Stochastic Processes in Cell Biology II: Supplementary material

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August 20, 2024

Chapter 13
Self-organization and assembly of cellular structures

A. Mean field theory for interacting particle systems

Large systems of interacting particles arise in a wide range of applications in the natural and social sciences. For example, in physics the particles could represent electrons or ions in a plasma, molecules in passive or active fluids, or galaxies in a cosmological model. On the other hand, particles in biological applications tend to be micro-organisms such as cells or bacteria that can exhibit non-trivial aggregation phenomena such as motility-based phase separation (see Sect. 15.7). Finally, in economics or social sciences, particles typically represent individual "agents". A major challenge is how to reduce the complexity of such systems. A classical approach is to derive a macroscopic model that provides a continuous description of the dynamics in terms of global densities evolving according to non-linear partial differential equations. Such kinetic formulations date back to the foundations of statistical mechanics and the Boltzmann equation of dilute gases interacting via direct collisions. In recent years, however, much of the focus has been on the mean field limit of particles with long range or collisionless interactions. Two paradigmatic examples are interacting Brownian particles in the overdamped regime and the Kuramoto model of coupled phase oscillators (see Sect. 15.5).

The classical Dean-Kawasaki (DK) equation is a stochastic partial differential equation (SPDE) that describes fluctuations in the global density of N over-damped Brownian particles with positions $\mathbf{X}_j(t) \in \mathbb{R}^d$ at time t [21, 31]. Within the context of non-equilibrium statistical physics, the DK equation is commonly combined with dynamical density functional theory (DDFT) in order to derive hydrodynamical models of interacting particle systems [37, 4, **?**, 61]. It is an exact equation for the global density (or empirical measure) in the distributional sense, and plays an important role in the stochastic and numerical analysis of interacting particle systems [23, 32, 33, 24, 25, 27, 16]. There is also considerable mathematical interest in the rigorous stochastic analysis of the mean field limit $N \to \infty$ for overdamped Brownian particles with weak interactions, see for example Refs. [43, 29, 46, 13, 14]. In particular, if the initial positions of the N particles are independent and identically distributed, then for a wide range of systems it can be proven that ρ converges in distribution to the solution of the McKean-Vlasov (MV) equation [39]; the latter is a nonlocal nonlinear Fokker-Planck (FP) equation for the mean field density. The interacting particle system is said to satisfy the propagation of chaos property. The MV equation can also be derived directly from the DK equation by taking expectations with respect to the independent white noise processes and imposing a mean field ansatz. The MV equation is of interest in its own right, since it can support multiple stationary solutions and associated phase transitions [54, 55]. This has been explored in various configurations, including double-well confinement and Curie-Weiss (quadratic) pairwise interactions on $\mathbb{R}$ [22, 20, 45], and interacting particles on a torus [15, 11]. A well-known example of the latter is the stochastic Kuramoto model of interacting phase oscillators with sinusoidal coupling and quenched disorder due to the random distribution of natural frequencies [34, 53, 1]. The well-known continuum model for the density of phase oscillators [49, 52, 17, 18] is precisely the MV equation for the global density in the mean field limit $N \to \infty$, whose existence can be proven rigorously using propagation of chaos [19].

A.1 Weakly interacting Brownian particles and the McKean-Vlasov equation

Consider N overdamped Brownian particles in $\mathbb{R}^d$. Let $\mathbf{X}_j(t) \in \mathbb{R}^d$ denote the position of the jth particle at time t, $j = 1,\ldots,N$. We assume that the particles are subject to a common external conservative force $\mathbf{F}(\mathbf{x}) = -\boldsymbol{\nabla} V(\mathbf{x})$ and interact via a pairwise potential K. That is, the force on a particle at $\mathbf{x}$ due to a particle at $\mathbf{y}$ is $-\boldsymbol{\nabla} K(\mathbf{x}-\mathbf{y})$, where differentiation is with respect to $\mathbf{x}$. The particle positions $\mathbf{X}_j(t)$ evolve according to the SDE[1]

$$d\mathbf{X}_j(t) = -\frac{1}{\gamma}\left[\boldsymbol{\nabla} V(\mathbf{X}_j(t)) + \frac{1}{N}\sum_{k=1}^{N} \boldsymbol{\nabla} K(\mathbf{X}_j(t) - \mathbf{X}_k(t))\right]dt + \sqrt{2D}d\mathbf{W}_j(t) \quad \text{(A.1)}$$

where $\mathbf{W}_j$ is a vector of independent Wiener processes. Following the "hydrodynamic" formulation of Ref. [21], we define the global density (or empirical measure)

$$\rho(x,t) = \frac{1}{N}\sum_{j=1}^{N} \delta(\mathbf{x} - \mathbf{X}_j(t)), \quad \text{(A.2)}$$

and introduce an arbitrary smooth test function $f(\mathbf{x})$ of compact support. It follows that

$$\frac{1}{N}\sum_{j=1}^{N} f(\mathbf{X}_j(t)) = \int_{\mathbb{R}^d} \rho(\mathbf{x},t) f(\mathbf{x}) d\mathbf{x}, \quad \text{(A.3)}$$

