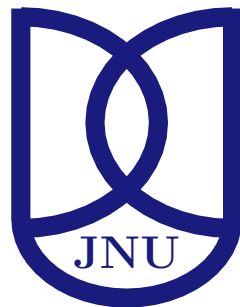


Hydrodynamics of Flocking: Continuum Models of Active Brownian Particles

A thesis
submitted in partial fulfillment
of the requirements for the award of the degree of
Doctor of Philosophy

Sunil Kumar Yadav

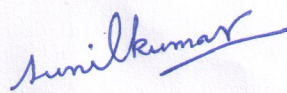


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Jawaharlal Nehru University
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January 2019

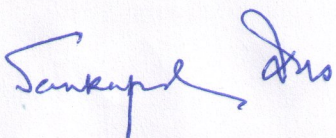
Declaration

I hereby declare that the work reported in this thesis is entirely original and has been carried out by me in the School of Physical Sciences, Jawaharlal Nehru University, New Delhi under supervision of Prof. Shankar P. Das. I further declare that it has not formed the basis for the award of any degree, diploma, associateship or similar title of any university or institution.

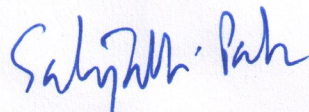
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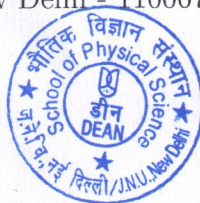
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Dedicated to
My Parents

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Publications

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2. “*Field-theoretic model for dynamics of active Brownian particles*”, Sunil Kumar Yadav, and Shankar P. Das, accepted for publication in AIP Conf. Proc. (2018).
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4. “*Positive entropy production and its implications on the equations of hydrodynamics for active matter*”, Sunil Kumar Yadav, and Shankar P. Das, preprint 2018.

Contents

1	Introduction	1
1.1	Active matter	1
1.2	Active matter hydrodynamics	4
1.3	Notion of coarse-graining	6
1.4	Toner-Tu model: Self-driven fluid model	9
1.5	Microscopic approaches to continuum dynamics of active systems	11
1.6	Outline of the thesis	12
2	Hydrodynamic description of a simple fluid	14
2.1	Time-reversible balance equations	15
2.2	Local equilibrium average	17
2.3	The Euler equations: Reversible dynamics	19
2.3.1	The Galilean invariance	23
2.4	Dissipative hydrodynamics	25
2.5	Discussion	27
	Appendix	28
2.A	Momentum density equation	28
2.B	Energy density equation	30

3	Hydrodynamic equations for coarse-grained fields	31
3.1	Brownian motion	32
3.1.1	Passive particles motion	32
3.2	Fokker-Planck dynamics	38
3.3	Smoluchowski dynamics	39
3.4	Coarse-grained equations	42
3.4.1	Coarse-grained equations for Smoluchowski case	44
3.4.2	Coarse-grained equations for Fokker-Planck case	49
3.5	Active particles Brownian motion	50
3.6	Discussion	51
4	Dynamic renormalization group analysis	53
4.1	The Navier-Stokes equation	55
4.2	Renormalization group method	56
4.2.1	Viscosity renormalization	59
4.2.2	Renormalization of noise strength	62
4.2.3	Rescaling of variables and recursion relation	64
4.2.4	Spectral energy density	67
4.3	A review on dynamic RG analysis of Toner-Tu equations	68
4.4	Discussion	73
	Appendix	75
4.A	Viscosity renormalization	75
4.B	Renormalization of noise strength	79
5	Fluctuating hydrodynamic approach to flocking	81
5.1	The microscopic model	83
5.1.1	The individual particle dynamics	84
5.1.2	The equations of motion for collective densities	86

5.2	Coarse-graining microscopic equations	87
5.2.1	Averaging reversible part	90
5.2.2	Averaging irreversible part	90
5.2.3	Hydrodynamic equations	94
5.3	Discussion	95
Appendix		98
5.A	The dissipative part	98
6	Implications of the field-theoretic equations	102
6.1	Breaking of Galilean invariance	103
6.2	Entropy production rate	106
Appendix		113
6.A	Identity	113
7	Summary of key issues	115

Chapter 1

Introduction

1.1 Active matter

The objective of this thesis is to understand the collective dynamical behavior of elements of active matter systems from the microscopic basis using the tools of statistical mechanics. Active matter describes systems which consist of a large number of self-driven or active particles (Marchetti *et al.*, 2013). The constituents of active systems are able to move on its own using their internal energy or ambient free energy and collectively generate organized motion. Fig (1.2) illustrates the collective motion of active particles. The particles in active matter systems are able to self-produce energy and hence responsible for the non-equilibrium state of the system. Active systems are different from the field driven systems or other nonequilibrium systems in a manner that field acts at the level of each element rather than at the boundaries of the system. Examples of these systems mainly consist of living organisms ranging from microscopic to macroscopic scales, e.g., insect swarms, bacteria (Budrene & Berg, 1991; Sokolov & Aranson, 2009), motor proteins (Kruse & Jülicher, 2003), mammal herds, fish schools, bird flocks (Bialek *et al.*, 2012). Some examples can also be found in man-made systems like

synthetic active systems (e.g., light activated colloids), robotic systems (Turgut *et al.*, 2008), artificial microswimmers (Bechinger *et al.*, 2016), etc. Study of active systems have various applications in biological systems, traffic dynamics (Helbing, 2001), glassy dynamics (Angelini *et al.*, 2011; Berthier & Kurchan, 2013), etc. Depending on the symmetry and momentum conservation law active systems are divided into the following category (Marchetti *et al.*, 2013):

(a) **Symmetry.** Systems can be classified into polar and apolar (or nematic) according to the orientation order of the active particles. Polar system consists of polar particles which have distinct head and tail, e.g., bacteria, birds, mammals, etc. Apolar particles which have symmetric head and tail form the nematic ordering. Nematic ordering can also be formed by polar particles which orient themselves in randomly opposite direction from ordered phase. Polar ordering is characterized by vector order parameter while nematic ordering by tensor order parameter. We classify one more active system containing isotropic active particles such as spheres which do not show orientational order on macroscopic scale for an isotropic interaction but show fascinating non-equilibrium phenomena due to self-propelling nature of particles (Fily & Marchetti, 2012; Redner *et al.*, 2013).

(b) **Conservation laws.** We classify the systems as wet or dry respectively according to the conservation or non-conservation of the momentum for a particular model of a system. Examples of wet active systems are cell cytoskeleton (Bendix *et al.*, 2008) and swimming bacteria in bulk suspensions (Dombrowski *et al.*, 2004) where motion is identical to viscous flow of a fluid and total momentum of the system is conserved. Dry systems describe a collection of self-driven particles in an inert medium or on a substrate which only provides friction. Momentum is not conserved due to friction on the substrate. Examples of dry systems contain mammal herds on land, vibrated granular rods on a plate, bacteria gliding on a

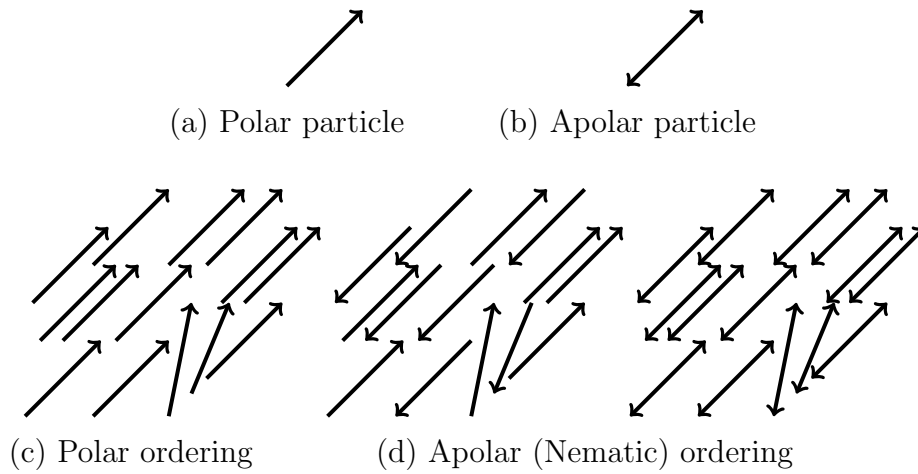


Figure 1.1: Schematic representation of active particles and their ordering state (a) Polar particle: asymmetric head-tail. (b) Apolar particle: symmetric head-tail. (c) Polar ordering of polar particles, mean velocity is non-zero. (d) Apolar ordering of polar as well as apolar particles, mean velocity is zero in this case.

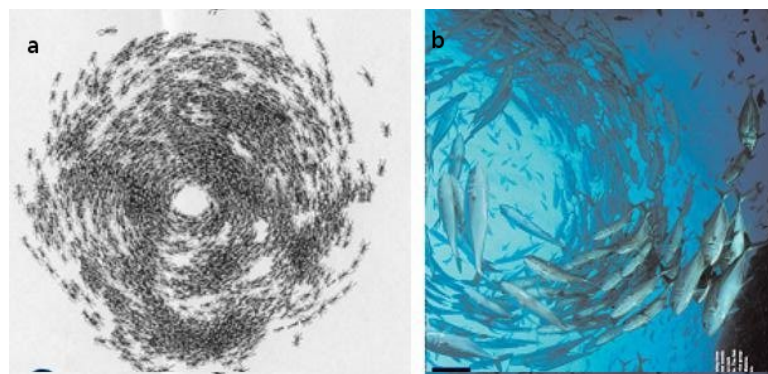


Figure 1.2: Collective motion of active particles (a) ants vortices (b) vortices formed by fish. Taken from (Vicsek & Zafeiris, 2012).

substrate, etc.

1.2 Active matter hydrodynamics

To study the dynamical properties of any system at large length and time scales, hydrodynamic approach is utilized (Forster, 1975; Hansen & McDonald, 1986). To discuss the dynamics we need to identify the scales of both length and time. Conventionally wavelengths is compared with the mean free path ℓ and times with mean collision time τ . With this identification wavenumber-frequency plane may be divided into three region. If ω and k denote angular frequency and wave vector respectively, then the region given by the inequalities $\omega\tau \ll 1$, $k\ell \ll 1$ defines the hydrodynamic regime. The two other region $\omega\tau \approx 1$, $k\ell \approx 1$ and $\omega\tau \gg 1$, $k\ell \gg 1$ denote kinetic regime and free-particle regime respectively. In hydrodynamic regime, the fluid is fully described by the local values of the thermodynamic quantities, whose evolution is determined by the hydrodynamic equations. In this thesis, we are mainly concerned with the hydrodynamic regime. Hydrodynamic description for active matter systems are obtained from the following approaches:

(a) **Phenomenological.** This approach is based on the symmetry and conservation law of the system. Phenomenological approach was first applied by Toner and Tu for dry active system (animal herds on land, bird flock etc.) in 1995, later it was extended by others (Ramaswamy, 2017, 2010; Ramaswamy & Simha, 2006; Simha & Ramaswamy, 2002) for different active systems. Hydrodynamic equations for relevant macroscopic variables are written down directly containing all terms which are not ruled out by symmetry of the problem. A more practical consideration while implementing the phenomenological approach is that we assume that the nonequilibrium steady state of the active system arises due to a small driving force on a system which has attained thermal equilibrium state.

(b) **Entropy production.** Concepts of Entropy production rate near equilibrium is utilized for the hydrodynamic description of active polar gel. Standard procedure of obtaining entropy production rate (De Groot & Mazur, 1984) for dissipative system are extended to the case of active polar systems to obtain the dynamical equations in terms of hydrodynamic fields (de Gennes & Prost, 1993; Joanny *et al.*, 2007; Jülicher *et al.*, 2018; Kruse *et al.*, 2004). This process involves choosing appropriate fields and writing down conservation laws corresponding to conserved quantities of a system. Next step follows identifying the generalized fluxes and conjugate forces which define the rate of entropy production and dissipation in the system. The reactive and dissipative fluxes of the system then defined by knowing the time reversal behavior of the fluxes and forces. Using a general expansion and writing down all terms allowed by symmetry as well as considering time reversal signature, the fluxes are expressed in terms of forces. Dropping non-relevant terms obtains the dynamical equations for the system which are valid near equilibrium. These equations are useful to analyze the macroscopic dynamical behavior of the system.

(c) **Coarse-graining of microscopic equation.** Hydrodynamic equations are obtained by coarse-graining microdynamic equations (Baskaran & Marchetti, 2008; Bertin *et al.*, 2013; Ihle, 2011; Yadav & Das, 2018; Yang & Marchetti, 2015). Analogous to the passive particle systems, we write down the microscopic equations for active systems for a particular model. New terms are added into the microscopic equations arising due to the activity of particles. Using the tools of statistical mechanics (Dorfman, 1999; Mazenko, 2006; Zubarev *et al.*, 1997; Zwanzig, 2001) we obtain the closed form of hydrodynamic equations in terms of slow variables. In this description, parameters such as transport coefficients in the macroscopic equations are related to the microscopic parameters which can be directly linked to experimentally accessible quantities.

1.3 Notion of coarse-graining

Phenomena happening in Nature depends on scale (energies, lengths). Depending on the energy scale or length scale, many levels of description of a system exists . Each level can be described by the dynamical equations for the variables appropriate at that level. There are systems such as complex fluids, biological systems etc. of which important properties can be described without atomic level description. Generally, we call this scale of description as mesoscopic scale which is higher level description than microscopic scale or fine-grain level. Hydrodynamics is such type of description. On the other hand, thermodynamics gives the macroscopic level description of a system where dynamical variables become time independent and there is no dynamical equations. At microscopic level, a system has many degrees of freedom. To study the system properties at more coarser level, we average out some degrees of freedom which are not useful to describe the system at coarse-grained level. Thus coarse-graining is a process in which we average out the ‘irrelevant’ degrees of freedom. To construct the simplified model which can be easily tractable by simulation or analytical approach, coarse-grained methods are useful. These methods are applied to formulate an effective theory (Amit, 1999; Chaikin & Lubensky, 1995; Kardar, 2007) which allows us to characterize the behavior of the system without specifying all the hidden causes which are responsible for the system state changes. This approach is widely used in the study of critical phenomena and renormalization group analysis (Ma, 1973; Wilson, 1971a, 1971b; Wilson & Kogut, 1974) where we need different length scale description to characterize the system. The coarse-graining procedure is different for different level of description of the system. One can go from lower level to higher level description by coarse-graining process but the reverse is not possible. Higher level description cannot describe the phenomena occurring at lower level. Below we give general idea of coarse-graining (Mazenko, 2002) using a specific

example.

We consider a system at a fine-grained (FG) level with the characteristic length scale l_{fg} is described by the Hamiltonian H_{fg} . Equilibrium state of the system is determined by the Boltzmann-type probability distribution P_{fg} as

$$P_{fg} \sim \exp\{-\beta H_{fg}\}, \quad (1.1)$$

where β represents the inverse of temperature of the system. If we want to know the properties of the system at mesoscale or higher length scale l_{cg} (say) which is much bigger than the l_{fg} , we need to obtain the coarse-grained probability P_{cg} corresponding to Eq. (1.1). We denote the coarse-grained Hamiltonian by H_{cg} . We assume that the P_{cg} has the Boltzmann-type distribution and given by

$$P_{cg} \sim \exp\{-\beta H_{cg}\}. \quad (1.2)$$

The normalization constants for both the distributions (1.1) and (1.2) will not be same. The Hamiltonian H_{cg} is effective Hamiltonian which has less degrees of freedom than the microscopic Hamiltonian H_{fg} . To demonstrate the idea behind averaging out the degrees of freedom, we consider here a probability distribution function $P(x_1, x_2)$ corresponding to the continuous random variables x_1 and x_2 defined in the range $-\infty < x_1, x_2 < +\infty$. The average of any function $f(x_1, x_2)$ is given by

$$\langle f(x_1, x_2) \rangle = \int dx_1 dx_2 P(x_1, x_2) f(x_1, x_2). \quad (1.3)$$

Next, we consider a the joint probability distribution $P'(\bar{x}_1, \bar{x}_2)$ which determines the probability that the variables x_1 has value \bar{x}_1 and x_2 has the value \bar{x}_2 . We define $P'(\bar{x}_1, \bar{x}_2)$ as

$$P'(\bar{x}_1, \bar{x}_2) = \langle \delta(\bar{x}_1 - x_1) \delta(\bar{x}_2 - x_2) \rangle. \quad (1.4)$$

The above relation is obtained in the following form

$$P'(\bar{x}_1, \bar{x}_2) = \int dx_1 dx_2 P(x_1, x_2) \delta(\bar{x}_1 - x_1) \delta(\bar{x}_2 - x_2) = P(\bar{x}_1, \bar{x}_2). \quad (1.5)$$

From the above result we see that the distribution function P' has the same number of degrees of freedom as the previous distribution function P has before averaging. Thus we consider a bit different distribution function which involves the average of stochastic variables x_1 and x_2 and given by the following relation

$$P'(\bar{x}) = \langle \delta(\bar{x} - \frac{1}{2}(x_1 + x_2)) \rangle = \int dx_1 dx_2 P(x_1, x_2) \delta(\bar{x} - \frac{1}{2}(x_1 + x_2)). \quad (1.6)$$

Applying the change of variables $\bar{x} = \frac{1}{2}(x_1 + x_2)$ and $r = x_1 - x_2$, we obtain the following form of the above expression

$$P'(\bar{x}) = \int dr P\left(\bar{x} - \frac{r}{2}, \bar{x} + \frac{r}{2}\right). \quad (1.7)$$

To evaluate the above integral, we need to know the explicit form of the distribution function P . Here we assume that P has the Gaussian form given as

$$P(x_1, x_2) = \left(\frac{\alpha}{2\pi}\right) \exp\left\{-\frac{\alpha}{2}(x_1^2 + x_2^2)\right\}, \quad (1.8)$$

where α is a constant. Now the the P' in Eq. (1.7) is obtained as

$$P'(\bar{x}) = \left(\frac{\alpha}{\pi}\right)^{1/2} \exp\{-\alpha\bar{x}^2\}. \quad (1.9)$$

Here the coarse-grained probability distribution has reduced degrees of freedom and the normalization constant is changed by a factor of 2. This example can be generalized to N stochastic variables. If $\hat{f}(\mathbf{x}, t)$ is a function which is microscopic, i.e., depends on all the phase space coordinates $\{\mathbf{r}_\alpha, \mathbf{p}_\alpha\}$ with $\alpha = 1..N$,

1.4 Toner-Tu model: Self-driven fluid model

of the particles in a microscopic description. Note that this dependence is implicit and indicated by the hat and (\mathbf{x}, t) is only an external label of space and time. Coarse graining in the present context means averaging over the phase space coordinates and getting a $f(\mathbf{x}, t)$ free of all phase space coordinates. So in doing the average we need an ensemble description. Generally one will expect a non-equilibrium ensemble since the flocking system is out of equilibrium. Here we make an approximation and assume weak departure. Thus we use the local equilibrium description. How to get that? There we use the Gibbsian description and replace fixed thermodynamic properties which would describe complete equilibrium with space dependent quantities. This defines the local equilibrium. Finally in forming Partial differential equations for the coarse-grained densities we do a leading order expansion in gradients of these local thermodynamic properties, i.e., we assume that in local equilibrium these quantities are not sharply changing in space. The idea of coarse-graining discussed here are utilized to obtain the coarse-grained description of active and passive particle systems from micro-dynamics in the subsequent chapters.

1.4 Toner-Tu model: Self-driven fluid model

The first theoretical model for the dynamics of polar active particles was proposed by Toner and Tu in 1995 (Toner & Tu, 1995). Using the symmetry and conservation laws they have obtained the continuum description of the model which includes the physics of numerical simulation model introduced by Vicsek (Vicsek *et al.*, 1995). In this model, active particles move on a substrate which provides only friction as a consequence momentum is not conserved. Thus the only conserved quantity is the number density, assuming that active particles such as birds do not die or reproduce. The system - be it flock of birds or swarms

1.4 Toner-Tu model: Self-driven fluid model

of bacteria is described in terms of field equations with smooth spatio-temporal dependence. The relevant fields here are the local density $\rho(\mathbf{x}, t)$ and velocity $\mathbf{v}(\mathbf{x}, t)$ whose time evolution equations are given by the following set of equations

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0, \quad (1.10)$$

$$\begin{aligned} \partial_t \mathbf{v} + \lambda (\mathbf{v} \cdot \nabla) \mathbf{v} &= (\tilde{\alpha} - \tilde{\beta} |\mathbf{v}|^2) \mathbf{v} - \nabla P + D_1 \nabla (\nabla \cdot \mathbf{v}) \\ &+ D_2 \nabla^2 \mathbf{v} + D_3 (\mathbf{v} \cdot \nabla)^2 \mathbf{v} + \mathbf{f}, \end{aligned} \quad (1.11)$$

where the coefficients $\tilde{\beta}$, D_1 , D_2 and D_3 are positive. Under specific circumstances the equations can lead to a situation, instead of a disordered state where average velocity is zero, to the spontaneous breaking of rotational invariance with a non-zero mean velocity $|\mathbf{v}| = \sqrt{\tilde{\alpha}/\tilde{\beta}}$. The parameter λ in the above equation is not equal to one due to the absence of Galilean invariance of the model. Pressure P in the velocity field equation is obtained by Taylor series expansion of the density ρ about mean density ρ_0 and given by the expression

$$P = \sum_{n=1}^{\infty} \sigma_n (\rho - \rho_0)^n,$$

with σ_n 's as expansion coefficients. \mathbf{f} is noise which is assumed to be white Gaussian with variance given as

$$\langle f_i(\mathbf{r}, t) f_j(\mathbf{r}', t') \rangle = \Delta \delta_{ij} \delta^d(\mathbf{r} - \mathbf{r}') \delta(t - t'),$$

where Δ is a constant. The unknown coefficients $\tilde{\alpha}$, $\tilde{\beta}$, λ , σ_n , and $D_{1,2,3}$ are functionals of the scalar fields ρ and $|\mathbf{v}|^2$.

1.5 Microscopic approaches to continuum dynamics of active systems

Here we review some approaches which are already proposed by various people to obtain coarse-grained equations for active matter systems from the microscopic starting point for the different models of active system (Marchetti *et al.*, 2013). The first microscopic description using Boltzmann approach to obtain hydrodynamic equations for self-driven particle is given by Bertin *et al.* for vicsek model (Czirk *et al.*, 1997; Vicsek *et al.*, 1995). They obtained closed form of hydrodynamic equations of mass density field and momentum density field starting from Boltzmann equations for the particle dynamics followed by Fourier transforming the equations near transition point. These equations are derived for the two dimensional case. The Boltzmann approach used by Bertin *et al.* is restricted to low density limit and cannot effectively describe the high density structure of the particles. To overcome this difficulty, Thomas Ihle (Ihle, 2011) used the Enskog-type kinetic theory to obtain the coarse-grained description for the same model. Instead of a bilinear collision, his approach considers multibody collisions. The transport coefficients of the equations are expressed in terms of multibody integrals whose analytical solutions cannot be obtained in many cases. Therefore only numerical values of the coefficients of equations can be determined. In his later publication (Ihle, 2015), he considers the binary collision analogous to the Bertin *et al.* approach and obtain simple form of transport coefficients which are valid in the large density limit. Nevertheless, more exploration of these models are needed to describe the dynamical properties above two dimensions.

A different kind of approach to obtain continuum equations was presented by Baskaran and Marchetti for a more realistic model (Baskaran & Marchetti, 2008). They have considered the non-zero particle size model in which particles interact

via excluded volume interactions. Starting from Smoluchowski dynamics, they have obtained coarse-grained equations for the density field, polarization vector field and nematic (tensor) order field in two dimensions. Though the microscopic equations have a noise term, the coarse-grained equations are deterministic. In Chapter 5, we have proposed a method to obtain coarse-grained equations for polar active particles. The continuum dynamics is obtained in terms of stochastic partial differential equations which contain a multiplicative noise term.

1.6 Outline of the thesis

This thesis is about the study of flocking behavior of active particle systems using hydrodynamic approach. Particularly, we will focus on models of active Brownian particles and obtain the hydrodynamic description. Newtonian mechanics and theory of Brownian motion provide appropriate tools to describe the dynamical behavior of such type of systems from the microscopic origin. Continuum equations are similar in some ways to the Navier-Stokes equations for simple compressible fluid. In Chapter 2, we obtain macroscopic hydrodynamic equations for ordinary fluid in which constituent particles follow reversible Newtonian dynamics. We define the microscopic (fine-grained) phase-space densities of the system in terms of sums of delta functions. Continuum field equations are obtained by coarse-graining the time evolution of microscopic phase-space densities. This chapter forms the basis for obtaining hydrodynamic equations from the microscopic origin.

For a system of passive Brownian particles in a fluid, dynamics is described by Langevin equation with a simple additive noise term. The microscopic dynamics is dissipative and equation is not invariant under time reversal. Microscopic model does not conserve momentum. Coarse-grained description of this model

is presented in Chapter 3. Notion of Brownian motion for active particles also introduced in this chapter.

Renormalization group (RG) provides essential tools to deal a system with many length scales. Under RG transformation, a system with many degrees of freedom is easily transformed to fewer effective degrees of freedom. RG methods have been very useful to extract important properties of a system, e.g., long distance behavior of correlation functions, without solving full equations characterizing the system. In chapter 4, we discuss the dynamic renormalization group analysis of the Navier-Stokes equation in which the reversible convective nonlinearity play major role. Dynamic RG methods discussed in this chapter are useful to study the phase behavior in active matter systems.

Chapter 5 deals with the hydrodynamic description for polar active particles from the microscopic starting point. We extend the idea of Brownian dynamics to model our system at microscopic level. The model, which we have considered, do not conserve momentum and energy due to friction of background medium. As a consequence of momentum conservation violation, equations break Galilean invariance, i.e., they do not remain invariant from one frame to the moving coordinate frame. In Chapter 6, we have elaborated the implications of the continuum model discussed in Chapter 5. We conclude our work in Chapter 7.

Chapter 2

Hydrodynamic description of a simple fluid

Hydrodynamic equations of a fluid provide the basic foundation to formulate the continuum equations of motion for active matter systems. In this chapter, we discuss the dynamics of a simple fluid. If we focus on the motion of the fluid particles, we will observe that there are intermolecular collisions resulting in a rapid motion. For classical fluids, the mean time interval of collisions, in many cases, may be of the order of $10^{-15}s$ to $10^{-10}s$ which decreases with increasing density. The corresponding mean free path, i.e., the mean distance traveled by particles in successive collisions, also decreases with increasing density. The disorderly dynamics of fluid particle system contains some collective modes whose relaxation time is much longer than those for fast modes of the system. Hydrodynamic behavior of the fluid is given in terms of such slow modes. Microscopic conservation laws and some symmetry breaking of microscopic Hamiltonian are mainly responsible for the existence of the slow modes. A fluid at the microscopic level is described in terms of the actual position and momenta coordinate of the constituent particles. The microscopic conservation laws for the fluid system are

2.1 Time-reversible balance equations

the densities of mass, momentum, and energy. Microscopically, these quantities are defined in terms of the phase-space variables involving sums of delta functions. When these quantities are coarse-grained over microscopic scales, they give rise to smoothly varying density fields whose time evolution gives the dynamical equations for the fluid system. Dynamics of an ideal fluid is described by time-reversible equations whereas equations describing normal fluid have reversible as well as dissipative part. First, we obtain the microscopic equations corresponding to the microscopic conserved densities of mass, momentum, and energy. Next, we average them over suitable ensemble to get the continuum equations of motion. Methods of obtaining fluctuating hydrodynamic equations described in this chapter form the basis of further discussion in the subsequent chapters.

