fluctuations $g_{\leftarrow\leftarrow} \sim 1$, whereas the right-oriented particles, due to small $\kappa_{\rightarrow}$, mostly only experience orientation flips, which tends to create greater number fluctuations ($g_{\rightarrow\rightarrow} > 1$). These greater fluctuations, in turn, lead to more particles aligning to the right. This interpretation is supported by dynamical simulations of a small periodic system of three sites with hopping (see Appendix D).

The spontaneous emergence of $\phi > 0$ has interesting consequences for the efficiency in the case $\Delta W > 0$. Below the transition point, $r_x < 0$, so there is no work done. Above the transition point, the population prefers to orient itself uphill. If in addition $r_{x,\rightarrow} > 0$ (for $\Delta W > 0$), then the system can convert chemical energy to work.

In Fig. 11, we show the efficiency and entropy generation rate as a function of the opposing mechanical force. In this example, the chemomechanical coupling rates are large compared to the futile chemical reaction and the passive mechanical hopping rates, i.e., the tight-coupling limit. Efficiency (entropy generation rate) will decrease (increase) even further as these loss processes increase. We see that incomplete particle alignment, futile chemical reactions, and passive mechanical hopping rates all reduce efficiency. As expected, entropy generation is minimized when $\eta = 0$ for a finite opposing force.

When ΔW is small, similar to Fig. 10, ϕ can randomly take on negative values. In this case, $r_x < 0$ and the efficiency cannot be defined. This explains the missing values in Fig. 11(b) when $\Delta \bar{W} < 0.7$. In these cases, the particles all flow downhill, and the entropy generation is large [see points with $\sigma/\gamma k_B > 150$ in Fig. 11(c)] as all the chemical energy is simply dissipated as heat rather than used to produce work. For $\beta'_\gamma \rho < 2$, $\phi = 0$. As a consequence, efficiency is zero and entropy generation monotonically increases with ΔW . In Fig. 12, we also show the well-known trade-off between mechanical power and efficiency [65]. In contrast to

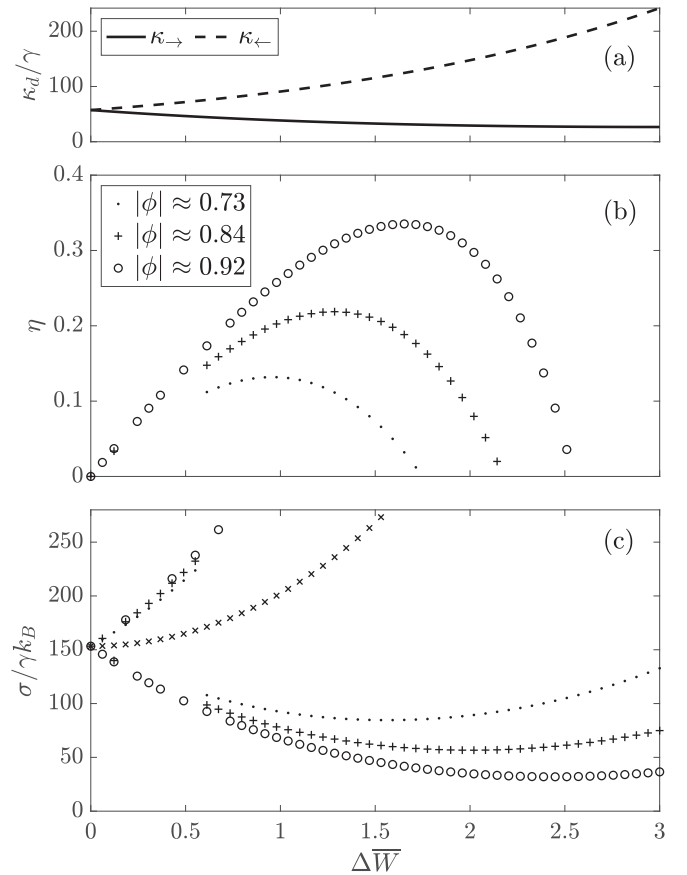


FIG. 11. κ_d [panel (a)], efficiency [panel (b)], and entropy generation rate [panel (c)] as a function of opposing mechanical force $\Delta \bar{W} = \Delta W/k_B T$. In panels (b) and (c), we show values for $\beta'_\gamma \rho = 6$ (o), $\beta'_\gamma \rho = 4$ (+), $\beta'_\gamma \rho = 3$ (·), and $\beta'_\gamma \rho = 0.4$ (×). Other parameters are $\chi_0 = v_{1,2}^0 = v_{2,3}^0 = v_{3,1}^0 = 0.001\gamma$, $\zeta_{1,2}^0 = 20\gamma$, $\zeta_{2,3}^0 = \zeta_{3,1}^0 = 10\gamma$, $\Delta\mu = -3k_B T$, and $\rho = 2$.