[1] In the original formulation of Ref. [21] the interaction potential is not scaled by a factor $1/N$ and the global density is taken to be $\rho(x,t) = \sum_{j=1}^{N} \delta(\mathbf{x} - \mathbf{X}_j(t))$. It is necessary to include the factor $1/N$ in order to apply a mean field ansatz.

and

$$\left[\int_{\mathbb{R}^d} d\mathbf{x}\, f(\mathbf{x}) \frac{\partial \rho(\mathbf{x},t)}{\partial t}\right] dt = \frac{1}{N}\sum_{j=1}^{N} df(X_j(t)).$$

Using Itô's lemma (see Sect. 2.2), we find that

$$\begin{aligned}&\int_{\mathbb{R}^d} d\mathbf{x}\, f(\mathbf{x}) \frac{\partial \rho(\mathbf{x},t)}{\partial t} \qquad \text{(A.4)}\\ &= \int_{\mathbb{R}^d} d\mathbf{x} \left[\frac{\sqrt{2D}\boldsymbol{\nabla} f(\mathbf{x})}{N} \cdot \sum_{j=1}^{N} \rho_j(x,t)\boldsymbol{\xi}_j(t) + \rho(\mathbf{x},t)\left(D\boldsymbol{\nabla}^2 f(\mathbf{x}) - \boldsymbol{\nabla} f(\mathbf{x})\cdot \mathcal{V}[\mathbf{x},t,\rho]\right)\right.,\end{aligned}$$

where $\rho_j(\mathbf{x},t) = \delta(\mathbf{x} - \mathbf{X}_j(t))$, $d\mathbf{W}_j(t) = \boldsymbol{\xi}_j(t)dt$, and

$$\mathcal{V}[\mathbf{x},t,\rho] = \frac{1}{\gamma}\left[\boldsymbol{\nabla} V(\mathbf{x}) + \int_{\mathbb{R}^d} d\mathbf{y}\, \rho(\mathbf{y},t)\boldsymbol{\nabla} K(\mathbf{x}-\mathbf{y})\right]. \qquad \text{(A.5)}$$

Integrating by parts the various terms involving derivatives of f and using the fact that f is arbitrary yields the following SPDE for ρ:

$$\frac{\partial \rho(\mathbf{x},t)}{\partial t} = -\sqrt{\frac{2D}{N^2}}\sum_{j=1}^{N} \boldsymbol{\nabla}\cdot\left[\rho_j(\mathbf{x},t)\boldsymbol{\xi}_j(t)\right] + D\boldsymbol{\nabla}^2\rho(\mathbf{x},t) + \boldsymbol{\nabla}\cdot\left(\rho(\mathbf{x},t)\mathcal{V}[\mathbf{x},t,\rho]\right). \qquad \text{(A.6)}$$

As it stands, equation (A.6) is not a closed equation for ρ due to the noise terms. Following Ref. [21], we introduce the space-dependent Gaussian noise term

$$\xi(\mathbf{x},t) = -\frac{1}{N}\sum_{j=1}^{N} \boldsymbol{\nabla}\cdot\left[\rho_j(\mathbf{x},t)\boldsymbol{\xi}_j(t)\right], \qquad \text{(A.7)}$$

with zero mean and the correlation function

$$\langle \xi(\mathbf{x},t)\xi(\mathbf{y},t')\rangle = \frac{\delta(t-t')}{N^2}\sum_{j=1}^{N} \boldsymbol{\nabla}_{\mathbf{x}}\cdot\boldsymbol{\nabla}_{\mathbf{y}}\left(\rho_j(\mathbf{x},t)\rho_j(\mathbf{y},t)\right).$$

Since $\rho_j(\mathbf{x},t)\rho_j(\mathbf{y},t) = \delta(\mathbf{x}-\mathbf{y})\rho_j(\mathbf{x},t)$, it follows that

$$\langle \xi(\mathbf{x},t)\xi(\mathbf{y},t')\rangle = \frac{1}{N}\delta(t-t')\boldsymbol{\nabla}_{\mathbf{x}}\cdot\boldsymbol{\nabla}_{\mathbf{y}}\left(\delta(\mathbf{x}-\mathbf{y})\rho(\mathbf{x},t)\right).$$

Finally, we introduce the global density-dependent noise field

$$\widehat{\xi}(\mathbf{x},t) = \frac{1}{\sqrt{N}}\boldsymbol{\nabla}\cdot\left(\eta(\mathbf{x},t)\sqrt{\rho}(\mathbf{x},t)\right), \qquad \text{(A.8)}$$

where $\eta(\mathbf{x},t)$ is a global white noise field whose components satisfy

$$\langle \eta^{\sigma}(\mathbf{x},t)\eta^{\sigma'}(\mathbf{y},t')\rangle = \delta(t-t')\delta(\mathbf{x}-\mathbf{y})\delta_{\sigma,\sigma'}. \tag{A.9}$$