2.1 Time-reversible balance equations

The microscopic densities, in terms of phase-space coordinates of the particles, at a given point \mathbf{x} and time t are given by

$$\hat{\rho}(\mathbf{x}, t) = \sum_{\alpha} m \delta(\mathbf{x} - \mathbf{x}_{\alpha}(t)), \quad (2.1)$$

$$\hat{\mathbf{g}}(\mathbf{x}, t) = \sum_{\alpha} \mathbf{p}_{\alpha} \delta(\mathbf{x} - \mathbf{x}_{\alpha}(t)), \quad (2.2)$$

$$\hat{e}(\mathbf{x}, t) = \sum_{\alpha} e_{\alpha} \delta(\mathbf{x} - \mathbf{x}_{\alpha}(t)). \quad (2.3)$$

The quantities $\hat{\rho}(\mathbf{x}, t)$, $\hat{\mathbf{g}}(\mathbf{x}, t)$, and $\hat{e}(\mathbf{x}, t)$ denote microscopic mass density, momentum density, and energy density respectively. These are the five conserved densities of the system. In the definition of microscopic energy density, the quan-

2.1 Time-reversible balance equations

tity e_α is defined as

$$e_\alpha = p_\alpha^2/(2m) + \sum_{\beta \neq \alpha} U(x_{\alpha\beta}).$$

Hat on these quantities represents their phase-space dependence. The time evolution equations of the above five microscopic densities are obtained as (Appendix)

$$\frac{\partial \hat{\rho}}{\partial t} + \nabla \cdot \hat{\mathbf{g}} = 0, \quad (2.4)$$

$$\frac{\partial \hat{g}_i}{\partial t} + \sum_j \nabla_j \hat{\sigma}_{ij} = 0, \quad (2.5)$$

$$\frac{\partial \hat{e}}{\partial t} + \nabla \cdot \hat{\mathbf{j}}^e = 0. \quad (2.6)$$

The respective currents, mass current density $\hat{\mathbf{g}}$, momentum current density (or stress tensor) $\hat{\sigma}_{ij}$, and energy current density $\hat{\mathbf{j}}^e$ are given by

$$\hat{\mathbf{g}}(\mathbf{x}) = \sum_{\alpha} \mathbf{p}_\alpha \delta(\mathbf{x} - \mathbf{x}_\alpha), \quad (2.7)$$

$$\hat{\sigma}_{ij}(\mathbf{x}) = \sum_{\alpha} \frac{p_\alpha^i p_\alpha^j}{m} \delta(\mathbf{x} - \mathbf{x}_\alpha) + \frac{1}{2} \sum_{\alpha \neq \beta} \Pi_{\alpha\beta}^{ij} \Omega_{\alpha\beta}, \quad (2.8)$$

$$\hat{\mathbf{j}}_i^e(\mathbf{x}) = \sum_{\alpha} e_\alpha \frac{p_\alpha^i}{m} \delta(\mathbf{x} - \mathbf{x}_\alpha) + \frac{1}{4} \sum_{\alpha \neq \beta} \sum_j \Pi_{\alpha\beta}^{ij} \left(\frac{p_\alpha^j}{m} + \frac{p_\beta^j}{m} \right) \Omega_{\alpha\beta}, \quad (2.9)$$

where we have defined the quantities $\Pi_{\alpha\beta}^{ij}$ and $\Omega_{\alpha\beta}$ as

$$\Pi_{\alpha\beta}^{ij} = (\mathbf{x}_{\alpha\beta} \cdot \mathbf{F}_{\alpha\beta}) \hat{x}_{\alpha\beta}^i \hat{x}_{\alpha\beta}^j, \quad (2.10)$$

$$\Omega_{\alpha\beta} = \int_0^1 d\omega \delta(\mathbf{x} - \mathbf{x}_\alpha + \omega \mathbf{x}_{\alpha\beta}). \quad (2.11)$$

$\mathbf{F}_{\alpha\beta}$ is the interaction force between the particles α and β . The quantity $\Omega_{\alpha\beta}$ is symmetric under the exchange of particle indices α, β , i.e., $\Omega_{\alpha\beta} = \Omega_{\beta\alpha}$. The

2.2 Local equilibrium average

tensor quantity $\Pi_{\alpha\beta}^{ij}$, defined in Eq. (2.10), is also symmetric under the exchange of particle indices α, β as well as Cartesian coordinate indices i, j . It is obvious from Eq. (2.8) that stress tensor σ_{ij} is symmetric, i.e., $\hat{\sigma}_{ij} = \hat{\sigma}_{ji}$. The five microscopic continuity equations deduced above are exact and do not contain any dissipative part. They preserve time-reversal symmetry and are non-local. Only for small values of $x_{\alpha\beta}$ potential is nonzero, we approximate $\Omega_{\alpha\beta}$ as $\delta(\mathbf{x} - \mathbf{x}_\alpha)$ which gives the local form of the currents as

$$\hat{\sigma}_{ij}(\mathbf{x}) = \sum_{\alpha} \left\{ \frac{p_{\alpha}^i p_{\alpha}^j}{m} + \frac{1}{2} \sum_{\alpha \neq \beta} \Pi_{\alpha\beta}^{ij} \right\} \delta(\mathbf{x} - \mathbf{x}_{\alpha}), \quad (2.12)$$

$$\hat{\mathbf{j}}_i^e(\mathbf{x}) = \sum_{\alpha} \left\{ e_{\alpha} \frac{p_{\alpha}^i}{m} + \frac{1}{4} \sum_{\alpha \neq \beta} \sum_j \Pi_{\alpha\beta}^{ij} \left(\frac{p_{\alpha}^j}{m} + \frac{p_{\beta}^j}{m} \right) \right\} \delta(\mathbf{x} - \mathbf{x}_{\alpha}). \quad (2.13)$$

2.2 Local equilibrium average

In the above section, we have obtained time-reversible microscopic equations for the set of five conserved densities $\{\hat{\rho}(\mathbf{x}, t), \hat{\mathbf{g}}(\mathbf{x}, t), \hat{e}(\mathbf{x}, t)\}$. Here we discuss averaging process applicable to nonequilibrium systems (Zubarev *et al.*, 1997) by extending the ideas of equilibrium averaging (Huang, 1987; McQuarrie, 2000). We visualize that at any time the nonequilibrium system may be divided into many cells of intermediate size. Size of these cells are assumed in such a way that each individual cell can be treated as thermodynamic subsystem with their surroundings and any thermodynamic quantities inside the cell varies very slowly. This assumption makes it possible to define local thermodynamic quantity which vary from one cell to another but uniform inside each cell. Equilibrium distribution function for a set of extensive variable $\{\Phi\} = \{H, N, \mathbf{p}, \dots\}$ is obtained as

$$f_{eq}(\mathbf{x}^N, \mathbf{p}^N) = \mathcal{Z}^{-1} \exp \{-\beta(H - \mu N + \mathbf{p} \cdot \mathbf{v})\}, \quad (2.14)$$

2.2 Local equilibrium average

where \mathcal{Z}^{-1} is the normalization constant. The conjugate variable corresponding to total energy, number of particle, and momentum are temperature, chemical potential, and velocity respectively and represented by the set $\{\bar{\Phi}\} = \{\beta, \mu, \mathbf{v}\}$. Using the same analogy, the distribution function for nonuniform densities $\hat{\mathbf{w}} \equiv \{\hat{e}, \hat{\mathbf{g}}, \hat{n}\}$ is given by

$$f_{le}(\Gamma_N, t) = Q_l^{-1} \exp \left\{ - \int d\mathbf{x} \beta(\mathbf{x}, t) \left[\hat{e}(\mathbf{x}) - \mathbf{v}(\mathbf{x}, t) \cdot \hat{\mathbf{g}}(\mathbf{x}) - (\mu(\mathbf{x}, t) - \frac{1}{2} m v^2(\mathbf{x}, t)) \hat{n}(\mathbf{x}) \right] \right\}, \quad (2.15)$$

where Γ_N is phase point described by $6N$ variables $\{\mathbf{x}_1, \mathbf{p}_1, \dots, \mathbf{x}_N, \mathbf{p}_N\}$, and $\hat{n}(\mathbf{x})$ is the number density given as $\hat{n}(\mathbf{x}) = \sum_{\alpha} \delta(\mathbf{x} - \mathbf{x}_{\alpha}(t))$ which is related to mass density $\hat{\rho}(\mathbf{x})$ by $\hat{\rho}(\mathbf{x}) = m \hat{n}(\mathbf{x})$. For unit mass $\hat{n}(\mathbf{x})$ and $\hat{\rho}(\mathbf{x})$ are same. The quantity Q_l^{-1} is the normalization constant given by the following relation

$$Q_l = Tr \left[\exp \left\{ - \int d\mathbf{x} \sum_{\{\psi\}} w_{\psi}(\mathbf{x}, t) \hat{\psi}(\mathbf{x}) \right\} \right]. \quad (2.16)$$

The local density $\hat{\psi}(\mathbf{x})$ is defined by the extensive variable Ψ as

$$\Psi = \int d\mathbf{x} \hat{\psi}(\mathbf{x}), \quad (2.17)$$

and w_{ψ} is corresponding local thermodynamic property (intensive variable). The local equilibrium average of $\hat{\psi}(\mathbf{x})$ is given by the relation

$$\langle \hat{\psi}(\mathbf{x}) \rangle_{le} = - \frac{\delta \ln Q_l(t)}{\delta w_{\psi}(\mathbf{x}, t)}. \quad (2.18)$$

2.3 The Euler equations: Reversible dynamics

w_ψ corresponding to set $\hat{\psi} \equiv \{\hat{n}, \hat{\mathbf{g}}, \hat{e}\}$ are obtained as

$$\begin{aligned} w_n &= -\beta(\mathbf{x}, t) \left[\mu(\mathbf{x}, t) - \frac{1}{2} m v^2(\mathbf{x}, t) \right], \\ w_{\mathbf{g}} &= -\beta(\mathbf{x}, t) \mathbf{v}(\mathbf{x}, t), \quad w_e = -\beta(\mathbf{x}, t). \end{aligned} \quad (2.19)$$

The set of local thermodynamic variables $\{\beta(\mathbf{x}, t), \mu(\mathbf{x}, t), \mathbf{v}(\mathbf{x}, t)\}$, analogous to the equilibrium case, represents the local temperature, local chemical potential, and local velocity respectively. Nonequilibrium average of local density $\hat{\psi}$ is approximated as the average over local equilibrium distribution,

$$\psi(\mathbf{x}, t) = \langle \hat{\psi}(\mathbf{x}) \rangle_{ne} \approx \langle \hat{\psi}(\mathbf{x}) \rangle_{le}. \quad (2.20)$$

The averaged local densities $\psi(\mathbf{x}, t)$ have smooth spatial and temporal dependence. We call them as hydrodynamic fields. The coarse-grained equations corresponding to microscopic densities $\hat{\psi}(\mathbf{x}, t) = \{\hat{\rho}, \hat{\mathbf{g}}, \hat{e}\}$ are given as

$$\frac{\partial \psi(\mathbf{x}, t)}{\partial t} + \nabla \cdot \mathbf{J}_\psi = 0, \quad (2.21)$$

with the corresponding macroscopic currents \mathbf{J}_ψ which are given by the local equilibrium average of the microscopic currents (defined in Eqs. (2.7) - (2.9)), i.e., $\langle \hat{\mathbf{g}} \rangle_{le}$, $\langle \hat{\sigma}_{ij} \rangle_{le}$ and $\langle \hat{\mathbf{j}}^e \rangle_{le}$.

2.3 The Euler equations: Reversible dynamics

Euler equations describe the dynamics of a perfect fluid or ideal fluid (Landau & Lifshitz, 1963). To obtain Euler equations of the hydrodynamics, we need to average the microscopic balance Eqs. (2.4) - (2.6) over nonequilibrium ensemble by utilizing the concept of Gibbsian ensemble. The set of averaged local densities

2.3 The Euler equations: Reversible dynamics

denoted by $\{\rho(\mathbf{x}, t), \mathbf{g}(\mathbf{x}, t), e(\mathbf{x}, t)\}$ have smooth dependence on space and time. The macroscopic equations of hydrodynamics are obtained corresponding to these slow conserved densities (Das, 2011).

To coarse-grain the microscopic Eqs. (2.4) - (2.6), we consider the fluid from a comoving frame with local velocity $\mathbf{v}(\mathbf{x}, t)$ so that fluid appears at rest in the vicinity of point \mathbf{x} at time t . The moving frame is denoted by prime. In locally moving frame, we take conserved densities $\{\hat{\rho}'(\mathbf{x}), \hat{g}'(\mathbf{x}), \hat{e}'(\mathbf{x})\}$ and corresponding currents $\{\hat{g}'(\mathbf{x}), \hat{\sigma}'(\mathbf{x}), \hat{\mathbf{J}}'^e(\mathbf{x})\}$. In moving frame, the position and momentum coordinates of the particles are defined by the canonical transformation from the rest frame as

$$\mathbf{p}_\alpha = \mathbf{p}_\alpha + m\mathbf{v}(\mathbf{x}'_\alpha) \text{ and } \mathbf{x}_\alpha = \mathbf{x}'_\alpha. \quad (2.22)$$

Using the transformation rule (2.22), the following relations of the microscopic densities in the two frames are obtained:

$$\hat{\rho}(\mathbf{x}) = \hat{\rho}'(\mathbf{x}), \quad (2.23)$$

$$\hat{\mathbf{g}}(\mathbf{x}) = \hat{\mathbf{g}}'(\mathbf{x}) + \hat{\rho}'(\mathbf{x})\mathbf{v}(\mathbf{x}), \quad (2.24)$$

$$\hat{e}'(\mathbf{x}) = \hat{e}'(\mathbf{x}) + \frac{1}{2}\hat{\rho}'(\mathbf{x})v^2(\mathbf{x}) + \hat{\mathbf{g}}'(\mathbf{x}) \cdot \mathbf{v}(\mathbf{x}). \quad (2.25)$$

Transformation for the currents $\hat{\sigma}'_{ij}(\mathbf{x})$ and $\hat{\mathbf{J}}'^e(\mathbf{x})$ are obtained as

$$\hat{\sigma}'_{ij}(\mathbf{x}) = \hat{\sigma}'_{ij}(\mathbf{x}) + \hat{g}'_j(\mathbf{x})v_i(\mathbf{x}) + \hat{\rho}'(\mathbf{x})v_i(\mathbf{x})v_j(\mathbf{x}), \quad (2.26)$$

$$\begin{aligned} \hat{\mathbf{J}}^e(\mathbf{x}) &= \hat{\mathbf{J}}'^e(\mathbf{x}) + \left[\hat{e}'(\mathbf{x}) + \mathbf{v}(\mathbf{x}) \cdot \hat{\mathbf{g}}'(\mathbf{x}) + \frac{1}{2}\hat{\rho}'(\mathbf{x})v^2(\mathbf{x}) \right] \mathbf{v}(\mathbf{x}) \\ &+ \frac{1}{2}\hat{\mathbf{g}}'(\mathbf{x})v^2(\mathbf{x}) + \hat{\sigma}' \cdot \mathbf{v}(\mathbf{x}). \end{aligned} \quad (2.27)$$

2.3 The Euler equations: Reversible dynamics

The transformation rule obtained in Eq. (2.27) holds for short range potential. Heat current, $\hat{\mathbf{J}}^e(\mathbf{x})$, for short range potential is defined by Eq. (2.13). Transformed form of distribution function is obtained as

$$f_{le}(\Gamma'_N; t) = Q_l^{-1} \exp \left\{ - \int d\mathbf{x} \beta(\mathbf{x}, t) [\hat{e}'(\mathbf{x}) - \mu(\mathbf{x}, t) \hat{n}'(\mathbf{x})] \right\}. \quad (2.28)$$

Local equilibrium average of mass density is given by

$$\langle \hat{\rho}(\mathbf{x}, t) \rangle_{le} = \rho(\mathbf{x}, t) = \langle \hat{\rho}'(\mathbf{x}, t) \rangle_{le}. \quad (2.29)$$

Currents $\hat{\mathbf{g}}'(\mathbf{x})$ and $\hat{\mathbf{J}}'^e(\mathbf{x})$ are antisymmetric in momentum their local equilibrium averages $\langle \hat{\mathbf{g}}'(\mathbf{x}) \rangle_{le}$ and $\langle \hat{\mathbf{J}}'^e(\mathbf{r}) \rangle_{le}$ with respect to $f_{le}(\Gamma'_N, t)$ will be zero

$$\langle \hat{\mathbf{g}}'(\mathbf{x}) \rangle_{le} = 0, \quad \langle \hat{\mathbf{J}}'^e(\mathbf{x}) \rangle_{le} = 0. \quad (2.30)$$

The average of microscopic stress tensor, $\hat{\sigma}'_{ij}$, and energy density, \hat{e}' , are nonzero and respectively related to the local thermodynamic pressure $P(\mathbf{x}, t)$ and internal energy density $\varepsilon(\mathbf{x}, t)$ of the fluid as

$$\langle \hat{\sigma}'_{ij} \rangle_{le} = \delta_{ij} P(\mathbf{x}, t), \quad (2.31)$$

$$\langle \hat{e}' \rangle_{le} = \varepsilon(\mathbf{x}, t). \quad (2.32)$$

Next, using the relations (2.29)-(2.32), we obtain the averages of microscopic

2.3 The Euler equations: Reversible dynamics

currents and energy density as

$$\mathbf{g} = \langle \hat{\mathbf{g}} \rangle_{le} = \rho \mathbf{v}, \quad (2.33)$$

$$\sigma_{ij} = \langle \hat{\sigma}_{ij} \rangle_{le} = \delta_{ij} P + \rho v_i v_j, \quad (2.34)$$

$$\mathbf{J}^e = \langle \hat{\mathbf{J}}^e \rangle_{le} = \left\{ \varepsilon(\mathbf{x}, t) + \frac{1}{2} \rho v^2 + P \right\} \mathbf{v}, \quad (2.35)$$

$$e(\mathbf{x}, t) = \langle \hat{e}(\mathbf{x}, t) \rangle_{le} = \varepsilon(\mathbf{x}, t) + \frac{1}{2} \rho(\mathbf{x}, t) v^2(\mathbf{x}, t). \quad (2.36)$$

Now substituting the coarse-grained currents (2.33)-(2.35) in Eq. (2.21), we get the Euler equations of hydrodynamics

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{g} = 0, \quad (2.37)$$

$$\frac{\partial g_i}{\partial t} + \sum_j \nabla_j \left(\frac{g_i g_j}{\rho} \right) + \nabla_i P = 0, \quad (2.38)$$

$$\frac{\partial e}{\partial t} + \nabla \cdot \left[(e + P) \frac{\mathbf{g}}{\rho} \right] = 0. \quad (2.39)$$

Above coarse-grained equations are dissipation free and preserve time-reversal symmetry. In this dynamics, we have not considered any processes which cause energy dissipation. Heat exchange and internal frictional force or viscosity between fluid layers cause energy loss. In the ideal fluid motion, viscosity and thermal conductivity do not play any role. The ideal fluid motion is considered adiabatic since the heat exchange between distinct parts of the fluid as well as between fluid and surroundings is zero. In an adiabatic motion, there is no net production of entropy which implies that the entropy production rate $T(dS(\mathbf{x}, t)/dt)$ is equal to zero, where T is the temperature and $S(\mathbf{x}, t)$ is the total entropy of

2.3 The Euler equations: Reversible dynamics

the fluid in local equilibrium state defined as

$$S(\mathbf{x}, t) = -\langle \ln f_{le}(\Gamma_N, t) \rangle. \quad (2.40)$$

The entropy density $s(\mathbf{x}, t)$, whose spatial integral gives the total entropy $S(\mathbf{x}, t)$, satisfies the following continuity equation

$$\frac{\partial s}{\partial t} + \nabla \cdot (s\mathbf{v}) = 0, \quad (2.41)$$

where $s\mathbf{v}$ is the corresponding entropy current. In case of dissipative dynamics there will be positive production of entropy (Martin *et al.*, 1972).

2.3.1 The Galilean invariance

The convective nonlinear term $\nabla_j [g_i g_j / \rho]$ in Eq. (2.38) is responsible for maintaining the Galilean invariance of the hydrodynamic equations of motion obtained above. In order to elaborate this issue, we consider two frames S and S' moving relative to each other with constant velocity. We choose the S frame at rest in the laboratory and S' to be moving with constant velocity \mathbf{u} relative to S . The frame S' is the fluid rest frame when $\mathbf{u} = \mathbf{v}$, where \mathbf{v} is the fluid velocity. We put a prime on the quantities of the S' frame to distinguish the corresponding quantities of the S frame. The space-time coordinate of the two frame are related by the following transformation relation

$$\mathbf{x}' = \mathbf{x} - \mathbf{u}t, \quad t' = t, \quad (2.42)$$

and the velocity transformation rule is obtained as

$$\mathbf{v}'(\mathbf{x}', t) = \mathbf{v}(\mathbf{x}, t) - \mathbf{u}. \quad (2.43)$$

2.3 The Euler equations: Reversible dynamics

Using the transformation rule (2.42), we obtain the following relation

$$\nabla = \nabla', \quad \frac{\partial}{\partial t'} = \frac{\partial}{\partial t} + \mathbf{u} \cdot \nabla \quad (2.44)$$

Mass density is Galilean invariant, i.e., $\rho' = \rho$ and momentum density in two frame is related as $\mathbf{g}' = \mathbf{g} - \rho\mathbf{u}$. Using the transformation rules (2.42)-(2.44), it is straightforward to show that the continuity equation (2.37) and energy density equation (2.39) are invariant under Galilean transformation. Next, we focus on the momentum density equation (2.38). The time derivative of momentum density field \mathbf{g}' is obtained as

$$\frac{\partial g'_i}{\partial t'} = \frac{\partial g_i}{\partial t} + u_j \nabla_j g_i - u_i \frac{\partial \rho}{\partial t} - u_i u_j \nabla_j \rho, \quad (2.45)$$

and the convective term $\nabla_j [g_i g_j / \rho]$ in the primed frame is obtained as

$$\nabla'_j [g'_i g'_j / \rho'] = \nabla_j [g_i g_j / \rho] - u_j \nabla_j g_i - u_i \nabla_j g_j + u_i u_j \nabla_j \rho. \quad (2.46)$$

From Eqs. (2.45), (2.46) and using the continuity equation (2.37), we obtain

$$\frac{\partial g'_i}{\partial t'} + \nabla'_j [g'_i g'_j / \rho'] = \frac{\partial g_i}{\partial t} + \nabla_j [g_i g_j / \rho] \quad (2.47)$$

From the above relation, we see that the equation (2.38) is invariant under Galilean transformation and the nonlinear term $\nabla_j [g_i g_j / \rho]$ plays the crucial role to preserve the invariance. In Chapters 5 and 6, we will see that there are some active matter systems which violate the Galilean invariance.

2.4 Dissipative hydrodynamics

In the dissipative dynamics, irreversible transport coefficients like thermal conductivity and viscosity play essential role. Dissipative effects are included in a phenomenological way in the time evolution equations for the macroscopic densities. We add their contribution in terms of dissipative parts in the respective reversible currents as

$$\sigma_{ij} = \delta_{ij}P + \rho v_i v_j + \tilde{\sigma}_{ij}, \quad (2.48)$$

$$\mathbf{J}^e = \left\{ \varepsilon + \frac{1}{2}\rho v^2 + P \right\} \mathbf{v} + \tilde{\mathbf{J}}^e. \quad (2.49)$$

The entropy-production rate corresponding to dissipative dynamics described above is obtained as

$$T \frac{dS}{dt} = - \int d\mathbf{x} \left((\nabla_i v_j) \tilde{\sigma}_{ij} + \frac{\nabla T}{T} \cdot \tilde{\mathbf{J}}^e \right), \quad (2.50)$$

where we have ignored the terms of higher order in gradients of \mathbf{v} or T . Next, to have positive entropy-production rate for the irreversible process, $\tilde{\sigma}_{ij}$ and $\tilde{\mathbf{J}}^e$ must have the following form

$$\tilde{\sigma}_{ij} = -\eta_{ijkl} \nabla_k v_l, \quad (2.51)$$

$$\tilde{J}_i^e = -\kappa_{ij} \nabla_j T, \quad (2.52)$$

where repeated indices are summed over. Forth and second rank tensors in Eqs. (2.51) and (2.52) represent viscosity and thermal conductivity respectively. For

an isotropic system viscosity and thermal conductivity tensors are simplified as,

$$\eta_{ijkl} = \eta(\delta_{ik}\delta_{jl} + \delta_{ij}\delta_{kl}) + \left(\zeta - \frac{2\eta}{3}\right)\delta_{ij}\delta_{kl}, \quad (2.53)$$

$$\kappa_{ij} = \delta_{ij}\kappa, \quad (2.54)$$

where η is shear viscosity and ζ is bulk viscosity. The dissipative hydrodynamic equations corresponding to the coarse-grained mass density, momentum density and energy density are obtained as

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{g} = 0, \quad (2.55)$$

$$\frac{\partial g_i}{\partial t} + \sum_j \nabla_j \left(\frac{g_i g_j}{\rho} \right) + \nabla_i P - \left(\zeta + \frac{1}{3}\eta \right) \nabla_i (\nabla \cdot \mathbf{v}) - \eta \nabla^2 v_i = 0, \quad (2.56)$$

$$\frac{\partial e}{\partial t} + \nabla \cdot \left[(e + P) \frac{\mathbf{g}}{\rho} \right] - \kappa \nabla^2 T = 0. \quad (2.57)$$

Continuity Eq. (2.55) does not have any dissipative part in it and is invariant under time reversal. Using the nonlinear relation (2.33) and Eq. (2.56), we obtain the following equation for the velocity field

$$\rho \left(\frac{\partial v_i}{\partial t} + (\mathbf{v} \cdot \nabla) v_i \right) = -\nabla_i P + \left(\zeta + \frac{1}{3}\eta \right) \nabla_i (\nabla \cdot \mathbf{v}) + \eta \nabla^2 v_i. \quad (2.58)$$

The above equation with the mass density Eq. (2.56) and energy density Eq. (2.57) are the Navier-Stokes equations of fluid dynamics. These equations provide a complete description of the long-distance long-time dynamics of the fluid. For an incompressible fluid, the mass density becomes constant in time and space which follows that $\nabla_j v_j = 0$. Eq. (2.58) for an incompressible fluid reduces to

the form

$$\frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla) \mathbf{v} = -\frac{\nabla P}{\rho_0} + \nu_0 \nabla^2 \mathbf{v}, \quad (2.59)$$

where $\nu_0 = \eta/\rho_0$ with ρ_0 as the constant density, denotes the kinematic viscosity. The above equation describes the flow of an incompressible fluid. This equation is fully deterministic, i.e., it does not contain any stochastic or random part. The second nonlinear term on the right-hand side of the above equation, as described in section (2.3.1), maintains the Galilean invariance of the equation of motion.

2.5 Discussion

The Euler equations of hydrodynamics follow from the averaging of the microscopic equations over local equilibrium distribution function. These equations describe the adiabatic motion of the fluid which has zero viscosity. The entropy production rate is zero which signifies the time-reversal symmetry of the equations. The dissipative extension of the Euler equations are the Navier-Stokes equations. Dissipative terms are obtained in a phenomenological manner. Positive definiteness of entropy production rate allows us to obtain the dissipative form of fluxes which lead to the time irreversible hydrodynamic equations of the fluid.

Appendix

2.A Momentum density equation

Taking the time derivative of momentum density $\hat{\mathbf{g}}$ defined in Eq. (2.2), we obtain

$$\begin{aligned}
\frac{\partial \hat{g}_i}{\partial t} &= \sum_{\alpha} \nabla_{\mathbf{x}_{\alpha}} \delta(\mathbf{x} - \mathbf{x}_{\alpha}) \cdot \dot{\mathbf{x}}_{\alpha} p_{\alpha}^i + \sum_{\alpha} \dot{p}_{\alpha}^i \delta(\mathbf{x} - \mathbf{x}_{\alpha}) \\
&= - \sum_j \nabla_j \sum_{\alpha} \frac{p_{\alpha}^i p_{\alpha}^j}{m} \delta(\mathbf{x} - \mathbf{x}_{\alpha}) \\
&\quad - \frac{1}{2} \sum_{\alpha \neq \beta} \{ \delta(\mathbf{x} - \mathbf{x}_{\beta}) - \delta(\mathbf{x} - \mathbf{x}_{\alpha}) \} F_{\alpha\beta}^i, \tag{2.A.1}
\end{aligned}$$

where $\mathbf{F}_{\alpha\beta}$ is interaction force between particles α and β and $F_{\alpha\beta}^i = -F_{\beta\alpha}^i$. To simplify the second term of above equation, we manipulate it like the following way

$$\begin{aligned}
&\{ \delta(\mathbf{x} - \mathbf{x}_{\beta}) - \delta(\mathbf{x} - \mathbf{x}_{\alpha}) \} F_{\alpha\beta}^i \\
&= \left\{ \int_0^1 d\omega \sum_j \frac{\partial}{\partial x^j} \delta(\mathbf{x} - \mathbf{x}_{\alpha} + \omega \mathbf{x}_{\alpha\beta}) \right\} x_{\alpha\beta}^j F_{\alpha\beta}^i \\
&= \sum_j \nabla_j \left\{ \int_0^1 d\omega \delta(\mathbf{x} - \mathbf{x}_{\alpha} + \omega \mathbf{x}_{\alpha\beta}) x_{\alpha\beta}^j F_{\alpha\beta}^i \right\} \\
&= \nabla_j [\Omega_{\alpha\beta} \Pi_{\alpha\beta}^{ij}], \tag{2.A.2}
\end{aligned}$$

2.A Momentum density equation

where $\Omega_{\alpha\beta} = \int_0^1 d\omega \delta(\mathbf{x} - \mathbf{x}_\alpha + \omega \mathbf{x}_{\alpha\beta})$ and $\Pi_{\alpha\beta}^{ij} = x_{\alpha\beta}^j F_{\alpha\beta}^i$. The quantity $\Pi_{\alpha\beta}^{ij}$ can be written as

$$\Pi_{\alpha\beta}^{ij} = x_{\alpha\beta}^j F_{\alpha\beta}^i = (\mathbf{x}_{\alpha\beta} \cdot \mathbf{F}_{\alpha\beta}) \hat{x}_{\alpha\beta}^i \hat{x}_{\alpha\beta}^j. \quad (2.A.3)$$

It is obvious that the quantities $\Omega_{\alpha\beta}$ and $\Pi_{\alpha\beta}^{ij}$ are symmetric under exchange of particle indices α, β and coordinate indices i, j . Now Eq. (2.A.1) is obtained as

$$\begin{aligned} \frac{\partial \hat{g}_i}{\partial t} &= - \sum_j \nabla_j \left\{ \sum_\alpha \frac{p_\alpha^i p_\alpha^j}{m} \delta(\mathbf{x} - \mathbf{x}_\alpha) + \frac{1}{2} \sum_{\alpha \neq \beta} \Omega_{\alpha\beta} [(\mathbf{x}_{\alpha\beta} \cdot \mathbf{F}_{\alpha\beta}) \hat{x}_{\alpha\beta}^i \hat{x}_{\alpha\beta}^j] \right\} \\ &= - \sum_j \nabla_j \hat{\sigma}_{ij} \end{aligned}$$

or

$$\frac{\partial \hat{g}_i}{\partial t} + \sum_j \nabla_j \hat{\sigma}_{ij} = 0,$$

where stress tensor $\hat{\sigma}_{ij}$ is given by

$$\hat{\sigma}_{ij}(\mathbf{x}, t) = \sum_\alpha \frac{p_\alpha^i p_\alpha^j}{m} \delta(\mathbf{x} - \mathbf{x}_\alpha) + \frac{1}{2} \sum_{\alpha \neq \beta} \Omega_{\alpha\beta} (\mathbf{x}_{\alpha\beta} \cdot \mathbf{F}_{\alpha\beta}) \hat{x}_{\alpha\beta}^i \hat{x}_{\alpha\beta}^j \quad (2.A.4)$$

or

$$\hat{\sigma}_{ij}(\mathbf{x}, t) = \sum_\alpha \frac{p_\alpha^i p_\alpha^j}{m} \delta(\mathbf{x} - \mathbf{x}_\alpha) + \frac{1}{2} \sum_{\alpha \neq \beta} \Omega_{\alpha\beta} \Pi_{\alpha\beta}^{ij}. \quad (2.A.5)$$

Symmetry property, $\hat{\sigma}_{ij} = \hat{\sigma}_{ji}$, of the microscopic stress tensor is the consequence of conservation of angular momentum of the system.