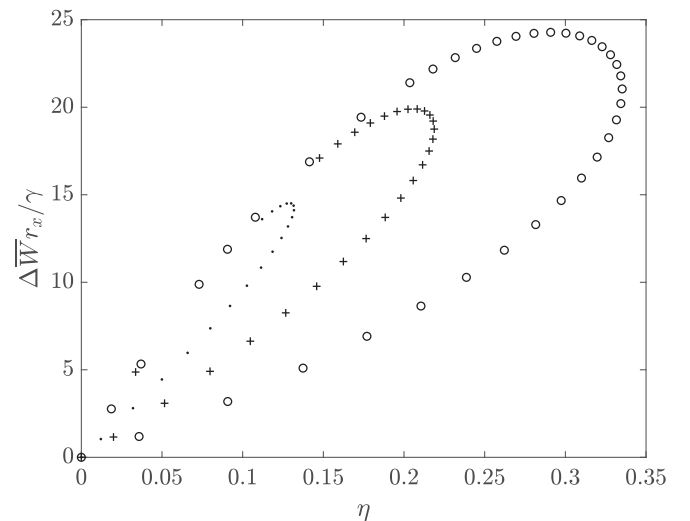


FIG. 12. Mechanical output power $\Delta W r_x$ vs efficiency. Parameters are the same as Fig. 11.

the single-molecule results, we show how collective effects impact this trade-off.

As noted in Sec. IV, a finite opposing mechanical force ($\Delta W > 0$) results in an unequal chemical drift for each particle orientation ($r_{y,\rightarrow} \neq r_{y,\leftarrow}$). Above the threshold ($\phi > 0$), this results in a reduction in the overall magnitude of the collective chemical drift $|r_y|$. Thus, the magnitude of the chemical reaction rate also depends on the outcome of the spontaneous collective effect.

VII. CONCLUSION

We have investigated the nonequilibrium state of a simple 1D lattice model of oriented Brownian particles with an explicit coupling to a chemical degree of freedom and an external macroscopic force. This model provides insights into the relationship between the emergence of collective behavior, the chemomechanical conversion process, and the development of macroscopic forces in active matter. The steady-state drift and number fluctuations of this model are explored in all parameter regimes. Especially interesting results are given as follows: (1) Collective alignment requires both sufficiently large alignment interactions and hopping; (2) collective alignment of particles does not require chemomechanical coupling and can occur with passive hopping alone; and (3) for the alignment interactions considered here [see Eq. (18)], if chemomechanical coupling is present, particles will spontaneously align uphill against the macroscopic force and production of work. These features have interesting consequences for active matter and its relation to living matter. In particular, (3) provides a mechanism for active matter to spontaneously produce macroscopic forces on its environment.

Our work points the way for a number of interesting future directions. The coarse-grained mean-field equations [Eqs. (74) and (75)] of the 1D model could be extended to 2D using the approach used in Refs. [26,27] to make a connection to hydrodynamic treatments and experiments while still retaining the chemical coupling elements. It would also be interesting to explore the nature of the changes in the phase transition [26] that occur with $\Delta W \neq 0$. In addition, the lattice model could be extended to include repulsive particle-particle interactions to explore the impact of blocking effects [27,45,58,59]. Here, we showed that an externally imposed force can alter the chemical reaction rate and efficiency; we expect that blocking interactions will have a similar effect. Other types of alignment interactions could also be investigated. Here, we show that a specific type of alignment interaction [i.e., Eq. (18)] leads to particles spontaneously aligning uphill against an opposing force. It would be interesting to see whether this behavior is universal or specific to this case. Finally, as we have formulated this system using creation and annihilation operators for classical identical particles, there are interesting parallels with quantum many-body systems that may enable a deeper physical understanding of active matter. This formulation also enables the use of powerful theoretical tools from quantum theory beyond those explored here such as perturbative expansions of observable quantities [53].

