

# Thermodynamically Consistent Coarse-graining: from Interacting Particles to Fields via Second Quantization

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We systematically derive an exact coarse-grained description for interacting particles with thermodynamically consistent stochastic dynamics, applicable across different observation scales, the mesoscopic and the macroscopic. We implement the coarse-graining procedure using the Doi–Peliti field theory, which preserves microscopic noise effects on the meso/macro scale. The exact mapping reveals the key role played by Poissonian particle occupancy statistics. We show the implications of the exact coarse-graining method using a prototypical flocking model, namely the active Ising model, which exhibits a mismatch between the microscopic and macroscopic mean-field coarse-grained descriptions. Our analysis shows that the high- and low-density regimes are governed by two different coarse-grained equations. In the low-density regime, noise effects play a prominent role, leading to a first-order phase transition. In contrast, the second-order phase transition occurs in the high-density regime. Due to the exact coarse-graining methods, our framework also opens up applicability to systematically analyze noise-induced phase transitions in other models of reciprocally and non-reciprocally interacting particles.

## 1. INTRODUCTION

The dynamics of microscopic particles have been qualitatively well understood using a coarse-grained macroscopic/mesoscopic field-theoretical description for an order parameter [1–5]. This methodology is based on delineating the order parameter, and it relies on symmetries and conservation laws: a *top-down approach* towards mean-field dynamics of the order parameter. The field-theoretical physical description of many-body particle systems has been overwhelmingly successful in encapsulating the universal physical properties of different microscopic systems. For example, the critical phenomena in equilibrium systems [2], non-equilibrium systems such as reaction-diffusion systems [3], and chemical reaction networks [6]. The path integral formulations that incorporate fluctuations have been studied, namely the Martin-Siggia-Rose functional [7] and the Bausch-Janssen-Wagner-deDominicis functional [8–10]. However, they incorporate close-to-equilibrium Gaussian fluctuations around the mean-field dynamics of the order parameter: again a *top-down approach* towards fluctuations.

Despite its success, the field-theoretical description has major drawbacks [1–5]. First, a field theory contains multiple control parameters without a systematic and transparent connection to the microscopic control parameters of the system under consideration, which are usually only a few. Second, an effective coarse-grained description lumps together microscopic degrees of freedom that do not necessarily have the same dynamic and thermodynamic properties. Therefore, these field theories are usually not thermodynamically consistent because an exact connection to a microscopic system is missing, which impedes a field-theoretic formulation of the stochastic thermodynamics of the system under consideration, in particular, the computation of the *thermodynamic* entropy production [11]. Third, the coarse-

grained phenomenological description utilizes the mean-field assumption, which completely ignores microscopic noise effects. This approximation has been shown to exhibit a huge qualitative and quantitative mismatch between microscopic and coarse-grained descriptions. For example, the prototypical flocking model, the active Ising model [12, 13]. The AIM has a first-order phase transition from the disordered to the ordered phase [12, 13]. In contrast, the macroscopic coarse-grained description predicts a second-order phase transition from the disordered to the ordered phase [12, 13]. Incorporating noise effects for particle occupancy has been shown to successfully bridge the microscopic and coarse-grained physical description in the low-density regime; however, it fails in the high-density regime [14]. In addition, noise effects play a key role in not only the correctness of the phase diagram but also the exact quantification of thermodynamic dissipation across different observation scales. This highlights the importance of incorporating noise effects for a dynamic and thermodynamically consistent description across different observable scales. Fourth, the focus has been on the non-equilibrium dynamics of non-interacting (ideal) particles modelled using ideal reaction-diffusion systems or chemical reaction networks, but the majority of real-world particles are interacting (non-ideal). This implies that a tool similar to reaction-diffusion systems and chemical reaction networks for studying the dynamics and thermodynamics of out-of-equilibrium interacting particles is missing. *Bottom-up approaches* to a coarse-grained description have been explored [15–19], but are susceptible to one or more of the aforementioned drawbacks.

To remedy aforementioned drawbacks, a *bottom-up approach* is necessary, which we present here for a generic class of interacting particle systems, comprising non-equilibrium systems with reciprocal and non-reciprocal interactions [11], that preserves microscopic noise and the thermodynamical consistency on the macroscale/mesoscale. Here, we systematically elaborate on the technical aspects of the coarse-graining procedure for the interacting parti-

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cles and obtain the corresponding mesoscopic/macroscale Langevin description for the stochastic particle number/density fields. Thermodynamically consistent coarse-graining allows us to identify the Local detailed balance condition (LDB) on the mesoscale/macroscale, which preserves the thermodynamically-consistent formulation of microscopic particles [11]. Moreover, in contrast to simulating the microscopic Master equation, simulating the coarse-grained microscopic/macroscale Langevin equations for the particle number/density greatly decreases computational requirements. We use the Doi–Peliti field theory (DPFT) technique to implement the coarse-graining procedure [20–28]. We obtain an exact large deviation rate functional for the stochastic dynamics of interacting particles. DPFT exactly quantifies the microscopic fluctuation in the coarse-grained description because of its second quantized nature. We implement and derive the coarse-graining procedure for the thermodynamically consistent non-reciprocally interacting particles. However, it can be easily modified to any system of interacting particles that does not necessarily satisfy the thermodynamic consistency condition, but requires microscopic noise effects incorporated in the coarse-grained description. Using *bottom-up approach* to microscopic transitions, an exact path integral formalism for discrete state systems is derived in Ref. [29–31], and the dynamic and thermodynamic implications of Poissonian transitions for far-from-equilibrium systems are detailed.

## 2. MICROSCOPIC DESCRIPTION

### 2.1. Dynamics

We consider a lattice gas model with lattice spacing  $l$  and continuous-time dynamics. The lattice spacing is assumed to be one, unless stated otherwise. Physically, this corresponds to choosing the microscopic diffusive length scale as a measurement unit. Here, we study the discrete space description; however, the continuous space limit is obtained by taking an infinitesimally small lattice spacing. Each particle has a type index  $\gamma$  and a lattice index  $\#$ .  $N_i^\#$  denotes the number of particles of type  $i$  at the lattice site index  $\#$ .  $\{N\}$  denotes the lattice configuration specified by the particle occupancy vector. The dimension of  $\{N\}$  is the product of the number of lattice sites and the particle types. The microscopic Boltzmann weight  $\epsilon_i^\#$  for the type  $i$  particle at the lattice site  $\#$  is divided into its

reciprocal and non-reciprocal parts,  $\epsilon_i^r$  and  $f_i^{nr}$ , respectively [11].

$$\epsilon_i^r = \beta \sum_{j \neq i} v_{ij}^r N_j^\# + \beta v_{ii}^r (N_i^\# - 1), \quad f_i^{nr} = \beta \sum_j v_{ij}^{nr} N_j^\#. \quad (1)$$

$v_{ij}^r$  quantifies the microscopic Boltzmann weight due to the reciprocal interaction between the particle types  $i$  and  $j$  [11]. Similarly,  $v_{ij}^{nr}$  quantifies the microscopic Boltzmann weight due to the non-reciprocal interaction experienced by the particle of type  $i$  due to the particle of type  $j$ . Importantly, by construction, the symmetry  $v_{ij}^r = v_{ji}^r$  and the anti-symmetry  $v_{ij}^{nr} = -v_{ji}^{nr}$  are satisfied [11].  $v_{ij}^r, v_{ij}^{nr} > 0$  ( $v_{ij}^r, v_{ij}^{nr} < 0$ ) signify a repulsive (an attractive) interaction.  $v_{ij} = v_{ij}^r + v_{ij}^{nr}$  quantifies the total interaction coefficient.

$\Delta_{\gamma\gamma'}^\#$  denotes a reactive transition of type  $\gamma'$  to  $\gamma$  at the lattice site  $\#$ . The reactive transition changes the lattice occupancy vector  $\{N\} \rightarrow \{N + \Delta_{\gamma\gamma'}^\#\}$ . Similarly,  $\Delta_i^{\tilde{D}\#}$  denotes a diffusive transition of the particle of type  $i$  at the lattice site  $\#$  along the direction  $\tilde{D}$ . The diffusive transition changes the lattice occupancy vector  $\{N\} \rightarrow \{N + \Delta_i^{\tilde{D}\#}\}$ .  $k_{\gamma\gamma'}^\#$  denotes the reactive transition rate to change the particle type from  $\gamma$  to  $\gamma'$  at the lattice site  $\#$ . Similarly,  $k_i^{\tilde{D}\#}$  denotes the diffusive transition rate of the particle type  $i$  along the direction vector  $\tilde{D}$ . Reactive and diffusive transition rates are related to the microscopic Boltzmann weight eq. (1). The exact expressions read:

$$k_{\gamma\gamma'}^\# = d_{\gamma\gamma'} e^{\epsilon_{\gamma\gamma'}^\#}, \quad k_i^{\tilde{D}\#} = d_i^{\tilde{D}} e^{\epsilon_i^{\tilde{D}\#}}. \quad (2)$$

Here,  $d_{\gamma\gamma'}$  and  $d_i^{\tilde{D}}$  are the constants that quantify the reactive and diffusive transition rates, respectively.  $\{\Delta_{\gamma\gamma'}^\#\}$  and  $\{\Delta_i^{\tilde{D}\#}\}$  denote the set of all reactive and diffusive transitions, respectively. Thus, the system satisfies the Local Detailed Balance condition [11].

### A. Master equation

The probability of a configuration  $\{N\}$  at time  $t$  is denoted by  $P_{\{N\}}(t)$ . The Master Equation for the evolution of  $P_{\{N\}}(t)$  reads:

$$\partial_t P_{\{N\}}(t) = \sum_{\{\Delta_{\gamma\gamma'}^\#\}} \underbrace{\left( k_{\gamma\gamma'}^\# (\{N + \Delta_{\gamma\gamma'}^\#\}) P_{\{N + \Delta_{\gamma\gamma'}^\#\}} - k_{\gamma\gamma'}^\# (\{N\}) P_{\{N\}} \right)}_{-j_{\gamma\gamma'}^\#(\{N\})} + \sum_{\{\Delta_i^{\tilde{D}\#}\}} \underbrace{\left( k_i^{\tilde{D}\#} (\{N + \Delta_i^{\tilde{D}\#}\}) P_{\{N + \Delta_i^{\tilde{D}\#}\}} - k_i^{\tilde{D}\#} (\{N\}) P_{\{N\}} \right)}_{-j_i^{\tilde{D}\#}(\{N\})}, \quad (3)$$

Here,  $j_{\gamma\gamma'}^\#(\{N\})$  and  $j_i^{\tilde{D}\#}(\{N\})$  quantify the net probability

outflow due to the transitions  $\Delta_{\gamma\gamma'}^\#$  and  $\Delta_i^{\tilde{D}\#}$ , respectively.

### 3. COARSE-GRAINING: MICROSCOPIC TO MESOSCOPIC

The microscopic stochastic description requires tracking all possible configurations in the  $\{N\}$  space. We aim to formulate a coarse-grained mesoscopic description of the average particle occupancy, which fluctuates stochastically. This reduces the complexity of tracking the mesoscopic dynamics compared to the Master Equation.