2.B Energy density equation

Taking the time derivative of microscopic energy density \hat{e} defined by Eq. (2.3), we obtain

$$\frac{\partial \hat{e}}{\partial t} = -\nabla_{\mathbf{x}} \cdot \sum_{\alpha} \delta(\mathbf{x} - \mathbf{x}_{\alpha}) \frac{\mathbf{p}_{\alpha}}{m} e_{\alpha} + \sum_{\alpha} \dot{e}_{\alpha} \delta(\mathbf{x} - \mathbf{x}_{\alpha}). \quad (2.B.1)$$

From the expression, $e_{\alpha} = p_{\alpha}^2/(2m) + (1/2)\sum_{\beta \neq \alpha} u(x_{\alpha\beta})$, its derivative \dot{e}_{α} is obtained as

$$\dot{e}_{\alpha} = \frac{1}{2} \sum_{\alpha \neq \beta} \mathbf{F}_{\alpha\beta} \cdot \left(\frac{\mathbf{p}_{\alpha}}{m} + \frac{\mathbf{p}_{\beta}}{m} \right).$$

Using the above expression for \dot{e}_{α} , Eq. (2.B.1) is obtained as

$$\begin{aligned} \frac{\partial \hat{e}}{\partial t} = & -\sum_i \nabla_i \left\{ \sum_{\alpha} \frac{p_{\alpha}^i}{m} e_{\alpha} \delta(\mathbf{x} - \mathbf{x}_{\alpha}) \right. \\ & \left. + \frac{1}{4} \sum_j \sum_{\alpha \neq \beta} \left(\frac{p_{\alpha}^j}{m} + \frac{p_{\beta}^j}{m} \right) [\Omega_{\alpha\beta} \Pi_{\alpha\beta}^{ij}] \right\} \end{aligned} \quad (2.B.2)$$

or

$$\frac{\partial \hat{e}}{\partial t} = -\nabla \cdot \hat{\mathbf{J}}^e. \quad (2.B.3)$$

Chapter 3

Hydrodynamic equations for coarse-grained fields

In the previous chapter, we have discussed the hydrodynamics of a simple fluid in which particles follow Newtonian dynamics. Hydrodynamic equations are obtained corresponding to the local density fields. They follow from the time reversible microscopic equations which do not contain any dissipative or random noise part. In the process of obtaining macroscopic equations dissipative terms are added phenomenologically by utilizing the notion of entropy production rate. Here we consider the case when microscopic dynamics will be irreversible and particles follow Brownian dynamics. Microscopic momentum is not conserved in this model. In this chapter, we discuss the coarse-grained description for passive particles only to facilitate the description of the method to be applied in the subsequent chapter for active particles.

In the following section, we give brief discussion on the Brownian dynamics for passive particles by considering the simplest form of Langevin equation. In the subsequent sections, we discuss the two different cases for the dynamics of passive Brownian particles: the Fokker-Planck case, and Smoluchowski case. The

coarse-grained form of equations for the two cases are obtained in terms of the hydrodynamic field equations. The idea of Brownian motion for active particles also discussed at the end of this chapter.

3.1 Brownian motion

3.1.1 Passive particles motion

Brownian motion illustrates the erratic motion of a large particle (Brownian particle) suspended in fluids. Irregular motion of the big particle is due to the continuous random collision of surrounding fluid particles. The theory of Brownian motion was first explained by Einstein and Smoluchowski and further developed by Langevin and others (Chandrasekhar, 1949; Einstein, 1949; Frey & Kroy, 2005). Here we describe briefly the Einstein's explanation on Brownian motion followed by Langevin description.

Einstein proposed that the suspended particle is big enough to be observed by a microscope and small enough to perform the Brownian motion without affected by the gravity. N particles having number density n suspended in a background fluid are treated to behave like as an ideal gas for small particle density. These particles, when trying to leave their container, exert osmotic pressure $p = nk_B T$ on the wall of container. One assumes that a force K acts on each immersed particles and in dynamic equilibrium, K is independent of time. Equilibrium condition, in one dimension, requires force balance relation

$$nK - \partial p / \partial x = 0. \tag{3.1}$$

Now if one considers spherical Brownian particles having radius r and suspended in a fluid of viscosity η , then the drift velocity of particles, due to the force K , is

given as $nK/(6\pi\eta r)$. And next, the diffusion current for suspended particles for diffusion constant D is given by $-D\partial n/\partial x$. In dynamic equilibrium, sum of drift and diffusion current vanishes. Using this fact and the force balance condition (3.1), one obtains $D = k_B T/(6\pi\eta r)$ which is the Stokes-Einstein relation that relates the two macroscopic hydrodynamic coefficients D and η .

Next, we will discuss the probabilistic interpretation of diffusion equation for Brownian particles. We assume that motion of a single Brownian particle is not affected by the motion of all other particles as well as movement of the same particle after different time intervals is mutually independent for reasonable time intervals. Particle density at position x and time $t + \tau$ is expressed as the function of particle at time t by the relation

$$n(x, t + \tau) = \int_{-\infty}^{+\infty} n(x + \varepsilon, t) \phi(\varepsilon) d\varepsilon, \quad (3.2)$$

where $\phi(\varepsilon)$ follows the properties $\phi(\varepsilon) = \phi(-\varepsilon)$ and $\int_{-\infty}^{+\infty} \phi(\varepsilon) = 1$. In modern language, $\phi(\varepsilon)$ is termed as the jump probabilities (Gardiner, 1989). On Taylor expansion of Eq. (3.2) with respect to τ and ε , and comparing both sides we obtain the following diffusion equation

$$\frac{\partial n}{\partial t} = D \frac{\partial^2 n}{\partial x^2}, \quad (3.3)$$

where the D is the diffusion coefficient obtained by

$$\frac{1}{2\tau} \int_{-\infty}^{+\infty} d\varepsilon \varepsilon^2 \phi(\varepsilon) = \langle \delta x^2 \rangle / (2\tau) = D, \quad (3.4)$$

which gives the relation

$$\langle x^2(t) \rangle = 2Dt, \quad (3.5)$$

where $\langle x^2(t) \rangle$ is the mean square displacement of the Brownian particle in a time

interval t . Eq. (3.5) is termed as Einstein relation which tells the distance traveled by the Brownian particle in a given interval of time. This relation is based on the assumptions that at time $t = 0$ each particle's coordinate system have the same origin and distribution follows the Gaussian form. From the above results have seen that the discrete random processes generate smooth behavior on macroscale. Below we will discuss the Langevin formulation of Brownian motion.

Langevin description

In order to discuss the dynamics in terms of Langevin equation, we consider mass of Brownian particle m , velocity $u(t)$ at time t . Langevin assumed that the force acting on the Brownian particle is given by two parts. First part is deterministic part which is the frictional force proportional to the velocity of the particle and in opposite direction. The second part is stochastic force, $\xi(t)$, which results from the random collision of the surrounding particles. The motion of the Brownian particle in one dimension is given by the following equation:

$$\frac{dx}{dt} = u, \quad m \frac{du}{dt} + \zeta_0 u = F(x) + \xi(t). \quad (3.6)$$

Here $F(x)$ is the external force resulting from the spatial derivative of total external potential of the system. $\xi(t)$ is assumed to be Gaussian white noise with its mean zero and variance given by

$$\langle \xi(t)\xi(t') \rangle = 2\bar{D}\delta(t - t'), \quad (3.7)$$

where \bar{D} is the noise strength. For $F(x) = 0$, we obtain, from Eq. (3.6), the velocity autocorrelation function given as

$$C(t, t') = \frac{\bar{D}}{2\zeta_0} e^{-\zeta_0|t-t'|} + e^{-\zeta_0(t+t'-2t_0)} \left[C(t_0, t_0) - \frac{\bar{D}}{2\zeta_0} \right]. \quad (3.8)$$

If we assume that Brownian particle system is in equilibrium at temperature T , initial velocity distribution follow Maxwell-Boltzmann statistics giving the equal time correlation function as

$$C(t_0, t_0) = \langle v_0^2 \rangle = k_B T, \quad (3.9)$$

where we have taken particle mass m to be unity. In equilibrium state, equal time velocity correlation $C(t, t)$ should be time independent satisfying the following condition

$$k_B T - \frac{\bar{D}}{2\zeta_0} = 0. \quad (3.10)$$

Using the above condition we obtain \bar{D} as

$$\bar{D} = 2\zeta_0 k_B T. \quad (3.11)$$

Therefore noise correlation (3.7), using the relation (3.11), is given by

$$\langle \xi(t)\xi(t') \rangle = 2\zeta_0 k_B T \delta(t - t'). \quad (3.12)$$

In the long time limit (for large t and t'), Brownian particle equilibrates at temperature T and Eq. (3.8) becomes independent of the initial time t_0 giving the following relation for the velocity autocorrelation function as

$$C(t, t') = k_B T e^{-\zeta_0 |t - t'|}. \quad (3.13)$$

The above equation depends on time difference between t and t' and hence is time translation invariant.

The root mean square (rms) displacement of the large particle can be obtained by integrating the Eq. (3.13) with respect to time. Since velocity of the particle

is related to its position by $u = dx/dt$, we can write Eq. (3.13) as

$$\left\langle \frac{d}{dt}x(t) \frac{d}{dt'}x(t') \right\rangle = k_B T e^{-\zeta_0 |t-t'|}. \quad (3.14)$$

Integrating the above equation at time t and t' gives the following relation

$$\langle \Delta(t) \Delta(t') \rangle = k_B T \int_{t_0}^t d\tau \int_{t_0}^{t'} d\tau' e^{-\zeta_0 |\tau-\tau'|}, \quad (3.15)$$

where we have defined $\Delta(t) = (x(t) - x(t_0))$. For the equal time case $t = t'$, we obtain

$$\langle \Delta^2(t) \rangle = 2k_B T \zeta_0^{-1} \left[t - t_0 \zeta_0^{-1} \left(e^{-\zeta_0(t-t_0)} - 1 \right) \right]. \quad (3.16)$$

Now we discuss two limiting cases of the above equation. If we consider very short time such that $\zeta_0^{-1}(t - t_0) \ll 1$, the rms displacement of the particle can be obtained as

$$\langle (x(t) - x(t_0))^2 \rangle^{1/2} = (k_B T)^{1/2} (t - t_0) = u_0 (t - t_0). \quad (3.17)$$

Here rms displacement is linearly proportional to time. This type of motion of the particle corresponds to free particle behaviour. Further if we consider long time limit such that $\zeta_0^{-1}(t - t_0) \gg 1$, we can write

$$\langle (x(t) - x(t_0))^2 \rangle = 2k_B T \zeta_0^{-1} (t - t_0) = 2\bar{D}(t - t_0), \quad (3.18)$$

which shows that mean square displacement is linearly dependent on time. This is the Einstein relation. We have discussed this relation in Eq. (3.4). The diffusion coefficient \bar{D} is related to the frictional coefficient by $\bar{D} = k_B T \zeta_0^{-1}$. The frictional drag ζ_0 on a spherical Brownian particle of radius r , in a liquid

having shear viscosity η is given by Stokes' law $\zeta_0 = 6\pi r\eta$. We can write diffusion coefficient in terms of viscosity as

$$\bar{D} = \frac{k_B T}{6\pi r\eta}. \quad (3.19)$$

The above relation is Stokes-Einstein relation which we have discussed in the Einstein's explanation of Brownian motion in the above subsection. The main difference between the two approaches is that Langevin applied the Newton's second law to write particles equation of motion in terms of stochastic forces with time scale separation while Einstein's approach is based on entirely a probabilistic description of motion of the particles and using reasonable assumptions on probability functions one reaches the Stokes-Einstein relation.

The phenomena of Brownian motion is not limited to only passive particle systems it is also applicable to explain the mechanics of active systems. For example, the mechanism of protein synthesis inside an Eukaryotic cell can be explained using the stochastic dynamical motion of Brownian particle (Frey & Kroy, 2005). One of the important process involved in protein synthesis is that ribosomes inside the cell perform motion from one codon to another codon on the one dimensional filament to transport genetic information. To understand the transport mechanism we consider a Brownian particle doing random walk in one dimension under the influence of a asymmetric potential (shawtooth-type potential). When the potential is off, the particle perform free random walk but when potential is on particle perform net motion in one direction due to the asymmetric nature of the potential. Therefore, we can say that Brownian motion provides a vital force to influence transport mechanism inside the cell. Here the important point is that the energy for this kind of motion do not involve thermal energy as in usual passive particle Brownian motion.

3.2 Fokker-Planck dynamics

We consider a system of N Brownian particles all having the same mass m . Motion of α -th Brownian particle for $\alpha = 1, \dots, N$, is described in terms of position and momentum coordinates $\{\mathbf{x}_\alpha, \mathbf{p}_\alpha\}$. Time evolution of position \mathbf{x}_α and momentum \mathbf{p}_α is given by the following equations

$$m \frac{dx_\alpha^i(t)}{dt} = p_\alpha^i(t), \quad (3.20)$$

$$\frac{dp_\alpha^i(t)}{dt} = -\nabla_\alpha^i \sum_{\nu=1, N}^{\nu \neq \alpha} U(\mathbf{x}_\alpha(t) - \mathbf{x}_\nu(t)) - \frac{\zeta}{m} p_\alpha^i + \eta_\alpha^i(t), \quad (3.21)$$

where the Roman index i denotes the Cartesian coordinates. The quantity ζ/m is dissipative coefficient having dimension inverse of time and $U(\mathbf{x}_\alpha(t) - \mathbf{x}_\nu(t))$ is interaction potential between particles α and ν . We assume that interaction potential depends on the magnitude of separation between particles only, i.e., $U = U(|\mathbf{x}|)$. The quantity η_α on the right-hand side of Eq. (3.21) is the random white noise on the particle α . Its correlation is related to the dissipative coefficient ζ via fluctuation-dissipation theorem as

$$\langle \eta_\alpha^i(t) \eta_\beta^j(t') \rangle = 2k_B T \zeta \delta_{\alpha\beta} \delta_{ij} \delta(t - t'). \quad (3.22)$$

The collective modes for Fokker-Planck dynamics are mass density field $\hat{\rho}(\mathbf{x}, t)$ and momentum density field $\hat{\mathbf{g}}(\mathbf{x}, t)$ defined by

$$\hat{\rho}(\mathbf{x}, t) = \sum_{\alpha=1}^N m \delta(\mathbf{x} - \mathbf{x}_\alpha(t)), \quad (3.23)$$

$$\hat{g}_i(\mathbf{x}, t) = \sum_{\alpha=1}^N p_\alpha^i \delta(\mathbf{x} - \mathbf{x}_\alpha). \quad (3.24)$$

3.3 Smoluchowski dynamics

Using the definition (3.23) for mass density and definition (3.24) for momentum density, closed time evolution equations for density fields are obtained as (Nakamura & Yoshimori, 2009)

$$\frac{\partial \hat{\rho}}{\partial t} + \nabla \cdot \hat{\mathbf{g}} = 0, \quad (3.25)$$

$$\begin{aligned} \frac{\partial \hat{g}_i(\mathbf{x}, t)}{\partial t} &= -\zeta \hat{g}_i(\mathbf{x}, t) - \nabla_j \hat{\Gamma}_{ij}(\mathbf{x}, t) \\ &\quad - \hat{\rho}(\mathbf{x}, t) \nabla_x^i \int dx' U(\mathbf{x} - \mathbf{x}') \hat{\rho}(\mathbf{x}', t) + \hat{\theta}_i(\mathbf{x}, t), \end{aligned} \quad (3.26)$$

where we have defined $\hat{\Gamma}_{ij}(\mathbf{x}, t)$ and noise $\hat{\theta}_i(\mathbf{x}, t)$ as

$$\hat{\Gamma}_{ij}(\mathbf{x}, t) = \sum_{\alpha=1}^N \frac{p_{\alpha}^i p_{\alpha}^j}{m} \delta(\mathbf{x} - \mathbf{x}_{\alpha}), \quad (3.27)$$

$$\hat{\theta}_i(\mathbf{x}, t) = \sum_{\alpha=1}^N \eta_{\alpha}^i(t) \delta(\mathbf{x} - \mathbf{x}_{\alpha}). \quad (3.28)$$

The noise $\hat{\theta}_i$ is multiplicative in nature with zero mean and correlation given by

$$\langle \hat{\theta}_i(\mathbf{x}, t) \hat{\theta}_j(\mathbf{x}', t') \rangle = 2k_B T \zeta \hat{\rho}(\mathbf{x}, t) \delta_{ij} \delta(\mathbf{x} - \mathbf{x}') \delta(t - t'). \quad (3.29)$$

3.3 Smoluchowski dynamics

In the Smoluchowski dynamics of interacting Brownian particles, we consider that system is strongly overdamped by the frictional force. In this situation, momentum fluctuations become very fast as compared to the time evolution of the position coordinates. Momentum thermalizes rapidly and distribution becomes nearly Maxwellian within a short time. Thus particle coordinates $\{\mathbf{x}_{\alpha}\}$ alone is sufficient to describe the dynamics of the system. Here time scale of interest

3.3 Smoluchowski dynamics

is much longer than Brownian relaxation time m/ζ , i.e., the time scale of momentum damping. Smoluchowski dynamics is obtained by adiabatic elimination (Kampen, 1985) of the momentum of the Brownian particle in the Fokker-Planck description. As a result of adiabatic elimination the contribution of inertia term in Eq. (3.21) vanishes. Therefore, in case of additive noise simply neglecting the inertia term obtains the Smoluchowski description. If we assume the noise η_α to be multiplicative, merely ignoring the inertia term will not give the correct Smoluchowski dynamics. In this case, other standard methods are used to eliminate the fast relaxing variable of the dynamics. Some of the methods are discussed in the review article (Kampen, 1985). Neglecting the time derivative of momentum on the left-hand side of Eq. (3.21), we obtain the following equation of motion for the α -th particle

$$\zeta \frac{dx_\alpha^i(t)}{dt} = - \sum_{\nu=1, N}^{\nu \neq \alpha} \nabla_\alpha^i U(\mathbf{x}_\alpha(t) - \mathbf{x}_\nu(t)) + \eta_\alpha^i(t). \quad (3.30)$$

The collective mode corresponding to Smoluchowski dynamics is the mass density defined in Eq. (3.23). For a fix number of particles, N , of the system, mass density is conserved quantity. In order to obtain time evolution of density field $\hat{\rho}$ (Dean, 1996), we consider chain rule of stochastic differential equation in Itô calculus (Øksendal, 1992; Risken, 1989) for a set of random variable $r_\alpha(t)$ ($\alpha = 1, \dots, N$) satisfying the following differential equation

$$\dot{r}_\alpha(t) = q_\alpha(\mathbf{r}, t) + s_{\alpha\beta} \Gamma_\beta(t), \quad (3.31)$$

where variance of white noise Γ_α is defined as $\langle \Gamma_\alpha(t) \Gamma_\beta(t') \rangle = 2\delta_{\alpha\beta} \delta(t - t')$. Here the noise Γ_α is considered to be additive, i.e., $s_{\alpha\beta}$ does not depend on the variable $r_\alpha(t)$. For multiplicative noise, interpretation of the first-order stochastic differential equation (3.31) cannot be given uniquely. In this case the quantity

3.3 Smoluchowski dynamics

$s_{\alpha\beta}$, which will depend on $r_\alpha(t)$, need to be evaluated. Mainly, there are Itô and Stratonovich rules for integration of multiplicative noise which we call the interpretation of the multiplicative noise. Itô interpretation evaluate the quantity $s_{\alpha\beta}$ at the initial time whereas Stratonovich rule evaluates it at the mean of initial and final time. Most of the time it is difficult to choose appropriate interpretation for multiplicative noise. This problem is termed as the Itô-Stratonovich dilemma (Gardiner, 1989; Mortensen, 1969). For additive noise case both the interpretations give the same result. The Stratonovich interpretation uses standard rules of calculus while Itô interpretation deals with the different rules of calculus to evaluate integrals and derivatives. The Langevin equations, describing the dynamics of Brownian particles, considered here have additive noise and hence free from the Itô-Stratonovich dilemma. Brownian motion with additive noise can be extended to multiplicative noise case with proper interpretation of the noise (Kuroiwa & Miyazaki, 2014).

The stochastic differential equation corresponding to Eq. (3.31) for the variable $f(\{r_\alpha\})$, using the Itô rule, is obtained as

$$\dot{f} = \sum_{\alpha} \frac{\partial f}{\partial r_{\alpha}} \dot{r}_{\alpha} + \sum_{\alpha, \beta, \nu} \frac{1}{2} \frac{\partial^2 f}{\partial r_{\alpha} \partial r_{\beta}} s_{\alpha\nu} s_{\beta\nu}. \quad (3.32)$$

We apply the above chain rule for the variable \mathbf{x}_{α} ($\alpha = 1, \dots, N$) for the corresponding differential Eq. (3.30). We identify the function f as

$$f(\mathbf{x}_{\alpha}) \equiv \hat{\rho}(\mathbf{x}, t) = \sum_{\alpha=1}^N \delta(\mathbf{x} - \mathbf{x}_{\alpha}(t)) = \sum_{\alpha=1}^N \hat{\rho}_{\alpha}(\mathbf{x}, t). \quad (3.33)$$

In the above definition we have taken mass m to be unity for simplicity of the notation. Using Eqs. (3.32) and (3.33), time evolution of the density ρ is obtained

as

$$\begin{aligned} \frac{\partial \hat{\rho}(\mathbf{x}, t)}{\partial t} &= \zeta^{-1} \left[\beta^{-1} \nabla^2 \hat{\rho}(\mathbf{x}, t) + \nabla \cdot \left\{ \hat{\rho}(\mathbf{x}, t) \nabla \int dx' U(\mathbf{x} - \mathbf{x}') \hat{\rho}(\mathbf{x}', t) \right\} \right] \\ &\quad + \hat{\Upsilon}(\mathbf{x}, t), \end{aligned} \quad (3.34)$$

where $\beta^{-1} = k_B T$. The random noise $\hat{\Upsilon}(\mathbf{x}, t)$ in the above equation is defined as

$$\hat{\Upsilon}(\mathbf{x}, t) = -\nabla \cdot \sum_{\alpha=1}^N (\hat{\rho}_\alpha(\mathbf{x}, t) \boldsymbol{\eta}_\alpha(t)). \quad (3.35)$$

The noise correlation is given by

$$\begin{aligned} \langle \hat{\Upsilon}(\mathbf{x}, t) \hat{\Upsilon}(\mathbf{x}', t') \rangle &= 2\zeta \beta^{-1} \sum_{\alpha=1}^N \nabla_x \cdot \nabla_{x'} \{ \hat{\rho}_\alpha(\mathbf{x}, t) \hat{\rho}_\alpha(\mathbf{x}', t') \} \delta(t - t') \\ &= 2\zeta \beta^{-1} \nabla_x \cdot \nabla_{x'} \{ \delta(\mathbf{x} - \mathbf{x}') \hat{\rho}(\mathbf{x}, t) \} \delta(t - t'), \end{aligned} \quad (3.36)$$

where ∇_x and $\nabla_{x'}$ denotes derivative operator with respect to components \mathbf{x} and \mathbf{x}' respectively. To simplify the above term, we have used the following property of delta function

$$\sum_{\alpha=1}^N \hat{\rho}_\alpha(\mathbf{x}, t) \hat{\rho}_\alpha(\mathbf{x}', t') = \delta(\mathbf{x} - \mathbf{x}') \hat{\rho}(\mathbf{x}, t) = \delta(\mathbf{x} - \mathbf{x}') \hat{\rho}(\mathbf{x}', t'). \quad (3.37)$$

3.4 Coarse-grained equations

We have obtained, in the above sections, exact time evolution equations for the collective densities $\hat{\rho}$ and $\{\hat{\rho}, \hat{\mathbf{g}}\}$ for the Smoluchowski and Fokker-Planck cases respectively. The collective densities, in a general representation $\hat{\psi}(\mathbf{x}, t)$ and the respective currents $\hat{\mathbf{J}}_\psi$ are related by the continuity equation, $\partial_t \hat{\psi} + \nabla \cdot \hat{\mathbf{J}}_\psi = 0$. The microscopic densities are defined as a sum of delta functions; they cannot be directly related to experimental outcomes. We need to average these

3.4 Coarse-grained equations

microscopic equations over a suitable ensemble to obtain time evolution equations describing the physical properties of the system. The microscopic densities $\hat{\psi}$ depend on phase-space variable. In averaging process, their dependence on phase-space variable are integrated out. We average the microscopic densities $\hat{\psi}(\mathbf{x}, t)$ over nonequilibrium ensemble. The averaged densities $\psi(\mathbf{x}, t)$, i.e., $\psi(\mathbf{x}, t) = \langle \hat{\psi}(\mathbf{x}, t) \rangle_{ne}$, have smooth behavior over time and space. The microscopic equations for $\hat{\psi}(\mathbf{x}, t)$ when averaged over suitable nonequilibrium ensemble results the macroscopic equations for smoothly varying density fields $\psi(\mathbf{x}, t)$ in terms of the respective coarse-grained currents $\mathbf{J}_\psi = \langle \hat{\mathbf{J}}_\psi \rangle_{ne}$. The average of local variable $\hat{\psi}$ over nonequilibrium state is approximated to the average over local equilibrium distribution, i.e., $\psi(\mathbf{x}, t) = \langle \hat{\psi}(\mathbf{x}) \rangle_{ne} \approx \langle \hat{\psi}(\mathbf{x}) \rangle_{le}$. The averaged equations for collective densities form the closed equations of fluctuating nonlinear hydrodynamics.

In chapter 2, we have discussed the averaging process over local equilibrium ensemble by extending the idea of equilibrium Gibbsian ensemble. To average the microscopic equations corresponding to collective modes of the system, we adopt the same procedure. We consider the fluid from a comoving frame with local velocity $\mathbf{v}(\mathbf{x}, t)$ so that fluid appears at rest in the vicinity of point \mathbf{x} at time t . The position and momentum coordinates of the particles in moving frame are related to the rest frame by the canonical transformation rule defined in Eq. (2.22). The microscopic mass and momentum densities between primed (locally moving) and unprimed frame (laboratory rest frame) are related by Eqs. (2.23) and (2.24) respectively. The local equilibrium distribution function f_{le} at temperature $T(= \beta^{-1})$ in the primed frame is obtained as

$$f_{le}(\Gamma'_N; t) = Q_l^{-1} \exp \left\{ - \int d\mathbf{x} \beta [H' - \mu(\mathbf{x}, t) \rho'(\mathbf{x})] \right\} \equiv Q_l^{-1} \exp \left(- \beta \tilde{H}' \right), \quad (3.38)$$

where H' is the Hamiltonian in the local rest frame, Γ'_N is the phase-space co-

ordinates in the primed frame and μ is the local chemical potential. The equal time momentum density autocorrelation in the local rest frame is obtained as

$$\langle \hat{g}'_i(\mathbf{x}, t) \hat{g}'_i(\mathbf{x}', t) \rangle = \beta^{-1} \delta(\mathbf{x} - \mathbf{x}') \delta_{ij} \langle \hat{\rho}(\mathbf{x}, t) \rangle_{le}, \quad (3.39)$$

which follows the equipartition law of energy.

3.4.1 Coarse-grained equations for Smoluchowski case

We average Eq. (3.34) over local equilibrium distribution function f_{le} , defined in Eq. (3.38), to obtain time evolution equation for density field $\rho(\mathbf{x}, t)$ which has smooth spatial and temporal dependence (Das & Yoshimori, 2013). For Smoluchowski dynamics, the macroscopic density $\rho(\mathbf{x}, t)$ is the only slow mode, i.e., the hydrodynamic field. On averaging Eq. (3.34), we obtain

$$\begin{aligned} \frac{\partial \rho(\mathbf{x}, t)}{\partial t} &= \bar{D} \left[\nabla^2 \rho(\mathbf{x}, t) + \nabla \cdot \left\{ \int dx' \{ \nabla U'(\mathbf{x} - \mathbf{x}') \} \langle \rho(\mathbf{x}, t) \hat{\rho}(\mathbf{x}', t) \rangle_{le} \right\} \right] \\ &+ \Upsilon(\mathbf{x}, t), \end{aligned} \quad (3.40)$$

where $\bar{D} = 1/(\beta\zeta)$ and $U' = \beta U$. To obtain average of the second term on the right-hand side (RHS) of Eq. (3.40), we introduce here the operator \hat{O} which is defined for the N particle system as

$$i\hat{O} = \sum_{\alpha=1}^N \left[\frac{\partial H}{\partial \mathbf{p}_\alpha} \frac{\partial}{\partial \mathbf{x}_\alpha} - \frac{\partial H}{\partial \mathbf{x}_\alpha} \frac{\partial}{\partial \mathbf{p}_\alpha} \right]. \quad (3.41)$$

It should be noted that \hat{O} is the Liouville operator for the Newtonian system. The standard Hamiltonian H for N particle system is defined by

$$H = \sum_{\alpha=1}^N \frac{\mathbf{p}_\alpha^2}{2m} + U(\mathbf{x}_1, \dots, \mathbf{x}_N). \quad (3.42)$$

Operation of \hat{O} on the microscopic mass density $\hat{\rho}$ gives the following relation

$$i\hat{O}\hat{\rho} = -\nabla \cdot \hat{\mathbf{g}} = \frac{\partial \hat{\rho}}{\partial t}. \quad (3.43)$$

Operating \hat{O} on momentum density $\hat{\mathbf{g}}$ and using the definition (3.24), we obtain

$$\begin{aligned} i\hat{O}\hat{g}'_i(\mathbf{x}) &= \sum_{\alpha=1}^N \frac{p'_\alpha{}^i}{m} \frac{\partial p'_\alpha{}^j}{\partial \mathbf{x}_\alpha} \delta(\mathbf{x} - \mathbf{x}_\alpha) - \frac{\partial U}{\partial \mathbf{x}_\alpha} \delta(\mathbf{x} - \mathbf{x}_\alpha) \\ &= -\sum_j \nabla_j \sum_{\alpha=1}^N p'_\alpha{}^i p'_\alpha{}^j \delta(\mathbf{x} - \mathbf{x}_\alpha) \\ &\quad - \int d\mathbf{x}' (\nabla_i U(\mathbf{x} - \mathbf{x}')) \hat{\rho}(\mathbf{x}, t) \hat{\rho}(\mathbf{x}', t) \end{aligned} \quad (3.44)$$

Next, we average the above equation over local equilibrium distribution f_{le} which is symmetric in momentum \mathbf{p}'_α . In order to obtain the average of the first term on the RHS of the above equation, we use the relation $p'^j_\alpha = m^{-1}(\partial \tilde{H}' / \partial p'^j_\alpha)$ and perform the integration by parts with respect to p'^j_α . This gives the average of first term as $k_B T \delta_{ij} m^{-1} \nabla_j \rho(\mathbf{x})$. Using the above argument, local equilibrium average of the equation (3.44) is given by

$$\begin{aligned} \langle -i\hat{O}\hat{g}'_i(\mathbf{x}) \rangle &= k_B T \nabla_i \rho(\mathbf{x}, t) \\ &\quad + \int d\mathbf{x}' (\nabla_i U(\mathbf{x} - \mathbf{x}')) \langle \hat{\rho}(\mathbf{x}, t) \hat{\rho}(\mathbf{x}', t) \rangle_{le}. \end{aligned} \quad (3.45)$$

Again the integral $\langle -i\hat{O}\hat{g}'_i(\mathbf{x}) \rangle$ is evaluated by integration by parts and using the property $i\hat{O}H = 0$ as

$$\begin{aligned} \langle -i\hat{O}\hat{g}'_i(\mathbf{x}) \rangle &= \int d\Gamma \hat{g}'_i Q_l^{-1} i\hat{O} e^{-\beta \tilde{H}'} \\ &= \int d\mathbf{x}' \mu(\mathbf{x}') \langle \hat{g}'_i(\mathbf{x}) i\hat{O}\hat{\rho}'(\mathbf{x}) \rangle_{le} \end{aligned}$$

or

$$\langle -i\hat{O}\hat{g}'_i(\mathbf{x}) \rangle = \rho(\mathbf{x})\nabla_i\mu(\mathbf{x}), \quad (3.46)$$

where we have used Eqs. (3.39) and (3.43) in obtaining the above result. Further, we establish the link between local chemical potential and Helmholtz free energy functional of coarse-grained density field. Grand potential Ω , corresponding to grand canonical ensemble, has the equilibrium relation

$$\Omega = -PV = F - G$$

In density functional formalism (Ramakrishnan & Yussouff, 1979) above relation is written as

$$F[\rho(\mathbf{x})] \equiv \Omega[\rho(\mathbf{x})] + \int d\mathbf{x}\mu(\mathbf{x})\rho(\mathbf{x}) \quad (3.47)$$

Grand potential is minimized at equilibrium density and we write this result in terms of the functional variational principle as $[\partial\Omega/\partial\rho(\mathbf{x})] = 0$. Therefore, from the relation (3.47) we obtain,

$$\frac{\delta F[\rho]}{\delta\rho(\mathbf{x})} = \mu(\mathbf{x}). \quad (3.48)$$

The above relation allows us to write the first and second term on the RHS of Eq. (3.40) in a compact form as $\bar{D}\rho\nabla_i[\delta F[\rho]/\delta\rho(\mathbf{x})]$.