DATA AVAILABILITY

The data that support the findings of this article are openly available [66].

APPENDIX A: NO-HOPPING CASE

It is useful to write the evolution operator in Eq. (63) in terms of the Jordan-Schwinger angular momentum representation

$$\hat{\mathcal{L}} = \gamma e^{\frac{1}{2}\beta_\gamma N} \left[\left(\hat{J}_+ - \frac{N}{2} + \hat{J}_z \right) e^{\beta_\gamma \hat{J}_z} + \left(\hat{J}_- - \frac{N}{2} - \hat{J}_z \right) e^{-\beta_\gamma \hat{J}_z} \right], \quad (\text{A1})$$

where

$$\hat{J}_z = \frac{1}{2}(\hat{n}_\rightarrow - \hat{n}_\leftarrow), \quad (\text{A2})$$

$$\hat{J}_+ = \hat{A}_\rightarrow^\dagger \hat{A}_\leftarrow, \quad (\text{A3})$$

$$\hat{J}_- = \hat{A}_\leftarrow^\dagger \hat{A}_\rightarrow. \quad (\text{A4})$$

We also define $\hat{J}_x = \frac{1}{2}(\hat{J}_+ + \hat{J}_-)$ and $\hat{J}_y = \frac{1}{2i}(\hat{J}_+ - \hat{J}_-)$. A complete set of states are then given by the eigenstates of $\hat{J}^2 = \hat{J}_x^2 + \hat{J}_y^2 + \hat{J}_z^2$ and $\hat{J}_z$: $\hat{J}^2|j, m\rangle = j(j+1)|j, m\rangle$ and $\hat{J}_z|j, m\rangle = m|j, m\rangle$, where $j = \frac{N}{2}$. These states are related to the number states introduced in Sec. V by $|n_\rightarrow, N - n_\rightarrow\rangle = |j = N/2, m = n_\rightarrow - N/2\rangle$.

Defining the rotation operator about the y direction by $\hat{R}_y(\phi) = e^{-i\phi\hat{J}_y}$, we note the relations $\hat{R}_y^{-1}(\frac{\pi}{2})\hat{J}_x\hat{R}_y(\frac{\pi}{2}) = \hat{J}_z$, $\hat{R}_y^{-1}(\frac{\pi}{2})\hat{J}_z\hat{R}_y(\frac{\pi}{2}) = -\hat{J}_x$. Using these relations and definitions (A3) and (A4), it is straightforward to show that

$$\hat{R}_y^{-1}\left(\frac{\pi}{2}\right)(\hat{J}_\pm \pm \hat{J}_z)\hat{R}_y\left(\frac{\pi}{2}\right) = \hat{J}_z \pm \hat{J}_\mp, \quad (\text{A5})$$

$$\hat{R}_y^{-1}\left(\frac{\pi}{2}\right)(\hat{J}_\pm \mp \hat{J}_z)\hat{R}_y\left(\frac{\pi}{2}\right) = \hat{J}_z \pm \hat{J}_\pm. \quad (\text{A6})$$

Using the Baker-Campbell-Hausdorff formula, it is also possible to show that

$$e^{-k\hat{J}_z(\hat{J}_z \pm 1)}\hat{J}_\pm e^{k\hat{J}_z(\hat{J}_z \pm 1)} = e^{\mp 2k\hat{J}_z}\hat{J}_\pm, \quad (\text{A7})$$

where k is an arbitrary constant.

We are now in a position to prove Eqs. (65) and (66). In the angular momentum representation, these have the form

$$\langle Q_0 | = \langle j, j | \hat{R}_y^{-1}\left(\frac{\pi}{2}\right) = \frac{1}{2j} \sum_{m=-j}^j \binom{2j}{j+m}^{1/2} \langle j, m |, \quad (\text{A8})$$

$$|P_0\rangle = \mathcal{N} e^{\beta_\gamma \hat{J}_z} \hat{R}_y\left(\frac{\pi}{2}\right) |j, j\rangle, \quad (\text{A9})$$

where the normalization factor $\mathcal{N}$ is determined by $\langle Q_0 | P_0 \rangle = 1$ and we have used the Wigner small d -matrix to expand $\langle Q_0 |$ in the angular momentum states in Eq. (A8), which coincides