#### 3.1. Doi-Peliti field theory

##### A. Introduction

DPFT utilizes the second quantized to classical many-body systems [20–28, 32]. Due to its second quantized formulation, DPFT incorporates the discreteness of the microscopic system in the mesoscopic description. Moreover, DPFT has obtained the mesoscopic description using a Poissonian measure over the microscopic particle occupancy. The phenomenological coarse-grained mean-field description does not account for Poissonian fluctuations or microscopic discreteness. Poissonian occupancy has prominent importance in the low-particle density limit. In this regime, the coarse-grained mean-field description fails due to the importance of Poissonian noise [13, 14]. Importantly, it qualitatively and quantitatively affects the thermodynamic dissipation [11]. Hence, it has prominent importance for the thermodynamically consistent coarse-graining.

##### B. Doi representation

The second quantized state for the  $N_i^\#$  number of the type  $i$  particles at the lattice site  $\#$  is denoted by  $|N_i^\#\rangle$ , and the corresponding dual  $\langle N_i^\#|$  [20–22]. The second quantized states satisfy the following ladder operator relations,

$$(\hat{n}_i^\#)^\dagger |N_i^\#\rangle = |N_i^\# + 1\rangle, \quad \hat{n}_i^\# |N_i^\#\rangle = N_i^\# |N_i^\# - 1\rangle, \quad (4)$$

The creation (annihilation) operators  $(\hat{n}_i^\#)^\dagger (\hat{n}_i^\#)$  acting on  $|N_i^\#\rangle$  increase (decrease) the occupancy state by 1. Analogously, the number operator  $\hat{N}_i^\# = (\hat{n}_i^\#)^\dagger \hat{n}_i^\#$  satisfies  $(\hat{n}_i^\#)^\dagger \hat{n}_i^\# |N_i^\#\rangle = N_i^\# |N_i^\#\rangle$ . In contrast to the quantum notation, the classical notation asymmetrically distributes the eigenvalue  $N_i^\#$  over the creation and annihilation operators. The consequence of combinatorics is that there are  $N_i^\#$  different possibilities of annihilating a particle, but only 1 possibility of creation.

### C. Second Quantized Hamiltonian

The second quantized Hamiltonian for  $\Delta_{\gamma\gamma'}^\#$  and  $\Delta_i^{\bar{\mathcal{D}}\#}$  is given by [20–22]:

$$\begin{aligned} \hat{H}_i^{\bar{\mathcal{D}}\#} &= d_i \left[ (\hat{n}_i^\#)^\dagger - (\hat{n}_i^{\bar{\mathcal{D}}\#})^\dagger \right] \left[ \hat{n}_i^\# e^{\epsilon_i^\# + \frac{1}{2} \bar{\mathcal{D}} \cdot \tilde{f}_i^{sp}} - \hat{n}_i^{\bar{\mathcal{D}}\#} e^{\epsilon_i^{\bar{\mathcal{D}}\#} - \frac{1}{2} \bar{\mathcal{D}} \cdot \tilde{f}_i^{sp}} \right], \\ \hat{H}_{\gamma\gamma'}^\# &= d_{\gamma\gamma'} \left[ (\hat{n}_{\gamma'}^\#)^\dagger - (\hat{n}_{\gamma'}^{\bar{\mathcal{D}}\#})^\dagger \right] \left[ \hat{n}_{\gamma'}^\# e^{\epsilon_{\gamma'}^\# - \frac{1}{2} f_{\gamma\gamma'}^{ch}} - \hat{n}_{\gamma'}^{\bar{\mathcal{D}}\#} e^{\epsilon_{\gamma'}^{\bar{\mathcal{D}}\#} + \frac{1}{2} f_{\gamma\gamma'}^{ch}} \right]. \end{aligned} \quad (5)$$

The total second quantized Hamiltonian  $\hat{H}$  for all possible transitions is:

$$\hat{H} = \hat{H}^{\mathcal{R}} + \hat{H}^{\mathcal{D}}. \quad (6)$$

Here,  $\hat{H}^{\mathcal{R}} = \sum_{\{\Delta_{\gamma\gamma'}^\#\}} \hat{H}_{\gamma\gamma'}^\#$  and  $\hat{H}^{\mathcal{D}} = \sum_{\{\Delta_i^{\bar{\mathcal{D}}\#}\}} \hat{H}_i^{\bar{\mathcal{D}}\#}$  are the reactive and diffusive contributions, respectively.

#### D. The coherent state and master equation

The coherent state  $|\phi_i^\#\rangle$  for the type  $i$  particle at  $\#$  and its dual counterpart  $\langle (\phi_i^\#)^*|$  are defined as:

$$|\phi_i^\#\rangle = e^{\phi_i^\# (\hat{n}_i^\#)^\dagger} |0\rangle, \quad \langle (\phi_i^\#)^*| = \langle 0| e^{(\phi_i^\#)^* \hat{n}_i^\#}. \quad (7)$$

The Taylor series expansions of it are  $|\phi_i^\#\rangle = \sum_l \frac{(\phi_i^\#)^l ((\hat{n}_i^\#)^\dagger)^l}{l!} |0\rangle$  and  $\langle (\phi_i^\#)^*| = \langle 0| \sum_l \frac{((\phi_i^\#)^*)^l (\hat{n}_i^\#)^l}{l!}$ . It has an inherent probabilistic interpretation, namely  $|\phi_i^\#\rangle = \sum_l P(l) |N_i^\#\rangle$ . Thus,  $P(l) = (\phi_i^\#)^l / l!$  gives a realization of the Poissonian distribution for the particle occupancy [33]. Importantly,  $(\hat{n}_i^\#)^\dagger |\phi_i^\#\rangle = \phi_i^\# |\phi_i^\#\rangle$  and  $\langle (\phi_i^\#)^*| \hat{n}_i^\# = \langle (\phi_i^\#)^*| (\phi_i^\#)^*$ , therefore,  $\phi_i^\#$  is the eigenvalue of the coherent state. Therefore, the inner product of any operator using the coherent state is equivalent to taking the Poisson probability measure for the particle occupancy. The expectation value of an operator  $\hat{O}$  over the Poissonian occupancy probability measure is defined as  $\langle \hat{O} \rangle = \langle \{\phi^*\} | \hat{O} | \{\phi\} \rangle / \langle \{\phi^*\} | \{\phi\} \rangle$ . The composite coherent state for the whole lattice is defined as:

$$|\{\phi\}\rangle = \prod_{i,\#} |\phi_i^\#\rangle \quad \langle \{\phi\}| = \prod_{i,\#} \langle \phi_i^\#|. \quad (8)$$

In eq. (8),  $\otimes$  denotes the tensor product of the coherent states for all types of particles and lattice indices. The ladder operators commute for particles of different types; thus,  $|\{\phi\}\rangle$  is the tensor product of  $|\phi_i^\#\rangle$  over all types of particles and lattice indices.

The time-dependent Schrödinger equation  $\partial_t |\{\phi\}\rangle = -\hat{H} |\{\phi\}\rangle$  for the coherent state is equivalent to the master eq. (3) for  $P_{\{N\}}(t)$ . This formulates the analogue between the classical many-body systems and its second quantized quantum representation.

### E. Normal ordering

Computing the expectation values for the operators (relevant physical quantities) becomes a cumbersome task using the second-quantized methods. To simplify this computation, one needs to obtain the normal ordered form  $: \hat{O} :$  of the operator  $\hat{O}$ . In the normal ordered form, the creation and annihilation operators are replaced by the eigenvalues of  $|\{\phi\}\rangle$ ,

$$\begin{aligned} : \hat{H}_{YY'}^\# : &= d_{YY'} \left[ (\hat{\eta}_Y^\#)^\dagger - (\hat{\eta}_{Y'}^\#)^\dagger \right] \left[ e^{\sum_j \hat{N}_j^\# (e^{\beta v_{Yj}} - 1) - \frac{1}{2} f_{YY'}^{ch}} \hat{\eta}_Y^\# - e^{\sum_j \hat{N}_j^\# (e^{\beta v_{Y'j}} - 1) + \frac{1}{2} f_{YY'}^{ch}} \hat{\eta}_{Y'}^\# \right], \\ : \hat{H}_i^{\tilde{D}\#} : &= d_i \left[ (\hat{\eta}_i^\#)^\dagger - (\hat{\eta}_i^{\tilde{D}\#})^\dagger \right] \left[ e^{\sum_j \hat{N}_j^\# (e^{\beta v_{ij}} - 1) - \frac{1}{2} f_{YY'}^{ch}} \hat{\eta}_i^\# - e^{\sum_j \hat{N}_j^{\tilde{D}\#} (e^{\beta v_{ij}} - 1) + \frac{1}{2} f_{YY'}^{ch}} \hat{\eta}_i^{\tilde{D}\#} \right]. \end{aligned} \quad (9)$$

### 3.2. The mesoscopic Doi-Peliti Action

#### A. The mesoscopic Doi-Peliti Lagrangian

In DPFT, the mesoscopic description of eq. (3) is obtained using the mesoscopic Doi-Peliti action  $\mathcal{S}_{DP}$ . It is constructed using the coherent state path integral approach [20–23, 32].  $\mathcal{S}_{DP}$  is obtained by computing an expectation value of the transition Hamiltonian in eq. (6) over the coherent state.  $\mathcal{S}_{DP}$  is rewritten as an integral of a Lagrangian,  $\mathcal{S}_{DP}[\{\phi^*, \phi\}] = \int_{t_i}^{t_f} dt \mathcal{L}[\{\phi^*, \phi\}]$ . The exact expression for  $\mathcal{L}[\{\phi^*, \phi\}]$  obtained using eq. (6) reads [20–23, 32]:

$$\mathcal{L}[\{\phi^*, \phi\}] = \left\{ -\langle \partial_t \{\phi^*\} | \{\phi\} \rangle + \frac{\langle \{\phi^*\} | \hat{H} | \{\phi\} \rangle}{\langle \{\phi^*\} | \{\phi\} \rangle} \right\}. \quad (10)$$

in particular  $(\hat{\eta}_i^\#)^\dagger \rightarrow \phi_i^\#$  and  $\hat{\eta}_i^\# \rightarrow (\phi_i^\#)^*$ . The reason is that the coherent state is an eigenvector of the creation operator with eigenvalue  $\phi_i^\#$ . Thus,  $\langle \hat{O} \rangle$  is computed trivially using the normal ordered form. For the non-interacting particles, eq. (5) is normal ordered. In contrast, the interacting nature of the particles poses a challenge due to the exponential dependence of  $\hat{H}$  on the number operator  $\hat{N}_i^\# = (\hat{\eta}_i^\#)^\dagger \hat{\eta}_i^\#$ . The normal ordering of eq. (5) derived in appendix A reads:

In eq. (10), the first term corresponds to the evolution of the fields in time, the left-side of the master equation. The second term encapsulated the transition jumps, the RHS of the master equation. Defining the transition Hamiltonians  $\mathcal{H}_{YY'}^\#[\{\phi^*, \phi\}] = -\frac{\langle \{\phi^*\} | \hat{H}_{YY'}^\# | \{\phi\} \rangle}{\langle \{\phi^*\} | \{\phi\} \rangle}$ ,  $\mathcal{H}_i^{\tilde{D}\#}[\{\phi^*, \phi\}] = -\frac{\langle \{\phi^*\} | \hat{H}_i^{\tilde{D}\#} | \{\phi\} \rangle}{\langle \{\phi^*\} | \{\phi\} \rangle}$  and  $\mathcal{H}[\{\phi^*, \phi\}] = -\frac{\langle \{\phi^*\} | \hat{H} | \{\phi\} \rangle}{\langle \{\phi^*\} | \{\phi\} \rangle}$ . Using eq. (9), the Hamiltonian for  $\Delta_{YY'}^\#$  and  $\Delta_i^{\tilde{D}\#}$  are as follows:

$$\begin{aligned} \mathcal{H}_{YY'}^\#[\{\phi^*, \phi\}] &= -d_{YY'} \left[ (\phi_Y^\#)^* - (\phi_{Y'}^\#)^* \right] \left[ \phi_Y e^{\sum_j (\phi_j^\#)^* \phi_j^\# (e^{\beta v_{Yj}} - 1) - \frac{1}{2} f_{YY'}^{ch}} - \phi_{Y'} e^{\sum_j (\phi_j^\#)^* \phi_j^\# (e^{\beta v_{Y'j}} - 1) + \frac{1}{2} f_{YY'}^{ch}} \right], \\ \mathcal{H}_i^{\tilde{D}\#}[\{\phi^*, \phi\}] &= -d_i \left[ (\phi_i^\#)^* - (\phi_i^{\tilde{D}\#})^* \right] \left[ \phi_i e^{\sum_j (\phi_j^\#)^* \phi_j^\# (e^{\beta v_{ij}} - 1) - \frac{1}{2} f_{YY'}^{ch}} - \phi_i^{\tilde{D}\#} e^{\sum_j (\phi_j^{\tilde{D}\#})^* \phi_j^{\tilde{D}\#} (e^{\beta v_{ij}} - 1) + \frac{1}{2} f_{YY'}^{ch}} \right]. \end{aligned} \quad (11)$$

The transition probability measure  $\mathcal{P}[\{\phi^*, \phi\}]$  is obtained using  $\mathcal{S}_{DP}$  reads,

$$\mathcal{P}[\{\phi^*, \phi\}] = e^{-\mathcal{S}_{DP}[\{\phi^*, \phi\}]}. \quad (12)$$

The normalization factor for eq. (12) is obtained by imposing the probability conservation  $\int \mathbb{D}\{\phi^*\} \mathbb{D}\{\phi\} \mathcal{P}[\{\phi^*, \phi\}] = 1$ . Here,  $\mathbb{D}$  in eq. (12) represents the path integral over all realizations of the coherent state eigenvalues  $\{\phi\}$ . The eq. (12) formulates the path integral representation for stochastic dynamics.

#### B. Cole-Hopf Transform

The ladder operators are not a natural realization of the change of a physically quantifiable observable of the classical many-body system, in contrast to the quantum case. Thus, the coherent state path integral formalism leads to a scalar Lagrangian as a function of eigenvalues  $\phi$  and  $\phi^*$  of the coherent state, which is not related to a physical observable. To address this issue, one needs to deploy a canonical transformation called the Cole-Hopf transform [34–36]. It defines the relationship between the occupancy of the particles  $N_i^\#$  and  $\phi_i^\#$  and  $(\phi_i^\#)^*$ . The Cole-Hopf transform is defined as:

$$\phi_i^\# = N_i^\# e^{-\chi_i^\#}, \quad (\phi_i^\#)^* = e^{\chi_i^\#}. \quad (13)$$

The particle number is the eigenvalue of the number operator, therefore  $N_i^\# = (\phi_i^\#)^* \phi_i^\#$  is rather trivial.  $\chi_i^\#$  is referred to as a conjugate field, noise field, or bias field. It realizes the generator for the microscopic transition. For example, the transition  $\Delta_{\gamma\gamma'}^\#$  implies  $(\hat{\eta}_\gamma^\#)^\dagger \hat{\eta}_{\gamma'}^\# \rightarrow N_{\gamma'}^\# e^{\chi_{\gamma'}^\# - \chi_\gamma^\#}$ , where  $\chi_\gamma^\# - \chi_{\gamma'}^\#$  signifies conjugate field of the generator for the transition  $\Delta_{\gamma\gamma'}^\#$ . The change in the conjugate field due to the transition (stochastic or driven) represents the most-likelihood force that generates the transition. Note that  $\chi_i$  is an intensive field. Importantly, the Cole-Hopf transform also addresses imaginary noise for coarse-grained fields, which was identified as a problem asso-

ciated with obtaining a Langevin equation using DPFT [34–36].

### C. The mesoscopic Doi-Peliti Lagrangian in the occupancy-noise picture

Inserting the Cole-Hopf transform eq. (13) into eq. (11), the transition Hamiltonian is expressed in occupancy-noise fields.

$$\begin{aligned}\mathcal{H}_{\gamma\gamma'}^\# [\{N, \chi\}] &= d_{\gamma\gamma'} \left[ \left( e^{\chi_{\gamma'}^\# - \chi_\gamma^\#} - 1 \right) e^{\mu_{\gamma'}^\# - \frac{1}{2} \mathcal{F}_{\gamma\gamma'}^{ch}} + \left( e^{\chi_\gamma^\# - \chi_{\gamma'}^\#} - 1 \right) e^{\mu_{\gamma'}^\# + \frac{1}{2} \mathcal{F}_{\gamma\gamma'}^{ch}} \right], \\ \mathcal{H}_i^{\tilde{\mathcal{D}}} [\{N, \chi\}] &= d_i \left[ \left( e^{\chi_i^{\tilde{\mathcal{D}}} - \chi_i^\#} - 1 \right) e^{\mu_i^\# + \frac{1}{2} \tilde{\mathcal{D}} \cdot \tilde{F}_i^{sp}} + \left( e^{\chi_i^\# - \chi_i^{\tilde{\mathcal{D}}} } - 1 \right) e^{\mu_i^{\tilde{\mathcal{D}}} - \frac{1}{2} \tilde{\mathcal{D}} \cdot \tilde{F}_i^{sp}} \right].\end{aligned}\quad (14)$$

Where,  $\mu_i^\# = \ln N_i^\# + \sum_j \mathcal{V}_{ij} N_j^\#$  is the mesoscopic Boltzmann weight of the mesostate  $N_i^\#$ . The mesoscopic interaction coefficient  $\mathcal{V}_{ij} = (e^{\beta v_{ij}} - 1)$ . The non-linear dependence (renormalization) of  $\mathcal{V}_{ij}$  on  $v_{ij}$  is attributed to the Poissonian occupancy statistics. Importantly, for strongly interacting systems, incorporating the Poissonian mesostate occupancy is qualitatively more important. The simplification of eq. (10) leads to the Lagrangian in the density-noise picture.

$$\mathcal{L} [\{N, \chi\}] = \vec{\chi} \cdot \partial_t \vec{N} - \mathcal{H} [\{N, \chi\}]. \quad (15)$$

The eq. (15) reveals the more familiar structure between the Hamiltonian and the Lagrangian, justifying their previous definitions. The transition probability measure eq. (12) is reduced to,

$$\mathcal{P} [\{N, \chi\}] = e^{-S_{DP}[\{N, \chi\}]}, \quad (16)$$

with a normalization constraint  $\int \mathbb{D}\{N\} \mathbb{D}\{\chi\} \mathcal{P} [\{N, \chi\}] = 1$  for the probability conservation.  $\mathbb{D}$  represents the path integral over all realizations of occupancy  $\{N\}$  and conjugate noise fields  $\{\chi\}$ . Thus, the Cole-Hopf transformation  $\{\phi, \phi^*\} \rightarrow \{N, \chi\}$  illuminates the underlying physical structure.

### D. Mesoscopic Energy Functional and Interaction Coefficients

$\mu_i^\#$  is further decomposed into its reciprocal and non-reciprocal contributions such that  $\mu_i^\# = \mu_i^r + \mathcal{F}_i^{nr}$ . Where,  $\mu_i^r = \ln N_i^\# + \sum_j \mathcal{V}_{ij}^r N_j^\#$  and  $\mathcal{F}_i^{nr} = \sum_j \mathcal{V}_{ij}^{nr} N_j^\#$ . The decomposition of the interaction coefficient  $\mathcal{V}_{ij} = \mathcal{V}_{ij}^r + \mathcal{V}_{ij}^{nr}$ , by construction, satisfies  $\mathcal{V}_{ij}^r = \mathcal{V}_{ji}^r$  and  $\mathcal{V}_{ij}^{nr} = -\mathcal{V}_{ji}^{nr}$  [11]. Where,  $\mathcal{V}_{ij}^r = (\mathcal{V}_{ij} + \mathcal{V}_{ji})/2$ , which leads to  $\mathcal{V}_{ij}^r = (\cosh(\beta v_{ij}^{nr}) e^{\beta v_{ij}^r} - 1)$  and  $\mathcal{V}_{ij}^{nr} = (\mathcal{V}_{ij} - \mathcal{V}_{ji})/2$  leads to

$\mathcal{V}_{ij}^{nr} = \sinh(\beta v_{ij}^{nr}) e^{\beta v_{ij}^r}$ . The reciprocal part of the interaction between the mesostate  $N_i^\#$  and  $N_j^\#$  is derived from a single energy functional of the lattice. The energy functional for the reciprocal interactions reads,  $\mathcal{E}^{int} = \frac{1}{2} \sum_{i,j,\#} \mathcal{V}_{ij}^r N_i^\# N_j^\#$ . The decomposition of  $\mathcal{V}_{ij}$  into its reciprocal  $\mathcal{V}_{ij}^r$  and non-reciprocal  $\mathcal{V}_{ij}^{nr}$  parts is not unique. Subsequently,  $\mathcal{E}^{int}$  is also not unique. Choosing a particular decomposition is a gauge-fixing. Utilizing the reciprocal and non-reciprocal parts as the symmetric and antisymmetric interactions is the unique gauge fixing corresponding to the orthogonal decomposition [11]. This particular choice of the gauge fixing preserves the microscopic symmetry ( $v_{ij}^r = v_{ji}^r$  and  $v_{ij}^{nr} = -v_{ji}^{nr}$ ) on the mesoscale ( $\mathcal{V}_{ij}^r = \mathcal{V}_{ji}^r$  and  $\mathcal{V}_{ij}^{nr} = -\mathcal{V}_{ji}^{nr}$ ).

### E. Mesoscopic Local detailed balance condition

On the mesoscopic level, a microscopic reactive transition  $\Delta_{\gamma\gamma'}^\#$  generates a mesoscopic reactive transition  $N_{\gamma'}^\# \rightarrow N_\gamma^\#$  with transition rate  $\mathcal{K}_{\gamma\gamma'}^\#$ . Similarly, a microscopic diffusive transition  $\Delta_i^{\tilde{\mathcal{D}}}$  generates a mesoscopic diffusive transition  $N_i^\# \rightarrow N_i^{\tilde{\mathcal{D}}}$  with transition rate  $\mathcal{K}_i^{\tilde{\mathcal{D}}}$ . The mesoscopic Local detailed balance condition is obtained using the mesoscopic transition Hamiltonian eq. (14) [11].

$$\frac{\mathcal{K}_{\gamma\gamma'}^\#}{\mathcal{K}_{\gamma\gamma'}^\#} = e^{\mu_{\gamma'}^\# - \mu_\gamma^\# + \mathcal{F}_{\gamma\gamma'}^{ch}}, \quad \frac{\mathcal{K}_i^{\tilde{\mathcal{D}}}}{\mathcal{K}_i^{(\tilde{\mathcal{D}})^{-1}}} = e^{\mu_i^\# - \mu_i^{\tilde{\mathcal{D}}} + \tilde{\mathcal{D}} \cdot \tilde{F}_i^{sp}}. \quad (17)$$

Equation (17) is the thermodynamically consistent identification of the microscopic Local detailed balance condition on the mesoscale. Hence, all transition dynamics for  $\{N_i^\#\}$  are constrained/generated by the mesoscopic Boltzmann weights  $\{\mu_i^\#\}$ .