Next, the average of the third term on the RHS of Eq. (3.40) is obtained by taking the local equilibrium of Eq. (3.35) corresponding to the distribution function (3.38). Now using the relations (3.45), (3.46), and (3.48) we can write Eq. (3.40) as

$$\frac{\partial\rho(\mathbf{x}, t)}{\partial t} = \bar{D}\nabla \cdot \left\{ \rho\nabla \frac{\delta F}{\delta\rho} \right\} + \Upsilon(\mathbf{x}, t). \quad (3.49)$$

3.4 Coarse-grained equations

The noise correlation in the coarse-grained Eq. (3.49) is obtained by involving two step process. First, the microscopic noise $\hat{\theta}$ is averaged over different realizations of Brownian particles in local equilibrium distribution at constant temperature β^{-1} . As a result of above step, we obtain the coarse-grained noise θ . In the second step, at the same fixed temperature β^{-1} , we correlate the noise θ at two different space-time point.

$$\begin{aligned} \langle \Upsilon(\mathbf{x}, t) \Upsilon(\mathbf{x}', t') \rangle_{le} &= \langle \langle \hat{\Upsilon}(\mathbf{x}, t) \rangle_{le} \langle \hat{\Upsilon}(\mathbf{x}', t') \rangle_{le} \rangle \approx \langle \langle \hat{\Upsilon}(\mathbf{x}, t) \hat{\Upsilon}(\mathbf{x}', t') \rangle_{le} \rangle \\ &= 2\zeta\beta^{-1} \{ \nabla_x \rho(\mathbf{x}, t) \} \cdot \nabla_{x'} \delta(\mathbf{x} - \mathbf{x}') \delta(t - t'). \end{aligned} \quad (3.50)$$

In obtaining the above relation we have interchanged the averaging process which is essential for obtaining the closed form of noise correlation.

The free energy functional $F[\rho]$ in Eq. (3.49) is written as a sum of two parts,

$$F[\rho] = F_{id}[\rho] + F_{ex}[\rho], \quad (3.51)$$

where F_{id} denotes the ideal gas part contribution and F_{ex} symbolizes interaction or the excess part of the free energy. The noninteracting part F_{id} is obtained as

$$F_{id}[\rho] = \beta^{-1} \int d\mathbf{x} \rho(\mathbf{x}) \{ \ln(\lambda^3 \rho(\mathbf{x})) - 1 \}, \quad (3.52)$$

where $\lambda = h/(2\pi m k_B T)^{1/2}$ denotes the thermal wavelength. In general, excess part of the free energy is expressed as functional Taylor expansion in density fluctuations. Using the relation (3.52), Eq. (3.48) reduces to the form

$$\ln[\lambda^3 \rho(\mathbf{x})] - c^{(1)}(\mathbf{x}; [\rho]) = \beta \mu(\mathbf{x}), \quad (3.53)$$

3.4 Coarse-grained equations

where $c^{(1)}$ is the direct correlation function defined by

$$\beta^{-1}c^{(1)}(\mathbf{x}; [\rho]) = \frac{\delta F_{ex}[\rho]}{\delta \rho(\mathbf{x})}. \quad (3.54)$$

Using the above relation, the equilibrium density is obtained as

$$\rho(\mathbf{x}) = \rho_l \exp\{c^{(1)}(\mathbf{x}; [\rho]) - c_l\}, \quad (3.55)$$

where ρ_l and c_l are values of uniform liquid state corresponding to density ρ and direct correlation function $c^{(1)}$. In obtaining the above relation we have not considered any external field. Taylor expansion of $c^{(1)}(\mathbf{x}; [\rho])$ around uniform liquid state is obtained as

$$\begin{aligned} c^{(1)}(\mathbf{x}_1; [\rho]) &= c_l + \int d\mathbf{x}_2 c^{(2)}(\mathbf{x}_1, \mathbf{x}_2; \rho_l) \delta \rho(\mathbf{x}_2) \\ &+ \frac{1}{2} \int d\mathbf{x}_2 d\mathbf{x}_3 c^{(3)}(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3; \rho_l) \delta \rho(\mathbf{x}_2) \delta \rho(\mathbf{x}_3), \end{aligned} \quad (3.56)$$

where $\delta \rho(\mathbf{x}) = \rho(\mathbf{x}) - \rho_l$. Correlation functions $c^{(i)}$ in Eq. (3.56) is defined by

$$c^{(i)}(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_i; \rho_l) = \frac{\delta^i F[\rho]_{ex}}{\delta \rho(\mathbf{x}_1) \dots \delta \rho(\mathbf{x}_i)}. \quad (3.57)$$

First term on the RHS of Eq. (3.49) is obtained as

$$\rho(\mathbf{x}) \nabla_i \frac{\delta F[\rho]}{\delta \rho(\mathbf{x})} = \nabla_i \rho - \rho \nabla_i \int d\mathbf{x}' c^{(2)}(\mathbf{x}, \mathbf{x}'; \rho_l) \delta \rho(\mathbf{x}') + \dots \quad (3.58)$$

The quantity $c^{(2)}$ in the above equation is the Ornstein-Zernike direct correlation function. Ignoring the interacting part of the free energy gives only the first term on the RHS of Eq. (3.58) and diffusion Eq. (3.49) will be linear in this case with diffusion constant \bar{D} . On the other hand, if we keep the interaction part contribution and consider up to second term of the above equation, then,

in this case, the Fourier transform of diffusion constant $D(k)$ will be given by $D(k) = \bar{D}/S(k)$. Here $S(k)$ is the static structure factor.

3.4.2 Coarse-grained equations for Fokker-Planck case

Here we average Eqs. (3.25) and (3.26) over local equilibrium distribution. The coarse-grained equations are closed nonlinear stochastic differential equation for a set of macroscopic densities $\{\rho, \mathbf{g}\}$. These equations are termed as hydrodynamic equations. Eq. (3.25), after averaging gives the usual continuity equation

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{g} = 0. \quad (3.59)$$

Coarse-grained form of Eq. (3.26) is obtained as

$$\begin{aligned} \frac{\partial g_i}{\partial t} = & -\zeta g_i(\mathbf{x}, t) - \sum_j \nabla_j \langle \Gamma_{ij} \rangle_{le} \\ & - \int dx' (\nabla_i U(\mathbf{x} - \mathbf{x}')) \langle \hat{\rho}(\mathbf{x}, t) \hat{\rho}(\mathbf{x}', t) \rangle_{le} + \theta_i(\mathbf{x}, t). \end{aligned} \quad (3.60)$$

Using the transformation rule (2.22) and momentum symmetry (\mathbf{p} to $-\mathbf{p}$ symmetry) of the distribution function (3.38), average of the second term on the RHS of Eq. (3.60) is obtained as,

$$\langle \Gamma_{ij} \rangle_{le} = k_B T \nabla_i \rho(\mathbf{x}, t) + \nabla_j \left[\frac{g_i(\mathbf{x}, t) g_j(\mathbf{x}, t)}{\rho(\mathbf{x}, t)} \right]. \quad (3.61)$$

Using the above result and Eqs. (3.45), (3.46), and (3.48), we obtain

$$\frac{\partial g_i}{\partial t} + \nabla_j \left[\frac{g_i g_j}{\rho} \right] + \rho \nabla_i \frac{\delta F}{\delta \rho} + \zeta g_i = \theta_i(\mathbf{x}, t). \quad (3.62)$$

$\theta(\mathbf{x}, t)$ in the above equation is the multiplicative noise whose correlation is obtained as

$$\langle \theta_i(\mathbf{x}, t) \theta_j(\mathbf{x}', t') \rangle = 2\beta^{-1} \zeta \rho(\mathbf{x}, t) \delta_{ij} \delta(\mathbf{x} - \mathbf{x}') \delta(t - t'). \quad (3.63)$$

In obtaining the above relation, we have used the same approximation as was done in Eq. (3.50). The dissipative constant ζ in the forth term on the left-hand side of Eq. (3.62) should have ∇^2 operator associated with it to conserve momentum of the system.

3.5 Active particles Brownian motion

Here we discuss the active Brownian dynamics. The term ‘active’ means here that Brownian particles are able to move using their internal energy or ambient free energy. We consider that the internal energy production and dissipation occurs in three steps (Ebeling *et al.*, 1999; Romanczuk *et al.*, 2012; Schweitzer *et al.*, 1998). In the first step, they take energy from the environment and store it in an internal depot. In the second step, some kind of internal dissipation happens which is proportional to the internal energy. In the third step, conversion of internal energy into kinetic energy occurs and the rate of conversion is assumed to be function of actual particle velocities. In biological systems, the three step process can be easily understood. They take energy from the food (feeding). Some part of it dissipates in metabolic process happening inside the living entity. Next, they perform self-driven motion by consuming internal energy. The dynamics is obtained in the form of Langevin equation by introducing space and velocity dependent frictional coefficient which inherit the energy injection and dissipation feature of particles introduced above.

$$\frac{dx}{dt} = u, \quad m \frac{du}{dt} + \zeta(x, u)u = F(x) + \xi(t). \quad (3.64)$$

Depending on the models of active Brownian particles, the frictional coefficient $\zeta(x, u)$ can have different forms. For systems homogeneous in space, $\zeta(x, u)$ can be taken to be dependent on velocity only, i.e., $\zeta(x, u) = \zeta(u)$. Analogous to the standard Rayleigh and Helmholtz model developed for the theory of sound, the velocity dependent friction coefficient ζ can be expressed in terms of quadratic order in velocity, i.e., $\zeta(u) = -\zeta_0 + \zeta_2 u^2$. For $\zeta(u) < 0$, energy injection due to negative friction occurs implying that motion of slow particles will be accelerated and fast particles will be damped. For $\zeta(u) > 0$, dissipation dominates in the system. Due to energy injection and dissipation mechanism of the model, system is out of equilibrium and FDT relation does not hold (Steffenoni *et al.*, 2016).

3.6 Discussion

Here we have studied the coarse-grained description of the Brownian particles in the fluid for the two cases of the dynamics: The Fokker-Planck and the Smoluchowski. In case of Smoluchowski dynamics, the macroscopic dynamics is obtained in terms of time evolution of mass density field with a multiplicative noise in the equation. In Fokker-Planck dynamics, we have obtained closed time evolution equations of mass density and momentum density fields. They are the fluctuating nonlinear hydrodynamic equations of the system. The momentum density equation has the regular part and the multiplicative noise part. The density field equation is the continuity equation signifies the mass number conservation. The multiplicative noise in both cases (Fokker-Planck and Smoluchowski) of the coarse-grained description of the Brownian particles follows from the additive noise term in the microscopic equation.

Concept of Brownian motion can be extended to describe the motion of active particles such as living cells, bacteria, etc (Frey & Kroy, 2005). In case of active

motion, the frictional coefficient ζ_0 becomes nonlinear function of particle velocity and drives the system to out of equilibrium as a consequence the FDT relation does not hold. Thus this is a new kind of non-equilibrium system which is out of equilibrium due to the activity of the particles but not due to any external field. In Chapter 5, we will give hydrodynamic description of such type of (active) particles starting from microdynamic illustration.

Chapter 4

Dynamic renormalization group analysis

Renormalization group (RG) provides useful techniques to deal the hard problems in physics which include quantum field theory (Amit, 1999; Peterman, 1979), the Kondo effect (Wilson, 1975), critical phenomena (Ma, 1976; Stanley, 1971), etc. All of these problems involve a large number of degrees of freedom. In particular, RG has attained considerable success to study the problems in critical phenomena (Chang *et al.*, 1992; Halperin *et al.*, 1972, 1974; Hohenberg & Halperin, 1977). Such phenomena are specified by fluctuations on all length scales ranging from the molecular scale to macroscopic scale. Large scale fluctuations dominate when the system tends towards a phase transition. In the vicinity of a critical point, the system can exhibit anomalous static as well as dynamical properties. Static properties include the thermodynamic coefficients, single-time correlation functions which are determined by the averages over single-time equilibrium distribution function of particles. On the other hand, dynamical properties involves transport coefficients and relaxation rates, correlation functions with several time arguments, etc. These properties depend on equations of motion and are not

merely determined by single-time equilibrium distribution. Dynamical properties are sensitive to the evolution of the system due to multi-time dependence of the correlation functions of the system. The anomalies in the dynamical behavior of the system occur due to the appearance of long-wavelength correlations which cause the divergent relaxation times to conserved quantities and singular behavior in time correlation functions and transport coefficients. An isotropic ferromagnet is such kind of system whose critical dynamics is discussed in Ref. (Ma & Mazenko, 1975) using RG methods.

Navier-Stokes equation (NSE) of an incompressible fluid with a fluctuating forcing function are similar in some manner to many nonlinear spin models used in the study of critical phenomena. Identifying this similarity, Forster, Nelson, and Stephen (Forster *et al.*, 1977, 1976) adopted the RG methods useful in the study of critical dynamics to study the long-distance, long-time behavior of velocity correlations produced by the NSE, though their analysis does not discuss the properties of the fluid near its critical point. This was the pioneering work by Forster, Nelson, and Stephen to study the properties of a fluid using the dynamic renormalization group (DRG) techniques. The DRG has been a very useful in study of phase transition behavior including the order-disorder type transition seen in active matter (Chen *et al.*, 2018; Mishra *et al.*, 2010; Toner & Tu, 1998, 1995; Toner *et al.*, 2018). We present here a discussion of the Pioneering approach of Forster, Nelson, and Stephen of the application of the Dynamic RG approach for the case of a fluid of passive particles as a review material for our present discussion on the application of Nonlinear fluctuating hydrodynamics to understand the Toner-Tu theory for flocking.

4.1 The Navier-Stokes equation

The equations of motion (EOM) for velocity field $\mathbf{v}(\mathbf{x}, t)$ describing the dynamics of an incompressible fluid in the presence of fluctuating force $\mathbf{f}(\mathbf{x}, t)$ is given by the NSE

$$\partial_t \mathbf{v} + \lambda_0 (\mathbf{v} \cdot \nabla) \mathbf{v} = -\frac{\nabla p}{\rho} + \nu_0 \nabla^2 \mathbf{v} + \mathbf{f}, \quad (4.1)$$

where $p = p(\mathbf{x}, t)$ denotes the pressure, ρ denotes the mass density, ν_0 denotes the viscosity and λ_0 is perturbative parameter. Pressure p in the above equation enforces the incompressibility condition $\nabla \cdot \mathbf{v} = 0$. We consider the random force $\mathbf{f}(\mathbf{x}, t)$ purely solenoidal and its correlation in the Fourier space is given by

$$\langle f_i(\mathbf{k}, \omega) f_j(\mathbf{k}', \omega') \rangle = 2D_0(k) (2\pi)^{d+1} \delta(\mathbf{k} + \mathbf{k}') \delta(\omega + \omega') P_{ij}(\mathbf{k}), \quad (4.2)$$

where $\mathbf{f}(\mathbf{k}, \omega)$ is the Fourier transform of the random force $\mathbf{f}(\mathbf{x}, t)$ in space and time given as

$$\mathbf{f}(\mathbf{k}, \omega) = \int dx \int dt \mathbf{f}(\mathbf{x}, t) \exp i(\omega t - \mathbf{k} \cdot \mathbf{x}), \quad (4.3)$$

and $P_{ij}(\mathbf{k})$ is a transverse projection operator defined by

$$P_{ij}(\mathbf{k}) = \delta_{ij} - \hat{k}_i \hat{k}_j, \quad (4.4)$$

where $\hat{\mathbf{k}}$ denote the unit wavevector. We consider the following definition for forcing function $D(k)$

$$D(k) = \begin{cases} D_0 k^2 & \text{for } |\mathbf{k}| < \Lambda, \\ 0, & \text{else,} \end{cases} \quad (4.5)$$

where Λ is ultraviolet cutoff and constant $D_0 = \nu_0 k_B T / \rho$, with k_B denoting the Boltzmann constant, and T temperature of the system. The condition (4.5) for

$D(k)$ is defined as Model A in Ref. (Forster *et al.*, 1977). We will study the DRG of Model A in this chapter.

Eq. (4.1) is invariant under the Galilean transformation $\mathbf{v}(\mathbf{x}, t) \rightarrow \mathbf{v}'(\mathbf{x} - \mathbf{u}t, t) + \mathbf{u}$, where random force \mathbf{f} is assumed to be Galilean invariant separately. The isotropic fluid system conserve the momentum and this basic property of the system is responsible for the Galilean invariant EOM. In the active matter, there are various models of dry active systems (Ramaswamy, S. *et al.*, 2003; Vicsek & Zafeiris, 2012) which violate the above properties.

4.2 Renormalization group method

To implement the RG, we need to Fourier transform the velocity field Eq. (4.1). We write the l -th component of the transverse part of Eq. (4.1) in symmetric form as

$$\partial_t v_l + \frac{\lambda_0}{2}(P_{ln}\nabla_m(v_nv_m) + P_{lm}\nabla_n(v_mv_n)) = \nu_0\nabla^2 v_l + f_l, \quad (4.6)$$

where the transverse projection P_{ij} in real space is defined by $P_{ij}(\nabla) = \delta_{ij} - \nabla_i\nabla_j/\nabla^2$. In the above equation and rest of this chapter we follow the Einstein summation convention for the repeated indices. Fourier Transform of $v_i(\mathbf{x}, t)$, for $k < \Lambda$ is define by

$$v_i(\mathbf{x}, t) = \int_{k < \Lambda} \frac{d^d k}{2\pi^d} \frac{d\omega}{2\pi} v_i(\mathbf{k}, \omega) \exp i(\mathbf{k} \cdot \mathbf{x} - \omega t). \quad (4.7)$$

Now using definition (4.7), Fourier transform of Eq. (4.6) is obtained as

$$v_l(\mathbf{k}, \omega) = G_0(\mathbf{k}, \omega) f_l(\mathbf{k}, \omega) - \frac{i\lambda_0}{2} G_0(\mathbf{k}, \omega) P_{lmn}(\mathbf{k}) \int_{q, \Omega} v_m(\mathbf{q}, \Omega) v_n(\mathbf{k} - \mathbf{q}, \omega - \Omega), \quad (4.8)$$

where we have defined

$$G_0(\mathbf{k}, \omega) = (-i\omega + \nu_0 k^2)^{-1}, \quad (4.9)$$

and

$$P_{lmn}(\mathbf{k}) = P_{ln}(\mathbf{k})k_m + P_{lm}(\mathbf{k})k_n. \quad (4.10)$$

The Eq. (4.9) defines the zeroth order green function. The following convention is adopted for integral sign introduced in Eq. (4.8)

$$\int_{q, \Omega} \equiv \int_{q < \Lambda} \frac{d^d q}{(2\pi)^d} \int_{-\infty}^{+\infty} \frac{d\Omega}{2\pi}. \quad (4.11)$$

In absence of nonlinearity, zeroth order solution of Eq. (4.8) is given by

$$v_{l0}(\mathbf{k}, \omega) = G_0(\mathbf{k}, \omega) f_l(\mathbf{k}, \omega),$$

which gives zeroth order velocity autocorrelation function as

$$\langle v_{l0}(\mathbf{k}, \omega) v_{j0}(-\mathbf{k}, -\omega) \rangle = C_0(\mathbf{k}, \omega) P_{lj}(\mathbf{k}),$$

with $C_0(\mathbf{k}, \omega) = 2D_0 k^2 |G_0(\mathbf{k}, \omega)|^2$. The angular brackets on the left-hand side of the above expression denote the average over random noise.

RG process consists of two steps; the first step is coarse-graining or elimination of modes in which we average out the fast degrees of freedom and the second step involves rescaling of variables. Below we describe how to implement these two steps.

In a first step, we project EOM (4.8), which is defined for wavenumber belonging to interval $0 > k > \Lambda$, onto the phase-space spanned by the modes with $0 < k < \Lambda e^{-l}$ by eliminating the modes with $\Lambda e^{-l} < k < \Lambda$, and push

4.2 Renormalization group method

the leftover part into suitably redefined, partially renormalized noise. Here the parameter l denotes the measure of the degrees of freedom which have been eliminated. In the Second step, in the reduced EOM obtained from step one, we rescale the space, time, velocities and forces to restore the cutoff Λ and to preserve the form of EOM to the extent possible. In the two step process described above, parameters of the original EOM, $(\lambda_0, \nu_0, D_0) \equiv \mu_0$ (say) transformed to the l -dependent value $\mu(l) \equiv (\lambda(l), \nu(l), D(l))$. Next, the correlations functions at small wave numbers are calculated from the original equations of motion or from the new equations of motion leading to the homogeneity relation $C_{ij}(\mathbf{k}, \omega; \{\mu_0\}) = e^{fl} C_{ij}(e^l \mathbf{k}, e^{zl} \omega; \{\mu(l)\})$. Now this homogeneity relation can be used to obtain the infrared behaviour of correlation functions if the couplings flow to small fixed point value $\{\mu(\infty)\}$ under the iterations of the transformation described above. Below we use this process to evaluate long-wavelength velocity correlations generated by Navier-Stokes equation.

In order to perform the coarse-graining step, which is the first step of RG process, we decompose the velocity field $v_l(\mathbf{k}, \omega)$ into low and high wavenumber components as

$$v_l(\mathbf{k}, \omega) = v_l^<(\mathbf{k}, \omega) + v_l^>(\mathbf{k}, \omega), \quad (4.12)$$

where

$$v_l^<(\mathbf{k}, \omega) = \begin{cases} v_l(\mathbf{k}, \omega), & \text{for } 0 < k < \Lambda e^{-l}, \\ 0, & \text{else} \end{cases} \quad (4.13)$$

and

$$v_l^>(\mathbf{k}, \omega) = \begin{cases} v_l(\mathbf{k}, \omega), & \text{for } \Lambda e^{-l} < k < \Lambda, \\ 0, & \text{else} \end{cases}. \quad (4.14)$$

Similarly, the random force $f_l(\mathbf{k}, \omega)$ is decomposed into $f_l^<(\mathbf{k}, \omega)$ and $f_l^>(\mathbf{k}, \omega)$. Elimination of modes gives intermediate renormalization of the coefficients which are shown in the Fig.4.2 (Ma & Mazenko, 1975). We use here the term interme-

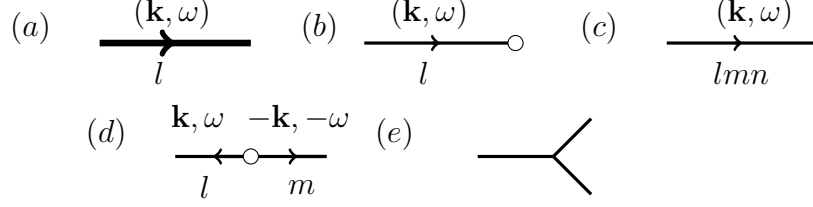


Figure 4.1: Graphical representation (a) denotes full solution $v_l(\mathbf{k}, \omega)$; (b) denotes $G_0(\mathbf{k}, \omega)f_l(\mathbf{k}, \omega)$; (c) denotes $G_0(\mathbf{k}, \omega)P_{lmn}(\mathbf{k})$; (d) denotes $C_0(\mathbf{k}, \omega)P_{lj}(\mathbf{k})$; (e) the three leg vertex denotes $-i\lambda/2$

diate for the renormalized coefficients of the reduced EOM before the rescaling. Graphs shown in Fig. 4.1 define the meaning of symbols. The three leg vertex graphs shown in Fig. 4.2(c) cancel each other and the nonlinear contribution to the renormalization of the parameter λ_0 vanishes, hence we obtain

$$\lambda_I = \lambda_0, \quad (4.15)$$

which is the general consequence of Galilean invariance.

4.2.1 Viscosity renormalization

After averaging out the $v_l^>$ part from the Eq. (4.8), we are left with EOM for $v_l^<$ which is shown in Fig.4.2(a). We have kept the terms up to second order in perturbative constant λ_0 . Below We show that averaging process contributes to the renormalization of viscosity coefficient. The algebraic equation corresponding to Fig.4.2(a) is given by

$$v_l^<(\mathbf{k}, \omega) = G_0^<(\mathbf{k}, \omega)f_l^<(\mathbf{k}, \omega) + 4G_0^<(\mathbf{k}, \omega) \left(\frac{-i\lambda_0}{2} \right)^2 P_{lmn}^<(\mathbf{k}) I_{mn\mu}(\mathbf{k}, \omega) v_\mu^<(\mathbf{k}, \omega), \quad (4.16)$$

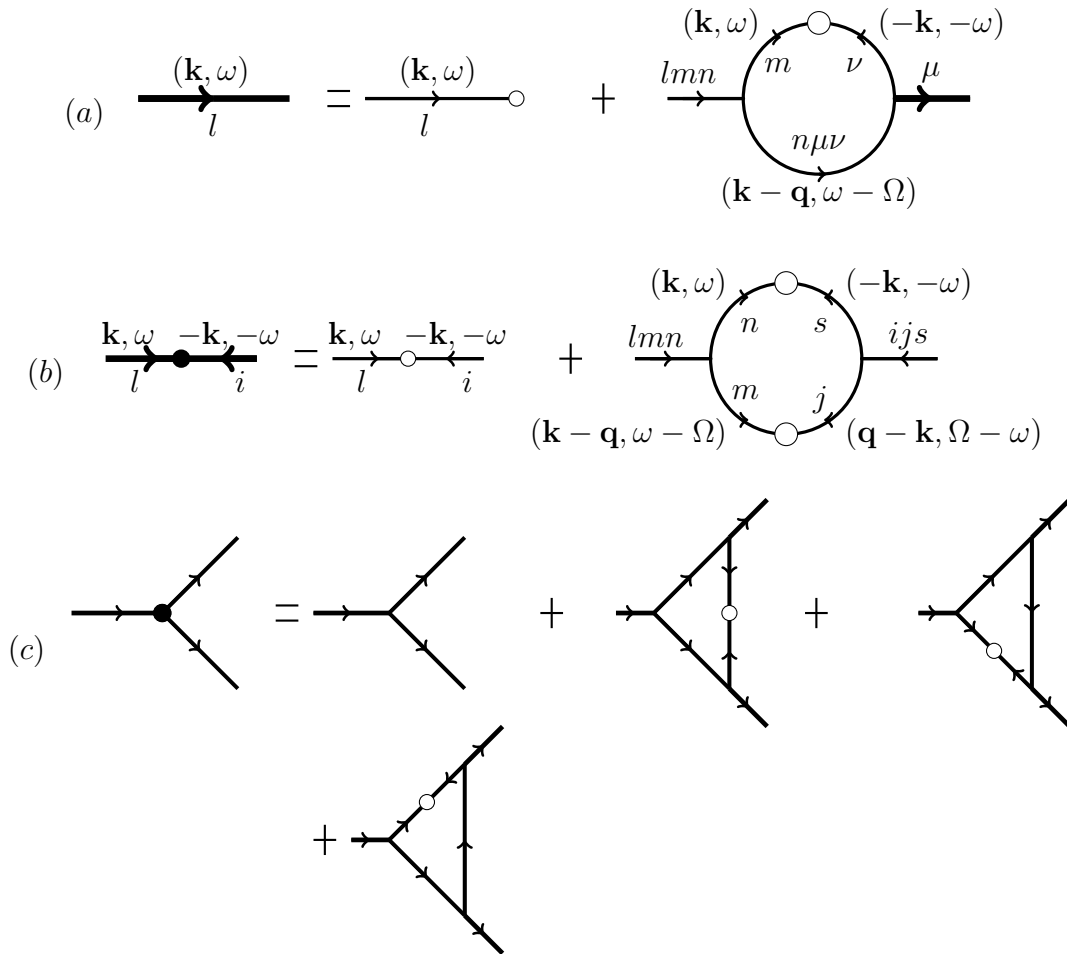


Figure 4.2: Graphs representing intermediate renormalization of coefficients to one-loop order (a) Renormalization of viscosity (b) Noise strength renormalization (c) Renormalization of parameter λ_0

where

$$I_{mn\mu}(\mathbf{k}, \omega) = \int_{q\Omega}^> G_0(\mathbf{k} - \mathbf{q}, \omega - \Omega) P_{n\mu\nu}(\mathbf{k} - \mathbf{q}) C_0(\mathbf{q}, \Omega) P_{m\nu}(\mathbf{q}). \quad (4.17)$$

The symbol $\int_{q\Omega}^>$ in Eq. (4.17) denotes $\int \frac{d^d q}{(2\pi)^d} \int_{-\infty}^{+\infty} \frac{d\Omega}{2\pi}$, where integration over q must be performed to the domain $\Lambda e^{-l} < q < \Lambda$ and $\Lambda e^{-l} < |\mathbf{k} - \mathbf{q}| < \Lambda$. The internal frequency integral is integrated from $-\infty$ to $+\infty$ for the above described range of wavenumber. It is not necessary to set any special cutoff for the frequency, since the propagators decay rapidly for sufficiently large value of frequency. The Eq. (4.16) can be rewritten in the following form

$$(-i\omega + k^2 \nu_I(\mathbf{k}, \omega)) v_l^<(\mathbf{k}, \omega) = f_l^<(\mathbf{k}, \omega), \quad (4.18)$$

where we define

$$\nu_I(\mathbf{k}, \omega) = \nu_0 + \Delta\nu(\mathbf{k}, \omega), \quad (4.19)$$

and correction term $\Delta\nu$ is given by

$$k^2 P_{l\mu}^<(\mathbf{k}) \Delta\nu(\mathbf{k}, \omega) = \lambda_0^2 P_{lmn}^<(\mathbf{k}) I_{mn\mu}(\mathbf{k}, \omega). \quad (4.20)$$

This shows elimination of mode $v_l^>$ modifies the viscous term. After performing integration, $I_{mn\mu}(\mathbf{k}, \omega)$, in the limit $k \rightarrow 0, \omega \rightarrow 0$, is obtained as (calculation is shown in the Appendix 4.A)

$$\begin{aligned} I_{mn\mu} = & \frac{D_0}{2\nu_0^2} k_\nu \left[\delta_{n\mu} \delta_{m\nu} \left(\frac{d^2 - 3}{d(d+2)} \right) \right. \\ & \left. + \frac{1}{d(d+2)} (\delta_{n\mu} \delta_{m\nu} + \delta_{nm} \delta_{\mu\nu}) \right] \frac{S_d}{(2\pi)^d} \int^> \frac{d^d q}{q^2}, \end{aligned} \quad (4.21)$$

4.2 Renormalization group method

where $S_d = 2\pi^{(d/2)}/\Gamma(d/2)$. Further, using the definition (4.10) for P_{lmn} and properties of projection operator we obtain (in the limit $k \rightarrow 0, \omega \rightarrow 0$)

$$k^2 P_{l\mu}^<(\mathbf{k}) \Delta\nu(0, 0) = k^2 P_{l\mu}^<(\mathbf{k}) \frac{\lambda_0^2 D_0}{\nu_0^2} A_d \frac{e^{(2-d)l} - 1}{2-d}, \quad (4.22)$$

where

$$A_d = \frac{d^2 - 2}{2d(d+2)} \frac{S_d}{(2\pi)^d}. \quad (4.23)$$

In obtaining the above integral, we have taken upper cutoff $\Lambda = 1$ for simplicity. Now intermediate renormalized viscosity is obtained as

$$\nu_I = \nu_0 + \Delta\nu(0, 0), \quad (4.24)$$

or

$$\nu_I = \nu_0 \left[1 + \bar{\lambda}_0^2 A_d \frac{e^{(2-d)l} - 1}{2-d} \right], \quad (4.25)$$

where $\bar{\lambda}_0 = \lambda_0 [D_0/\nu_0^3]^{1/2}$. This shows contribution to viscosity to one-loop order in Feynman graph illustrated in Fig. 4.2(a).