with Eq. (65). Operating to the left with $\hat{\mathcal{L}}$, we have

$$\langle Q_0 | \hat{\mathcal{L}} = \langle j, j | \hat{R}_y^{-1} \left(\frac{\pi}{2} \right) \hat{\mathcal{L}} \quad (\text{A10})$$

$$\propto \langle j, j | \hat{R}_y^{-1} \left(\frac{\pi}{2} \right) \left[\hat{J}_+ - \frac{N}{2} + \hat{J}_z \right] e^{\beta_\gamma \hat{J}_z} \\ + \langle j, j | \hat{R}_y^{-1} \left(\frac{\pi}{2} \right) \left[\hat{J}_- - \frac{N}{2} - \hat{J}_z \right] e^{-\beta_\gamma \hat{J}_z} \quad (\text{A11})$$

$$\propto \langle j, j | \left[\hat{J}_z - \frac{N}{2} + \hat{J}_- \right] \hat{R}_y^{-1} \left(\frac{\pi}{2} \right) e^{\beta_\gamma \hat{J}_z} \\ + \langle j, j | \left[\hat{J}_z - \frac{N}{2} - \hat{J}_- \right] \hat{R}_y^{-1} \left(\frac{\pi}{2} \right) e^{-\beta_\gamma \hat{J}_z}, \quad (\text{A12})$$

where the last line follows from Eqs. (A5) and (A6). As $\langle j, j | \hat{J}_z = j \langle j, j | = \frac{N}{2} \langle j, j |$ and $\langle j, j | \hat{J}_- = 0$, both terms in the last line vanish and $\langle Q_0 | \hat{\mathcal{L}} = 0$ as required.

Operating to the right with $\hat{\mathcal{L}}$, we have

$$\hat{\mathcal{L}} | P_0 \rangle \propto \hat{\mathcal{L}}^\gamma e^{\beta_\gamma \hat{J}_z^2} \hat{R}_y \left(\frac{\pi}{2} \right) | j, j \rangle \quad (\text{A13})$$

$$\propto \left[\hat{J}_+ - \frac{N}{2} + \hat{J}_z \right] e^{\beta_\gamma \hat{J}_z} e^{\beta_\gamma \hat{J}_z^2} \hat{R}_y \left(\frac{\pi}{2} \right) | j, j \rangle \\ + \left[\hat{J}_- - \frac{N}{2} - \hat{J}_z \right] e^{-\beta_\gamma \hat{J}_z} e^{\beta_\gamma \hat{J}_z^2} \hat{R}_y \left(\frac{\pi}{2} \right) | j, j \rangle \quad (\text{A14})$$

$$\propto e^{\beta_\gamma \hat{J}_z} e^{\beta_\gamma \hat{J}_z^2} \left[\hat{J}_- - \frac{N}{2} + \hat{J}_z \right] \hat{R}_y \left(\frac{\pi}{2} \right) | j, j \rangle \\ + e^{-\beta_\gamma \hat{J}_z} e^{\beta_\gamma \hat{J}_z^2} \left[\hat{J}_+ - \frac{N}{2} - \hat{J}_z \right] \hat{R}_y \left(\frac{\pi}{2} \right) | j, j \rangle \quad (\text{A15})$$

$$\propto e^{\beta_\gamma \hat{J}_z} e^{\beta_\gamma \hat{J}_z^2} \hat{R}_y \left(\frac{\pi}{2} \right) \left[\hat{J}_z - \frac{N}{2} - \hat{J}_+ \right] | j, j \rangle \\ + e^{-\beta_\gamma \hat{J}_z} e^{\beta_\gamma \hat{J}_z^2} \hat{R}_y \left(\frac{\pi}{2} \right) \left[\hat{J}_z - \frac{N}{2} + \hat{J}_+ \right] | j, j \rangle, \quad (\text{A16})$$

where the second line follows from Eq. (A7) and the third from Eqs. (A5) and (A6). As $\hat{J}_z | j, j \rangle = j | j, j \rangle = \frac{N}{2} | j, j \rangle$ and $\hat{J}_+ | j, j \rangle = 0$, both terms in the last line vanish and $\hat{\mathcal{L}} | P_0 \rangle = 0$ as required.