#### 4. COARSE-GRAINING: MESOSCOPIC TO MACROSCOPIC

The mesoscopic description is suitable for systems that exhibit a finitely small number of particles per lattice site. In addition, the increasing number of particles suppresses the importance of the microscopic fluctuations in the observable mesoscopic quantity. Thus, the particle number and the transition current scale as  $O(N)$ , in comparison, fluctuations scale as  $O(1)$ . In the limit of the number of large particles per lattice site, we define the macrostate density field  $\rho_i(\vec{r}) = N_i^\#/\Omega$ . Here, the density  $\rho_i$  is defined in accordance with the Large Deviation Theory [37], where the intensive variable  $\rho_i$  is  $O(1)$  and its fluctuations are  $O(1/\Omega)$ . Hence, the lattice index is converted to the spatial position vector  $\vec{r}$ .  $\Omega$  quantifies the average number of particles per lattice site. Thus,  $\rho_i$  is defined as an intensive finite variable; compared to  $N_i^\#$ , which is an extensive variable. This macroscopic limit is an inherent assumption in the formulation of the chemical reaction networks and active matter models, that relies on the van Kampen closure expansion [38]. Here, we have rather demonstrated this as a coarse-graining step from the mesoscopic to the macroscopic description.

##### 4.1. Scale-invariance and renormalization

###### A. Equilibrium Thermodynamics: Energy functional and Boltzmann weights

The macroscopic interaction energy functional obeys the extensive scaling in  $\Omega$ . Thus, it satisfies  $\Omega E^{int} = \mathcal{E}^{int}$ , similar to the scaling between  $\rho_i$  and  $N_i$ . It leads to the scaling between the macroscopic  $V_{ij}^r$  and the mesoscopic  $\mathcal{V}_{ij}^r$  interaction coefficients,  $V_{ij}^r = \Omega \mathcal{V}_{ij}^r$ . Hence,  $V_{ij}^r = \Omega \left( \cosh(\beta v_{ij}^{nr}) e^{\beta v_{ij}^r} - 1 \right)$ . The macroscopic energy functional reads,  $E^{int} = \frac{1}{2} \int_{\vec{r}} d\vec{r} \sum_{i,j} V_{ij}^r \rho_i \rho_j$ . Thus, the reciprocal macroscopic Boltzmann weight  $\mu_i^r$  for the density field  $\rho_i$  is  $\mu_i^r = \ln(\rho_i) + \sum_j V_{ij}^r \rho_j$ . Here, the first and second terms are the Boltzmann entropic contribution due to the degeneracy of the macrostate and the reciprocal interactions, respectively. Writing  $\mu_i = \delta E / \delta \rho_i$  as a gradient of the energy functional, we obtain the total energy functional  $E = E^{int} - S^b$ , where  $S^b = -\sum_i \rho_i \ln(\rho_i/e)$  is the Boltzmann entropic contribution. The macroscopic Boltzmann weight  $\mu_i$  for the density field  $\rho_i$  is  $\mu_i = \ln(\rho_i) + \sum_j V_{ij} \rho_j$ , where  $V_{ij} = V_{ij}^r + V_{ij}^{nr}$ . Such that  $\mu_i = \mu_i^r + F_i^{nr}$  is satisfied with  $F_i^{nr} = \sum_j V_{ij}^{nr} \rho_j$  quantifying the non-reciprocal part of  $\mu_i$ .

The microscopic interaction coefficients  $v_{ij}$  are  $O(1/\Omega)$ . This enforces the microscopic Boltzmann weight  $\epsilon_i^\#$  as an intensive physical quantity. Subsequently, this ensures that  $V_{ij}, \mathcal{V}_{ij} \propto O(1/\Omega)$ , physically this ensures the extensive scaling of the interaction energy functional across the observable scales; the microscopic, mesoscopic, and macroscopic. From a thermodynamic point of view, the thermodynamically consistent models need to ensure the intensive Boltzmann weights that lead to the extensive interaction energy.

This important feature is usually overlooked in lattice gas models, where the interaction energy might scale super-/sub-extensively. Here, the requirement of a thermodynamically consistent framework across the scale requires careful treatment.

###### B. Non-equilibrium dynamics: The dynamical rate functional

Similarly to the energy functional, the macroscopic Doi-Peliti action  $\mathcal{S}_{DP}[\{\rho, \chi\}]$  follows the scaling in  $\Omega$ . The scaling is  $\Omega \mathcal{S}_{DP}[\{\rho, \chi\}] = \mathcal{S}_{DP}[\{N, \chi\}]$ ,  $\Omega \mathcal{L}[\{\rho, \chi\}] = \mathcal{L}[\{N, \chi\}]$  and  $\Omega \mathcal{H}[\{\rho, \chi\}] = \mathcal{H}[\{N, \chi\}]$ . This is trivially verified by substituting  $\Omega \rho_i(\vec{r}) = N_i^\#$  in eqs. (14) and (15). Hence, the macroscopic Lagrangian and Hamiltonian are obtained by  $N_i^\# \rightarrow \rho_i$ ,  $\chi_i^\# \rightarrow \chi_i$ ,  $\mu_i^\# \rightarrow \mu_i$ . The macroscopic transition probability measure  $\mathcal{P}[\{\rho, \chi\}]$  is reduced to the following,

$$\mathcal{P}[\{\rho, \chi\}] = e^{-\Omega \mathcal{S}_{DP}[\{\rho, \chi\}]}. \quad (18)$$

Here,  $\Omega$  plays the role of the large deviation parameter. Hence,  $\mathcal{P}[\{\rho, \chi\}]$  converges to the path of the most likelihood obtained by extremizing  $\mathcal{S}_{DP}[\{\rho, \chi\}]$ . Importantly,  $\mathcal{L}[\{\rho, \chi\}]$  is the same rate functional as that previously obtained to delineate the orthogonal decomposition symmetry of the EPR [39–55]. Our novel formulation generalizes its existence to the non-reciprocal systems. Its thermodynamically consistent framework enables the correct identification of the EPR discussed in Ref [11]. In addition to the  $\Omega$ , for the externally driven systems, the observable time-integrated current scales with the observation time  $\tau$ . This further leads to the scaling  $\mathcal{S}_{DP}[\{\rho, \chi\}] = \tau \tilde{\mathcal{S}}_{DP}[\{\rho, \chi\}]$  and  $\mathcal{L}[\{\rho, \chi\}] = \tau \tilde{\mathcal{L}}[\{\rho, \chi\}]$  [29, 30]. Hence, it quantifies the dynamical rate functional for the transition dynamics [37, 56].

###### C. Dynamics: Macroscopic Local detailed balance condition

Analogous to Mesoscopic LDB eq. (17), the macroscopic LDB is obtained using the macroscopic transition Hamiltonian  $\mathcal{H}[\{\rho, \chi\}]$ . It reads,

$$\frac{K_{\gamma\gamma'}}{K_{\gamma'\gamma}} = e^{\mu_{\gamma'} - \mu_{\gamma} + F_{\gamma\gamma'}^{ch}}, \quad \frac{K_i^{\vec{\mathcal{D}}}}{K_i^{(\vec{\mathcal{D}})^{-1}}} = e^{\mu_i - \mu_i^{\vec{\mathcal{D}}} + \vec{\mathcal{D}} \cdot \vec{F}_i^{sp}}. \quad (19)$$

where,  $K_{\gamma\gamma'}$  is the reactive transition rate  $\rho_{\gamma'} \rightarrow \rho_{\gamma}$  and its reverse transition rate  $K_{\gamma'\gamma}$  for  $\rho_{\gamma'} \rightarrow \rho_{\gamma}$ , defined between the density macrostates. Similarly,  $K_i^{\vec{\mathcal{D}}}$  is the diffusive transition rate for the density field  $\rho_i$  in the direction  $\vec{\mathcal{D}}$ . The transition affinities for the reactive and diffusive transitions are defined as,  $A_{\gamma\gamma'} = \mu_{\gamma'} - \mu_{\gamma} + F_{\gamma\gamma'}^{ch}$ , and  $A_i^{\vec{\mathcal{D}}} = \mu_i - \mu_i^{\vec{\mathcal{D}}} + \vec{\mathcal{D}} \cdot \vec{F}_i^{sp}$ , respectively.

#### 4.2. Hamilton-Jacobi equation: Minimum action principle

The eq. (18) implies convergence to the most likely path in the limit  $\Omega \rightarrow \infty$ . The first-order variation of  $\mathcal{S}_{DP}[\{\rho, \chi\}]$  leads to  $\delta\mathcal{S}_{DP}[\{\rho, \chi\}]$ . The instanton equation obtained reads,

$$\begin{aligned}\partial_t \rho_i &= \partial_{\chi_i} \mathcal{H}[\{\rho, \chi\}], \\ \partial_t \chi_i &= -\partial_{\rho_i} \mathcal{H}[\{\rho, \chi\}].\end{aligned}\quad (20)$$

The eq. (20) with  $\chi_i = 0$  gives the deterministic continuity equation for  $\rho_i$ . The non-trivial solution of eq. (20) ( $\chi_i \neq 0$ ) corresponds to the instanton. Here, the instanton corresponds to the minimum action path that gives the trajectory of the transition from one attractor to another attractor. Due to the violation of time-reversal symmetry, the instanton does not necessarily coincide with the gradient-descent dynamics of the energy functional.

Here, we are rather interested in the fluctuating dynamics of the macrostate confined to the basin of attraction of the fixed point. Thus, we aim to incorporate the Gaussian fluctuations of transitions. The second-order variation  $\delta^2\mathcal{S}_{DP}[\{\rho, \chi\}]$  around the minimal action path encapsulates the Gaussian fluctuations due to the transitions. The amplitude of the Gaussian fluctuations is equal to the curvature of the Hamiltonian, hence,

$$T_{YY'} = -\partial_{\chi_Y} \partial_{\chi_{Y'}} \mathcal{H}[\{\rho, \chi\}]|_{\chi=0}. \quad (21)$$

$T_{YY'}$  and  $T_i^{\mathcal{D}}$  correspond to the variance of the noise due to transitions  $\Delta_{YY'}$  and  $\Delta_i^{\mathcal{D}}$ , respectively. The deterministic transition current in eq. (20) could further be decomposed into its individual transition currents  $J_{YY'} = \partial_{\chi_Y - \chi_{Y'}} \mathcal{H}[\{\rho, \chi\}]|_{\chi=0}$ . The derivation of eqs. (20) and (21) is detailed in appendix B. This formulates the stochastic continuity equation for the macrostate/mesostate. Its further analysis is detailed in section 4.4.3. The higher-order variations of the Doi-Peliti action satisfy  $\delta^n \mathcal{S}_{DP}[\{\rho, \chi\}] \propto O(1/\Omega^{n-1})$ . Thus,  $\Omega \rightarrow \infty$  corresponds to the deterministic limit where the deterministic continuity eq. (20) suffices. For significantly large values of  $\Omega$ ,  $\delta^2\mathcal{S}_{DP}[\{\rho, \chi\}]$  gives the dominant contribution to the transition noise, which effectively incorporates the Gaussian fluctuations due to microscopic transitions. The mesoscopic systems prone to Poissonian transition noise need a careful treatment of the Poissonian noise [29].