It can be checked that the Gaussian noises ξ and $\widehat{\xi}$ have the same correlation functions and are thus statistically identical. We thus obtain the classical DK equation [21, 31]

$$\frac{\partial \rho(\mathbf{x},t)}{\partial t} = \sqrt{\frac{2D}{N}}\boldsymbol{\nabla}\cdot\left[\sqrt{\rho(\mathbf{x},t)}\boldsymbol{\eta}(\mathbf{x},t)\right] + D\boldsymbol{\nabla}^2\rho(\mathbf{x},t) + \boldsymbol{\nabla}\cdot\bigg(\rho(\mathbf{x},t)\mathcal{V}[\mathbf{x},t,\rho]\bigg) \tag{A.10}$$

Although equation (A.10) is exact in the weak sense, it is highly singular. Moreover, averaging with respect to the Gaussian white noise processes results in a moment closure problem for the one-particle density $\langle\rho\rangle$. That is, setting $p(\mathbf{x},t) = \Big\langle \rho(\mathbf{x},t)\Big\rangle$, we have

$$\begin{aligned}\frac{\partial p(\mathbf{x},t)}{\partial t} &= D\boldsymbol{\nabla}^2 p(\mathbf{x},t) + \frac{1}{\gamma}\boldsymbol{\nabla}\cdot\bigg(p(\mathbf{x},t)\boldsymbol{\nabla}V(\mathbf{x})\bigg)\\ &\quad + \frac{1}{\gamma}\boldsymbol{\nabla}\cdot\bigg(\int_{\mathbb{R}^d}\boldsymbol{\nabla}K(\mathbf{x}-\mathbf{y})\Big\langle\rho(\mathbf{x},t)\rho(\mathbf{y},t)\Big\rangle\bigg).\end{aligned} \tag{A.11}$$

As it stands, $p(\mathbf{x},t)$ couples to the two-point correlation function, which in turn couples to the three-point correlation function etc. Therefore, we now take the thermodynamic limit $N\to\infty$ under the mean field ansatz

$$\Big\langle\rho(\mathbf{x},t)\rho(\mathbf{y},t)\Big\rangle = \Big\langle\rho(\mathbf{x},t)\Big\rangle\Big\langle\rho(\mathbf{y},t)\Big\rangle = p(\mathbf{x},t)p(\mathbf{y},t). \tag{A.12}$$

This yields the deterministic MV equation

$$\frac{\partial p(\mathbf{x},t)}{\partial t} = D\boldsymbol{\nabla}^2\phi(\mathbf{x},t) + \boldsymbol{\nabla}\cdot\bigg(p(\mathbf{x},t)\mathcal{V}[\mathbf{x},t,p]\bigg). \tag{A.13a}$$

with

$$\mathcal{V}[\mathbf{x},t,p] = \frac{1}{\gamma}\left[\boldsymbol{\nabla}V(\mathbf{x}) + \int_{\mathbb{R}^d} d\mathbf{y}\, p(\mathbf{y},t)\boldsymbol{\nabla}K(\mathbf{x}-\mathbf{y})\right]. \tag{A.13b}$$

The derivation of classical MV equation [39], and the validity of the mean field ansatz can be proven using propagation of chaos [43, 29, 46, 13, 14]. The latter is essentially a version of the law of large numbers, so that simulations for large but finite N generate macroscopic quantities that are consistent with solutions to the deterministic MV equation up to $O(1/\sqrt{N})$ errors.

A.2 Stationary solutions of the 1D McKean-Vlasov equation

A classical result in statistical physics is that for a finite system of overdamped Brownian particles subject to conservative forces, the corresponding linear Fokker-Planck (FP) equation has a unique stationary solution given by the Boltzmann distribution. More specifically, the joint probability density $p(\mathbf{x}_1,\ldots,\mathbf{x}_N,t)$ evolves according to the multivariate FP equation

$$\frac{\partial p}{\partial t} = D\sum_{j=1}^N \boldsymbol{\nabla}_j^2 p + \frac{1}{\gamma}\sum_{j=1}^N \boldsymbol{\nabla}_j\cdot(\boldsymbol{\nabla}_j U(\mathbf{x}_1,\ldots,\mathbf{x}_N)p), \tag{A.14}$$

where $\boldsymbol{\nabla}_j$ indicates differentiation with respect to $\mathbf{x}_j$, and

$$U(\mathbf{x}_1,\ldots,\mathbf{x}_N) = \sum_{j=1}^N V(\mathbf{x}_j) + \frac{1}{2N}\sum_{j,k=1}^N K(\mathbf{x}_j-\mathbf{x}_k). \tag{A.15}$$