4.2.2 Renormalization of noise strength

Renormalization of noise strength is shown graphically in Fig. 4.2(b). We write its corresponding algebraic equation given as

$$\begin{aligned} 2D_I(\mathbf{k}, \omega) k^2 P_i^<(\mathbf{k}) &= 2D_0 k^2 P_i^<(\mathbf{k}) \\ &+ 2 \left(\frac{-i\lambda_0}{2} \right)^2 P_{lmn}^<(\mathbf{k}) P_{ijs}^<(-\mathbf{k}) J_{mjns}(\mathbf{k}, \omega), \end{aligned} \quad (4.26)$$

where

$$J_{mjns}(\mathbf{k}, \omega) = \int_{q\Omega}^> C_0(\mathbf{k} - \mathbf{q}, \omega - \Omega) C_0(\mathbf{q}, \Omega) P_{mj}(\mathbf{k} - \mathbf{q}) P_{ns}(\mathbf{q}). \quad (4.27)$$

The above integral is evaluated (Appendix 4.B) as

$$\begin{aligned}
 J_{mjns} &= \frac{D_0^2}{\nu_0^3} \left[\delta_{mj} \delta_{ns} \left(\frac{d^2 - 3}{d(d+2)} \right) \right. \\
 &\quad \left. + \frac{1}{d(d+2)} (\delta_{mn} \delta_{js} + \delta_{ms} \delta_{jn}) \right] \frac{S_d}{(2\pi)^d} \int^> \frac{d^d q}{q^2}. \quad (4.28)
 \end{aligned}$$

The product of operators $P_{lmn}^<(\mathbf{k})P_{ijs}^<(-\mathbf{k})$ in Eq. (4.26) is obtained as

$$\begin{aligned}
 P_{lmn}^<(\mathbf{k})P_{ijs}^<(-\mathbf{k}) &= - \left[P_{lm}^<(\mathbf{k})P_{ij}^<(\mathbf{k})k_n k_s + P_{lm}^<(\mathbf{k})P_{is}^<(\mathbf{k})k_n k_j \right. \\
 &\quad \left. + P_{ln}^<(\mathbf{k})P_{ij}^<(\mathbf{k})k_m k_s + P_{ln}^<(\mathbf{k})P_{is}^<(\mathbf{k})k_m k_j \right], \quad (4.29)
 \end{aligned}$$

where we have used the property $P_{ijs}(-\mathbf{k}) = -P_{ijs}(\mathbf{k})$. Now using Eqs.(4.28) and (4.29) we obtain

$$J_{mjns}P_{lmn}^<(\mathbf{k})P_{ijs}^<(-\mathbf{k}) = -4k^2 P_{li}^<(\mathbf{k}) \frac{D_0^2}{\nu_0^3} A_d \frac{S_d}{(2\pi)^d} \int^> \frac{d^d q}{q^2}. \quad (4.30)$$

Using result of Eq. (4.30) in Eq. (4.26), renormalized noise strength is obtained as

$$D_I = D_0 \left[1 + \bar{\lambda}_0^2 A_d \frac{e^{(2-d)l} - 1}{2-d} \right]. \quad (4.31)$$

From Eq. (4.25) and (4.31) we see that ν_0 and D_0 renormalize in the same way. This is a consequence of fluctuation-dissipation theorem which relates noise strength to viscosity coefficient.

4.2.3 Rescaling of variables and recursion relation

After elimination of modes $v_l^>$, reduced equation of motion in the wavenumber range $0 < k < \Lambda e^{-l}$ takes the form

$$\begin{aligned}
v_l^<(\mathbf{k}, \omega) &= G_r(\mathbf{k}, \omega)(f_l^<(\mathbf{k}, \omega) + \Delta f_l) \\
&\quad - \frac{i\lambda_0}{2} G_r(\mathbf{k}, \omega) P_{lmn}(\mathbf{k}) \int_{q\Omega} v_m^<(\mathbf{q}, \Omega) v_n^<(\mathbf{k} - \mathbf{q}, \omega - \Omega) \\
&\quad + O(v^<)^3,
\end{aligned} \tag{4.32}$$

where

$$G_r(\mathbf{k}, \omega) = (-i\omega + \nu_l k^2)^{-1}. \tag{4.33}$$

Next, in order to compare the reduced EOM to original EOM, we need to rescale it which is the second step of RG. Rescaled variables are defined as

$$\mathbf{k}' = \mathbf{k}e^l, \tag{4.34}$$

$$\omega' = \omega e^{\alpha(l)}, \tag{4.35}$$

$$\mathbf{v}^<(\mathbf{k}, \omega) = \zeta(l) \mathbf{v}'(\mathbf{k}, \omega), \tag{4.36}$$

where k' is defined in the interval $0 < k' < \Lambda$ and variables $\alpha(l)$ and $\zeta(l)$ are to be determined. Now the EOM (4.32) in terms of scaled variables takes the form

$$\begin{aligned}
\mathbf{v}'_l(\mathbf{k}', \omega') &= G_r(\mathbf{k}', \omega') f'_l(\mathbf{k}', \omega') \\
&\quad - \frac{i\lambda(l)}{2} G_r(\mathbf{k}', \omega') P_{lmn}(\mathbf{k}') \int v'_n(\mathbf{k}' - \mathbf{q}', \omega' - \Omega') \\
&\quad \times v'_m(\mathbf{q}', \Omega') \frac{d^d q'}{(2\pi)^d} \frac{d\Omega'}{2\pi},
\end{aligned} \tag{4.37}$$

where

$$f'_l(\mathbf{k}', \omega') = f_l(\mathbf{k}, \omega) \zeta^{-1}(l) e^{\alpha(l)}, \quad (4.38)$$

$$G_r(\mathbf{k}', \omega') = [-i\omega' + \nu(l)k'^2]^{-1}, \quad (4.39)$$

$$\nu(l) = \nu_I e^{\alpha(l)-2l}, \quad (4.40)$$

$$\lambda(l) = \lambda_0 \zeta(l) e^{-(d+l)l}. \quad (4.41)$$

In order to obtain recursion relation for noise strength D , we write the noise correlation from the intermediate Eq. (4.32) as

$$\langle f'_{iI}(\mathbf{k}, \omega) f'_{jI}(\mathbf{k}_1, \omega_1) \rangle = 2D_I k^2 (2\pi)^{d+1} \delta(\mathbf{k} + \mathbf{k}_1) \delta(\omega + \omega_1) P_{ij}(\mathbf{k}), \quad (4.42)$$

which can be written in terms of rescaled variables as

$$\langle f'_{iI}(\mathbf{k}', \omega') f'_{jI}(\mathbf{k}'_1, \omega'_1) \rangle = 2D(l) k'^2 (2\pi)^{d+1} \delta(\mathbf{k}' + \mathbf{k}'_1) \delta(\omega' + \omega'_1) P_{ij}(\mathbf{k}'),$$

where

$$D(l) = e^{\alpha(l)-2l} D_I \left[\frac{\exp(\alpha(l) + \frac{1}{2}ld)}{\zeta(l)} \right]^2. \quad (4.43)$$

We analyse from Eqs. (4.25) and (4.31) that ν and D renormalize in similar way, this allows us to choose

$$\zeta(l) = \exp \left[\alpha(l) + \frac{1}{2}ld \right], \quad (4.44)$$

which gives us the l -dependent noise strength $D(l)$ as

$$D(l) = e^{\alpha(l)-2l} D_I. \quad (4.45)$$

4.2 Renormalization group method

Now using relation (4.44) for $\zeta(l)$, recursion relation (4.41) is obtained as

$$\lambda(l) = \lambda_0 \exp \left[\alpha(l) - \frac{l}{2}(d+2) \right]. \quad (4.46)$$

Next, using Eqs. (4.40), (4.45) and (4.46), we obtain differential recursion relation for $\nu(l)$, $D(l)$, and $\lambda(l)$ upto leading order in $\bar{\lambda}(l)$ as

$$\frac{d\nu(l)}{dl} = \nu(l) [z(l) - 2 + \bar{\lambda}^2(l)A_d], \quad (4.47)$$

$$\frac{dD(l)}{dl} = D(l) [z(l) - 2 + \bar{\lambda}^2(l)A_d], \quad (4.48)$$

$$\frac{d\lambda(l)}{dl} = \lambda(l) \left[-1 - \frac{d}{2} + z(l) \right]. \quad (4.49)$$

Here the function $z(l)$ is defined as

$$\alpha(l) = \int_0^l z(l') dl', \quad (4.50)$$

and the expansion parameter $\bar{\lambda}(l)$, in terms of $\nu(l)$, $D(l)$, and $\lambda(l)$, is obtained as

$$\bar{\lambda}(l) = \lambda(l) \left[\frac{D(l)}{\nu^3(l)} \right]^{1/2}. \quad (4.51)$$

The differential recursion relation for $\bar{\lambda}(l)$, using Eqs. (4.47), (4.48), and (4.49), is obtained as

$$\frac{d\bar{\lambda}(l)}{dl} = \frac{1}{2}\epsilon\bar{\lambda}(l) - A_d\bar{\lambda}^3(l), \quad (4.52)$$

with $\epsilon = 2 - d$. The above recursion relation is free from the arbitrary function $z(l)$.

Recursion relation (4.52) implies that, if $\epsilon < 0$, i.e., above two dimensions, parameter $\bar{\lambda}(l)$ tends to zero when $l \rightarrow \infty$. Same result follows in exactly two dimensions. Below two dimensions, i.e., for $\epsilon > 0$, $\bar{\lambda}(l)$ tends to stable a fixed

point for $\bar{\lambda} > 0$ as l tends towards sufficiently large value

$$\bar{\lambda}^* = (8\pi\epsilon)^{1/2}. \quad (4.53)$$

The above description follows from the solutions of the equation (4.52) obtained as

$$\bar{\lambda}(l) = \bar{\lambda}_0 e^{(\epsilon/2)l} \left[1 + 2A_d \bar{\lambda}_0^2 \frac{e^{\epsilon l} - 1}{\epsilon} \right]^{-1/2}. \quad (4.54)$$

In order to make $D(l)$ and $\nu(l)$ fixed at their initial values, i.e., independent from l , we choose arbitrary function $z(l)$ as

$$z(l) = 2 - \bar{\lambda}^2(l) A_d. \quad (4.55)$$

In the above relation, $z(l)$ depends on the parameter $\bar{\lambda}(l)$ whose behavior we have discussed using Eq. (4.52) for large l in dimensions below and above $d = 2$ as well as in 2d. For $d \geq 2$, $z(l) \rightarrow 2$ as $l \rightarrow \infty$ and below two dimensions, $z(l) \rightarrow 2 - \epsilon/2$ for sufficiently large l .

4.2.4 Spectral energy density

Velocity autocorrelation function is defined by

$$C_{ij}(\mathbf{k}, \omega) = \frac{\langle v_i(\mathbf{k}, \omega) v_j(\mathbf{k}', \omega') \rangle}{(2\pi)^{d+1} \delta(\mathbf{k} + \mathbf{k}') \delta(\omega + \omega')}. \quad (4.56)$$

Using Eqs. (4.34)-(4.36), we can write

$$C_{ij}(\mathbf{k}, \omega; \lambda_0) = e^{\alpha(l)} C_{ij}(e^l \mathbf{k}, e^{\alpha(l)} \omega; \bar{\lambda}(l)). \quad (4.57)$$

The left-hand side of the above equation is difficult to calculate if $\bar{\lambda}(l)$ is large. In the previous section, we have seen that, for $d \geq 2$, $\bar{\lambda}(l)$ tends to zero and $z(l)$

4.3 A review on dynamic RG analysis of Toner-Tu equations

tends to fixed value 2 for sufficiently large l . This allows us to obtain C_{ij} in terms of scaling function as

$$C_{ij}(\mathbf{k}, \omega; \lambda_0) = P_{ij}(\mathbf{k})k^{-z}g(\omega/k^z). \quad (4.58)$$

Spectral energy density $E(k)$ is obtained from Eq. (4.58) as

$$E(k) = k^{d-1} \int Tr C_{ij}(\mathbf{k}, \omega) \frac{d\omega}{2\pi}. \quad (4.59)$$

Since $\int Tr C_{ij}(\mathbf{k}, \omega) d\omega/2\pi$ is constant in small k limit in any dimensions, this implies that $E(k)$ is proportional to k^{d-1} . In three dimensions, this behaves as k^2 in accordance with the equipartition theorem (Huang, 1987). Depending on the various forms of forcing function $D(k)$, different result can be obtained for $E(k)$ which we have not discussed here. The forcing function $D(k)$ which we have considered in the present analysis, vanishes as wave number $k \rightarrow 0$.

4.3 A review on dynamic RG analysis of Toner-Tu equations

Here we summarize some important results on RG calculation of Toner-Tu equation. The time evolution equation for density field $\rho(\mathbf{x}, t)$ and velocity field $\mathbf{v}(\mathbf{x}, t)$ are given by the following set of equations

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0, \quad (4.60)$$

$$\begin{aligned} & \partial_t \mathbf{v} + \lambda_1 (\mathbf{v} \cdot \nabla) \mathbf{v} + \lambda_2 (\nabla \cdot \mathbf{v}) \mathbf{v} + \lambda_3 \nabla (|\mathbf{v}|^2) \\ & = (\tilde{\alpha} - \tilde{\beta} |\mathbf{v}|^2) \mathbf{v} - \nabla P + D_1 \nabla (\nabla \cdot \mathbf{v}) + D_2 \nabla^2 \mathbf{v} + D_3 (\mathbf{v} \cdot \nabla)^2 \mathbf{v} + \mathbf{f}, \end{aligned} \quad (4.61)$$

4.3 A review on dynamic RG analysis of Toner-Tu equations

where the coefficients $\tilde{\beta}$, D_1 , D_2 and D_3 are positive. The coefficient $\tilde{\alpha} > 0$ leads to the spontaneous breaking of rotational invariance with a non-zero mean velocity $|\mathbf{v}| = \sqrt{\tilde{\alpha}/\tilde{\beta}}$. The disordered state is characterized by $\tilde{\alpha} < 0$ with zero mean velocity. The $\lambda_{1,2,3}$ in the above equation are the nonzero phenomenological parameters specifying the Galilean invariance violation of the equation. Pressure P in the velocity field equation is obtained by Taylor series expansion of the density ρ about mean density ρ_0 given as

$$P = \sum_{n=1}^{\infty} \sigma_n (\rho - \rho_0)^n, \quad (4.62)$$

with σ_n as expansion coefficient. \mathbf{f} is noise which is assumed to be white Gaussian with variance given as

$$\langle f_i(\mathbf{r}, t) f_j(\mathbf{r}', t') \rangle = \Delta \delta_{ij} \delta^d(\mathbf{r} - \mathbf{r}') \delta(t - t'), \quad (4.63)$$

where Δ is a constant. The unknown coefficients $\tilde{\alpha}$, $\tilde{\beta}$, λ , σ_n , and $D_{1,2,3}$ are functionals of the scalar fields ρ and $|\mathbf{v}|^2$.

Since the velocity field in equation (4.61) is not slow variable. To discuss the long time and distance dynamics, we need to write the hydrodynamic equations corresponding to slow component of the velocity field. For this purpose $\mathbf{v}(\mathbf{x}, t)$ is decomposed into the longitudinal and the transverse part as $\mathbf{v}(\mathbf{x}, t) = (v_0 + \delta v_{||})\hat{x}_{||} + \mathbf{v}_{\perp}$, where \mathbf{v}_{\perp} represents the of the velocity fluctuations perpendicular to mean direction of the flock, v_0 represents the average value of the velocity and chosen to be equal to $\sqrt{\tilde{\alpha}/\tilde{\beta}}$. Now the Toner-Tu equations are written in terms of \mathbf{v}_{\perp} , by ignoring the irrelevant terms, as

$$\frac{\partial \delta \rho}{\partial t} + \rho_0 (\nabla_{\perp} \cdot \mathbf{v}_{\perp}) + \nabla_{\perp} \cdot (\delta \rho \mathbf{v}_{\perp}) + v_0 \partial_{||} \delta \rho = D_{\rho} \partial_{||}^2 \delta \rho, \quad (4.64)$$

4.3 A review on dynamic RG analysis of Toner-Tu equations

$$\begin{aligned} & \partial_t \mathbf{v}_\perp + \lambda_1 (\mathbf{v}_\perp \cdot \nabla_\perp) \mathbf{v}_\perp + \lambda_2 (\nabla_\perp \cdot \mathbf{v}_\perp) \mathbf{v}_\perp + \gamma \partial_\parallel \mathbf{v}_\perp \\ & = -\nabla_\perp P + D_1 \nabla_\perp (\nabla_\perp \cdot \mathbf{v}_\perp) + D_2 \nabla_\perp^2 \mathbf{v}_\perp + D_\parallel \partial_\parallel^2 \mathbf{v}_\perp + \mathbf{f}_\perp, \end{aligned} \quad (4.65)$$

where $\delta\rho = \rho - \rho_0$, $D_\rho = \sigma_1/(2\tilde{\alpha})$, $D_\parallel = D_2 + v_0^2 D_3$ and $\gamma = \lambda_1 v_0$. The definition of pressure in the above equation is the same as before.

Linear dynamics

To discuss the linear dynamics, Eqs. (4.64) and (4.65) are linearized in the $\delta\rho$ and \mathbf{v}_\perp . The equal time velocity autocorrelation function $C_{ij}(\mathbf{k}) = \langle v_i(\mathbf{k}, t) v_j(-\mathbf{k}, t) \rangle$ in linear case is obtained as

$$\begin{aligned} C_{ij}(\mathbf{k}) &= \int_{-\infty}^{+\infty} C_{ij}(\mathbf{k}, \omega) \frac{d\omega}{2\pi} \\ &= \frac{\Delta}{2} \left\{ \frac{P_{ij}^\perp(\mathbf{k})}{D_L k_\perp^2 + D_\parallel k_\parallel^2} + \frac{L_{ij}^\perp(\mathbf{k})}{D_2 k_\perp^2 + D_\parallel k_\parallel^2} \phi(\hat{\mathbf{k}}) \right\} \propto \frac{1}{k^2}, \end{aligned} \quad (4.66)$$

with $D_L = D_2 + D_3$. In the above equation $L_{ij}^\perp(\mathbf{k})$ and $P_{ij}^\perp(\mathbf{k})$ are the longitudinal and transverse projection operators respectively given by the expressions $\hat{k}_i^\perp \hat{k}_j^\perp$ and $(\delta_{ij}^\perp - L_{ij}^\perp)$. The function $\phi(\hat{\mathbf{k}})$ in the above expression depends on the direction $\hat{\mathbf{k}}$ of \mathbf{k} only but not on its magnitude (Toner & Tu, 1998). The above result shows long wavelength divergence of the equal time velocity correlations. The mean square velocity fluctuations in real space $\langle |\mathbf{v}_\perp(\mathbf{x}, t)|^2 \rangle$ will give more insight to the above argument

$$\begin{aligned} \langle |\mathbf{v}_\perp(\mathbf{x}, t)|^2 \rangle &= \int \frac{d^d k}{(2\pi)^d} \langle v_j(\mathbf{k}, t) v_j(-\mathbf{k}, t) \rangle \\ &= \frac{\Delta}{2} \int \frac{d^d k}{(2\pi)^d} \left\{ \frac{(d-2)}{D_L k_\perp^2 + D_\parallel k_\parallel^2} + \frac{\phi(\hat{\mathbf{k}})}{D_2 k_\perp^2 + D_\parallel k_\parallel^2} \right\}. \end{aligned} \quad (4.67)$$

4.3 A review on dynamic RG analysis of Toner-Tu equations

The wavevector integrals are restricted to the region $|\mathbf{k}_\perp| < \Lambda$, $-\infty \leq k_\parallel \leq +\infty$, where Λ is the ultraviolet cutoff defined by the inverse microscopic length characterized by the system, i.e., the interbird distance l_0 in this case. For $d \leq 2$, the second integral diverges when $|\mathbf{k}| \rightarrow 0$, i.e., towards infrared region. The ultraviolet divergence, $|\mathbf{k}| \rightarrow \infty$, for $d \geq 2$ is not relevant here since it is restricted by the cutoff Λ . From the above argument we see that, for $d \leq 2$, the velocity fluctuations are huge which destabilize the long range order similar to the case of equilibrium systems (Mermin & Wagner, 1966). Thus the linear dynamics of Toner-Tu model behaves like equilibrium system. Below we will discuss the effect of nonlinearities in the model.

Nonlinear dynamics

To see the effect of nonlinearities, i.e., how the model is different than the equilibrium model, we rescale the space, time and fields $\delta\rho$ and \mathbf{v}_\perp given as

$$\mathbf{x}_\perp \rightarrow b\mathbf{x}_\perp, \mathbf{x}_\parallel \rightarrow b^\zeta\mathbf{x}_\parallel, t \rightarrow b^z t, \mathbf{v}_\perp \rightarrow b^\chi\mathbf{v}, \delta\rho \rightarrow b^{\chi\rho}\delta\rho. \quad (4.68)$$

Our next step is to see how nonlinearities change upon rescaling by keeping the form of linear theory unchanged. We have seen in the linear dynamics (in Eq. (4.74)) that equal time correlation function is determined in terms of noise strength Δ and the diffusion coefficients $D_{1,2,\rho,\parallel}$ but not the other parameters. We will choose the scaling exponents such that these coefficients remain unchanged. After rescaling, the diffusion coefficients changed to $D_{1,2} \rightarrow b^{z-2}D_{1,2}$ and $D_{\rho,\parallel} = b^{z-2\zeta}D_{\rho,\parallel}$. These coefficients will remain unchanged if we choose $z = 2$ and $\zeta = 1$. Using the values of these exponents and noise correlation Eq. (4.63), we obtain the rescaled random force $\mathbf{f} \rightarrow b^{-1-d/2}\mathbf{f}$ which, in order to balance the linear terms in the \mathbf{v}_\perp in Eq. (4.65), gives $\chi = 1 - d/2$. For linear theory, χ is the roughness

4.3 A review on dynamic RG analysis of Toner-Tu equations

exponent. If we take L to be the length scale of the velocity fluctuations, then it scales like L^χ . For $d \leq 2$, the exponent is positive and velocity fluctuations grows without any restriction when L approaches very large value, i.e., when $L \rightarrow \infty$.

Upon rescaling the Eqs. (4.64) and (4.65), it is shown that the $\lambda_1(\mathbf{v}_\perp \cdot \nabla_\perp)\mathbf{v}_\perp$, $\lambda_2(\nabla_\perp \cdot \mathbf{v}_\perp)\mathbf{v}_\perp$ and $\sigma_2\nabla_\perp(\delta\rho^2)$ (in the pressure term) are the relevant nonlinearities for $d < 4$; and hence this implies that there will be breakdown of linear hydrodynamics below four dimensions. In case of simple fluid, linear breakdown of hydrodynamics occurs for $d \leq 2$. DRG analysis of Toner-Tu model predicts the correct behavior of equations for $2 \leq d \leq 4$.

The following coefficients of the linear theory are affected on the renormalization whose expressions are given by the following equations

$$D_{1,2,\rho}(\mathbf{k}) \propto \begin{cases} k_\perp^{z-2}, & \frac{k_\parallel}{\Lambda} \ll (\frac{k_\perp}{\Lambda})^\zeta, \\ k_\parallel^{(z-2)/\zeta}, & \frac{k_\parallel}{\Lambda} \gg (\frac{k_\perp}{\Lambda})^\zeta, \end{cases} \quad (4.69)$$

$$D_\parallel(\mathbf{k}) \propto \begin{cases} k_\perp^{z-2\zeta}, & \frac{k_\parallel}{\Lambda} \ll (\frac{k_\perp}{\Lambda})^\zeta, \\ k_\parallel^{z/\zeta-2}, & \frac{k_\parallel}{\Lambda} \gg (\frac{k_\perp}{\Lambda})^\zeta, \end{cases} \quad (4.70)$$

$$\Delta(\mathbf{k}) \propto \begin{cases} k_\perp^{z-\zeta-2\chi+1-d}, & \frac{k_\parallel}{\Lambda} \ll (\frac{k_\perp}{\Lambda})^\zeta, \\ k_\parallel^{(z-\zeta-2\chi+1-d)/\zeta}, & \frac{k_\parallel}{\Lambda} \gg (\frac{k_\perp}{\Lambda})^\zeta, \end{cases} \quad (4.71)$$

Here we see that all the coefficients depend only on k_\perp for $\frac{k_\parallel}{\Lambda} \ll (\frac{k_\perp}{\Lambda})^\zeta$ and k_\parallel for $\frac{k_\parallel}{\Lambda} \gg (\frac{k_\perp}{\Lambda})^\zeta$.

The scaling exponents cannot be calculated exactly for $2 < d \leq 4$ in one loop order calculation of the equations. This is due to the occurrence of the λ_2 nonlinearity in the equation of motion. For $\lambda_2 = 0$, exponents are calculated exactly with the following result

$$\zeta = (d+1)/5, \quad z = 2(d+1)/5, \quad \chi = (3-2d)/5 \quad (4.72)$$

In two dimensions, λ_2 nonlinearity disappears and scaling exponent are calculated exactly. Now, similar to the linear dynamics, we focus on the equal time velocity correlation function. In nonlinear case, the $C_{ij}(\mathbf{k})$ behave in the following manner

$$C_{ij}(\mathbf{k}) \propto \begin{cases} k_{\perp}^{z-\zeta-2\chi+1-d}, & \frac{k_{\parallel}}{\Lambda} \ll \left(\frac{k_{\perp}}{\Lambda}\right)^{\zeta}, \\ k_{\parallel}^{(z-\zeta-2\chi+1-d)/\zeta}, & \frac{k_{\parallel}}{\Lambda} \gg \left(\frac{k_{\perp}}{\Lambda}\right)^{\zeta}, \end{cases} \quad (4.73)$$

From the above expression, for $d < 4$ with the result $z < 2$ and $\zeta < 1$, we see that $C_{ij}(\mathbf{k})$ diverges more slowly than $1/k^2$. Below we obtain real space mean square velocity fluctuations as

$$\begin{aligned} \langle |\mathbf{v}_{\perp}(\mathbf{x}, t)|^2 \rangle &= \frac{1}{2} \int \frac{d^d k}{(2\pi)^d} \Delta(\mathbf{k}) \left\{ \frac{(d-2)}{D_L(\mathbf{k})k_{\perp}^2 + D_{\parallel}(\mathbf{k})k_{\parallel}^2} \right. \\ &\quad \left. + \frac{\phi(\hat{\mathbf{k}})}{D_2(\mathbf{k})k_{\perp}^2 + D_{\parallel}(\mathbf{k})k_{\parallel}^2} \right\}, \end{aligned} \quad (4.74)$$

which shows that fluctuations remain finite in real space.

4.4 Discussion

In the dynamic RG analysis of Navier-Stokes equation, we have discussed how transport coefficients have modified, and velocity correlation functions behave in the low wavenumber and frequency limit, i.e., in the limit $k \rightarrow 0$ and $\omega \rightarrow 0$. We have seen that nonlinear contribution to the renormalization of perturbative parameter λ_0 vanishes. This is due to the Galilean invariant equation of motion as a consequence to the momentum conservation. We have also discussed that viscosity coefficient and noise strength renormalized in the same way which is the significance of holding fluctuation-dissipation theorem (FDT) for the system.