The quadratic approximation of  $\mathcal{S}_{DP}$  in  $\chi_i$  leads to the Gaussian approximation of the transition noise, which is equivalent to the Onsager-Machlup functional [57, 58], the Martin-Siggia-Rose action [7], or the Bausch-Janssen-Wagner-de Dominicis action [8–10]. The Gaussian transition noise underestimates the thermodynamic cost compared to the Poissonian transition noise. Subsequently, it impacts the far-from-equilibrium optimal control formulation of stochastic thermodynamics compared to the close-to-equilibrium formulation [29–31]. Table I summarizes the different regimes for the transition and occupancy noise.

The nature of noise	Poissonian	Gaussian
Occupancy noise	$\mathcal{V}_{ij}$	$\mathcal{V}_{ij}$ expanded for small values of $\beta, v_{ij}$ up to $O((\beta v_{ij})^2)$
Transition noise	$\mathcal{S}_{DP}[\{N, \chi\}]$	$\mathcal{S}_{DP}$ expanded up to the quadratic terms in $\chi$

TABLE I. This table summarizes the implications of the noise. The noise in the occupancy statistics and transition statistics could either be Poissonian or Gaussian. For interacting systems, the Poissonian occupancy noise is reflected through the non-linear dependence (renormalization) of the microscopic interaction coefficients  $v_{ij}$  on the mesoscopic interaction coefficients  $\mathcal{V}_{ij}$ . The Gaussian approximation of the transition noise leads to the Langevin eqs. (22) and (25) for the fluctuating macro/mesostate. The thermodynamic implications of the Poissonian transition noise are detailed in Ref.[29–31].

#### 4.3. Generalized Macroscopic Fluctuating Dynamics

Using eqs. (20) and (21), the stochastic equation of motion for the macrostate  $\rho_i$  derived in appendices B and C reads,

$$\begin{aligned}\partial_t \rho_i &= -\nabla \cdot \vec{J}_i^{\mathcal{D}} - \sum_{i \in \{YY'\}} J_{YY'} + \sqrt{\frac{1}{\Omega}} \nabla \cdot \left( \sqrt{T_i^{\mathcal{D}}} \vec{\xi}_i^{\mathcal{D}} \right) \\ &\quad + \sqrt{\frac{1}{\Omega}} \sum_{i \in \{YY'\}} \sqrt{T_{YY'}^{\mathcal{R}}} \hat{\xi}_{YY'}^{\mathcal{R}},\end{aligned}\quad (22)$$

where,  $J_{YY'}$  and  $\vec{J}_i^{\mathcal{D}}$  are the transition currents for  $\Delta_{YY'}$  :  $\rho_{Y'} \rightarrow \rho_Y$  and  $\Delta_i^{\mathcal{D}} = \rho_i \rightarrow \rho_i^{\mathcal{D}}$ , respectively. Their exact expression for the transition currents derived in appendices B and C are,

$$\begin{aligned}\vec{J}_i^{\mathcal{D}} &= -D_i^{\mathcal{D}}(\{\rho\}) \nabla^{\mathcal{D}} \mu_i + \vec{J}_i^{sp}, \\ J_{YY'} &= 2D_{YY'}(\{\rho\}) \sinh\left(\frac{A_{YY'}}{2}\right).\end{aligned}\quad (23)$$

where,  $D_i(\{\rho\}) = \tilde{d}_i e^{\mu_i^r + F_i^{nr}}$  and  $D_{YY'}(\{\rho\}) = d_{YY'} e^{(\mu_Y + \mu_{Y'})/2}$  are the mobilities of the transitions  $\Delta_i^{\mathcal{D}}$  and  $\Delta_{YY'}$ , respectively. The transition mobilities incorporate the reciprocal and non-reciprocal microscopic interactions through  $\mu_i^r$  and  $F_i^{nr}$ . For ideal particles  $\mu_i = \log(\rho_i)$  and  $F_i^{nr} = 0$ , which reduces  $D_i(\{\rho\}) = \rho_i$  and  $D_{YY'}(\{\rho\}) = \sqrt{\rho_Y \rho_{Y'}}$ .  $\vec{\xi}_i^{\mathcal{D}}$  and  $\hat{\xi}_{YY'}^{\mathcal{R}}$  are the white Gaussian noise with unit variance and vanishing mean. The diffusive and reactive transition traffic derived in appendices B and C are,

$$T_i^{\mathcal{D}} = 2D_i^{\mathcal{D}}(\{\rho\}), \quad T_{YY'} = 2D_{YY'}(\{\rho\}) \cosh\left(\frac{A_{YY'}}{2}\right), \quad (24)$$

quantifies the variance of the fluctuations for transitions. For ideal particles  $\mu_i = \log(\rho_i)$  and  $F_i^{nr} = 0$  reduces  $T_i^{\mathcal{D}} = 2\rho_i$  and  $T_{YY'} = \rho_Y + \rho_{Y'}$ . Using eqs. (23) and (24), the fluctuation-response relation is satisfied between the currents and traffics,  $\partial J_{YY'}/\partial A_{YY'} = T_{YY'}/2$  and  $\partial \vec{J}_i^{\mathcal{D}}/\partial A_i^{\mathcal{D}} = T_i^{\mathcal{D}}/2$ .

Defining,  $\vec{\mathcal{D}} = \{\parallel, \perp\}$  for the diffusive transitions in the direction parallel and perpendicular to  $\vec{J}_i^{sp}$ , the simplified

form derived in appendix C reads  $-\nabla \cdot \vec{J}_i^{\vec{D}} = d_i^{\parallel} \Delta^{\parallel} e^{\mu_i} + d_i^{\perp} \Delta^{\perp} e^{\mu_i} + \nabla^{\parallel} \cdot \vec{J}_i^{sp}$ , where  $d_i^{\parallel} = d_i \cosh(f_i^{sp}/2)$  and  $d_i^{\perp} = d_i$ . The first and second terms give the diffusive currents in the direction parallel and perpendicular to the self-propulsion force.  $\vec{J}_i^{sp} = 2d_i e^{\mu_i} \sinh(f_i^{sp}/2)$  gives the macroscopic self-propulsion current. Defining the diffusion matrix;  $\mathbb{D}_i = \text{Diag}[d_i^{\parallel}, d_i^{\perp}]$ , the gradient vector;  $\vec{\nabla} = (\nabla^{\parallel}, \nabla^{\perp})$ , the mobility matrix;  $\mathbb{M}_i = \text{Diag}[d_i^{\parallel} e^{\mu_i}, d_i^{\perp} e^{\mu_i}]$ , the shorthand notation for  $-\nabla \cdot \vec{J}_i^{\vec{D}}$  is  $\vec{\nabla} \cdot \mathbb{M}_i \cdot \vec{\nabla} \mu_i$ .

The enhanced diffusion coefficient along the self-propulsion direction has been exhibited before [59, 60]. Importantly, the different transverse and longitudinal diffusion coefficients play a key role in the formation of the novel phases [61–65]. In addition,  $d_i^{\parallel} = d_i^{\perp}$  in the  $l \rightarrow 0$  limit oversimplifies the coarse-grained diffusive dynamics of the macrostate. For microscopic systems with an inherent finite diffusive length-scale, the anisotropic diffusion coefficient should be incorporated into the coarse-grained macroscopic description.

Multiplying eq. (22) by  $\Omega$ , one obtains the mesoscopic stochastic EOM for  $N_i^{\#}$ ,

$$\partial_t N_i^{\#} = -\nabla \cdot \vec{J}_i^{\vec{D}} - \sum_{i \in \{YY'\}} \mathcal{J}_{YY'}^{\#} + \nabla \cdot \left( \sqrt{\mathcal{T}_i^{\mathcal{D}}} \vec{\xi}_i^{\mathcal{D}} \right) + \sum_{i \in \{YY'\}} \sqrt{\mathcal{T}_{YY'}^{\#}} \hat{\xi}_{YY'}^{\mathcal{R}}. \quad (25)$$

The mesoscopic currents and traffic are analogous to eqs. (23) and (24) obtained by replacing  $\mu_i \rightarrow \mu_i^{\#}$  and  $\rho_i \rightarrow N_i^{\#}$ . In addition, the discrete Gradient and Laplacian operator is used in eq. (25), appendix C. In eq. (25), the variance of the noise appears to be  $O(1)$ , this apparent effect is attributed to considering the EOM for an extensive variable  $N_i^{\#}$ . In particular, eq. (25) is more useful than eq. (22) in the low-density regime, where the number of particles is finitely small, which makes the mean particle number (instead of density) a relevant physical parameter.

## 5. MULTI-BODY MICROSCOPIC INTERACTIONS

The microscopic interactions of the form eq. (1) lead to a quadratic macroscopic interaction energy functional  $E^{int}$ . However, for purely attractive microscopic reciprocal interactions  $v_{ij}^r < 0$  implies  $\mathcal{V}_{ij}^r, V_{ij}^r < 0$ . Therefore,  $E^{int}$  is not bounded from below. This means that to ensure the lower boundedness of  $E^{int}$ , we need to introduce higher-order multi-body interactions. To this end, we incorporate the repulsive interaction terms of higher order, which introduce additional terms to  $E^{int}$  of the form  $V_{ij}^4 \rho_i^2 \rho_j^2$ , such that  $V_{ij}^4 > 0$ . Here,  $V_{ij}^4$  is an extra macroscopic control parameter attributed to the higher-order microscopic repulsive interaction. Hence, effectively  $V_{ij}^r$  is reduced to the effective interaction coefficient  $V_{ij}^{eff} = V_{ij}^r + V_{ij}^4 \rho_i \rho_j$  with the effective interaction energy  $E^{int} = \frac{1}{2} V_{ij}^{eff} \rho_i \rho_j$ . For the higher values

of  $\rho_i$  and  $\rho_j$ ,  $V_{ij}^{eff} > 0$  is satisfied, thus,  $E^{int}$  is bounded from below. For the smaller values of  $\rho_i$  and  $\rho_j$ , the contribution due to  $V_{ij}^r$  dominates over the  $V_{ij}^4$  contribution. For  $i = j$ , one recovers the Ginzburg-Landau type higher-order interaction energy,  $E^{int} = \frac{1}{2} V_{ii}^r \rho_i^2 + \frac{1}{2} V_{ii}^4 \rho_i^4$ .

Note that we treat the higher-order multi-body repulsive interactions using the mean-field approximation. In the higher-density regime, where the importance of repulsive interactions becomes prominent, the discreteness of the particle number becomes less important. Thus, the mean-field approximation of higher-order multi-body interactions is physically justified. Moreover,  $V_{ij}^r$  captures the dominant-order Poissonian occupancy effect in the small particle number regime, further justifying the mean-field approximation of  $V_{ij}^4$ .

## 6. APPLICATIONS

### 6.1. Comparison to other coarse-graining methods

#### A. Kawasaki-Dean coarse-graining method for diffusive dynamics

For particles of type  $i$  and  $j$  with locally confined interactions, the diffusive dynamics of the density field eq. (25) reads,

$$\partial_t N_i = \Delta \left( N_i e^{N_j (e^{\beta v_{ij}} - 1)} \right) + \nabla \cdot \left( \sqrt{N_i e^{N_j (e^{\beta v_{ij}} - 1)}} \vec{\xi}_i^{\mathcal{D}} \right) \quad (26)$$

with diffusive mobility  $D_i = N_i e^{N_j (e^{\beta v_{ij}} - 1)}$  for  $N_i$ . We expand eq. (26) using Taylor series for small  $v_{ij}$ .  $O(1)$  approximation of diffusive mobility leads to diffusive mobility for non-interacting (ideal) fields  $D_i = N_i$ . Incorporating the first-order  $O(\beta v_{ij})$  approximation of the chemical potential gradient,  $\nabla \mu_i = (\nabla N_i)/N_i + \nabla(\beta v_{ij} N_j)$ . This simplifies the diffusive currents to,  $\vec{J}_i^{\vec{D}} = -D_i \nabla \mu_i = \nabla N_i + N_i \nabla(\beta v_{ij} N_j)$ .