equation (A.14) has the unique stationary solution

$$p = Z^{-1}\mathrm{e}^{-\beta U}, \quad Z = \int\left[\prod_{j=1}^N d\mathbf{x}_j\right]\mathrm{e}^{-\beta U(\mathbf{x}_1,\ldots,\mathbf{x}_N)}, \tag{A.16}$$

with $\beta = 1/(k_BT)$. (We are assuming that $Z<\infty$ for the given choice of potentials K and V.) The existence of a unique stationary density for the finite system reflects the fact that the dynamics is ergodic. However, ergodicity may break down in the thermodynamic limit $N\to\infty$, resulting in the coexistence of multiple stationary states and their associated phase transitions. This has been explored for an infinite system of interacting Brownian particles using the MV equation. (A.13) [54]. Examples include double-well confinement and Curie-Weiss (quadratic) interactions on $\mathbb{R}$ [22, 20, 45], and interacting particles on a torus [15, 11]. In the specific case of the Curie-Weiss potential $K(\mathbf{x}-\mathbf{y}) = \lambda(\mathbf{x}-\mathbf{y})^2/2$, the coupling term in the SDE (A.1) becomes $-\lambda(\mathbf{X}_j(t)-\overline{\mathbf{X}}(t))$ where $\overline{\mathbf{X}}(t) = N^{-1}\sum_{k=1}^N \mathbf{X}_k(t)$. It is an example of a cooperative coupling that tends to make the system relax towards the "center of gravity" of the multi-particle ensemble. If $V(\mathbf{x})$ is given by a multi-well potential then there is competition between the cooperative interactions and the tendency of particles to be distributed across the different potential wells according to the classical Boltzmann distribution. Here we explore stationary solutions by considering a 1D version of the MV equation (A.13) with Curie-Weiss coupling:

$$\frac{\partial p(x,t)}{\partial t} = D\frac{\partial^2 p(x,t)}{\partial x^2} + \frac{\partial}{\partial x}\left(p(x,t)\mathcal{V}[x,t,p]\right), \tag{A.17}$$

with

$$\mathcal{V}[x,t,p] = \frac{1}{\gamma}\left[V'(x) + \lambda\int_{-\infty}^{\infty}(x-y)p(y,t)dy\right]. \tag{A.18}$$

The steady state version of equation (A.17) is $J_0'(x) = 0$,where

$$J_0(x) := -D\frac{\partial p_0(x)}{\partial x} - \beta D p_0(x)\left(V'(x) + \lambda \int_{-\infty}^{\infty}(x-y)p_0(y)dy\right).$$

(We use the subscript 0 to indicate no resetting.) The integral term reduces to $\lambda(x - \langle y \rangle)$ with $\langle y \rangle = \int_0^\infty y p_0(y)dy$. Suppose, for the moment, that $\langle y \rangle = \ell$ for some fixed ℓ, which then acts as a parameter of the density p_0. The normalizability of $p_0(x)$ implies that $J_0(\pm\infty) = 0$ and so $J_0(x) = 0$ for all x. It follows that, for fixed ℓ, the stationary density is given by a Boltzmann distribution:

$$p_0 = p_0(x;\ell) = Z(\ell)^{-1}\exp\left(-\beta[V(x) + \lambda x^2/2 - \ell\lambda x]\right). \tag{A.19}$$

The factor $Z(\ell)$ ensures the normalization $\int_0^\infty p_0(x;\ell)dx = 1$. The unknown parameter ℓ is determined by imposing the self-consistency condition

$$\ell = m_0(\ell) \equiv \int_{-\infty}^{\infty} x p_0(x;\ell)dx. \tag{A.20}$$

The number of equilibrium solutions is then equal to the number of solutions of equation (A.20). First, consider the quadratic confining potential $V(x) = \nu x^2/2$, $\nu > 0$. We have

$$Z(\ell) = \int_{-\infty}^{\infty} \mathrm{e}^{-\beta[(\nu+\lambda)x^2/2 - \ell\lambda x]}dx = \sqrt{\frac{2\pi}{\beta[\nu+\lambda]}}\mathrm{e}^{\beta\ell^2\lambda^2/2[\nu+\lambda]}, \tag{A.21}$$

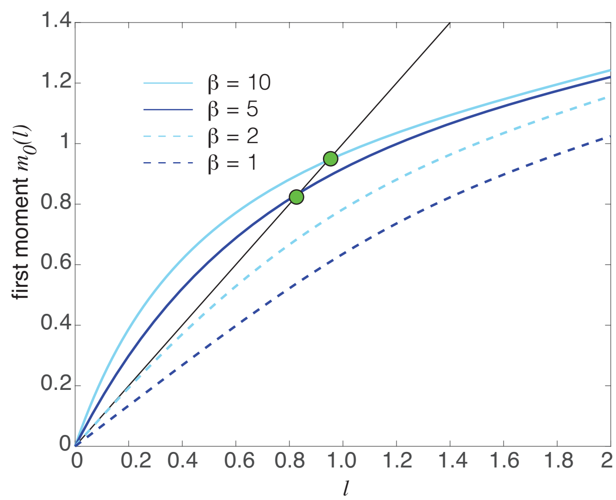

Fig. 13.1: Stationary solution of the 1D McKean-Vlasov equation (A.17) for $V(x) = x^4/4 - x^2/2$. Plot of the first moment $m_0(\ell)$ as a function of ℓ and various inverse temperatures β. The nonzero intercepts with the diagonal determine the positive definite solution ℓ_0. We also take $\lambda = 1$.