APPENDIX B: BOGOLIUBOV-LIKE TREATMENT

Making the substitution in Eqs. (69) and (70) and expanding to zeroth order in the δ modes, we have $\rho = \sum_{m,d} \alpha_{m,d}^\dagger \alpha_{m,d}$ and the evolution operator, Eq. (21), becomes

$$\hat{\mathcal{L}}_R^{(0)} = \sum_d \alpha_d^\dagger L_{0,d} \alpha_d + \gamma (\alpha_{\rightarrow}^\dagger - \alpha_{\leftarrow}^\dagger) \\ \times \left(e^{\frac{1}{2} \beta'_\gamma \rho (1+\phi)} \alpha_{\leftarrow} - e^{\frac{1}{2} \beta'_\gamma \rho (1-\phi)} \alpha_{\rightarrow} \right), \quad (\text{B1})$$

where $\sum_m \alpha_{m,\pm}^\dagger \alpha_{m,\pm} = (1 \pm \phi)$. It is now straightforward to see how this can be made equal to zero by the procedure described in Sec. VIA.

The terms first order in the δ modes vanish. Expanding the evolution operator, Eq. (21), to quadratic order in the δ modes and transforming to the k modes [mirroring Eqs. (33) and (34)]:

$$\delta \hat{b}_{k,l,d} = \frac{1}{\sqrt{M_x}} \sum_{n,m} (U_{k,d}^{-1})_{m,l} e^{-ikn} \delta \hat{a}_{n,m,d}, \quad (\text{B2})$$

$$\delta \hat{b}_{k,l,d}^\dagger = \frac{1}{\sqrt{M_x}} \sum_{n,m} (U_{k,d})_{l,m} e^{+ikn} \delta \hat{a}_{n,m,d}^\dagger, \quad (\text{B3})$$

the evolution operator can then be written as

$$\hat{\mathcal{L}}_R^{(2)} = \sum_{k,l} \delta b_{k,l}^\dagger M_{k,l} \delta b_{k,l}, \quad (\text{B4})$$

$$\delta b_{k,l} = [\delta \hat{b}_{k,l,\rightarrow}, \delta \hat{b}_{k,l,\leftarrow}, \delta \hat{b}_{-k,l,\rightarrow}, \delta \hat{b}_{-k,l,\leftarrow}], \quad (\text{B5})$$

$$\delta b_{k,l}^\dagger = [\delta \hat{b}_{k,l,\rightarrow}^\dagger, \delta \hat{b}_{k,l,\leftarrow}^\dagger, \delta \hat{b}_{-k,l,\rightarrow}^\dagger, \delta \hat{b}_{-k,l,\leftarrow}^\dagger], \quad (\text{B6})$$

where $M_{k,l}$ is a 4×4 matrix. The key nonzero elements are

$$M_{k,l}^{11} = \lambda_{k,l,\rightarrow} + M_{k,l}^{21}, \quad (\text{B7})$$

$$M_{k,l}^{21} = \delta_{k,0} \gamma e^{\frac{1}{2} \beta'_\gamma \rho} \left[\frac{1}{2} e^{\frac{1}{2} \beta'_\gamma \rho \phi} \beta'_\gamma \rho (1 - \phi) \delta_{1,l} - e^{-\frac{1}{2} \beta'_\gamma \rho \phi} \right], \quad (\text{B8})$$

$$M_{k,l}^{22} = \lambda_{k,l,\leftarrow} + M_{k,l}^{12}, \quad (\text{B9})$$

$$M_{k,l}^{12} = \delta_{k,0} \gamma e^{\frac{1}{2} \beta'_\gamma \rho} \left[\frac{1}{2} e^{-\frac{1}{2} \beta'_\gamma \rho \phi} \beta'_\gamma \rho (1 + \phi) \delta_{1,l} - e^{\frac{1}{2} \beta'_\gamma \rho \phi} \right]. \quad (\text{B10})$$

The 4×4 matrix M_{kl} has two nonzero eigenvalues and can be diagonalized to give

$$\hat{\mathcal{L}}_R^{(2)} = \sum_{k,l} (\Omega_{k,l,-} \delta \hat{c}_{k,l,-}^\dagger - \delta \hat{c}_{k,l,-} + \Omega_{k,l,+} \delta \hat{c}_{k,l,+}^\dagger + \delta \hat{c}_{k,l,+}), \quad (\text{B11})$$

where

$$\Omega_{k,l,\pm} = \frac{1}{2} (M_{k,l}^{11} + M_{k,l}^{22}) \pm \frac{1}{2} \sqrt{(M_{k,l}^{11} - M_{k,l}^{22})^2 + 4 M_{k,l}^{12} M_{k,l}^{21}} \quad (\text{B12})$$

and the new modes $\delta \hat{c}_{k,l,d}^\dagger$ and $\delta \hat{c}_{k,l,d}$ are linear combinations of the original b modes.