This reduces eq. (26) in the small interaction regime to the Kawasaki-Dean equation [15, 16],

$$\partial_t N_i = \Delta N_i + \nabla \cdot [N_i \nabla(\beta v_{ij} N_j)] + \nabla \cdot (\sqrt{N_i} \vec{\xi}_i^{\mathcal{D}}) \quad (27)$$

Substituting  $N_i = \rho(x)$ ,  $v_{ij} = v(x - y)$  and  $N_j = \rho(y)$ , adding to the interaction neighborhood  $y$ , eq. (27) is exactly equal to the Kawasaki-Dean equation [15, 16]. Importantly, this highlights that spatially extended interactions are trivially incorporated by including non-local contributions to the microscopic Boltzmann weight. In conclusion, eq. (26) is the Langevin equation for the particle occupancy of strongly interacting particles, namely, the generalized Kawasaki-Dean equation. The

In the Kawasaki-Dean eq. (27), the fluctuations of the density fields depend on density, and interactions do not play any role. Despite its wide applicability, eq. (27) does not address this physical problem, particularly important for strongly interacting particles. In addition, the fluctuation response relation for interacting fields is easily accessible with



eq. (26). In contrast to eq. (27), where even if the fluctuation-response relation is formulated, it is the same for both the non-interacting (ideal) and interacting particles.

### B. Classical Stochastic Path Integral formalism for reactive transition dynamics

We highlight the importance of the exact coarse-graining procedure by comparing our results with the classical stochastic path integral formalism (CSPIF) in Ref.[34], which has been extensively utilized as a preferred coarse-graining method for interacting particles. To this end, we consider only two species of particles that interact in a single volume, which is equivalent to  $N$  spins, which can take pos-

itive (+) and negative (−) values, ferromagnetically interacting with the strength  $v/N$  ( $v > 0$ ). Particles with the same/opposite spins attract/repel each other. Hence, the microscopic interaction rules are defined as  $v_{++} = v_{--} = -v/N$  and  $v_{+-} = v_{-+} = v/N$ .

We have defined the total particle number  $N = N_+ + N_-$  (which is a constant) and magnetization  $M = N_+ - N_-$ . For this microscopic system, the exact coarse-grained EOM eq. (25) reads,

$$\begin{aligned}\partial_t N_+ &= \mathcal{J}_{+-} + \sqrt{\mathcal{T}_{+-}} \hat{\xi}_{+-}^R \\ \partial_t N_- &= -\mathcal{J}_{+-} - \sqrt{\mathcal{T}_{+-}} \hat{\xi}_{+-}^R\end{aligned}\quad (28)$$

with the spin-flipping transition current  $\mathcal{J}_{+-}$  and traffic  $\mathcal{T}_{+-}$

$$\begin{aligned}\mathcal{J}_{+-} &= d_{+-} \left( e^{N \left( \cosh \left[ \frac{\beta v}{N} \right] - 1 \right)} \right) \left[ N \sinh \left( M \sinh \left[ \frac{\beta v}{N} \right] \right) - M \cosh \left( M \sinh \left[ \frac{\beta v}{N} \right] \right) \right] \\ \mathcal{T}_{+-} &= d_{+-} \left( e^{N \left( \cosh \left( \frac{\beta v}{N} \right) - 1 \right)} \right) \left[ N \cosh \left( M \sinh \left[ \frac{\beta v}{N} \right] \right) - M \sinh \left( M \sinh \left[ \frac{\beta v}{N} \right] \right) \right]\end{aligned}\quad (29)$$

Here, the mesoscopic interaction coefficients  $\mathcal{V}_{++} = \mathcal{V}_{--} = e^{-\beta v/N} - 1$  and  $\mathcal{V}_{+-} = \mathcal{V}_{-+} = e^{\beta v/N} - 1$  were used to derive the reactive transition current in eq. (29).

Using CSPIF, the coarse-grained EOM for the spin-flipping dynamics has the same structure as eq. (28), with a different spin-flipping current ( $J_{+-}^{CSPIF}$ ) and traffic ( $T_{+-}^{CSPIF}$ ), which read [34],

$$\begin{aligned}J_{+-}^{CSPIF} &= d_{+-} \left[ N \sinh \left( \frac{\beta v M}{N} \right) - M \cosh \left( \frac{\beta v M}{N} \right) \right] \\ T_{+-}^{CSPIF} &= d_{+-} \left[ N \cosh \left( \frac{\beta v M}{N} \right) - M \sinh \left( \frac{\beta v M}{N} \right) \right]\end{aligned}\quad (30)$$

The small  $\beta v/N$  approximation for hyperbolic functions:  $\sinh(\beta v/N) = \beta v/N$ , using this mean field approximation for the particle occupancy, we find that eq. (30) is a deterministic limit of the exact EOM eq. (29).

For large values of  $\beta v M/N$ , which means small  $N$ , large  $\beta, v$  and  $M > 0$  (i.e. in the ordered phase of the FM model), the differences between eqs. (29) and (30) have substantial consequences: eq. (29) then predicts a much larger current and much larger fluctuations (traffic) in the vicinity  $M \approx N$  (i.e. close to the FM ordered state). The origin of this discrepancy is the mean field approximation of the particle numbers  $N_+$  and  $N_-$  in CSPIF, which treats the stochastic variable as a deterministic quantity. Within DPFT, this issue is carefully handled by construction, due to the requirement of normal-ordering needed to simplify from the second-quantized formalism to the coherent state path integral. For non-interacting particles or transition rates that do not depend on particle occupancy, the mean-field treatment of transition rates using CSPIF is equivalent to DPFT.

### 6.2. Active Ising Model

Flocking models exhibit a first-order transition from ordered to disordered phase, accompanied by an intermediate phase-co-existence regime [12, 13]. The width of the coexistence regime reduces with increasing total density, such that the limit of infinite total density corresponds to a second-order transition. The Active Ising Model (AIM) is a prototypical, most simplified flocking model that encapsulates the above-mentioned physical characteristics of flocking models [12, 13]. However, the coarse-grained description of AIM derived in Ref.[12, 13] fails in the low-particle-number regime. The order and onset of the phase transition are incorrectly predicted. Here, we highlight the importance of the role that microscopic interaction coefficients, Poissonian particle occupancy, and the exact coarse-graining methods developed play.

AIM models flocking with only two types of particles, positive (+) and negative (−), with self-propulsion direction along + and − horizontal axes, respectively. The microscopic alignment is modelled with the attractive/repulsive interaction between the same/different types of particles. Thus,  $v_{++}, v_{--} < 0$  and  $v_{+-}, v_{-+} > 0$  [66]. In the AIM, the particles can undergo diffusive or reactive transitions. The reactive transitions are thermodynamically consistent. In contrast to the thermodynamically consistent diffusive transitions formulated in this paper, in the original AIM, the particles have constant diffusive transition rates in addition to the biased self-propulsion [11]. In the following, we elaborate on two regimes corresponding to the low- and high-density regimes of AIM, because different microscopic interaction coefficient rules govern them. This difference will play a crucial role in fulfilling the physical mismatch between the low- and high-

density regimes.

### A. Low density regime

In the low-density regime, the minimum number of interacting particles is one. Hence, the low-density limit corresponds to the microscopic interaction coefficients  $v_{+-} =$

$v_{-+} = 1$  and  $v_{++} = v_{--} = -1$ . This leads to mesoscopic interaction coefficients,  $\mathcal{V}_{+-} = \mathcal{V}_{-+} = e^\beta - 1$  and  $\mathcal{V}_{++} = \mathcal{V}_{--} = e^{-\beta} - 1$  with mesoscopic Boltzmann weights  $\mu_+^\# = \log(N_+^\#) - \sinh(\beta)M^\# + (\cosh(\beta) - 1)N^\#$  and  $\mu_-^\# = \log(N_-^\#) + \sinh(\beta)M^\# + (\cosh(\beta) - 1)N^\#$ . here, we denote the total number and magnetization of particles by  $N^\# = N_+^\# + N_-^\#$  and  $M^\# = N_+^\# - N_-^\#$ , respectively. The EOM eq. (25) for the mean particle number at each lattice site reads:

$$\begin{aligned} \partial_t N_+^\# &= -\nabla \cdot \tilde{\mathcal{J}}_+^{\tilde{\mathcal{D}}} + \mathcal{J}_{+-}^\# + \nabla \cdot \left( \sqrt{\mathcal{T}_+^{\mathcal{D}}} \tilde{\xi}_+^{\mathcal{D}} \right) + \sqrt{\mathcal{T}_{+-}^{\mathcal{R}}} \tilde{\xi}_{+-}^{\mathcal{R}} \\ \partial_t N_-^\# &= -\nabla \cdot \tilde{\mathcal{J}}_-^{\tilde{\mathcal{D}}} - \mathcal{J}_{+-}^\# + \nabla \cdot \left( \sqrt{\mathcal{T}_-^{\mathcal{D}}} \tilde{\xi}_-^{\mathcal{D}} \right) - \sqrt{\mathcal{T}_{+-}^{\mathcal{R}}} \tilde{\xi}_{+-}^{\mathcal{R}} \\ \mathcal{J}_{+-}^\# &= d_{+-} \left( e^{N^\# (\cosh(\beta) - 1)} \left[ N^\# \sinh(M^\# \sinh[\beta]) - M^\# \cosh(M^\# \sinh[\beta]) \right] \right) \\ \mathcal{T}_{+-}^\# &= d_{+-} \left( e^{N^\# (\cosh(\beta) - 1)} \left[ N^\# \cosh(M^\# \sinh[\beta]) - M^\# \sinh(M^\# \sinh[\beta]) \right] \right) \end{aligned} \quad (31)$$

The thermodynamically inconsistent diffusive transition rates involve the modification of the diffusive mobilities  $D_+^{\mathcal{D}} = dN_+^\#$  and  $D_-^{\mathcal{D}} = dN_-^\#$ . Hence,  $-\nabla \cdot \tilde{\mathcal{J}}_+^{\tilde{\mathcal{D}}} = d^\parallel \Delta^\parallel N_+^\# + d^\perp \Delta^\perp N_+^\# - 2d \sinh\left(\frac{f_{sp}}{2}\right) \nabla^\parallel N_+^\#$  and  $-\nabla \cdot \tilde{\mathcal{J}}_-^{\tilde{\mathcal{D}}} = d^\parallel \Delta^\parallel N_-^\# + d^\perp \Delta^\perp N_-^\# + 2d \sinh\left(\frac{f_{sp}}{2}\right) \nabla^\parallel N_-^\#$ . The deterministic part of EOM eq. (31) is equivalent to the one obtained in Ref.[14], where it was obtained by introducing Poissonian statistics into the density. But eq. (31) is also valid for higher values of  $f_{sp}$  and incorporates stochasticity using multiplicative noise, going beyond the formulations in Ref.[14]. The linear stability analysis of faster reactive transition currents exhibits a first-order phase transition from the ordered to disordered phase and an intermediate coexistence regime [14]. In contrast, the mean-field hydrodynamic EOM fails to capture the ordered-to-disordered first-order phase transition [13].