and equation (A.20) becomes

$$\ell = Z(\ell)^{-1} \int_0^\infty x e^{-\beta[(\nu+\lambda)x^2/2-\ell\lambda x]} dx = \frac{1}{\lambda\beta} \frac{\partial \log Z(\ell)}{\partial \ell} = \frac{\ell\lambda}{\nu+\lambda}. \tag{A.22}$$

It follows that $\ell = 0$ and

$$p_0(x;0) = \sqrt{\frac{\beta[\nu+\lambda]}{2\pi}} \exp\left(-\beta(\nu+\lambda)x^2/2\right). \tag{A.23}$$

Hence, the interactions simply modify the effective strength of the quadratic potential.

The situation is more complicated when $V(x)$ has at least two minima, because the tendency of the Boltzmann distribution to localize around both minima competes with the cooperative effects of the Curie-Weiss potential. As an example, consider the double-well potential $V(x) = x^4/4 - x^2/2$. Although it is no longer possible to analytically solve the corresponding self-consistency equation (A.20), one can prove that there exists a phase transition at a critical temperature T_c such that $\ell = 0$ for $T > T_c$ and $\ell = \pm\ell_0 \neq 0$ for $T < T_c$ [22, 20, 45]. This is illustrated in Fig. 13.1 by plotting the first moment function $m(\ell)$ for different values of β. We find numerically that $\beta_c \approx 2$ when $\lambda = 1$, which is consistent with the critical point obtained in Refs. [22, 20].

A.3 Dynamical density functional theory (DDFT)

One of the crucial assumptions of mean field theory is that the particles are weakly interacting, In particular, the pairwise interaction potential K in equation (A.1) is scaled by the factor $1/N$. In the absence of this scaling, equation (A.11) becomes

$$\begin{aligned}\frac{\partial u(\mathbf{x},t)}{\partial t} &= D\boldsymbol{\nabla}^2 u(\mathbf{x},t) + \frac{1}{\gamma}\boldsymbol{\nabla}\cdot\Big(u(\mathbf{x},t)\boldsymbol{\nabla}V(\mathbf{x})\Big) \\ &\quad + \frac{1}{\gamma}\boldsymbol{\nabla}\cdot\left(\int_{\mathbb{R}^d} \boldsymbol{\nabla}K(\mathbf{x}-\mathbf{y})\Big\langle \rho(\mathbf{x},t)\rho(\mathbf{y},t)\Big\rangle\right),\end{aligned} \tag{A.24}$$

where

$$u(\mathbf{x},t) = \langle \rho(\mathbf{x},t)\rangle = \left\langle \sum_{j=1}^N \delta(\mathbf{x}-\mathbf{X}_j(t))\right\rangle. \tag{A.25}$$

The exact mean field limit no longer exists. However, one can use an alternative method to achieve moment closure of equation (A.11) for the one-body density, which is known as dynamical density functional theory (DDFT) [37, 4, **?**, 61]. A crucial assumption of DDFT is that the relaxation of the system is sufficiently slow such that the pair correlation function can be equated with that of a corresponding equilibrium system at each point in time [61]. This allows one to approximate equation (A.24) by the closed equation

$$\frac{\partial u(\mathbf{x},t)}{\partial t} = -\nabla \cdot \mathbf{J}(\mathbf{x},t), \tag{A.26}$$

where

$$\mathbf{J}(\mathbf{x},t) = -D\left\{\nabla u(\mathbf{x},t) + \beta u(\mathbf{x},t)\nabla[V(\mathbf{x}) + \mu^{\mathrm{ex}}(\mathbf{x},t)]\right\}, \tag{A.27}$$

Here

$$\mu^{\mathrm{ex}}(\mathbf{x},t) = \frac{\delta F^{\mathrm{ex}}[u(\mathbf{x},t)]}{\delta u(\mathbf{x},t)}, \tag{A.28}$$

and $F^{\mathrm{ex}}[u]$ is the equilibrium excess free energy functional with the equilibrium density profiles replaced by non-equilibrium ones. One of the features of DDFT is that $F^{\mathrm{ex}}[u]$ is independent of the actual external potential. Note that equation (A.26) is a version of the generalized Fick's law derived in Box 13A using linear response theory.