It is useful to consider the $k = 0, l = 1$ mode where $\Omega_{0,1,+} = 0$ and

$$\Omega_{0,1,-} = -\gamma e^{\frac{1}{2} \beta'_\gamma \rho} \cosh \left(\frac{1}{2} \beta'_\gamma \rho \phi \right) \\ \times \{ 2 + \beta'_\gamma \rho [\phi \tanh \left(\frac{1}{2} \beta'_\gamma \rho \phi \right) - 1] \} \quad (\text{B13})$$

$$= -\gamma e^{\frac{1}{2} \beta'_\gamma \rho} \cosh \left(\frac{1}{2} \beta'_\gamma \rho \phi \right) [2 + \beta'_\gamma \rho (\phi^2 - 1)], \quad (\text{B14})$$

where in the second line we have used Eq. (72). Let us consider the solution $\phi = 0$. Equation (B14) tells us that this solution becomes unstable, i.e., $\Omega_{0,1,-} > 0$ —leading to

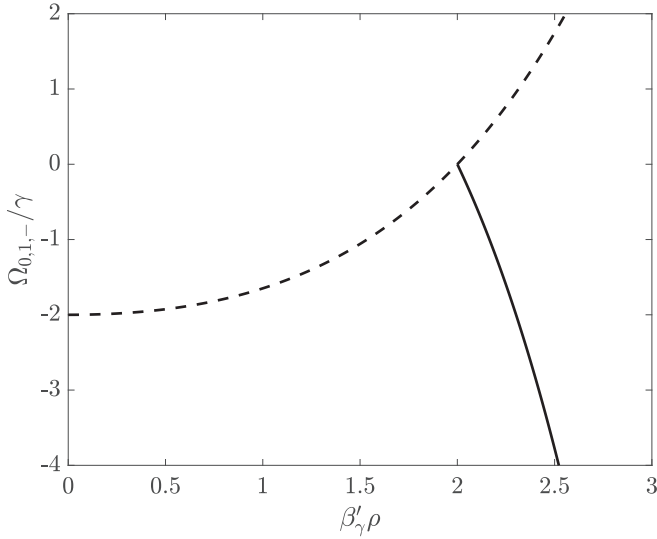


FIG. 13. $\Omega_{0,1,-}$ as a function of $\beta'_\gamma \rho$ for $\phi = 0$ (dashed line) and $\phi \neq 0$ (solid line). This shows the instability of the $\phi = 0$ solution when $\beta'_\gamma \rho > 2$.

exponential growth—when $\beta'_\gamma \rho > 2$. In contrast, the two solutions $\phi \neq 0$ are stable for $\beta'_\gamma \rho > 2$. To see this, we plot $\Omega_{0,1,-}$ versus $\beta'_\gamma \rho$ in Fig. 13 where we have solved Eq. (73) to find $\phi \neq 0$.

APPENDIX C: CURRENT IN THE DECOUPLING APPROXIMATION

Using the decoupling approximation [Eqs. (77) and ((82), we can derive, for example,

$$\begin{aligned} \langle j_{n,m,\rightarrow}^x \rangle_{ss} &= \chi^+ \langle q_0 | n+1 \hat{a}_{n+1,m,\rightarrow}^\dagger | p_0 \rangle_{n+1} \langle q_0 | n \hat{a}_{n,m,\rightarrow} | p_0 \rangle_i \\ &\quad - \chi^- \langle q_0 | n \hat{a}_{n,m,\rightarrow}^\dagger | p_0 \rangle_n \langle q_0 | n+1 \hat{a}_{n+1,m,\rightarrow} | p_0 \rangle_{n+1}. \end{aligned} \quad (C1)$$

Under the simplifications described in Sec. VIB, this becomes

$$\langle j_{n,m,\rightarrow}^x \rangle_{ss} = \sqrt{\rho} \langle \hat{A}_\rightarrow \rangle [(\chi^+ - \chi^-)(U_{0,d})_{1,m}]. \quad (C2)$$

Summing over n and m (and calculating the steady-state currents for the other directions and orientations), it is straightforward to show that drift has the same form as Eqs. (1) and (2) with $\phi = ((\langle \hat{A}_\rightarrow \rangle - \langle \hat{A}_\leftarrow \rangle)/\sqrt{\rho})$.