As Navier-Stokes equation for simple fluid describe the liquid phase of water not its solid phase, similarly hydrodynamic equations for polar active particles

obtained by Toner and Tu (Toner & Tu, 1998, 1995), describes only one phase of a flock out of many possible phases (Toner *et al.*, 2005; Tu, 2000). Toner-Tu equations unify the features of Navier-Stokes equation for a normal compressible fluid as well as a relaxational time-dependent Ginsburg-Landau model for spins in an isotropic ferromagnet. Toner and Tu showed that linear theory breaks down in spatial dimensions $d < 4$ analogous to the equilibrium fluid where breakdown occurs in dimensions below $d = 2$. The linear dynamics of the flock shows the long-wavelength fluctuations in the velocity correlation functions. These fluctuations are strong enough to demolish the long-range order in spatial dimensions $d \leq 2$. Convective nonlinearities play crucial role to stabilize the long-range order in two dimensions. The FDT and Galilean invariance both are violated in Toner-Tu equations. Lack of Galilean invariance allows extra convective nonlinear terms in the equations for $d > 2$. Up to one loop order calculation, they were not able to predict the exact phase of the flock and calculate the scaling exponents exactly for dimensions $2 < d < 4$. They have discussed the three possible phases of the flock on the basis of one loop-order RG analysis of equations. Two loop order calculation can provide the information about exact phase of the flock. Full RG analysis of Toner-Tu equation is still needed which may lead to a new universality class.

To elaborate the discussion on fluctuating hydrodynamic equations of flocking (Toner & Tu, 1998, 1995), we have presented here the details of dynamic RG analysis of the Navier-Stokes equation as was done in the seminal work of Forster, Nelson, and Stephen (Forster *et al.*, 1977, 1976). In Chapter 5, we will discuss some specific comments on the continuum equations for flocking along the lines of the analysis presented here.

Appendix

4.A Viscosity renormalization

We evaluate integral $I_{mn\mu}$ given by Eq. (4.17) as

$$I_{mn\mu}(\mathbf{k}, \omega) = \int_{q\Omega}^> G_0(\mathbf{k} - \mathbf{q}, \omega - \Omega) P_{n\mu\nu}(\mathbf{k} - \mathbf{q}) C_0(\mathbf{q}, \Omega) P_{m\nu}(\mathbf{q}), \quad (4.A.1)$$

where

$$\int_{q,\Omega} \equiv \int_{q<\Lambda}^> \frac{d^d q}{(2\pi)^d} \int_{-\infty}^{+\infty} \frac{d\Omega}{2\pi},$$

and

$$G_0(\mathbf{k}, \omega) = (-i\omega + \nu_0 k^2)^{-1}.$$

First, we evaluate frequency integral of Eq. (4.A.1) (we denote it by symbol I_Ω)

$$\begin{aligned} I_\Omega &= \int_{-\infty}^{+\infty} \frac{d\Omega}{2\pi} G_0^>(\mathbf{k} - \mathbf{q}, \omega - \Omega) |G_0^>(\mathbf{q}, \Omega)|^2 \\ &= \int_{-\infty}^{+\infty} \frac{d\Omega}{2\pi} \frac{1}{-i(\omega - \Omega) + \nu_0 |\mathbf{k} - \mathbf{q}|^2} \frac{1}{\Omega^2 + (\nu_0 q^2)^2}, \end{aligned} \quad (4.A.2)$$

or

$$I_\Omega = \int_{-\infty}^{+\infty} \frac{d\Omega}{2\pi} \frac{1}{\beta + i\Omega} \frac{1}{\Omega^2 + \alpha^2},$$

4.A Viscosity renormalization

where we have defined $-i(\omega - \Omega) + \nu_0|\mathbf{k} - \mathbf{q}|^2 = \beta$ and $\nu_0 q^2 = \alpha$. After performing the integral over frequency, I_Ω obtains the following result

$$\begin{aligned}
 I_\Omega &= \frac{1}{2\pi(\beta^2 - \alpha^2)} \left[\pi \frac{\beta + \alpha}{\alpha} - 2\pi \right] \\
 &= \frac{1}{2\alpha(\beta + \alpha)} \\
 &= \frac{1}{2\nu_0 q^2 (-i\omega + \nu_0|\mathbf{k} - \mathbf{q}|^2 + \nu_0 q^2)}. \tag{4.A.3}
 \end{aligned}$$

Now using (4.A.3) in Eq. (4.A.1) we obtain

$$I_{mn\mu}(\mathbf{k}, \omega) = \frac{D_0}{\nu_0} \int_q^> \frac{P_{n\mu\nu}(\mathbf{k} - \mathbf{q}) P_{m\nu}(\mathbf{q})}{(-i\omega + \nu_0|\mathbf{k} - \mathbf{q}|^2 + \nu_0 q^2)}. \tag{4.A.4}$$

To proceed further, we replace $\mathbf{q} \rightarrow \mathbf{q} + \frac{\mathbf{k}}{2}$ and obtain the above expression in the limit $\omega \rightarrow 0, k \rightarrow 0$ as

$$I_{mn\mu}(\mathbf{k}, \omega) = \frac{D_0}{2\nu_0^2} \int_q^> \frac{P_{n\mu\nu}(\frac{\mathbf{k}}{2} - \mathbf{q}) P_{m\nu}(\mathbf{q} + \frac{\mathbf{k}}{2})}{q^2},$$

or

$$\begin{aligned}
 I_{mn\mu}(\mathbf{k}, \omega) &= \frac{D_0}{2\nu_0^2} \int_q^> \frac{1}{q^2} \left[\frac{k_\nu}{2} P_{n\mu}(\frac{\mathbf{k}}{2} - \mathbf{q}) P_{m\nu}(\mathbf{q} + \frac{\mathbf{k}}{2}) \right. \\
 &\quad - q_\nu P_{n\mu}(\frac{\mathbf{k}}{2} - \mathbf{q}) P_{m\nu}(\mathbf{q} + \frac{\mathbf{k}}{2}) \\
 &\quad + \frac{k_\mu}{2} P_{n\nu}(\frac{\mathbf{k}}{2} - \mathbf{q}) P_{m\nu}(\mathbf{q} + \frac{\mathbf{k}}{2}) \\
 &\quad \left. - q_\mu P_{n\nu}(\frac{\mathbf{k}}{2} - \mathbf{q}) P_{m\nu}(\mathbf{q} + \frac{\mathbf{k}}{2}) \right]. \tag{4.A.5}
 \end{aligned}$$

To simplify the above expression, we obtain the following relation up to linear order in k

$$\frac{k_\nu}{2} P_{m\nu}(\frac{\mathbf{k}}{2} + \mathbf{q}) = -q_\nu P_{m\nu}(\mathbf{q} + \frac{\mathbf{k}}{2}). \tag{4.A.6}$$

Next, we simplify the following expression from the Eq. (4.A.5) as

$$P_{n\nu}\left(\frac{\mathbf{k}}{2} - \mathbf{q}\right)P_{m\nu}\left(\mathbf{q} + \frac{\mathbf{k}}{2}\right) = \left[\delta_{n\nu} - \frac{\left(\frac{k}{2} - q\right)_n \left(\frac{k}{2} - q\right)_\nu}{\left|\frac{\mathbf{k}}{2} - \mathbf{q}\right|^2} \right] \\ \times \left[\delta_{m\nu} - \frac{\left(\frac{k}{2} + q\right)_m \left(\frac{k}{2} + q\right)_\nu}{\left|\frac{\mathbf{k}}{2} - \mathbf{q}\right|^2} \right]$$

Upto linear order in k we obtain

$$P_{n\nu}\left(\frac{\mathbf{k}}{2} - \mathbf{q}\right)P_{m\nu}\left(\mathbf{q} + \frac{\mathbf{k}}{2}\right) \approx \delta_{nm} - \frac{q_n q_m}{q^2} - \frac{k_n q_m}{2q^2} + \frac{q_n k_m}{2q^2},$$

or

$$P_{n\nu}\left(\frac{\mathbf{k}}{2} - \mathbf{q}\right)P_{m\nu}(\mathbf{q}) = P_{nm}(\mathbf{q}) - \frac{k_n q_m}{2q^2} + \frac{q_n k_m}{2q^2}.$$

The last two terms are symmetric and opposite in sign. On integration, sum of contribution of the two terms will be zero. This allows us to obtain the above relation as

$$P_{n\nu}\left(\frac{\mathbf{k}}{2} - \mathbf{q}\right)P_{m\nu}(\mathbf{q}) = P_{nm}(\mathbf{q}). \quad (4.A.7)$$

Now using the relation (4.A.6) and (4.A.7) and neglecting the terms having no contribution to the renormalized viscosity in the the limit $k \rightarrow 0, \omega \rightarrow 0$, Eq. (4.A.5) is obtained as

$$I_{mn\mu}(\mathbf{k}, \omega) = k_\nu \frac{D_0}{2\nu_0^2} \int^> \frac{1}{q^2} [P_{n\mu}(\mathbf{q})P_{m\nu}(\mathbf{q})] \quad (4.A.8)$$

or

$$\begin{aligned}
I_{mn\mu}(\mathbf{k}, \omega) &= k_\nu \frac{D_0}{2\nu_0^2} \int^> \frac{1}{q^2} [\delta_{n\mu} \delta_{m\nu} - \delta_{n\mu} \hat{q}_m \hat{q}_\nu - \delta_{m\nu} \hat{q}_n \hat{q}_\mu + \hat{q}_n \hat{q}_\mu \hat{q}_m \hat{q}_\nu] \\
&= k_\nu \frac{D_0}{2\nu_0^2} \int^> \frac{1}{q^2} \left[\delta_{n\mu} \delta_{m\nu} - \frac{1}{d} \delta_{n\mu} \delta_{m\nu} - \frac{1}{d} \delta_{m\nu} \delta_{n\mu} \right. \\
&\quad \left. + \frac{1}{d(d+2)} (\delta_{n\mu} \delta_{m\nu} + \delta_{n\nu} \delta_{m\mu} + \delta_{mn} \delta_{\mu\nu}) \right] \\
&= k_\nu \frac{D_0}{2\nu_0^2} \int^> \frac{1}{q^2} \left[\delta_{n\mu} \delta_{m\nu} \left(1 - \frac{2}{d} + \frac{1}{d(d+2)} \right) \right. \\
&\quad \left. + \frac{1}{d(d+2)} (\delta_{n\nu} \delta_{m\mu} + \delta_{mn} \delta_{\mu\nu}) \right]. \tag{4.A.9}
\end{aligned}$$

Using the above result, the term on the right-hand side of Eq. (4.20) of the main text is obtained as

$$\begin{aligned}
P_{lmn}^<(\mathbf{k}) I_{mn\mu}(\mathbf{k}, \omega) &= \frac{D_0}{2\nu_0^2} k_\nu [P_{lm}^<(\mathbf{k}) k_n + P_{ln}^<(\mathbf{k}) k_m] \\
&\quad \times \left[\delta_{n\mu} \delta_{m\nu} \left(1 - \frac{2}{d} + \frac{1}{d(d+2)} \right) \right. \\
&\quad \left. + \frac{1}{d(d+2)} (\delta_{n\nu} \delta_{m\mu} + \delta_{mn} \delta_{\mu\nu}) \right] \int^> \frac{1}{q^2} \\
&= \frac{D_0}{2\nu_0^2} \left[P_{l\mu}^<(\mathbf{k}) k^2 \left(1 - \frac{2}{d} + \frac{1}{d(d+2)} \right) \right. \\
&\quad \left. + P_{l\mu}^<(\mathbf{k}) k^2 \frac{1}{d(d+2)} \right] \int^> \frac{1}{q^2} \\
&= P_{l\mu}^<(\mathbf{k}) k^2 \frac{D_0}{\nu_0^2} \frac{d^2 - 2}{2d(d+2)} \frac{S_d}{(2\pi)^d} \int^> \frac{d^d q}{q^2} \\
&= P_{l\mu}^<(\mathbf{k}) k^2 \frac{D_0}{\nu_0^2} A_d \int^> \frac{d^d q}{q^2}, \tag{4.A.10}
\end{aligned}$$

where

$$A_d = \frac{d^2 - 2}{2d(d+2)} \frac{S_d}{(2\pi)^d}, \tag{4.A.11}$$

with $S_d = 2\pi^{(d/2)}/\Gamma(d/2)$.

4.B Renormalization of noise strength

We take the integral $J_{mrrns}(\mathbf{k}, \omega)$ defined by equation (4.27) in the main text

$$J_{mjns}(\mathbf{k}, \omega) = \int_{q\Omega}^> C_0(\mathbf{k} - \mathbf{q}, \omega - \Omega) C_0(\mathbf{q}, \Omega) P_{mj}(\mathbf{k} - \mathbf{q}) P_{ns}(\mathbf{q}). \quad (4.B.1)$$

First, we evaluate frequency integral by defining

$$\begin{aligned} J_\Omega &= \int_{-\infty}^{+\infty} \frac{d\Omega}{2\pi} C_0(\mathbf{k} - \mathbf{q}, \omega - \Omega) C_0(\mathbf{q}, \Omega) \\ &= 4D_0^2 \int_{-\infty}^{+\infty} \frac{d\Omega}{2\pi} \frac{|\mathbf{k} - \mathbf{q}|^2}{(\omega - \Omega)^2 + \nu_0^2 |\mathbf{k} - \mathbf{q}|^4} \frac{q^2}{\Omega^2 + \nu_0^2 q^4}. \end{aligned} \quad (4.B.2)$$

From Eq. (4.26) we see that integral J_{mrrns} is multiplied by a factor of quadratic order in k . In evaluating the above integral we neglect the higher order term in k . Now in the limit $k \rightarrow 0, \omega \rightarrow 0$, we obtain

$$J_\Omega = 4D_0^2 \int_{-\infty}^{+\infty} \frac{d\Omega}{2\pi} \frac{q^4}{(\Omega^2 + \nu_0^2 q^4)^2}, \quad (4.B.3)$$

by defining $\alpha = \nu_0 q^2$, above integral is written as

$$J_\Omega = 4D_0^2 \int_{-\infty}^{+\infty} \frac{d\Omega}{2\pi} \frac{q^4}{[(\Omega + i\alpha)(\Omega - i\alpha)]^2}, \quad (4.B.4)$$

J_Ω , after performing frequency integral is obtained as

$$J_\Omega = \frac{1}{\nu_0^3 q^6}. \quad (4.B.5)$$

Now using the above result in Eq. (4.B.1) and performing the integration over direction of $\hat{\mathbf{q}}$ of \mathbf{q} for fixed $|\mathbf{q}|$, we obtain

4.B Renormalization of noise strength

$$\begin{aligned}
J_{mjns} &= \frac{D_0^2}{\nu_0^3} \int^> \frac{1}{q^2} \left[\delta_{mj} \delta_{ns} \left(1 - \frac{2}{d} + \frac{1}{d(d+2)} \right) \right. \\
&\quad \left. + \frac{1}{d(d+2)} (\delta_{mn} \delta_{js} + \delta_{ms} \delta_{jn}) \right]. \tag{4.B.6}
\end{aligned}$$

Next, To evaluate the second term on the right-hand side of Eq. (4.26), we consider the following relation

$$\begin{aligned}
P_{lmn}^<(\mathbf{k}) P_{ijs}^<(\mathbf{k}) &= \left[P_{lm}^<(\mathbf{k}) P_{ij}^<(\mathbf{k}) k_n k_s + P_{lm}^<(\mathbf{k}) P_{is}^<(\mathbf{k}) k_n k_j \right. \\
&\quad \left. + P_{ln}^<(\mathbf{k}) P_{ij}^<(\mathbf{k}) k_m k_s + P_{ln}^<(\mathbf{k}) P_{is}^<(\mathbf{k}) k_m k_j \right]. \tag{4.B.7}
\end{aligned}$$

Now using the property of projection operator $P_{lj}(\mathbf{k}) P_{ji}(\mathbf{k}) = P_{li}(\mathbf{k})$, we obtain from (4.B.6) and (4.B.7)

$$\begin{aligned}
J_{mjns} P_{lmn}^<(\mathbf{k}) P_{ijs}^<(\mathbf{k}) &= \frac{D_0^2}{\nu_0^3} \left[2k^2 P_{l\mu}^<(\mathbf{k}) \left(1 - \frac{2}{d} + \frac{1}{d(d+2)} \right) \right. \\
&\quad \left. + k^2 P_{l\mu}^<(\mathbf{k}) \frac{2}{d(d+2)} \right] \int^> \frac{1}{q^2} \\
&= 4k^2 P_{l\mu}^<(\mathbf{k}) \frac{D_0^2}{\nu_0^3} \frac{d^2 - 2}{2d(d+2)} \frac{S_d}{(2\pi)^d} \int^> \frac{d^d q}{q^2} \\
&= 4k^2 P_{l\mu}^<(\mathbf{k}) \frac{D_0^2}{\nu_0^3} A_d \int^> \frac{d^d q}{q^2}. \tag{4.B.8}
\end{aligned}$$

Chapter 5

Fluctuating hydrodynamic approach to flocking

Collective, organized motion of a large number of living entities exhibit striking phenomena which occur in nature from microscale to large-length scale. Some of the examples are flocks of birds, mammal herds, schools of fish, bacterial colony, etc. The collective motion of these elements is termed as ‘flocking’. The study of these systems falls under the evolving branch of physics ‘active matter’. Active matter systems are intrinsically out of equilibrium, i.e., without applying any external field or perturbation on the system. The study of these systems attracted the great interest to scientists after the pioneering work of Vicsek *et al.*, (1995), who first identified that flocks are the nonequilibrium dynamical systems. Flock elements of the Vicsek model are considered as point-particles all moving with constant speed. The velocity vector of an individual element is treated as the magnetic spin in a ferromagnetic system. Thus the flocks show some analogy with the magnetic systems studied in the theory of phase transitions in statistical mechanics. The main difference between these two is that flocks are the nonequilibrium system in which birds are moving while the spins in ferromag-

netic systems are static. Due to this difference, flocking systems shows intriguing properties in terms of phase transitions which are not seen in equilibrium systems. In section 5.1, we will review the Vicsek model.

Coarse-grained description of the flocking system can be obtained either by symmetry consideration or by deriving particle-based models. Coarse-grained equations in terms of hydrodynamic field equations are useful to study the long-distance and long-time properties of a many-particle system in equilibrium (Forster *et al.*, 1977) as well as in out of equilibrium (Kardar *et al.*, 1986). Hydrodynamic equations for the flocking of active particles have been proposed by Toner and Tu on the basis of symmetry and conservation laws (Toner & Tu, 1998, 1995). Their model showed a nonequilibrium phase-transition from a disordered state to a state of long-range order. The Toner-Tu equations, though successful in explaining important dynamical phenomena, misses some essential microscopic details. The hydrodynamic coefficients like viscosities, diffusivities cannot be determined in terms of the microscopic parameters of the dynamics. If we start the description from the microscopic point to obtain coarse-grained description, we can easily relate the microscopic parameter of the dynamics to the macroscopic parameters which can be directly linked to the experimentally accessible quantities.

In this chapter, we give the coarse-grained description for polar active particles from a microscopic starting point. The active systems considered here are specified by short-range interactions. A particular element in the flock is influenced by the neighboring elements within a specific distance which is much smaller than the size of the flock. We consider that the surrounding medium in which particles move is inert which provides only friction and therefore momentum of the system is not conserved. We write down the microscopic Langevin equation with an additive noise. We obtain the microscopic equations for collective densities

corresponding to the microscopic Langevin equation. The collective modes for the system are the microscopic mass density and momentum density. For a fixed number of particles, mass density is conserved. We average the equations for collective densities over a suitable ensemble to obtain macroscopic hydrodynamic equations corresponding to mass density field and momentum density fields. The momentum field equation obtained in this manner contains a multiplicative noise whose microscopic origin is the additive noise term in the Langevin equation.

5.1 The microscopic model

Generally, microscopic dynamics of particles in a complex fluid is described by the Langevin equation with noise. To discuss the dynamics of polar active particles of the flock, we follow a similar approach. Since the active particles are self-driven, the Langevin equation describing the dynamics of such type of particles should have energy pumping terms (or active terms) other than dissipative and random noise terms (Schweitzer, 2003). The concept of universality class introduced with respect to the condensed matter physics and critical phenomena specify that systems having the same general characteristics are expected to behave similarly. Therefore, before discussing our microscopic model, we find it useful first to review the Vicsek model (Vicsek *et al.*, 1995) which is the simplest discrete model of self-propelled particles (e.g., birds) in two dimensions. We consider $\mathbf{r}_\alpha(t)$ is the position and $\hat{\theta}_\alpha(t)$ be the respective direction of the α -th element of the flock at discrete time t in a two dimensional plane. During the time step τ particle's position is updated according to

$$\mathbf{r}_\alpha(t + \tau) = \mathbf{r}_\alpha(t) + \tau \mathbf{v}_\alpha(t), \quad (5.1)$$

where particle velocities $\mathbf{v}_\alpha(t + \tau) = v_0(\cos \hat{\theta}_\alpha(t), \sin \hat{\theta}_\alpha(t))$ have fixed magnitude v_0 . Direction update of the particle α is determined by

$$\hat{\theta}_\alpha(t + \tau) = \bar{\theta}_\alpha + \eta_\alpha(t), \quad (5.2)$$

where the direction $\bar{\theta}_\alpha$ denotes the average of all vectors $\mathbf{v}_\beta(t)$ over all neighbors β lying within a circle of radius R_0 around the α -th particle and given by the expression as $\bar{\theta}_\alpha = \arctan(\sum_\beta \sin(\hat{\theta}_\beta) / \sum_\beta \cos(\hat{\theta}_\beta))$. The variable η_α in the Eq. (5.2) is random noise which have short-range correlations. This model characterizes that there is no preferred direction of motion of birds, i.e., all directions are equally likely. Spontaneous continuous symmetry breaking occurs in transition to a collective motion from the disordered state to ordered state. The only conservation law for this model is the total number of particles, and particularly it is to be noted that momentum is not conserved. Vicsek model is the ideal flocking model for self-driven particles. Realistic features of this model are discussed in Refs. (Cavagna *et al.*, 2015; Couzin *et al.*, 2002; Ginelli & Chaté, 2010; Grégoire & Chaté, 2004; Levine *et al.*, 2000); and in all of these, the basic structure of the dynamical equations are same. Time evolution of velocity vector is described by a Langevin-type equation containing terms of random noise and alignment force due to interactions between local neighbors. The first coarse-grained description for the two-dimensional Vicsek model has been obtained by Bertin *et al.*, (2006, 2009) using the Boltzmann approach.

5.1.1 The individual particle dynamics

We consider here a flock of N elements each having the same mass m . Generally, microscopic dynamics of the α -th element of the flock is described in terms of its respective position and momentum coordinates $\{\mathbf{x}_\alpha, \mathbf{p}_\alpha\}$ with $\alpha = 1, \dots, N$.

We will work here with the time evolution of momentum coordinate of the α -th element given by the Langevin equation as

$$\frac{dp_{\alpha}^i(t)}{dt} = -\nabla_{\alpha}^i \sum_{\nu} U(\mathbf{x}_{\alpha}(t) - \mathbf{x}_{\nu}(t)) - \sum_{\nu} \zeta_{\alpha\nu}^{ij}(\mathbf{p}_{\nu}) p_{\nu}^j + \xi_{\alpha}^i(t) \quad (5.3)$$

In the above expression, the Latin indices i, j denote the Cartesian components ranging from 1 to dimensionality d , the Greek indices α and ν denote the different elements of the flock of N elements. Operator ∇_{α}^i denotes the derivative with respect to the i -th component of \mathbf{x}_{α} and U is the two-body interaction potential. In the above equation and rest of this chapter we follow the Einstein summation convention for repeated Latin indices. The first term on the right-hand side (RHS) of the Eq. (5.3) represents the reversible part while the second term denotes the irreversible or the dissipative part. A salient characteristic of the Eq. (5.3), describing the dynamics of α -th element, is that the dissipative coefficient $\zeta_{\alpha\nu}^{ij}(\mathbf{p}_{\nu})$ is dependent on momentum \mathbf{p}_{α} and the frictional drag on the α -th element depends on its own velocity, as well as those of its neighbors. The third term $\xi_{\alpha}^i(t)$ on the RHS of the above equation denotes the stochastic part or noise. The noise $\xi_{\alpha}^i(t)$ is considered to be additive in nature. Its correlation is defined by

$$\langle \xi_{\alpha}^i(t) \xi_{\nu}^j(t') \rangle_{\text{F}} = 2\Gamma_{\alpha\nu}^{ij} \delta(t - t'), \quad (5.4)$$

where $\Gamma_{\alpha\nu}^{ij}$ is symmetric matrix and the subscript F on the angular bracket represents the average over the fast degrees of freedom in the dynamics.

5.1.2 The equations of motion for collective densities

To describe dynamics at collective level, we define microscopic mass and momentum densities $\hat{\rho}(\mathbf{x}, t)$ and $\hat{\mathbf{g}}(\mathbf{x}, t)$ as

$$\hat{\rho}(\mathbf{x}, t) = \sum_{\alpha=1}^N m \delta(\mathbf{x} - \mathbf{x}_\alpha(t)), \quad (5.5)$$

$$\hat{\mathbf{g}}(\mathbf{x}, t) = \sum_{\alpha=1}^N \mathbf{p}_\alpha \delta(\mathbf{x} - \mathbf{x}_\alpha(t)). \quad (5.6)$$

In order to obtain the time evolution equation for collective density $\hat{\rho}(\mathbf{x}, t)$ we take time derivative of Eq. (5.5)

$$\frac{\partial \hat{\rho}}{\partial t} = \sum_{\alpha} m \nabla_{\mathbf{x}_\alpha} \delta(\mathbf{x} - \mathbf{x}_\alpha) \cdot \dot{\mathbf{x}}_\alpha.$$

Using the property $\nabla_{\mathbf{x}} f(\mathbf{x} - \mathbf{x}') = -\nabla_{\mathbf{x}'} f(\mathbf{x} - \mathbf{x}')$, we obtain

$$\frac{\partial \hat{\rho}}{\partial t} + \nabla \cdot \hat{\mathbf{g}} = 0, \quad (5.7)$$

with $\hat{\mathbf{g}}$ identified as current for mass density. Similarly to obtain equations of motion for collective mode $\hat{\mathbf{g}}(\mathbf{x}, t)$ we take time derivative of Eq. (5.6)

$$\begin{aligned} \frac{\partial \hat{g}_i}{\partial t} &= \sum_{\alpha} \nabla_{\mathbf{x}_\alpha} \delta(\mathbf{x} - \mathbf{x}_\alpha) \cdot \dot{\mathbf{x}}_\alpha p_\alpha^i + \sum_{\alpha} \frac{dp_\alpha^i(t)}{dt} \delta(\mathbf{x} - \mathbf{x}_\alpha) \\ &= -\nabla_j \sum_{\alpha} \frac{p_\alpha^i p_\alpha^j}{m} \delta(\mathbf{x} - \mathbf{x}_\alpha) + \sum_{\alpha} \frac{dp_\alpha^i(t)}{dt} \delta(\mathbf{x} - \mathbf{x}_\alpha). \end{aligned} \quad (5.8)$$

Using Eq. (5.3) in (5.8), we obtain the time evolution for $\hat{g}_i(\mathbf{x}, t)$ as

$$\frac{\partial}{\partial t} \hat{g}_i(\mathbf{x}, t) + \hat{V}_i(\mathbf{x}, t) + \hat{\mathcal{F}}_i(\mathbf{x}, t) = \hat{\theta}_i(\mathbf{x}, t). \quad (5.9)$$

5.2 Coarse-graining microscopic equations

The left-hand side (LHS) of the above equation has the reversible and irreversible terms, denoted by $\hat{V}_i(\mathbf{x}, t)$ and $\hat{\mathcal{F}}_i(\mathbf{x}, t)$ respectively, arises from the corresponding contributions in the microscopic equation (5.3). The time reversible part $\hat{V}_i(\mathbf{x}, t)$ contains two terms resulting from the time derivatives acting on the function $\delta(\mathbf{x} - \mathbf{x}_\alpha)$ and momentum coordinate \mathbf{p}_α . The reversible part $\hat{V}_i(\mathbf{x}, t)$ and dissipative part $\hat{\mathcal{F}}_i(\mathbf{x}, t)$ of Eqn. (5.9) are obtained as

$$\hat{V}_i = \nabla_j \left[\sum_{\alpha} p_{\alpha}^i p_{\alpha}^j \delta(\mathbf{x} - \mathbf{x}_{\alpha}) \right] + \hat{\rho}(\mathbf{x}, t) \nabla_i \int d\mathbf{x}' U(\mathbf{x} - \mathbf{x}') \hat{\rho}(\mathbf{x}', t), \quad (5.10)$$

$$\hat{\mathcal{F}}_i = \sum_{\alpha, \nu} \zeta_{\alpha\nu}^{ij}(\mathbf{p}_{\nu}) p_{\nu}^j \delta(\mathbf{x} - \mathbf{x}_{\alpha}). \quad (5.11)$$

The fluctuating part $\hat{\theta}_i(\mathbf{x}, t)$ on the RHS of Eqn. (5.9), originating from the noise ξ_{α} of Eqn. (5.3), is obtained as

$$\hat{\theta}_i(\mathbf{x}, t) = \sum_{\alpha} \xi_{\alpha}^i \delta(\mathbf{x} - \mathbf{x}_{\alpha}). \quad (5.12)$$

Using Eq.(5.4) for the correlation of white noise $\xi_{\alpha}^i(t)$ and by applying translational invariance, variance of the noise $\hat{\theta}$ is obtained as

$$\langle \hat{\theta}_i(\mathbf{x}, t) \hat{\theta}_j(\mathbf{x}', t') \rangle_{\text{F}} = \Gamma_0 \delta_{ij} \hat{\rho}(\mathbf{x}') \delta(\mathbf{x} - \mathbf{x}') \delta(t - t'), \quad (5.13)$$

where, for the isotropic system, we have taken a local approximation for the symmetric matrix $\Gamma_{\alpha\nu}^{ij}(\mathbf{x}) \equiv \delta_{ij} \delta_{\alpha\nu} \Gamma_0 \delta(\mathbf{x})$ with Γ_0 as a constant.

5.2 Coarse-graining microscopic equations

The microscopic Eqs. (5.7) and (5.9) for the set of collective densities $\hat{\rho}$ and $\{\hat{\rho}, \hat{\mathbf{g}}\}$ when averaged over suitable nonequilibrium ensemble obtain the macro-

5.2 Coarse-graining microscopic equations

scopic equations for smoothly varying density fields. We define the nonequilibrium ensemble average of the microscopic densities by

$$\langle \hat{\rho}(\mathbf{x}, t) \rangle_{\text{ne}} = \rho(\mathbf{x}, t), \quad (5.14)$$

$$\langle \hat{\mathbf{g}}(\mathbf{x}, t) \rangle_{\text{ne}} = \mathbf{g}(\mathbf{x}, t). \quad (5.15)$$

The time evolution equations for coarse-grained density fields $\rho(\mathbf{x}, t)$ and $\mathbf{g}(\mathbf{x}, t)$ give rise to the macroscopic hydrodynamic equations describing the dynamics of polar active particles.