A.4 McKean-Vlasov equation for the classical Kuramoto model

One of the most studied interacting particle systems is the Kuramoto model of weakly-coupled, near identical limit-cycle oscillators with a sinusoidal phase interaction function [34, 53, 1]. The deterministic version of the model takes the form of a system of nonlinear phase equations

$$\frac{d\theta_j}{dt} = \omega_j + \frac{\lambda}{N}\sum_{k=1}^{N}\sin(\theta_k - \theta_j), \tag{A.29}$$

where $\theta_j(t) \in [0,2\pi]$ is the phase of the jth oscillator with natural frequency ω_j, and $\lambda \geq 0$ is the coupling strength. The frequencies ω_j are typically assumed to be distributed according to a probability density $g(\omega)$ with (i) $g(-\omega) = g(\omega)$ and (ii) $g(0) \geq g(\omega)$ for all $w \in [0,\infty)$. Without loss of generality, one can always take $g(\omega)$ to have zero mean by going to a rotating frame if necessary. One method for investigating the collective behavior of the Kuramoto model is to assume that it has a well-defined mean field limit $N \to \infty$ involving a continuum of oscillators distributed on the circle [52, 17, 18]. Let $\sigma_0(\theta,t,\omega)$ denote the fraction of oscillators with natural frequency ω that lie between θ and $\theta + d\theta$ at time t with

$$\int_0^{2\pi} \sigma_0(\theta,t,\omega)d\theta = 1. \tag{A.30}$$

More precisely, $\sigma_0(\theta,t,\omega)$ is a population density that is conditioned on the natural frequency of the oscillators, see below. Since the total number of oscillators is fixed,

σ evolves according to the continuity or Liouville equation

$$\frac{\partial \sigma_0}{\partial t} = -\frac{\partial}{\partial \theta}(\sigma_0 v_0), \tag{A.31}$$

where

$$v_0(\theta,t,\omega) = \omega + \lambda \int_0^{2\pi} d\theta' \int_{-\infty}^{\infty} d\omega' \sin(\theta' - \theta)\sigma_0(\theta',t,\omega')g(\omega'). \tag{A.32}$$

It is also possible to consider a stochastic version of the Kuramoto model [49]. If $\Theta_j(t) \in [0,2\pi)$ denotes the stochastic phase of the jth oscillator at time t, then the corresponding SDE is

$$d\Theta_j(t) = \left[\omega_j + \frac{\lambda}{N}\sum_{k=1}^{N} \sin(\Theta_k(t) - \Theta_j(t))\right]dt + \sqrt{2D}dW_j(t) \tag{A.33}$$

for $j = 1,\ldots,N$, where $W_j(t)$ is an independent Wiener process. The corresponding continuum model now takes the form of a nonlinear FP equation on the circle:

$$\frac{\partial \sigma_0}{\partial t} = -\frac{\partial}{\partial \theta}(\sigma_0 v_0) + D\frac{\partial^2 \sigma_0}{\partial \theta^2}. \tag{A.34}$$

An alternative interpretation of the SDE (A.33) is a system of Brownian particles on an N-torus with pairwise coupling and quenched disorder due to the random distribution of natural frequencies. It follows that Eq. (A.34) is equivalent to the corresponding MV equation for the global density in the mean field limit. The existence of the latter has been proven rigorously using propagation of chaos [19], and has been extended to a wider class of interacting particle systems on the torus [11, 46]. The mean field limit also applies to the deterministic Kuramoto model in the case of an ensemble of initial conditions. The next step is to introduce the global density or empirical measure

$$\rho(\theta,t,\omega) = \frac{1}{N}\sum_{j=1}^{N} \delta(\theta - \Theta_j(t))\delta(\omega - \omega_j). \tag{A.35}$$

It is important to note that the stochastic density ρ is distinct from the deterministic density σ_0 for the noiseless Kuramoto model. Moreover, the former has the normalization

$$\int_0^{2\pi} \rho(\theta,t,\omega)d\theta = \frac{1}{N}\sum_{j=1}^{N} \delta(\omega - \omega_j). \tag{A.36}$$

Taking expectations with respect to the quenched random frequencies, we have

$$\mathbb{E}[\rho(\theta,t,\omega)] = \frac{1}{N}\sum_{j=1}^{N}\delta(\theta-\Theta_j(t))\mathbb{E}[\delta(\omega-\omega_j)]$$
$$= \frac{g(\omega)}{N}\sum_{j=1}^{N}\delta(\theta-\Theta_j(t)), \tag{A.37}$$

which implies that $\int_0^{2\pi}\mathbb{E}[\rho(\theta,t,\omega)]d\theta = g(\omega)$. Consider an arbitrary smooth test function $f:[0,2\pi]\times\mathbb{R}\to\mathbb{R}$ with

$$f(\Theta_j(t),\omega_j) = \int_0^{2\pi}d\theta\int_{\mathbb{R}}d\omega\rho_j(\theta,t,\omega)f(\theta,\omega), \tag{A.38}$$

and

$$\left[\int_0^{2\pi}d\theta\int_{\mathbb{R}}d\omega f(\theta,\omega)\frac{\partial\rho_j(\theta,t,\omega)}{\partial t}\right]dt = df(\Theta_j,\omega_j).$$