APPENDIX D: DYNAMICAL SIMULATION OF SMALL SYSTEM

To understand the competition between hopping and nonlinear interactions, we perform a dynamical simulation of a small periodic system of $N = 6$ particles on $M_x = 3$ sites. The evolution operator has the form

$$\begin{aligned} \mathcal{L}_R &= \sum_n [(\hat{A}_{n+1,\rightarrow}^\dagger - \hat{A}_{n,\rightarrow}^\dagger) \kappa_\rightarrow \hat{A}_{n,\rightarrow} \\ &\quad + (\hat{A}_{n-1,\leftarrow}^\dagger - \hat{A}_{n,\leftarrow}^\dagger) \kappa_\leftarrow \hat{A}_{n,\leftarrow} \\ &\quad + \gamma (\hat{A}_{n,\leftarrow}^\dagger - \hat{A}_{n,\rightarrow}^\dagger) (e^{\beta_\gamma \hat{n}_\leftarrow} \hat{A}_{n,\rightarrow} - e^{\beta_\gamma \hat{n}_\rightarrow} \hat{A}_{n,\leftarrow})], \end{aligned} \quad (D1)$$

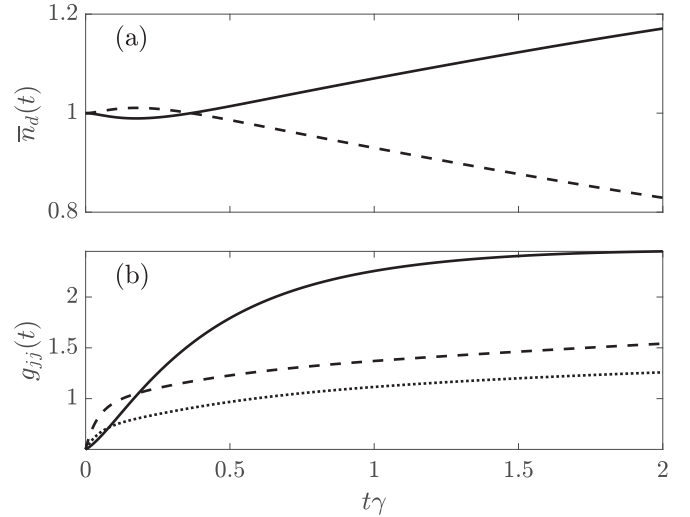


FIG. 14. Number [panel (a)] and number fluctuations [panel (b)] of $\rightarrow$ (solid line) and $\leftarrow$ (dashed line) oriented particles as a function of time for the small periodic system given by Eq. (D1). In panel (b), we also show the number fluctuations of the symmetric mode $\frac{1}{\sqrt{2}}(\hat{A}_{1,\rightarrow} + \hat{A}_{1,\leftarrow})$ (dotted line), which increase from zero due to the hopping between sites. Parameters are $N = 6$, $\kappa_\leftarrow = 10\gamma$, $\kappa_\rightarrow = \gamma/10$, and $\beta_\gamma = 0.9$.

with periodic boundary conditions. The left-hand ground state is given by $\langle Q_0 | \propto \langle \{0\} | (\sum_{n,d} \hat{A}_{n,d})^N$. We propagate the state of the system $|P(t)\rangle$ forward in time using Eq. (8) from the initial state $|P(0)\rangle \propto \prod_{n=1}^3 [\frac{1}{\sqrt{2}}(\hat{A}_{n,\rightarrow}^\dagger + \hat{A}_{n,\leftarrow}^\dagger)]^2 |\{0\}\rangle$. We put $\kappa_\leftarrow > \kappa_\rightarrow$ and evaluate the time evolution of the following quantities: $\bar{n}_d(t) = \langle Q_0 | \hat{n}_{1,d} | P(t) \rangle$ and $g_{ij}(t) = \langle Q_0 | \hat{A}_{1,i}^\dagger \hat{A}_{1,j}^\dagger \hat{A}_{1,i} \hat{A}_{1,j} | P(t) \rangle / \bar{n}_i(t) \bar{n}_j(t)$ [cf. Eqs. (28) and (28)], where we have dropped the site index as the sites are identical.