The microscopic densities depend on phase-space variable. In averaging process, their dependence on phase-space variable are integrated out. In order to coarse-grain the equations, we define an appropriate probability distribution function by assuming that system has reached a state of local equilibrium and root mean square of the momentum is constant. To make the averaging process simple, we consider the fluid from a co-moving frame having local velocity $\mathbf{v}(\mathbf{x}, t)$ so that fluid appears at rest in the vicinity of point \mathbf{x} at time t . Quantities in moving frame will be denoted by prime. In locally moving frame, we take collective densities $\{\hat{\rho}'(\mathbf{x}), \hat{\mathbf{g}}'(\mathbf{x})\}$. The position and momentum coordinates in moving frame are linked to the rest frame by following canonical transformation

$$\mathbf{x}_\alpha = \mathbf{x}'_\alpha \text{ and } \mathbf{p}_\alpha = \mathbf{p}_\alpha + m\mathbf{v}(\mathbf{x}'_\alpha). \quad (5.16)$$

Using the above transformation rule we relate the microscopic densities in the locally moving to the rest frame as

$$\hat{\rho}(\mathbf{x}) = \hat{\rho}'(\mathbf{x}), \quad (5.17)$$

$$\hat{\mathbf{g}}(\mathbf{x}) = \hat{\mathbf{g}}'(\mathbf{x}) + \hat{\rho}'(\mathbf{x})\mathbf{v}(\mathbf{x}). \quad (5.18)$$

5.2 Coarse-graining microscopic equations

Using the ideas of Gibbsian ensemble and the transformation rule (5.16), local equilibrium distribution function in the primed frame is obtained as

$$f_{\text{le}}(\Gamma'_N, t) = Q_l^{-1} \exp \left[-\beta \left\{ H' - \int d\mathbf{x} \mu(\mathbf{x}, t) \hat{\rho}'(\mathbf{x}) \right\} \right], \quad (5.19)$$

where Γ'_N represents the phase-space coordinates and Q_l is the normalization constant for the distribution function f_{le} . The β factor on the RHS of Eq. (5.19) is related to the average kinetic energy $\epsilon_0 = d/(2\beta)$ in d dimensions. H' is the Hamiltonian in the local rest frame and $\mu(\mathbf{x})$ denotes the local chemical potential. Local equilibrium averages of the quantities with respect to the distribution f_{le} will be denoted by angular brackets $\langle \dots \rangle$.

Local equilibrium average of Eq. (5.18), using the fact that the distribution function has \mathbf{p}' , $-\mathbf{p}'$ symmetry in the primed frame, gives the nonlinear relation $\mathbf{g} = \rho \mathbf{v}$ which defines the local velocity field $\mathbf{v}(\mathbf{x}, t)$ in terms of coarse-grained densities.

Coarse-grained form of the microscopic Eqs. (5.7) and (5.9) for the collective densities $\hat{\rho}$ and $\hat{\mathbf{g}}$ is obtained as

$$\frac{\partial \rho(\mathbf{x}, t)}{\partial t} + \nabla \cdot \mathbf{g}(\mathbf{x}, t) = 0, \quad (5.20)$$

$$\frac{\partial}{\partial t} g_i(\mathbf{x}, t) + V_i(\mathbf{x}, t) + \mathcal{F}_i(\mathbf{x}, t) = \theta_i(\mathbf{x}, t), \quad (5.21)$$

where we have defined $V_i = \langle \hat{V}_i \rangle$, $\mathcal{F}_i = \langle \hat{\mathcal{F}}_i \rangle$ and $\theta_i = \langle \hat{\theta}_i(\mathbf{x}, t) \rangle$ respectively as the local equilibrium averages of the reversible, irreversible, and fluctuating parts of the equation (5.9). The macroscopic mass density equation (5.20) is the usual continuity equation signifying the particle number conservation of the system. The correlation of noise $\theta(\mathbf{x}, t)$ in Eq. (5.21) is obtained by averaging Eq. (5.13)

5.2 Coarse-graining microscopic equations

over the same local equilibrium distribution,

$$\langle \theta_i(\mathbf{x}, t) \theta_j(\mathbf{x}', t') \rangle_{\text{F}} = \Gamma_0 \rho(\mathbf{x}') \delta_{ij} \delta(\mathbf{x} - \mathbf{x}') \delta(t - t'). \quad (5.22)$$

Explicit expressions for the averages $\langle \hat{V}_i \rangle$ and $\langle \hat{\mathcal{F}}_i \rangle$ will be obtained in the following sections and detailed calculation will be shown in the appendix.

5.2.1 Averaging reversible part

In order to obtain the coarse-grained form of the reversible part, we focus on the the second term \hat{V}_i on the LHS of Eq. (5.9). Its explicit expression is given by Eq. (5.10) which shows that it has the sum of contribution from two terms. The first term is quadratic in momentum \mathbf{p}_α and the second one is the interaction energy term. The average of first term gives rise to the standard convective nonlinear term in the velocity field \mathbf{v} and the average of the second term is obtained in terms of spatial derivative of the local chemical potential $\mu(\mathbf{x})$. Therefore, the local equilibrium average of \hat{V}_i is obtained as

$$V_i = \nabla_j \left[\frac{g_i(\mathbf{x}) g_j(\mathbf{x})}{\rho(\mathbf{x})} \right] + \rho(\mathbf{x}) \nabla_i \mu(\mathbf{x}). \quad (5.23)$$

5.2.2 Averaging irreversible part

Our next step follows the averaging of dissipative or the frictional term $\hat{\mathcal{F}}_i$ on the LHS of Eq. (5.9). $\hat{\mathcal{F}}_i$ is decomposed into two parts as

$$\hat{\mathcal{F}}_i(\mathbf{x}, t) = \hat{\mathcal{F}}_s^i(\mathbf{x}, t) + \hat{\mathcal{F}}_c^i(\mathbf{x}, t), \quad (5.24)$$

where the quantity $\hat{\mathcal{F}}_s^i$ represents the diagonal part or self-part defined for $\alpha = \nu$ and $\hat{\mathcal{F}}_c^i$ which is defined for $\alpha \neq \nu$ is the off-diagonal part or collective part. For

5.2 Coarse-graining microscopic equations

an isotropic system, the frictional coefficient $\zeta_{\alpha\nu}^{ij}(\mathbf{p}_\nu)$ in Eq. (5.11) is decomposed in the following form

$$\zeta_{\alpha\nu}^{ij}(\mathbf{p}_\nu) = \delta_{ij} \left[\delta_{\alpha\nu} \zeta_0(\mathbf{p}_\alpha) + (1 - \delta_{\alpha\nu}) \tilde{\zeta}_{\alpha\nu}(\mathbf{p}_\nu) \right]. \quad (5.25)$$

Next, we will assume that the total drag of a particular particle α on all of its neighboring particles ν becomes zero, i.e., $\sum_\nu \tilde{\zeta}_{\nu\alpha} = 0$. Having the above form (5.25) for $\zeta_{\alpha\nu}^{ij}(\mathbf{p}_\nu)$, the diagonal part $\hat{\mathcal{F}}_s^i$ is obtained as

$$\hat{\mathcal{F}}_s^i = \sum_\alpha \zeta_0(\mathbf{p}_\alpha) p_\alpha^i \delta(\mathbf{x} - \mathbf{x}_\alpha), \quad (5.26)$$

and the nondiagonal part $\hat{\mathcal{F}}_c^i$ is obtained in terms of gradient expansion as

$$\hat{\mathcal{F}}_c^i = \sum_{\alpha,\nu} \left[\tilde{\zeta}_{\alpha\nu}(\mathbf{p}_\nu) x_{\nu\alpha}^l \nabla_l + \frac{1}{2} \tilde{\zeta}_{\alpha\nu}(\mathbf{p}_\nu) x_{\nu\alpha}^k x_{\nu\alpha}^l \nabla_k \nabla_l + \dots \right] p_\nu^i \delta(\mathbf{x} - \mathbf{x}_\nu). \quad (5.27)$$

To proceed further, we need to obtain the momentum dependence of the frictional coefficients ζ_0 and $\tilde{\zeta}_{\alpha\nu}$ appearing on the RHS of Eq. (5.25). The dynamical nature of the active particles considered here allows us to choose these coefficients as momentum dependent (Yadav & Das, 2018). We consider their dependence on momentum up to quadratic order given as

$$\zeta_0(\mathbf{p}_\alpha) = \Delta_0 a_0 - b_{ln} p_\alpha^l p_\alpha^n, \quad (5.28)$$

$$\frac{1}{2} \tilde{\zeta}_{\alpha\nu}(\mathbf{p}_\nu) = \Delta_0 A_{\alpha\nu} - B_{\alpha\nu}^{ln} p_\nu^l p_\nu^n, \quad (5.29)$$

where the factor Δ_0 is defined by $\langle p_\alpha^i p_\alpha^j \rangle = \Delta_0 \delta_{ij}$. The set of phenomenological parameters, $\{a_0, b_{ln}\}$ introduced in Eq. (5.28) for the quantity $\zeta_0(\mathbf{p}_\alpha)$ are assumed to be independent of the particle label α for the isotropic system. The set of parameters $\{A_{\alpha\nu}, B_{\alpha\nu}^{ln}\}$ (for $\alpha \neq \nu$) introduced for the two body term $\tilde{\zeta}_{\alpha\nu}(\mathbf{p}_\nu)$

5.2 Coarse-graining microscopic equations

will depend only on the distance r (let) between two points for an isotropic translational invariant system. In Eqs. (5.28) and (5.29), we have ignored the linear term in momentum \mathbf{p} to preserve the $\mathbf{p}, -\mathbf{p}$ symmetry. We now focus on the averaging of the self-part $\hat{\mathcal{F}}_s^i$ defined in Eq. (5.26). Using the relation (5.28) for $\zeta_0(\mathbf{p}_\alpha)$, the self-part $\hat{\mathcal{F}}_s^i$ is obtained as

$$\hat{\mathcal{F}}_s^i = \sum_{\alpha} (\Delta_0 a_0 - b_{ln} p_{\alpha}^l p_{\alpha}^n) p_{\alpha}^i \delta(\mathbf{x} - \mathbf{x}_{\alpha}). \quad (5.30)$$

To obtain the local equilibrium average of the above expression, we first transform the momentum and position coordinates to the primed frame using the transformation rules (5.16) and then average it over distribution function (5.19). Since the distribution function is symmetric in momentum \mathbf{p} , therefore, the odd terms in momentum will vanish on averaging. After averaging, the coarse-grained expression for $\hat{\mathcal{F}}_s^i$ is obtained as

$$\mathcal{F}_s^i = \Delta_0 \tilde{a}_{ik} \rho(\mathbf{x}) v_k(\mathbf{x}) - m^2 b_{ln} v_l v_n \rho(\mathbf{x}) v_i(\mathbf{x}), \quad (5.31)$$

with $\tilde{a}_{ik} = (a_0 - b_{ll}) \delta_{ik} - 2b_{ik}$. For the isotropic system we can write $b_{ik} = \delta_{ik} b_0$, and the average \mathcal{F}_s^i takes the simple form,

$$\mathcal{F}_s^i = \{ \alpha_0 - \beta_0 |\mathbf{v}(\mathbf{x}, t)|^2 \} g_i(\mathbf{x}, t). \quad (5.32)$$

The parameters α_0 and β_0 are obtained as,

$$\alpha_0 = \Delta_0 \{ a_0 - (d+2)b_0 \}, \quad (5.33)$$

$$\beta_0 = m^2 b_0, \quad (5.34)$$

where d is the dimensionality of the space.

5.2 Coarse-graining microscopic equations

Next, we focus on the averaging of the off-diagonal term $\hat{\mathcal{F}}_c^i$, defined in Eq. (5.27), which is the many body part of the frictional coefficient $\hat{\mathcal{F}}_i$. The nondiagonal part $\hat{\mathcal{F}}_c^i$ is expressed in terms of gradient expansion up to second order in Eq. (5.27). The term linear in $x_{\nu\alpha}$ on the RHS of Eq. (5.27) will not contribute on averaging since due to the isotropic environment around each particle different contributions cancel out. Now using the relation (5.29), $\hat{\mathcal{F}}_c^i$ is obtained as

$$\hat{\mathcal{F}}_c^i = \nabla_k \nabla_l \sum_{\alpha\nu} \left[\Delta_0 A_{\alpha\nu} - B_{\alpha\nu}^{ln} p_\nu^l p_\nu^n \right] x_{\nu\alpha}^k x_{\nu\alpha}^l p_\nu^i \delta(\mathbf{x} - \mathbf{x}_\nu). \quad (5.35)$$

To average the above expression, we again transform the phase-space coordinates to the co-moving frame by applying the transformation rules (5.16) and then integrate out the momentum coordinates with respect to the distribution function (5.19). Further, to integrate out the position coordinates we need to evaluate the double summation over the configurational coordinates $\{\mathbf{x}_\alpha, \mathbf{x}_\nu\}$. This sum is performed in two step. In a first step, we sum over the difference $(\mathbf{x}_\alpha - \mathbf{x}_\nu)$ while holding the index ν fixed. Then, we use the translational invariance to make the sum independent of \mathbf{x}_ν and perform the summation on ν index separately. Now the average \mathcal{F}_c^i can be expressed in terms of tensors of rank two and four corresponding to the first and second terms on the RHS of Eq. (5.35). For the isotropic system, we obtain the following expression for the above argument

$$\left\langle \sum_{\alpha\nu} A_{\alpha\nu} x_{\nu\alpha}^i x_{\nu\alpha}^j \right\rangle_c = A_0 \delta_{ij}, \quad (5.36)$$

$$\left\langle \sum_{\alpha\nu} B_{\alpha\nu}^{ij} x_{\nu\alpha}^k x_{\nu\alpha}^l \right\rangle_c = B_0 \delta_{ij} \delta_{kl} + \frac{B'_0}{2} (\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}), \quad (5.37)$$

where the parameters A_0 , B_0 and B'_0 are the phenomenological constants related to the equal time correlation function of the system. They are evaluated using standard procedure for a particular model choice (Das & Dufty, 1992). The sub-

5.2 Coarse-graining microscopic equations

script c on the angular brackets denotes the integration with respect to position coordinates only while momentum coordinates are already integrated out. Now using the relations (5.36) and (5.37), average \mathcal{F}_c^i is obtained as

$$-\mathcal{F}_c^i = D_L \nabla^2 g_i + D_1 \nabla_i \nabla \cdot \mathbf{g} + D_2 \nabla^2 [|\mathbf{v}|^2 g_i] + D_2' \nabla_k \nabla_l [v_k v_l g_i], \quad (5.38)$$

where the dissipative coefficients, denoted by $D_{L,1,2}$, and D_2' , on the RHS of the above equation are obtained in terms of the phenomenological constants A_0 , B_0 , and B_0' and are explicitly shown in the Appendix. The cubic nonlinearity in velocity field $\mathbf{v}(\mathbf{x}, t)$ coupled with $\mathbf{g}(\mathbf{x}, t)$ on the RHS of Eq. (5.38) arises due to the quadratic dependence of momentum of the frictional coefficient.

5.2.3 Hydrodynamic equations

Using the relations (5.23), (5.32), and (5.38) for the averages V_i , \mathcal{F}_s^i , and \mathcal{F}_c^i respectively, we obtain the hydrodynamic equation for momentum density field as

$$\frac{\partial g_i}{\partial t} + \nabla_j \left[\frac{g_i g_j}{\rho} \right] + \rho \nabla_i \mu + \{ \alpha_0 - \beta_0 |\mathbf{v}|^2 \} g_i + L_{ij} g_j + \tilde{L}_{kl} [v_k v_l g_i] = \theta_i, \quad (5.39)$$

where dissipative matrices L_{ij} and \tilde{L}_{kl} in the above equation are obtained as

$$L_{ij} = D_L \delta_{ij} \nabla^2 + D_1 \nabla_i \nabla_j \quad \text{and} \quad \tilde{L}_{ij} = D_2 \delta_{ij} \nabla^2 + D_2' \nabla_i \nabla_j, \quad (5.40)$$

and the chemical potential $\mu(\mathbf{x})$ on the LHS of Eq. (5.39) is expressed in terms of the power series of the density fluctuations from its mean value ρ_0 as (Das, 2011)

$$\mu(\mathbf{x}) = \sum_{n=0}^{\infty} \sigma_n (\rho - \rho_0)^n, \quad (5.41)$$

with σ_n as the coefficient of expansion. Now using the nonlinear relation $\mathbf{g} = \rho\mathbf{v}$ and the continuity equation Eq. (5.20), Eq. (5.39) is obtained in terms of velocity field $\mathbf{v}(\mathbf{x}, t)$

$$\begin{aligned} \frac{\partial v_i}{\partial t} + \mathbf{v} \cdot \nabla v_i = & -\nabla_i \mu - \{\alpha_0 - \beta_0 |\mathbf{v}|^2\} v_i + D_L \nabla^2 v_i + D_1 \nabla_i \nabla \cdot \mathbf{v} \\ & + D_2 \nabla^2 [|\mathbf{v}|^2 v_i] + D'_2 \nabla_k \nabla_l [v_k v_l v_i] + f_i, \end{aligned} \quad (5.42)$$

where the correlation of the noise f_i is inversely proportional to the density ρ . In obtaining Eq. (5.42) for velocity field $\mathbf{v}(\mathbf{x}, t)$, we have assumed that terms containing the factors $(\nabla\rho)/\rho$ (Das, 2011) are negligible compared to the terms which are directly proportional to $\mathbf{v}(\mathbf{x}, t)$ or $\delta\rho(\mathbf{x}, t)$. Eq. (5.42) with the continuity equation (5.20) has the same form as the phenomenological equations obtained by Toner and Tu in the Refs. (Toner & Tu, 1998, 1995). The second term and the nonlinear cubic velocity terms in terms of gradient square on the RHS of Eq. (5.42) are absent in the Navier-Stokes equations for normal fluids. In this sense, we can call Eq. (5.42) the generalized Navier-Stokes equation which describes the dynamics of polar active particles. By choosing the certain coefficients zero in Eq. (5.39), we can recover the hydrodynamic equation for a normal fluid.

5.3 Discussion

We have obtained the coarse-grained equations of hydrodynamics for the active particles starting from the microscopic Brownian dynamics model. There are previous approaches to the microscopic derivations of hydrodynamic equations for active systems. Mainly, those are based on the Boltzmann and kinetic theory approaches (Ihle, 2016, 2011; Peshkov *et al.*, 2012a, 2012b). Authors have obtained deterministic hydrodynamic equations applicable in two dimensions. The starting point for our model is the microscopic Langevin equation with additive

noise. We have assumed that the drag or the frictional force between two elements of the flock is controlled by their respective velocity or momentum up to a characteristic length of the flock. This point plays the basic role in obtaining the coarse-grained hydrodynamic equations. The macroscopic hydrodynamic equations contain a noise term and are not restricted to two dimensions. The noise term is essential for the dynamic renormalization group analysis of the equation. The correlation of the noise depends on the density ρ , and therefore the noise has multiplicative nature. The numerical simulations on flocks performed by many authors showed that the dynamics and order-disorder transitions are mainly controlled by noise and density (Aldana *et al.*, 2007; Chaté *et al.*, 2008; Grégoire & Chaté, 2004; Vicsek *et al.*, 1995). But these numerical analyses still lacking supports from analytical approaches. The analytical form of the multiplicative noise obtained here will provide useful input to investigate the nature of phase transitions in flocks. The $1/\rho$ dependence of the correlation of noise f_i in Eq. (5.42) indicates that on increasing density the correlation will decrease. Therefore, the density-dependent multiplicative noise can control the dynamical transitions in the flock. The dissipative coefficients on the RHS of Eq. (5.42) are obtained in terms of the phenomenological parameters of the microscopic dynamics. Below we discuss some features of the important terms of Eq. (5.42) which are responsible for the characteristic dynamical behavior of active particles.

- The second term on the RHS of Eq. (5.42), i.e., $(\alpha_0 - \beta_0|\mathbf{v}|^2)v_i$ makes the mean velocity nonzero in the steady-state situation. This term is the signature of the self-propulsion nature of the particles. This term violates momentum conservation and breaks the Galilean invariance.
- The convective nonlinear term $(\mathbf{v}\cdot\nabla)v_i$ on the LHS of Eq. (5.42) do not contain any multiplicative factor. In the Ref. (Toner & Tu, 1998), this term is changed with the multiplicative factor(s) to break the Galilean invariance.

In our model, a multiplicative factor can be generated by changing the transformation rule at the microscopic level. We will discuss this issue in Chapter 6. Toner and Tu showed that this term is responsible for stable long-range order in two dimensions. They found that the long-wavelength velocity correlation is finite. In the equilibrium XY model, this term is absent, and there is no long-range order in two dimensions following the Mermin Wagner theorem (Mermin & Wagner, 1966).

- Eq. (5.42) contains additional nonlinear terms in $O(v^3)$ which are not present in Toner-Tu equations. We are hopeful that these nonlinearities can affect the nature of phase-transitions earlier studied in the Refs. (Toner, 2012; Toner & Tu, 1998, 1995). Here we discuss the key point to proceed for the dynamic renormalization group analysis of Eq. (5.42) on the basis of earlier analysis (Forster *et al.*, 1977; Toner & Tu, 1998, 1995). To simplify the complicated Eq. (5.42), we need to identify the slow modes for which hydrodynamic equations are justified. In this process, we express fluctuations in velocity field as $\mathbf{v} = (v_0 + \delta v_{\parallel})\hat{\mathbf{x}}_{\parallel} + \mathbf{v}_{\perp}$, where v_0 denotes the mean velocity, δv_{\parallel} represents velocity fluctuations along the mean direction of the flock, and \mathbf{v}_{\perp} denotes fluctuations perpendicular to the mean direction. Velocity fluctuations in the mean direction of the flock will be fast and perpendicular to mean direction will be slow. Thus δv_{\parallel} is regarded as the fast variable and \mathbf{v}_{\perp} as the slow variable. Now we write the equation of motion (5.42) in terms of slow modes \mathbf{v}_{\perp} by ignoring the irrelevant terms. Eq. (5.42) in terms of \mathbf{v}_{\perp} contains nonlinear terms like $D_2' v_0 (\nabla_{\perp} \cdot \mathbf{v}_{\perp}) \partial_{\parallel} v_{\perp}^i$ which are not present in the analysis of the Refs. (Toner, 2012; Toner & Tu, 1998). Further analysis needed to explore if these kinds of systems have fixed point and critical exponents different than the previously known systems and to check what will be the universality class of the transition.

Appendix

Here we describe in detail the averaging of the dissipative term $\hat{\mathcal{F}}_i$ on the RHS of Eq. (5.9). The averaging process of reversible term \hat{V}_i is similar as discussed in Chapter 3 in obtaining the field-theoretic description for the passive Brownian particle system.

5.A The dissipative part

The term $\hat{\mathcal{F}}_i$ of Eq. (5.9) is written as a sum of two terms denoted by $\hat{\mathcal{F}}_s^i$ and $\hat{\mathcal{F}}_c^i$ respectively. The first term $\hat{\mathcal{F}}_s^i$ arises from the diagonal part contribution ζ_0 of the frictional coefficient $\zeta_{\alpha\nu}^{ij}$. The second term $\hat{\mathcal{F}}_c^i$ is the many-body term which arises from the nondiagonal contribution $\tilde{\zeta}_{\alpha\nu}(\mathbf{p}_\nu)$ of the frictional coefficient. $\hat{\mathcal{F}}_i$ is written as

$$\hat{\mathcal{F}}_i(\mathbf{x}, t) = \hat{\mathcal{F}}_s^i(\mathbf{x}, t) + \hat{\mathcal{F}}_c^i(\mathbf{x}, t), \quad (5.A.1)$$

with

$$\hat{\mathcal{F}}_s^i = \sum_{\alpha} (\Delta_0 a_0 - b_{lm} p_{\alpha}^l p_{\alpha}^m) p_{\alpha}^i \delta(\mathbf{x} - \mathbf{x}_{\alpha}), \quad (5.A.2)$$

and

$$\hat{\mathcal{F}}_c^i = \nabla_k \nabla_l \sum_{\alpha\nu} \left[\Delta_0 A_{\alpha\nu} - B_{\alpha\nu}^{mn} p_{\nu}^m p_{\nu}^n \right] x_{\nu\alpha}^k x_{\nu\alpha}^l p_{\nu}^i \delta(\mathbf{x} - \mathbf{x}_{\nu}). \quad (5.A.3)$$

5.A The dissipative part

First, we focus on the averaging of the $\hat{\mathcal{F}}_s^i$, defined in (5.A.2), over the local equilibrium distribution function (5.19). We transform the phase-space coordinates to the primed frame and obtain the following expression for $\hat{\mathcal{F}}_s^i$

$$\begin{aligned}
\hat{\mathcal{F}}_s^i &= \sum_{\alpha} \left[a_0 \Delta_0 - b_{lm} (p_{\alpha}^l + m \mathbf{v}_l(\mathbf{x}'_{\alpha})) (p_{\alpha}^m + m \mathbf{v}_m(\mathbf{x}'_{\alpha})) \right] \\
&\quad \times (p_{\alpha}^i + m v_i(\mathbf{x}'_{\alpha})) \delta(\mathbf{x} - \mathbf{x}_{\alpha}) \\
&= \sum_{\alpha} \left[a_0 \Delta_0 (p_{\alpha}^i + m v_i(\mathbf{x}'_{\alpha})) - b_{lm} \left(p_{\alpha}^l p_{\alpha}^m p_{\alpha}^i \right. \right. \\
&\quad \left. \left. + m p_{\alpha}^l p_{\alpha}^i v_m(\mathbf{x}'_{\alpha}) + m p_{\alpha}^l p_{\alpha}^m v_i(\mathbf{x}'_{\alpha}) + m p_{\alpha}^m p_{\alpha}^i v_l(\mathbf{x}'_{\alpha}) \right. \right. \\
&\quad \left. \left. + m^2 p_{\alpha}^i v_l(\mathbf{x}'_{\alpha}) v_m(\mathbf{x}'_{\alpha}) + m^2 p_{\alpha}^l v_m(\mathbf{x}'_{\alpha}) v_i(\mathbf{x}'_{\alpha}) \right. \right. \\
&\quad \left. \left. + m^2 p_{\alpha}^m v_l(\mathbf{x}'_{\alpha}) v_i(\mathbf{x}'_{\alpha}) + m^3 v_l(\mathbf{x}'_{\alpha}) v_m(\mathbf{x}'_{\alpha}) v_i(\mathbf{x}'_{\alpha}) \right) \right] \delta(\mathbf{x} - \mathbf{x}'_{\alpha}).
\end{aligned}$$

Using the $\{\mathbf{p}', -\mathbf{p}'\}$ symmetry of the distribution function, the average of the above expression is obtained as

$$\begin{aligned}
\mathcal{F}_s^i &= \sum_{\alpha} \left[a_0 \Delta_0 v_i(\mathbf{x}) - \Delta_0 b_{lm} \left(\delta_{li} v_m(\mathbf{x}) + \delta_{lm} v_i(\mathbf{x}) + \delta_{mi} v_l(\mathbf{x}) \right) \right. \\
&\quad \left. - m^2 b_{lm} v_l(\mathbf{x}) v_m(\mathbf{x}) v_i(\mathbf{x}) \right] m \delta(\mathbf{x} - \mathbf{x}'_{\alpha}) \\
&= \Delta_0 [(a_0 - b_{ll}) \delta_{ik} - 2b_{ik}] \rho(\mathbf{x}) v_k(\mathbf{x}) - m^2 b_{lm} v_l v_m \rho(\mathbf{x}) v_i(\mathbf{x}). \quad (5.A.4)
\end{aligned}$$

For the isotropic system, we write the matrix $b_{ij} = \delta_{ij} b_0$ and obtain the above expression as

$$\mathcal{F}_s^i = \{\alpha_0 - \beta_0 |\mathbf{v}(\mathbf{x}, t)|^2\} g_i(\mathbf{x}, t), \quad (5.A.5)$$

where the constants α_0 and β_0 are obtained in terms of the phenomenological constants a_0 and b_0 as

$$\alpha_0 = \Delta_0 (a_0 - (d+2)b_0), \quad (5.A.6)$$

$$\beta_0 = m^2 b_0. \quad (5.A.7)$$

Further, we focus on the averaging of the off-diagonal or collective part $\hat{\mathcal{F}}_c^i$ of the dissipative term $\hat{\mathcal{F}}_i$. Since the off-diagonal part involves the many-body terms, its averaging is more complex than the self part $\hat{\mathcal{F}}_s^i$. First, we transform the phase-space variables of $\hat{\mathcal{F}}_c^i$ to the co-moving frame and then integrate out the momentum coordinates

$$\begin{aligned}
 \mathcal{F}_c^i &= \nabla_k \nabla_l \left\langle \sum_{\alpha\nu} [\Delta_0 A_{\alpha\nu} - B_{\alpha\nu}^{mn} (p'_\nu{}^m + m\mathbf{v}_m(\mathbf{x}'_\nu))(p'_\nu{}^n + m\mathbf{v}_n(\mathbf{x}'_\nu))] \right. \\
 &\quad \left. \times x_{\nu\alpha}^k x_{\nu\alpha}^l (p'_\nu{}^i + mv_i(\mathbf{x}'_\nu)) \delta(\mathbf{x} - \mathbf{x}_\nu) \right\rangle \\
 &= \nabla_k \nabla_l \left\langle \sum_{\alpha\nu} \left[\Delta_0 A_{\alpha\nu} v_i(\mathbf{x}_\nu) - B_{\alpha\nu}^{mn} \left\{ \Delta_0 (\delta_{mn} v_i(\mathbf{x}_\nu) + \delta_{im} v_n(\mathbf{x}_\nu) \right. \right. \right. \\
 &\quad \left. \left. \left. + \delta_{in} v_m(\mathbf{x}_\nu) \right) + m^2 v_m(\mathbf{x}_\nu) v_n(\mathbf{x}_\nu) v_i(\mathbf{x}_\nu) \right\} \right] \\
 &\quad \left. \times m \delta(\mathbf{x} - \mathbf{x}_\nu) x_{\nu\alpha}^k x_{\nu\alpha}^l \right\rangle_C, \tag{5.A.8}
 \end{aligned}$$

where subscript C on the angular bracket denotes the integration with respect to the position coordinates only while the momentum variables are already integrated out. Next, we perform the double summation over configurational coordinates $\{\mathbf{x}_\alpha, \mathbf{x}_\nu\}$ on the RHS of the above equation. First, we make the ν index fix at origin and sum over all values of the the difference vector $(\mathbf{x}_\alpha - \mathbf{x}_\nu)$ by using the translational invariance to make the sum independent of the particle index ν . The ν index is summed separately.

$$\begin{aligned}
 \mathcal{F}_c^i &= \nabla_k \nabla_l \left\langle \Delta_0 \left\{ \sum_{\alpha\nu} A_{\alpha\nu} x_{\nu\alpha}^k x_{\nu\alpha}^l \right\} \hat{\rho}(\mathbf{x}) v_i(\mathbf{x}) - \left\{ \sum_{\alpha\nu} B_{\alpha\nu}^{mn} x_{\nu\alpha}^k x_{\nu\alpha}^l \right\} \right. \\
 &\quad \times \left[\Delta_0 (\delta_{mn} v_i(\mathbf{x}) + \delta_{im} v_n(\mathbf{x}) + \delta_{in} v_m(\mathbf{x})) \right. \\
 &\quad \left. \left. + m^2 v_m(\mathbf{x}) v_n(\mathbf{x}) v_i(\mathbf{x}) \right] \hat{\rho}(\mathbf{x}) \right\rangle_C. \tag{5.A.9}
 \end{aligned}$$

5.A The dissipative part

Now we focus on the quantities within the curly brackets on the RHS of Eq. (5.A.9). They are the summations of the functions which depend on the distance between neighboring particles α , and ν , and are summed for all pairs. Using the isotropy, we approximate their local equilibrium average in terms of the parameters A_0 and $\{B_0, B'_0\}$ as

$$\left\langle \sum_{\alpha\nu} A_{\alpha\nu} x_{\nu\alpha}^k x_{\nu\alpha}^l \right\rangle_C = A_0 \delta_{kl}, \quad (5.A.10)$$

$$\left\langle \sum_{\alpha\nu} B_{\alpha\nu}^{pn} x_{\nu\alpha}^k x_{\nu\alpha}^l \right\rangle_C = B_0 \delta_{pn} \delta_{kl} + \frac{1}{2} B'_0 (\delta_{pk} \delta_{nl} + \delta_{pl} \delta_{nk}). \quad (5.A.11)$$

Putting back the values of above relations in Eq. (5.A.9), we obtain the local equilibrium average of $\hat{\mathcal{F}}_c^i$ given by

$$-\mathcal{F}_c^i = D_L \nabla^2 g_i + D_1 \nabla_i \nabla \cdot \mathbf{g} + D_2 \nabla^2 [|\mathbf{v}|^2 g_i] + D'_2 \nabla_k \nabla_l [v_k v_l g_i], \quad (5.A.12)$$

where the dissipative coefficients on the RHS of above equation are obtained in terms of the three phenomenological constants, A_0 , B_0 , and B'_0 as

$$D_L = \Delta_0 [(d+2)B_0 + B'_0 - A_0] \quad (5.A.13)$$

$$D_1 = 2\Delta_0 B'_0, \quad D_2 = B_0 m^2, \quad D'_2 = B'_0 m^2. \quad (5.A.14)$$

Chapter 6

Implications of the field-theoretic equations

In Chapter 2, we have discussed the hydrodynamic equations corresponding to the conservation of mass, momentum and energy for a normal fluid. They are the conventional Navier-Stokes equations (NSE) have rotational and translational invariance in space and time. NSE for normal fluid remain invariant when we transform the equations of motion from the rest frame to a moving coordinate frame (moving with constant velocity). The hydrodynamic equations for dry active systems of polar particles (Toner & Tu, 1998, 1995), which are the more generalized form of the historical NSE, lack in symmetries and conservation laws. In Chapter 5, we have obtained a coarse-grained description for such type of particles. In the first section of this chapter, we will discuss the Galilean invariance violation of these equations, and in the subsequent section, we analyze the signature of entropy production in the model.