Using Itô's lemma along analogous lines to the case of a Brownian gas, we find that

$$\int_0^{2\pi}d\theta\int_{\mathbb{R}}d\omega f(\theta,\omega)\frac{\partial\rho(\theta,t,\omega)}{\partial t}$$
$$= \int_0^{2\pi}d\theta\int_{\mathbb{R}}d\omega\left[\partial_\theta f(\theta,\omega)\frac{\sqrt{2D}}{N}\sum_{j=1}^{N}\rho_j(\theta,t,\omega)\xi_j(t)\right.$$
$$\left.+\rho(\theta,t,\omega)\left(D\partial_\theta^2 f(\theta,\omega)+\partial_\theta f(\theta,\omega)\mathcal{V}[\theta,t,\omega,\rho]\right)\right.,$$

where

$$\mathcal{V}[\theta,t,\omega,\rho] = \omega+\lambda\int_0^{2\pi}d\theta'\int_{\mathbb{R}}d\omega'\rho(\theta',t,\omega')\sin(\theta'-\theta). \tag{A.39}$$

Integrating by parts the various terms involving derivatives of f and using the fact that f is arbitrary yields the following SPDE for ρ:

$$\frac{\partial\rho(\theta,t,\omega)}{\partial t} = -\sqrt{\frac{2D}{N^2}}\sum_{j=1}^{N}\frac{\partial}{\partial\theta}\left[\rho_j(\theta,t,\omega)\xi_j(t)\right]+D\frac{\partial^2}{\partial\theta^2}\rho(\theta,t,\omega)$$
$$-\frac{\partial}{\partial\theta}\left(\rho(\theta,t,\omega)\mathcal{V}[\theta,t,\omega,\rho]\right) \tag{A.40}$$

Following along similar lines to the derivation of equation (A.10), we introduce the white noise term

$$\xi(\theta,t,\omega) = -\frac{1}{N}\sum_{j=1}^{N}\partial_\theta\left[\rho_j(\theta,t,\omega)\xi_j(t)\right], \tag{A.41}$$

which has zero mean and correlation function

$$\langle \xi(\theta,t,\omega)\xi(\theta',t',\omega')\rangle = \frac{1}{N^2}\delta(t-t')\sum_{j=1}^{N}\partial_\theta\partial_{\theta'}\bigg(\rho_j(\theta,t,\omega)\rho_j(\theta',t,\omega')\bigg).$$

Since $\rho_j(\theta,t,\omega)\rho_j(\theta',t,\omega') = \delta(\theta-\theta')\delta(\omega-\omega')\rho_j(\theta,t,\omega)$, it follows that

$$\langle \xi(\theta,t,\omega)\xi(\theta',t',\omega')\rangle = \frac{1}{N}\delta(t-t')\partial_\theta\partial_{\theta'}\bigg(\delta(\theta-\theta')\delta(\omega-\omega')\rho(\theta,t,\omega)\bigg).$$

Finally, we introduce the global density-dependent noise field

$$\widehat{\xi}(\theta,t,\omega) = \frac{1}{\sqrt{N}}\partial_\theta\bigg(\eta(\theta,t,\omega)\sqrt{\rho(\theta,t,\omega)}\bigg), \tag{A.42}$$

where $\eta(\theta,t,\omega)$ is a global white noise field whose components satisfy

$$\langle \eta(\theta,t,\omega)\eta(\theta',t',\omega')\rangle = \delta(t-t')\delta(\theta-\theta)\delta(\omega-\omega'). \tag{A.43}$$

It can be checked that the Gaussian noises ξ and $\widehat{\xi}$ have the same correlation functions and are thus statistically identical. We thus obtain the generalized DK equation for the stochastic Kuramoto model with resetting:

$$\begin{aligned}\frac{\partial\rho(\theta,t,\omega)}{\partial t} &= \sqrt{\frac{2D}{N}}\frac{\partial}{\partial\theta}\left[\sqrt{\rho(\theta,t,\omega)}\eta(\theta,t,\omega)\right] + D\frac{\partial^2}{\partial\theta^2}\rho(\theta,t,\omega)\\ &\quad - \frac{\partial}{\partial\theta}\bigg(\rho(\theta,t,\omega)\mathcal{V}[\theta,t,\omega,\rho]\bigg).\end{aligned} \tag{A.44}$$