### B. High density regime

In the high-density regime, each particle is surrounded by  $N \gg 1$  particles, where  $N$  is the average number of particles per lattice site. Hence, the microscopic interaction coefficients in the high-density limit are,  $v_{+-} = v_{-+} = 1/N$  and  $v_{++} = v_{--} = -1/N$ , which ensures that  $\mu_+$  and  $\mu_-$  are intensive [67]. This leads to  $V_{+-} = V_{-+} = \beta/\rho$  and  $V_{++} = V_{--} = -\beta/\rho$ . Thus,  $\mu_+ = \log(\rho_+) + \beta(\rho_- - \rho_+)/\rho$  and  $\mu_- = \log(\rho_-) + \beta(\rho_+ - \rho_-)/\rho$ , where the total density and magnetization are defined as  $\rho = \rho_+ + \rho_-$  and  $m = \rho_+ - \rho_-$ , respectively. The reactive transition currents read  $J_{+-} = \rho \sinh\left(\beta \frac{m}{\rho}\right) - m \cosh\left(\beta \frac{m}{\rho}\right)$ . The mean-field EOM

for the particle densities reads:

$$\begin{aligned} \partial_t \rho_+ &= d^\parallel \Delta^\parallel \rho_+ + d^\perp \Delta^\perp \rho_+ - 2d \sinh\left(\frac{f_{sp}}{2}\right) \nabla^\parallel \rho_+ + J_{+-} \\ \partial_t \rho_- &= d^\parallel \Delta^\parallel \rho_- + d^\perp \Delta^\perp \rho_- + 2d \sinh\left(\frac{f_{sp}}{2}\right) \nabla^\parallel \rho_- - J_{+-} \end{aligned} \quad (32)$$

The EOM eq. (32) are equal to the mean-field equations from Ref.[12, 13], with different transverse and longitudinal diffusion coefficients. Taking the  $l \rightarrow 0$  limit implies  $d_i^\parallel = d_i^\perp = \tilde{d}_i$ , which leads to the exact mean-field equations from Ref.[12]. The linear stability analysis of eq. (32) exhibits a second-order phase transition from ordered to disordered phase [12]. The fluctuations of dominant order ( $O(1/\sqrt{\Omega})$ ) to eq. (32) are incorporated using the multiplicative noise  $\sqrt{T_{+-}/\Omega} \tilde{\xi}_{+-}^{\mathcal{R}}$ , with  $T_{+-} = \rho \cosh\left(\beta \frac{m}{\rho}\right) - m \sinh\left(\beta \frac{m}{\rho}\right)$ .

In conclusion, our analysis reveals the key role that microscopic interaction coefficients play in bridging the low- and high-density regimes of AIM. In particular, the low-density and high-density regimes of the AIM belong to different universality classes of EOM, which results in first-order and second-order phase transitions from the disordered to ordered phase, respectively. Studied rigorously in Ref.[14] and Ref.[13], respectively.

## 7. CONCLUSION

We study a generic class of microscopic interacting particles that follows the thermodynamically consistent stochastic dynamics using the Master equation [11]. Using Doi-Peliti field theory, we implement the coarse-graining procedure to obtain Langevin dynamics of the mesoscopic (macroscopic) particle number (density). This procedure relies on computing an exact large deviation functional for interacting particle

systems. Importantly, DPFT encapsulates the impact of microscopic Poissonian particle occupancy fluctuations in the coarse-grained description. Using diffusive dynamics for interacting particles, we highlight the differences from the existing coarse-graining method, namely, the Kawasaki-Dean equation. Using reactive dynamics for interacting Ising spins, we highlight the differences between our approach and existing coarse-graining methods for interacting particles that do not account for Poissonian occupancy. Moreover, we show the importance of exact coarse-graining methods using a rigorously studied model, namely the Active Ising model (AIM). We show that the noise effects play a crucial role in quantifying the order of the phase transition in different density regimes (high and low density) of the Active Ising model. Our

coarse-graining procedure formulates a tool to study interacting particles using mesoscopic/macroscopic fields systematically. Importantly, this avoids the mean-field approximations by exactly incorporating Poissonian fluctuations of particle occupancy. This extends the importance of exact coarse-graining methods to practical applications by bridging the gap between experimental/numerical observations of microscopic systems using field-theoretical coarse-grained macroscopic/mesoscopic descriptions.

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## Appendix A: Coarse-Graining

### 1. Normal ordering the transition Hamiltonian: The derivation of eq. (9) from eq. (5)

The second quantized Hamiltonian for the reactive transition is reorganized to obtain the normal ordered form.

$$\begin{aligned}
 \hat{H}_{YY'}^\# &= d_{YY'} \left[ (\hat{\eta}_Y^\#)^\dagger - (\hat{\eta}_{Y'}^\#)^\dagger \right] \left[ \hat{\eta}_Y^\# e^{\epsilon_Y^\# - \frac{1}{2} f_{YY'}^{ch}} - \hat{\eta}_{Y'}^\# e^{\epsilon_{Y'}^\# + \frac{1}{2} f_{YY'}^{ch}} \right] \\
 &= d_{YY'} \left[ (\hat{\eta}_Y^\#)^\dagger - (\hat{\eta}_{Y'}^\#)^\dagger \right] \left[ \hat{\eta}_Y^\# e^{\left( \epsilon_{YY}^\# + \sum_{j \neq Y} \epsilon_{Yj}^\# \right) - \frac{1}{2} f_{YY'}^{ch}} - \hat{\eta}_{Y'}^\# e^{\left( \epsilon_{Y'Y'}^\# + \sum_{j \neq Y'} \epsilon_{Y'j}^\# \right) + \frac{1}{2} f_{YY'}^{ch}} \right] \\
 &= d_{YY'} \left[ (\hat{\eta}_Y^\#)^\dagger - (\hat{\eta}_{Y'}^\#)^\dagger \right] \left[ \hat{\eta}_Y^\# e^{\beta \left( v_{YY} (\hat{N}_Y^\# - 1) + \sum_{j \neq Y} v_{Yj} \hat{N}_j^\# \right) - \frac{1}{2} f_{YY'}^{ch}} - \hat{\eta}_{Y'}^\# e^{\beta \left( v_{Y'Y'} (\hat{N}_{Y'}^\# - 1) + \sum_{j \neq Y'} v_{Y'j} \hat{N}_j^\# \right) + \frac{1}{2} f_{YY'}^{ch}} \right].
 \end{aligned} \tag{A1}$$

The second quantized Hamiltonian has exponential density operator terms due to the interacting nature of particles. Following Ref. [68], the expression for the normal ordering of the exponential density operator reads:

$$e^{\lambda \hat{N}_i^\#} = : e^{\hat{N}_i^\# (e^\lambda - 1)} :. \tag{A2}$$

Which reduces the eq. (5) to eq. (9).

### 2. The derivation of eq. (14) from eq. (11)

$$\begin{aligned}
 -\mathcal{H}_{YY'}^\# [\{N, \chi\}] &= d_{YY'} \left[ e^{\chi_Y^\#} - e^{\chi_{Y'}^\#} \right] \left[ N_Y^\# e^{-\chi_Y^\#} e^{\sum_j N_j^\# \left( e^{\beta v_{Yj}} - 1 \right) - \frac{1}{2} f_{YY'}^{ch}} - N_{Y'}^\# e^{-\chi_{Y'}^\#} e^{\sum_j N_j^\# \left( e^{\beta v_{Y'j}} - 1 \right) + \frac{1}{2} f_{YY'}^{ch}} \right] \\
 &= d_{YY'} \left[ \left[ 1 - e^{\chi_{Y'}^\# - \chi_Y^\#} \right] N_Y^\# e^{\sum_j N_j^\# \left( e^{\beta v_{Yj}} - 1 \right) - \frac{1}{2} f_{YY'}^{ch}} + \left[ 1 - e^{\chi_Y^\# - \chi_{Y'}^\#} \right] N_{Y'}^\# e^{\sum_j N_j^\# \left( e^{\beta v_{Y'j}} - 1 \right) + \frac{1}{2} f_{YY'}^{ch}} \right] \\
 &= d_{YY'} \left[ \left[ 1 - e^{\chi_{Y'}^\# - \chi_Y^\#} \right] e^{\ln N_Y^\# + \sum_j N_j^\# \left( e^{\beta v_{Yj}} - 1 \right) - \frac{1}{2} f_{YY'}^{ch}} + \left[ 1 - e^{\chi_Y^\# - \chi_{Y'}^\#} \right] e^{\ln N_{Y'}^\# + \sum_j N_j^\# \left( e^{\beta v_{Y'j}} - 1 \right) + \frac{1}{2} f_{YY'}^{ch}} \right] \\
 &= d_{YY'} \left[ \left[ 1 - e^{\chi_{Y'}^\# - \chi_Y^\#} \right] e^{\mu_Y^\# - \frac{1}{2} \mathcal{F}_{YY'}^{ch}} + \left[ 1 - e^{\chi_Y^\# - \chi_{Y'}^\#} \right] e^{\mu_{Y'}^\# + \frac{1}{2} \mathcal{F}_{YY'}^{ch}} \right] \\
 &= d_{YY'} \left( \left[ 1 - e^{\chi_{Y'}^\# - \chi_Y^\#} \right] e^{\mu_Y^\# + \mathcal{F}_Y^{nr} - \frac{1}{2} \mathcal{F}_{YY'}^{ch}} + \left[ 1 - e^{\chi_Y^\# - \chi_{Y'}^\#} \right] e^{\mu_{Y'}^\# + \mathcal{F}_{Y'}^{nr} + \frac{1}{2} \mathcal{F}_{YY'}^{ch}} \right).
 \end{aligned} \tag{A3}$$

## Appendix B: Cummulants of the transition currents

The first and second cummulants of the transition currents are denoted by  $\mathcal{J}_\Delta$  and  $\mathcal{T}_\Delta$  respectively, and it is computed using  $\mathcal{H}$ . We adopt a shorthand notation  $\mathcal{J}_\Delta = \mathcal{J}_{YY'}^\#$ ,  $\mathcal{T}_\Delta = \mathcal{T}_{YY'}^\#$  and  $\Delta\chi = \chi_Y - \chi_{Y'}$  for  $\Delta_{YY'}^\#$ , and  $\mathcal{J}_\Delta = \mathcal{J}_i^{\vec{\mathcal{D}}^\#}$ ,  $\mathcal{T}_\Delta = \mathcal{T}_i^{\vec{\mathcal{D}}^\#}$  and  $\Delta\chi = \chi_i^{\vec{\mathcal{D}}^\#} - \chi_i^\#$  for  $\Delta_i^{\vec{\mathcal{D}}^\#}$ .

$$\begin{aligned}
 \mathcal{J}_\Delta &= \partial_{\Delta\chi} \Delta\mathcal{H}|_{\chi=0} = d_{YY'} \left( e^{\mu_Y^\# - \frac{1}{2} \mathcal{F}_{YY'}^{ch}} - e^{\mu_{Y'}^\# + \frac{1}{2} \mathcal{F}_{YY'}^{ch}} \right), \\
 \mathcal{T}_\Delta &= \partial_{\Delta\chi}^2 \Delta\mathcal{H}|_{\chi=0} = d_{YY'} \left( e^{\mu_Y^\# - \frac{1}{2} \mathcal{F}_{YY'}^{ch}} + e^{\mu_{Y'}^\# + \frac{1}{2} \mathcal{F}_{YY'}^{ch}} \right).
 \end{aligned} \tag{B1}$$