6.1 Breaking of Galilean invariance

The equations of motion for polar active particles violate momentum conservation due to the friction over static medium or substrate on which particles move. Thus, the equations of motion postulated for the dynamical description of these type of particles are written in such a manner to break Galilean invariance. The convective terms in Ref. (Toner & Tu, 1998) are multiplied by phenomenological parameter to break Galilean invariance. In Chapter 5, starting from the microscopic dynamics we have obtained the time evolution equations corresponding to mass density field $\rho(\mathbf{x}, t)$ and velocity field $\mathbf{v}(\mathbf{x}, t)$ for the active particle system. The convective term $(\mathbf{v} \cdot \nabla)\mathbf{v}$ in our velocity field equation is not changed by any multiplicative factor. A factor can be generated in this term by changing the transformation rule at microscopic level. We consider the following transformation relation between the laboratory rest frame and the moving frame (denoted by prime)

$$\mathbf{p}_\alpha = \mathbf{p}'_\alpha + \lambda m \mathbf{v}(\mathbf{x}'_\alpha), \quad \text{and} \quad \mathbf{x}_\alpha = \mathbf{x}'_\alpha, \quad (6.1)$$

where λ is a phenomenological constant. To obtain coarse-grained equations, we follow the same process as done in Chapter 5. We obtain time evolution equation for $\hat{\rho}$ and $\hat{\mathbf{g}}$ corresponding to the microscopic Eq. (5.3) (defined in Chapter 5) for the momentum of the α -th particle. Then we average these equations over local equilibrium ensemble to obtain the macroscopic equation.

Having the transformation rule (6.1), the relations of microscopic mass density and momentum in the two frames are obtained as

$$\hat{\rho}(\mathbf{x}) = \hat{\rho}'(\mathbf{x}), \quad (6.2)$$

$$\hat{\mathbf{g}}(\mathbf{x}) = \hat{\mathbf{g}}'(\mathbf{x}) + \lambda \hat{\rho}'(\mathbf{x}) \mathbf{v}(\mathbf{x}). \quad (6.3)$$

6.1 Breaking of Galilean invariance

Local equilibrium averages of Eqs. (6.2) and (6.3) over the distribution function (5.19) are given by

$$\langle \hat{\rho}(\mathbf{x}) \rangle_{le} = \rho(\mathbf{x}), \quad (6.4)$$

$$\langle \hat{\mathbf{g}}(\mathbf{x}) \rangle_{le} = \mathbf{g}(\mathbf{x}) = \lambda \rho(\mathbf{x}) \mathbf{v}(\mathbf{x}). \quad (6.5)$$

Time evolution equation of macroscopic mass density equation is obtained as

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{g} = 0. \quad (6.6)$$

In terms of \mathbf{v} field we can write

$$\frac{\partial \rho}{\partial t} + \lambda \nabla \cdot \mathbf{v} = 0. \quad (6.7)$$

Local equilibrium average of the self part is obtained by the relation

$$\mathcal{F}_s^i = \{ \alpha_0 - \lambda^2 \beta_0 |\mathbf{v}(\mathbf{x}, t)|^2 \} g_i(\mathbf{x}, t), \quad (6.8)$$

and the off-diagonal part is obtained as

$$-\mathcal{F}_c^i = D_L \nabla^2 g_i + D_1 \nabla_i \nabla \cdot \mathbf{g} + \lambda^2 D_2 \nabla^2 [|\mathbf{v}|^2 g_i] + \lambda^2 D'_2 \nabla_k \nabla_l [v_k v_l g_i]. \quad (6.9)$$

where the coefficients α_0 , β_0 are defined in Eqs. (5.33) and (5.34), respectively. The coefficients $D_{L,1,2}$ and D'_2 are defined in Eqs. (5.A.13)-(5.A.14) in the appendix of Chapter 5. The average of reversible part has the same form as obtained in Chapter 5 in the relation (6.5) and in this case momentum density is scaled by the factor λ . Using the above results, the momentum density field equation is

obtained as

$$\frac{\partial g_i}{\partial t} + \nabla_j \left[\frac{g_i g_j}{\rho} \right] + \rho \nabla_i \mu + \{ \alpha_0 - \lambda^2 \beta_0 |\mathbf{v}|^2 \} g_i + L_{ij} g_j + \lambda^2 \tilde{L}_{kl} [v_k v_l g_i] = \theta_i. \quad (6.10)$$

In eqn (6.6) and (6.10), \mathbf{g} is related to \mathbf{v} by the relation $\mathbf{g} = \lambda \rho \mathbf{v}$. The matrices L_{ij} and \tilde{L}_{ij} are defined by Eq. (5.40) in Chapter 5. Using the continuity Eq. (6.6) and Eq. (6.5), we obtain the following equation for velocity field

$$\begin{aligned} \frac{\partial v_i}{\partial t} + \lambda \mathbf{v} \cdot \nabla v_i &= -\nabla_i \mu - \left\{ \alpha_0 - \tilde{\beta}_0 |\mathbf{v}|^2 \right\} v_i + D_L \nabla^2 v_i + D_1 \nabla_i \nabla \cdot \mathbf{v} \\ &\quad + \tilde{D}_2 \nabla^2 [|\mathbf{v}|^2 v_i] + \tilde{D}'_2 \nabla_k \nabla_l [v_k v_l v_i] + f_i, \end{aligned} \quad (6.11)$$

where $\tilde{\beta}_0 = \lambda^2 \beta_0$, $\tilde{D}_2 = \lambda^2 D_2$, and $\tilde{D}'_2 = \lambda^2 D'_2$. In the above equation the expansion coefficients of the chemical potential μ , defined in Eq. (5.41), are scaled by one over λ factor. In obtaining the above equation we have ignored the terms having $\nabla \rho / \rho$ factors and kept the terms which are directly proportional to \mathbf{v} or $\delta \rho$. Under the transformation of $\mathbf{v} = \mathbf{v}' + \mathbf{v}_0$ and $\mathbf{x} = \mathbf{x}' + \mathbf{v}_0 t$, the continuity equation (6.7) and the above velocity field equation do not remain same, i.e., there is violation of Galilean invariance in the system. The second term on the left-hand side of the above equation breaks the Galilean invariance due to the λ factor which is not equal to one here. The other terms on the right-hand side (RHS) of the above equations also break the Galilean invariance signifying of momentum conservation violation of the system. In traditional Navier-Stokes equation, the standard convective term $(\mathbf{v} \cdot \nabla) \mathbf{v}$ does not have a multiplicative factor and the perturbative parameter λ_0 corresponding to this nonlinearity do not renormalize under renormalization group transformation (Chapter 4). This is due to the fact that graph corresponding to nonlinear contribution of λ_0 vanishes. But in the above case where λ is not equal to one, there will be nonlinear correction to this parameter. As discussed in chapter 5, we write Eqs. (6.6) and (6.11) in terms of

slow modes of the velocity fluctuations

$$\mathbf{v} = (v_0 + \delta v_{||})\hat{\mathbf{x}}_{||} + \mathbf{v}_{\perp},$$

where meaning of the symbols are the same as discussed there. Using the above decomposition and neglecting the irrelevant terms we get the following equations in terms of \mathbf{v}_{\perp}

$$\frac{\partial \delta \rho}{\partial t} + \lambda \rho_0 (\nabla_{\perp} \cdot \mathbf{v}_{\perp}) + \lambda \nabla_{\perp} \cdot (\delta \rho \mathbf{v}_{\perp}) + v_0 \lambda \partial_{||} \delta \rho = D_{\rho} \partial_{||}^2 \delta \rho, \quad (6.12)$$

$$\begin{aligned} & \partial_t \mathbf{v}_{\perp} + \lambda (\mathbf{v}_{\perp} \cdot \nabla_{\perp}) \mathbf{v}_{\perp} + \gamma \partial_{||} \mathbf{v}_{\perp} \\ &= -\nabla_{\perp} \mu + D_1 \nabla_{\perp} (\nabla_{\perp} \cdot \mathbf{v}_{\perp}) + \tilde{D}_L \nabla_{\perp}^2 \mathbf{v}_{\perp} + D_{||} \partial_{||}^2 \mathbf{v}_{\perp} \\ &+ \tilde{D}'_2 v_0 (\nabla_{\perp} \cdot \mathbf{v}_{\perp}) \partial_{||} \mathbf{v}_{\perp} + \mathbf{f}_{\perp}, \end{aligned} \quad (6.13)$$

where $\delta \rho = \rho - \rho_0$, $D_{\rho} = \sigma_1 / (2\tilde{\alpha})$, $\tilde{D}_L = D_L + v_0^2 \tilde{D}_2$, $D_{||} = D_L + v_0^2 (\tilde{D}_2 + \tilde{D}'_2)$ and $\gamma = \lambda v_0$. The definition of pressure in the above equation is the same as before. This equation has extra cubic nonlinearity in velocity, which was absent in earlier analysis, needs to be analyzed under renormalization group treatment to explore the phase behavior in the model.

6.2 Entropy production rate

In Chapter 2, we have utilized the concept of entropy production rate near equilibrium to obtain the hydrodynamic equations for simple fluid. Below we discuss in detail, how to evaluate entropy production rate for a simple fluid case which has attained a local equilibrium state. Some symbols and Meaning of the quantities used here are already defined in Chapter 2. We use Einstein summation

6.2 Entropy production rate

convention for repeated Cartesian indices. We extend this idea of entropy production rate to the continuum equations of active particles discussed in Chapter 5 to further explore the nature of dissipative coefficients of the equations. For easy access, we again define here the total entropy in local equilibrium state as

$$S = -\langle \ln f_{le}(\Gamma_N, t) \rangle. \quad (6.14)$$

Using relation (2.15) for f_{le} (defined in Chapter 2), $\ln f_{le}$ is obtained as

$$\ln f_{le} = -\ln Q_l - \int d\mathbf{x} \sum_{\{\psi\}} w_\psi(\mathbf{x}, t) \hat{\psi}(\mathbf{x}), \quad (6.15)$$

which gives entropy S as

$$S = \ln Q_l + \int d\mathbf{x} \sum_{\{\psi\}} w_\psi(\mathbf{x}, t) \psi(\mathbf{x}, t). \quad (6.16)$$

The entropy density $s(\mathbf{x}, t)$, from the above relation is obtained as

$$s(\mathbf{x}, t) = V^{-1} \ln Q_l + \sum_{\{\psi\}} w_\psi(\mathbf{x}, t) \psi(\mathbf{x}, t). \quad (6.17)$$

Next, we obtain the time derivative of $S(\mathbf{x}, t)$ as

$$\frac{\partial S}{\partial t} = \int d\mathbf{x} \sum_{\{\psi\}} w_\psi(\mathbf{x}, t) \frac{\partial \psi(\mathbf{x}, t)}{\partial t}. \quad (6.18)$$

Now using the relation (2.21), above relation is obtained as

$$\begin{aligned} \frac{\partial S}{\partial t} &= - \int d\mathbf{x} \sum_{\{\psi\}} w_\psi(\mathbf{x}, t) \nabla \cdot \mathbf{J}_\psi \\ &= \int d\mathbf{x} \sum_{\{\psi\}} \left\{ - \nabla \cdot (w_\psi(\mathbf{x}, t) \mathbf{J}_\psi) + \mathbf{J}_\psi \cdot \nabla w_\psi(\mathbf{x}, t) \right\}. \end{aligned} \quad (6.19)$$

6.2 Entropy production rate

For a set of densities $\hat{\psi}(\mathbf{x}, t) = \{\hat{n}, \hat{\mathbf{g}}, \hat{e}\}$ and corresponding $w_\psi \equiv \{-\beta(\mu - \frac{1}{2}mv^2), -\beta\mathbf{v}, \beta\}$, and the respective currents \mathbf{J}_ψ , we obtain

$$\begin{aligned}
\sum_{\{\psi\}} w_\psi J_\psi^i &= -\beta\left(\mu - \frac{1}{2}mv^2\right)nv_i - \beta v_j(P\delta_{ij} + \rho v_i v_j) + \beta(e + P)v_i \\
&= \left[\beta e - \beta v_j v_i - \beta\left(\mu - \frac{1}{2}mv^2\right)n\right]v_i \\
&= v_i \sum_{\{\psi\}} w_\psi(\mathbf{x}, t)\psi(\mathbf{x}, t).
\end{aligned} \tag{6.20}$$

Now using the relation (6.17) and (6.20), Eq. (6.19) is obtained as

$$\int d\mathbf{x} \left[\frac{\partial s}{\partial t} + \nabla \cdot (s\mathbf{v}) \right] = \int d\mathbf{x} \nabla \cdot (V^{-1} \ln Q_t \mathbf{v}) + \int d\mathbf{x} \sum_{\{\psi\}} \mathbf{J}_\psi \cdot \nabla w_\psi(\mathbf{x}, t). \tag{6.21}$$

The second term on the RHS of above equation is obtained as

$$\begin{aligned}
\sum_{\{\psi\}} \mathbf{J}_\psi \cdot \nabla w_\psi(\mathbf{x}, t) &= \left[-\beta n v_i \nabla_i \left(\mu - \frac{1}{2}mv^2 \right) - (P\delta_{ij} + \rho v_i v_j) \nabla_i (\beta v_j) \right] \\
&\quad + (e + P)v_i \nabla_i \beta \\
&= \beta \mathbf{v} \cdot [\nabla P - s \nabla T - n \nabla \mu] - \nabla \cdot (\beta P \mathbf{v}).
\end{aligned} \tag{6.22}$$

Analogous to the equilibrium case, the local quantities $P(\mathbf{x}, t)$, $T(\mathbf{x}, t)$, $\mu(\mathbf{x}, t)$, and $\mathbf{v}(\mathbf{x}, t)$, in the hydrodynamic regime, are the functionals of the conserved densities of mass, momentum, and energy. This allows us to use the Gibbs-Duhem relation $VdP - SdT = Nd\mu$ in the above equation. This makes the first term on the RHS of the above equation zero. We define the entropy production rate for the system as

$$R_{ep} = T \frac{d}{dt} \int d\mathbf{x} s(\mathbf{x}, t). \tag{6.23}$$

Now using relation (6.22) we obtain,

$$\begin{aligned}
 R_{ep} &= \beta^{-1} \int d\mathbf{x} \left[\frac{\partial s}{\partial t} + \nabla \cdot (s\mathbf{v}) \right] \\
 &= \beta^{-1} \int d\mathbf{x} \nabla \cdot (V^{-1}\Omega\mathbf{v}),
 \end{aligned} \tag{6.24}$$

with $\Omega = \ln Q_t - \beta PV$. The volume integral on the RHS of the above equation can be expressed as surface integral which is assumed to be zero in the absence of external perturbation. Therefore, for the reversible dynamics we obtain the following relation for the entropy density

$$\frac{\partial s}{\partial t} + \nabla \cdot \mathbf{J}_s = 0, \tag{6.25}$$

where the entropy current $\mathbf{J}_s = s\mathbf{v}$. For irreversible dynamics, the fluxes \mathbf{J}_ψ contain dissipative part. The flux corresponding to continuity equation for mass density, as discussed in Chapter 2, does not have any dissipative part. Now we evaluate the R_{sp} corresponding to the hydrodynamics equation for flocking obtained in chapter 5. We write it in the following compact notation

$$\frac{\partial g_i}{\partial t} + \nabla_j \tilde{\sigma}_{ij} = \tilde{f}_i + \theta_i. \tag{6.26}$$

The quantity $\tilde{\sigma}_{ij}$ is written as

$$\tilde{\sigma}_{ij} = \sigma_{ij}^R + \sigma_{ij}^D + \sigma_{ij}^{D'}, \tag{6.27}$$

where

$$\sigma_{ij}^R = \rho v_i v_j + \delta_{ij} P, \quad (6.28)$$

$$\sigma_{ij}^D = -\frac{D_L}{2} [\nabla_j g_i + \nabla_i g_j] - D_1 \delta_{ij} (\nabla \cdot \mathbf{g}), \quad (6.29)$$

$$\sigma_{ij}^{D'} = -\frac{D_2}{2} [\nabla_j (\mathbf{v}^2 g_i) + \nabla_i (\mathbf{v}^2 g_j)] - D_2' \nabla_l (v_l v_j g_i). \quad (6.30)$$

The third term f_i on the left-hand side of Eq. (6.26) is defined as

$$\tilde{f}_i = \{\alpha_0 - \beta_0 \mathbf{v}^2\} g_i. \quad (6.31)$$

Using Eq. (6.18) corresponding to reversible mass density equation, energy density equation (2.39) and momentum density equation (6.26), we can write

$$\begin{aligned} \frac{\partial S}{\partial t} &= \int d\mathbf{x} \sum_{\{\psi\}} w_\psi(\mathbf{x}, t) \frac{\partial \psi(\mathbf{x}, t)}{\partial t} \\ &= - \int d\mathbf{x} \left[-\beta \left(\mu - \frac{1}{2} m v^2 \right) \nabla \cdot \mathbf{g} - \beta v_i \nabla_j \sigma_{ij}^R + \beta \nabla \cdot \mathbf{j}_e^R \right] \\ &\quad - \int d\mathbf{x} \left[-\beta v_i \nabla_j (\sigma_{ij}^D + \sigma_{ij}^{D'}) \right] - \int d\mathbf{x} \beta v_i \tilde{f}_i - \int d\mathbf{x} \beta v_i \theta_i. \end{aligned} \quad (6.32)$$

The first integral in the above equation corresponds to the reversible contribution and is zero. The Entropy production rate, at constant temperature, due to irreversible parts of momentum density equation is given by

$$\begin{aligned} R_{ep} &= \int d\mathbf{x} \left[\frac{\partial s}{\partial t} + \nabla \cdot \mathbf{J}_s \right] \\ &= \int d\mathbf{x} v_i \left[\nabla_j (\sigma_{ij}^D + \sigma_{ij}^{D'}) - \tilde{f}_i - \theta_i \right]. \end{aligned} \quad (6.33)$$

6.2 Entropy production rate

We consider the average of the above relation over noise to obtain the constraint in dissipative coefficients. Now as a first approximation we take

$$R_{ep} = \int d\mathbf{x} v_i \left[-L_{ij}^0 v_j - \theta_i \right], \quad (6.34)$$

where $L_{ij}^0 = \rho[\alpha_0 - \beta_0 v^2] \delta_{ij}$ is the linear dissipation coefficient at zeroth-order. we write the above relation in a noise averaged form as

$$R_{ep} = \int d\mathbf{x} \left[-\langle v_i v_j L_{ij}^0 \rangle - \langle v_i \theta_i \rangle \right], \quad (6.35)$$

where the angular bracket represents average over noise.

Further, to evaluate the average over noise in the above equation, we consider that the probability distribution for the Gaussian noise θ is given by the following expression

$$P[\theta] = \frac{1}{z_\theta} e^{-\frac{1}{4} \sum_{ij} \int_{-\infty}^{+\infty} dt \theta_i(t) (\tilde{\Gamma}^{-1})_{ij} \theta_j(t)}, \quad (6.36)$$

where $\tilde{\Gamma}_{ij} = \rho \Gamma_{ij}$. The quantity z_θ is the normalization constant which ensures

$$\int P[\theta] D(\theta) = 1, \quad (6.37)$$

where $D(\theta) = \prod_i d\theta_i$. Now average of a quantity $A[\psi(\theta)]$, where ψ represents hydrodynamic fields, over noise is defined by

$$\langle A(\psi) \rangle = \int D(\theta) P[\theta] A[\psi(\theta)]. \quad (6.38)$$

Further, we use the above definition to obtain following relation

$$\int D(\theta) \frac{\delta}{\delta \theta_i} [P[\theta] A[\psi(\theta)]] = 0. \quad (6.39)$$

6.2 Entropy production rate

Using the above identity and distribution function (6.36), we obtain,

$$\langle A\theta_i \rangle = 2\tilde{\Gamma}_{ij} \left\langle \frac{\delta A}{\delta \theta_j} \right\rangle. \quad (6.40)$$

Next, we evaluate the average $\langle v_i \theta_i \rangle$, by using the identity $\delta g_i(t)/\delta \theta_j(t) = \frac{1}{2}\delta_{ij}$ (Appendix).

$$\langle v_i \theta_j \rangle = \Gamma_{ij} = \delta_{ij} \Gamma_0 \delta(\mathbf{x} - \mathbf{x}'). \quad (6.41)$$

To evaluate $\langle v_i v_j L_{ij} \rangle$, we take $\langle v_i v_j \rangle = \Delta_0 \delta_{ij}$, and obtain the following relation

$$\begin{aligned} \langle v_i v_j L_{ij}^0 \rangle &= \langle \rho(\alpha_0 v^2 - \beta_0 v^4) \rangle \\ &= \rho[\alpha_0 \langle v^2 \rangle - 3\beta_0 \langle v^2 \rangle^2] \\ &= \rho \Delta_0 [\alpha_0 - 3\beta_0 \Delta_0], \end{aligned} \quad (6.42)$$

where d is the dimensionality of the space. In obtaining the above relation we have assumed that at lowest order density is constant and unaffected by the averaging. Now using relations (6.35), (6.41) and (6.42) we obtain the following relation for positive entropy production rate

$$\rho \Delta_0 [\alpha_0 - 3\beta_0 \Delta_0] + \Gamma_0 d \leq 0, \quad (6.43)$$

The above relation can be written in scaled form as

$$\tilde{\Gamma}_0 \leq [3\tilde{\Delta}_0 - 1], \quad (6.44)$$

where $\tilde{\Gamma}_0 = \Gamma_0 (d/(\rho \Delta_0 \alpha_0))$ and $\tilde{\Delta}_0 = \Delta_0 (\beta_0/\alpha_0)$. This relation sets an upper limit to the noise.

Appendix

6.A Identity

Here we introduce the identity (Ma & Mazenko, 1975) which is used to evaluate the noise average in above chapter. Nonlinear Langevin equation for the dynamics of the variables $\{g_i\}$

$$\frac{\partial g_i(t)}{\partial t} = V_i[g] - L_i \frac{\partial F}{\partial g_i} + \theta_i(t), \quad (6.A.1)$$

where L_i are the transport coefficients and V_i is reversible part. Using partial integration we obtain

$$\begin{aligned} g_i(t) = & \sum_j \int_{-\infty}^{+\infty} dt' G_{ij}^0(t-t') L_i^{-1} \theta_j(t') + \sum_j \int_{-\infty}^{+\infty} dt' G_{ij}^0(t-t') h_j(t') \\ & + \sum_j \int_{-\infty}^{+\infty} dt' G_{ij}^0(t-t') N_j(t'; g), \end{aligned} \quad (6.A.2)$$

where h_j is the external field and N_j contains all nonlinear terms of equation. G_{ij}^0 is the zeroth order response function given by

$$G_{ij}^0(t-t') = \Theta(t-t') e^{-L_i(t-t')} \delta_{ij} L_i, \quad (6.A.3)$$

Now we apply chain rule of differentiation to obtain

$$\frac{\delta g_i(t)}{\delta \theta_j(t')} = L_i^{-1} G_{ij}^0(t - t') + \sum_{l,k} \int_{-\infty}^{+\infty} d\bar{t} G_{il}(t - \bar{t}) \frac{\delta N_l(\bar{t})}{\delta g_k(\bar{t})} \frac{\delta g_k(\bar{t})}{\delta \theta_j(t')} \quad (6.A.4)$$

In the second term of the above equation, all θ which appear in $g(\bar{t})$ will occur at a time less than or equal to \bar{t} , hence give rise the factor $\Theta(t - \bar{t})\Theta(\bar{t} - t')$. This term becomes zero for $t \geq \bar{t}$. Thus for $t = t'$, with the result $G_{ij}^0(t = t') = \frac{1}{2}\delta_{ij}L_i$, we obtain the relation

$$\frac{\delta g_i(t)}{\delta \theta_j(t)} = \frac{1}{2}\delta_{ij}. \quad (6.A.5)$$

Chapter 7

Summary of key issues

In this thesis, we have presented a systematic approach to obtain the coarse-grained description for the collective dynamics of polar active particles from the microscopic model of active Brownian particles. The continuum equations are obtained in terms of the coarse-grained densities and velocity fields which form the stochastic partial differential equations with multiplicative noise.

By coarse-graining the Langevin equation for the single particle dynamics, the time evolution of the velocity field $\mathbf{v}(\mathbf{x}, t)$ is obtained. The coarse-graining process is analogous to obtaining the hydrodynamics for simple fluids in local equilibrium description. The velocity field, in the local equilibrium description, is conjugate thermodynamic field to the total momentum of the system. Therefore, the analysis presented here provides the basic foundation to describe the active systems in a local equilibrium description. We have discussed the Galilean non-invariance of the hydrodynamic equations. This is directly linked to the momentum conservation violation of the model. In Chapter 1, we have discussed other approaches proposed by various authors to derive hydrodynamics from the microscopic models. Mainly, those are based on the Boltzmann and kinetic theory approaches as well as extensions of these two. But the hydrodynamic equations obtained there

are applicable for the two dimensional case and there is no noise term in the coarse-grained equations. Thus the equations cannot be analyzed along the lines of renormalization group methods which provides essential techniques to study the nature of phase transitions. In the present calculation, transport coefficients are obtained in terms of the statistical averages over an appropriate ensemble. These parameters can be expressed in terms of the equal time pair correlation functions which are averaged over different initial conditions of the flock. Below we list some of the key points

1. If the particle dynamics is reversible like in a Newtonian fluid, then irreversibility at the microscopic equations of hydrodynamics enters in a phenomenological manner through introduction of dissipative terms. In the present context microscopic dynamics is dissipative and the Brownian motion equations has dissipative and noise. Thus the difference in time scales of motion is introduced at the microscopic level. In a Newtonian dynamics case the separation in time scales and hence the justification of introducing noise is based on microscopic level conservation laws. Note that in the Brownian motion equation this time separation is simply introduced. Microscopic momentum conservation is not ensured.
2. The frictional coefficients in the microdynamic equations are not constants and are themselves momentum dependent. Their dependence is considered to be even function in momentum, and at lowest order it is taken to be in quadratic form. In general, it will depend on space also but we have considered homogeneity in space. The self part (diagonal part) of frictional coefficient is key in producing the non-gradient frictional terms $(\alpha - \beta \mathbf{v}^2)$. This term ensures the non-zero velocity in homogeneous state and also break the Galilean invariance.

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3. The values of the transport coefficients that appear in the hydrodynamic equations has constraint on their values for maintaining positive entropy production rate. Since fluctuation dissipation theorem is violated, relation between noise strength and dissipative coefficient cannot be obtained easily. We have obtained the inequality relation between the noise strength Γ_0 and transport coefficient α_0 and β_0 given as $\Gamma_0 \leq \frac{\Delta_0 \rho}{d} (3\beta_0 \Delta_0 - \alpha_0)$ setting an upper limit of noise.
 4. Breaking of Galilean invariance follows in a self-consistent manner when the same is assumed at microscopic level.
 5. The noise in the hydrodynamic equation itself is multiplicative in nature and this follows in a natural way. The fluctuation-dissipation theorem does not hold due to the nonequilibrium nature of the particles.

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