The results are shown in Fig. 14. $g_{\leftarrow\leftarrow}$ increases from 0 to ~ 1 on the fast $\kappa_\leftarrow$ timescale as expected. On a longer timescale, however, fluctuations $g_{\rightarrow\rightarrow} > 1$ and the particles evolve toward the long-term state where $\bar{n}_\rightarrow > \bar{n}_\leftarrow$. As discussed in Sec. VIB, the nonlinearity has the effect of aligning the particles with the smaller κ_d .

APPENDIX E: CONTINUOUS MEAN-FIELD EQUATIONS

The “Heisenberg” equations of motion for $\hat{n}_{n,m,d}$ are

$$\frac{d\hat{n}_{n,m,\rightleftharpoons}}{dt} = [\hat{n}_{n,m,\rightleftharpoons}, \hat{\mathcal{L}}_R] \quad (E1)$$

$$\begin{aligned} &= -(\hat{j}_{n,m,\rightleftharpoons}^x - \hat{j}_{n-1,m,\rightleftharpoons}^x) \\ &\quad - (\hat{j}_{n,m,\rightleftharpoons}^y - \hat{j}_{n-1,m\pm 1,\rightleftharpoons}^y) \\ &\quad - (\hat{j}_{n,m,\rightleftharpoons}^z - \hat{j}_{n,m-1,\rightleftharpoons}^z) \\ &\quad + \hat{a}_{n,m,\rightleftharpoons}^\dagger \hat{\gamma}_{n,m,\rightleftharpoons} \hat{a}_{n,m,\rightleftharpoons} \\ &\quad - \hat{a}_{n,m,\rightleftharpoons}^\dagger \hat{\gamma}_{n,m,\rightleftharpoons} \hat{a}_{n,m,\rightleftharpoons}. \end{aligned} \quad (E2)$$

The drift equations (22) and (23) can be derived from Eq. (E2) by taking the expectation value of each equation, multiplying by n (in the r_d^x case) or m (in the r_d^y case), and summing over all n and m accounting for periodic boundary conditions.

Here, we are interested in a mean-field coarse-grained description. Putting $\hat{a}_{n,m,d}^{\dagger}(t) \rightarrow 1$ and $\hat{a}_{n,m,d}(t) \rightarrow (U_{0,d})_{1,m} p_{n,d}(t)$ in line with Sec. VI A and summing over m yields

$$\begin{aligned} \frac{dp_{n,\rightleftharpoons}}{dt} &= (\chi^+ + \Xi_{\rightleftharpoons}^+) p_{n-1,\rightleftharpoons} + (\chi^- + \Xi_{\rightleftharpoons}^-) p_{n+1,\rightleftharpoons} \\ &\quad - \kappa_{\rightleftharpoons} p_{n,\rightleftharpoons} + \gamma (e^{\beta' p_{n,\rightleftharpoons}} p_{n,\rightleftharpoons} - e^{\beta' p_{n,\rightleftharpoons}} p_{n,\rightleftharpoons}), \end{aligned} \quad (\text{E3})$$

where κ_d is given by Eq. (76). Putting $\rho_d(x, t) = p_{n,d}(t)$ and taking the coarse-grain limit $\ell \rightarrow 0$, this becomes

$$\begin{aligned} \frac{\partial \rho_{\rightleftharpoons}(x)}{\partial t} &= -v_{\rightleftharpoons}^x \frac{\partial \rho_{\rightleftharpoons}(x)}{\partial x} + D_{\rightleftharpoons} \frac{\partial^2 \rho_{\rightleftharpoons}(x)}{\partial x^2} \\ &\quad + \gamma [e^{\beta' \rho_{\rightleftharpoons}(x)} \rho_{\rightleftharpoons}(x) - e^{\beta' \rho_{\rightleftharpoons}(x)} \rho_{\rightleftharpoons}(x)], \end{aligned} \quad (\text{E4})$$

where $v_d^x = \ell r_d^x$ and $D_d = \ell^2 \kappa_d / 2$. Defining $\rho(x) \equiv \rho_{\rightarrow}(x) + \rho_{\leftarrow}(x)$ and $m(x) \equiv \rho_{\rightarrow}(x) - \rho_{\leftarrow}(x)$ enables us to derive Eqs. (74) and (75).

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