The second cumulant of the current is given by the traffic [56]. Here, the traffic is defined as the symmetric part of the transition currents obtained by the modulus of the unidirectional

currents. The reactive and diffusive mean currents and traffic reads:

$$\begin{aligned}
 \mathcal{J}_{YY'}^\# &= d_{YY'} \left( e^{\mu_Y^\# - \frac{1}{2} \mathcal{F}_{YY'}^{ch}} - e^{\mu_{Y'}^\# + \frac{1}{2} \mathcal{F}_{YY'}^{ch}} \right), \\
 \mathcal{T}_{YY'}^\# &= d_{YY'} \left( e^{\mu_Y^\# - \frac{1}{2} \mathcal{F}_{YY'}^{ch}} + e^{\mu_{Y'}^\# + \frac{1}{2} \mathcal{F}_{YY'}^{ch}} \right), \\
 \mathcal{J}_i^{\vec{\mathcal{D}}^\#} &= d_{YY'} \left( e^{\mu_Y^\# - \frac{1}{2} \mathcal{F}_{YY'}^{ch}} - e^{\mu_{Y'}^\# + \frac{1}{2} \mathcal{F}_{YY'}^{ch}} \right), \\
 \mathcal{T}_i^{\vec{\mathcal{D}}^\#} &= d_{YY'} \left( e^{\mu_Y^\# - \frac{1}{2} \mathcal{F}_{YY'}^{ch}} + e^{\mu_{Y'}^\# + \frac{1}{2} \mathcal{F}_{YY'}^{ch}} \right).
 \end{aligned} \tag{B2}$$

Importantly, the  $n^{th}$  order cumulant  $\mathcal{J}_\Delta^n$  satisfies  $\mathcal{J}_\Delta^n = \partial_{\Delta\chi}^n \Delta\mathcal{H}|_{\chi=0}$ . Thus, the recursive relation between the current cummulants holds  $\mathcal{J}_\Delta^n = \mathcal{J}_\Delta^{n-2}$ . This enables utilizing Langevin(gaussian) approximation for the stochastic dynamics of the coarse-grained meso/macroscale valid for suffi-

ciently large  $\Omega$ . The mesoscopic systems prone to the poissonian transition fluctuations need a more systematic analysis [29, 30]. Here, our focus is on a valid coarse-grained macroscopic description, a regime in which transition fluctuations are gaussian.

### Appendix C: Diffusive transition Hamiltonian and current cumulants

#### 1. Mesoscopic Diffusion Hamiltonian

Here we consider the mesoscopic diffusive Hamiltonian

$$\begin{aligned} \mathcal{H}^{\mathcal{D}} [\{N_i^\#, \chi_i^\#\}] = \sum_{\#, i} d_i \Bigg[ & \left( e^{\chi_i^{\mathcal{D}^\parallel \#} - \chi_i^\#} - 1 \right) e^{\mu_i^\# + \frac{1}{2} f_i^{sp}} + \left( e^{\chi_i^\# - \chi_i^{\mathcal{D}^\parallel \#}} - 1 \right) e^{\mu_i^{\mathcal{D}^\parallel \#} - \frac{1}{2} f_i^{sp}} + \left( e^{\chi_i^{\mathcal{D}^\# \#} - \chi_i^\#} - 1 \right) e^{\mu_i^\# - \frac{1}{2} f_i^{sp}} + \left( e^{\chi_i^\# - \chi_i^{\mathcal{D}^\# \#}} - 1 \right) e^{\mu_i^{\mathcal{D}^\# \#} + \frac{1}{2} f_i^{sp}} \\ & + \left( e^{\chi_i^{\mathcal{D}^\perp \#} - \chi_i^\#} - 1 \right) e^{\mu_i^\#} + \left( e^{\chi_i^\# - \chi_i^{\mathcal{D}^\perp \#}} - 1 \right) e^{\mu_i^{\mathcal{D}^\perp \#}} + \left( e^{\chi_i^{\mathcal{D}^\top \#} - \chi_i^\#} - 1 \right) e^{\mu_i^\#} + \left( e^{\chi_i^\# - \chi_i^{\mathcal{D}^\top \#}} - 1 \right) e^{\mu_i^{\mathcal{D}^\top \#}} \Bigg] \end{aligned} \quad (\text{C1})$$

Where, we have utilized  $\mathcal{D}^\parallel \cdot \vec{f}^{sp} = f^{sp}$ ,  $\mathcal{D}^\# \cdot \vec{f}^{sp} = -f^{sp}$ ,  $\mathcal{D}^\perp \cdot \vec{f}^{sp} = 0$  and,  $\mathcal{D}^\top \cdot \vec{f}^{sp} = 0$ . Thus, the deterministic transition currents read,

$$\begin{aligned} \partial_{\chi_i^\#} \mathcal{H}^{\mathcal{D}} [\{N_i^\#, \chi_i^\#\}] |_{\{\chi\}=\{0\}} &= d_i \left[ -e^{\mu_i^\# + \frac{1}{2} f_i^{sp}} + e^{\mu_i^{\mathcal{D}^\parallel \#} - \frac{1}{2} f_i^{sp}} - e^{\mu_i^\# - \frac{1}{2} f_i^{sp}} + e^{\mu_i^{\mathcal{D}^\# \#} + \frac{1}{2} f_i^{sp}} - e^{\mu_i^\#} + e^{\mu_i^{\mathcal{D}^\perp \#}} - e^{\mu_i^\#} + e^{\mu_i^{\mathcal{D}^\top \#}} \right] \\ &= d_i \left[ \cosh \left( \frac{f_i^{sp}}{2} \right) \left( e^{\mu_i^{\mathcal{D}^\parallel \#}} + e^{\mu_i^{\mathcal{D}^\# \#}} - 2e^{\mu_i^\#} \right) + \sinh \left( \frac{f_i^{sp}}{2} \right) \left( e^{\mu_i^{\mathcal{D}^\perp \#}} - e^{\mu_i^{\mathcal{D}^\top \#}} \right) + e^{\mu_i^{\mathcal{D}^\perp \#}} + e^{\mu_i^{\mathcal{D}^\top \#}} - 2e^{\mu_i^\#} \right] \\ &= d_i \left[ \cosh \left( \frac{f_i^{sp}}{2} \right) \Delta^\parallel e^{\mu_i^\#} + 2 \sinh \left( \frac{f_i^{sp}}{2} \right) \nabla^\parallel e^{\mu_i^\#} + \Delta^\perp e^{\mu_i^\#} \right] \\ &= d_i \left[ \cosh \left( \frac{f_i^{sp}}{2} \right) \nabla^\parallel \left( e^{\mu_i^\#} \left[ \nabla^\parallel \mu_i^\# + 2 \tanh \left( \frac{f_i^{sp}}{2} \right) \right] \right) + \nabla^\perp \left( e^{\mu_i^\#} \nabla^\perp \mu_i^\# \right) \right] \end{aligned} \quad (\text{C2})$$

Where,  $\Delta^\parallel e^{\mu_i^\#}$  and  $\Delta^\perp e^{\mu_i^\#}$  are the discrete Laplacian operator in the direction parallel and perpendicular to the self-propulsion respectively.  $\nabla^\parallel e^{\mu_i^\#}$  is the gradient operator in the direction parallel to the self-propulsion. In the last line, we have decomposed the Laplacian operator into the gradient operator to obtain a more familiar form of the diffusive currents,  $\Delta^\parallel e^{\mu_i^\#} = \nabla^\parallel \cdot \left( e^{\mu_i^\#} \nabla^\parallel \mu_i^\# \right)$ . The last line helps identify the diffusive transition mobilities,  $D_i^{\mathcal{D}^\parallel} = d_i^\parallel e^{\mu_i^\#}$ ,  $D_i^{\mathcal{D}^\perp} = d_i^\perp e^{\mu_i^\#}$ , with  $d_i^\parallel = d_i \cosh \left( \frac{f_i^{sp}}{2} \right)$ ,  $d_i^\perp = d_i$ .  $\nabla \mu_i^\#$  is the thermodynamic force acting along the diffusive direction. Similarly, the variance of the transition fluctuations is given by the curvature

of the Hamiltonian,

$$-\partial_{\chi_i^\#} \partial_{\chi_i^\#} \mathcal{H}^{\mathcal{D}} [\{N_i^\#, \chi_i^\#\}] |_{\{\chi\}=\{0\}} = d_i \left[ e^{\mu_i^\# + \frac{1}{2} f_i^{sp}} + e^{\mu_i^{\mathcal{D}^\parallel \#} - \frac{1}{2} f_i^{sp}} \right] \quad (\text{C3})$$

#### 2. Macroscopic Diffusion Hamiltonian with infinitesimal lattice spacing

The eq. (C2) derived for the mesoscopic discrete lattice system holds for the macroscopic discrete lattice systems, by replacing  $\mu_i^\# \rightarrow \mu_i^\#$  and  $N_i^\# \rightarrow \rho_i^\#$ . In addition, the macroscopic continuous description is obtained by replacing the discrete

gradient and Laplacian operators with its continuous counterpart. The macroscopic continuous limit corresponds to the small lattice spacing  $l$ , instead of the unit lattice spacing in

eq. (C2). Thus,  $\mu_i^{\tilde{\mathcal{D}}} - \mu_i = l\nabla\mu_i \propto O(l)$ , similarly  $f_i^{sp} \propto O(l)$  which amounts to  $f_i^{sp} \rightarrow lf_i^{sp}$ . The macroscopic EOM is obtained by the transformation of gradient and Laplacian operators,  $\Delta \rightarrow l^2\Delta$  and  $\nabla \rightarrow l\nabla$ . Thus, the macroscopic counterpart of eq. (C2) reads:

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$$\partial_{\chi_i^*} \mathcal{H}^{\mathcal{D}} [\{\rho_i, \chi_i^*\}] = \tilde{d}_i \cosh\left(\frac{\tilde{f}_i^{sp}}{2}\right) \Delta^{\parallel} e^{\mu_i} + \frac{2\tilde{d}_i}{l} \sinh\left(\frac{\tilde{f}_i^{sp}}{2}\right) \nabla^{\parallel} e^{\mu_i} + \tilde{d}_i \Delta^{\perp} e^{\mu_i}, \quad (\text{C4})$$

where,  $\tilde{d}_i = d_i l^2$  and  $\tilde{f}_{sp} = lf_{sp}$ . The continuous limit leads to  $\tilde{d}_i = \lim_{l \rightarrow 0} d_i l^2$ ,  $f_i^{sp} = \lim_{l \rightarrow 0} \frac{2}{l} \sinh\left(\frac{\tilde{f}_i^{sp}}{2}\right)$  for small values of  $f_i^{sp}$ . In the continuous limit, the transverse and longitudinal diffusion coefficients are equal. The macroscopic self-propulsion current reads  $\tilde{J}_i^{sp} = 2d_i l \sinh\left(\frac{lf_i^{sp}}{2}\right)$ . Note that eq. (C4) is  $O(l^2)$ , the scaled microscope diffusion coefficient

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takes care of the macroscopic scaling of the small lattice spacing. Importantly, in the limit  $l \rightarrow 0$ ,  $\tilde{J}_i^{sp} = \tilde{d}_i f_i^{sp}$  leads to the linear relationship between the macroscopic self-propulsion current and the microscopic self-propulsion force. This underestimates the microscopic thermodynamic dissipation using the macroscopic continuous-space description.