As in the case of the DK equation (A.10), taking expectations with respect to the white noise processes results in a moment closure problem. However, assuming a mean field ansatz in the thermodynamic limit leads to the following deterministic MV equation for the mean field $\phi(\theta,t,\omega) = \Big\langle\rho(\theta,t,\omega)\Big\rangle$:

$$\frac{\partial\phi(\theta,t,\omega)}{\partial t} = D\frac{\partial^2}{\partial\theta^2}\phi(\theta,t,\omega) - \frac{\partial}{\partial\theta}\bigg(\phi(\theta,t,\omega)\mathcal{V}[\theta,t,\omega,\phi]\bigg) \tag{A.45}$$

As in the case of interacting Brownian particles, a stationary solution of the MV equation (A.45) has to be determined self-consistently. Now, however, the self-consistency condition involves the first circular moment

$$Z_1(t) = R(t)\mathrm{e}^{i\psi(t)} := \int_0^{2\pi} d\theta\int_{-\infty}^{\infty} d\omega\, \mathrm{e}^{i\theta}\phi(\theta,t,\omega), \tag{A.46}$$

rather than the first moment $\ell = \langle x\rangle$ for the Curie-Weiss potential, say. Substituting equation (A.46) into the MV equation (A.45) gives

$$\frac{\partial \phi(\theta,t,\omega)}{\partial t} = D\frac{\partial^2 \phi(\theta,t,\omega)}{\partial \theta^2} - \frac{\partial}{\partial \theta}\left[\Big(\omega + \lambda R(t)\sin(\psi(t)-\theta(t))\Big)\phi(\theta,t,\omega)\right]. \quad \text{(A.47)}$$

The amplitude $R(t)$ is a measure of the degree of synchronization with $R = 1$ signifying complete synchrony and $R = 0$ corresponding to the incoherent state $\phi(\theta,t,\omega) = g(\omega)/2\pi$, which is a solution of equation (A.45). In principle, one could now proceed by solving the time-independent version of (A.47) for fixed Z_1 and then substituting the resulting stationary solution $\phi_{Z_1}(\theta,\omega)$ into equation (A.46) to determine Z_1. However, the calculation of ϕ_{Z_1} is nontrivial since we no longer have a stationary Boltzmann distribution on the circle.

An alternative representation of the MV equation can be obtained by considering the Fourier series expansion

$$\phi(\theta,t,\omega) = \frac{g(\omega)}{2\pi}\left(1 + \sum_{m=1}^{\infty}\left[\phi_m(\omega,t)\mathrm{e}^{im\theta} + \text{c. c.}\right]\right), \quad \text{(A.48)}$$

with

$$\phi_m(\omega,t) = \langle \mathrm{e}^{-im\theta}\rangle := \int_0^{2\pi} \mathrm{e}^{-im\theta}\phi(\theta,t,\omega)\frac{d\theta}{2\pi}. \quad \text{(A.49)}$$

Solving the initial value problem for ϕ is then equivalent to solving an infinite hierarchy of equations for the coefficients ϕ_m:

$$\frac{\partial \phi_m}{\partial t} + im\omega\phi_m + \frac{\lambda m}{2}\left[\phi_{m+1}Z_1 - \phi_{m-1}Z_1^*\right], \quad \text{(A.50)}$$

with

$$Z_1(t) = \int_{-\infty}^{\infty} g(\omega)\phi_1^*(\omega,t)d\omega. \quad \text{(A.51)}$$

B. Active particles

A major topic of current interest within the general field of non-equilibrium systems is *active matter*, which is typically described in terms of a collection of elements that consume energy in order to move or to exert mechanical forces [47, 48, 51, 8]. Examples include animal flocks or herds [2], motility-based phase separation [12] (see Sect. 15.7), bacterial suspensions [26, 30], synthetically manufactured self-propelled colloids [42, 44, 9], and components of the cellular cytoskeleton (see Chap. 14). In many cases the individual particles have an intrinsic orientation and can exhibit long-range orientational interactions mediated by some sensing mechanism or by coupling hydrodynamically to the surrounding medium [56]. In order to gain theoretical insights into the behavior of active matter, it is often useful to consider simplified models of the individual particles, in particular, a run-and-tumble particle (RTP), an active Brownian particle (ABP) [51], or an active Ornstein-Uhlenbeck particle (AOUP) [38, 60]. These models provide an analytically tractable framework for studying self-organizing phenomena such as the accumulation of active particles at walls, which can occur even if inter-particle interactions are ignored [8]. Since RTP particles are covered extensively in Sect. 10.4, we focus here on the analysis of ABPs and AOUPs.

B.1 Active Brownian particle confined to a semi-infinite channel

Let $\mathbf{X}(t) \in \mathbb{R}^2$ and $\Theta(t) \in [0,2\pi]$ denote the position and orientation of an active particle in two dimensions. In the case of an RTP, the dynamics is described by the stochastic equation

$$\frac{d\mathbf{X}}{dt} = v_0 \mathbf{n}(\Theta(t)), \quad \mathbf{n}(\theta) = (\cos\theta, \sin\theta), \tag{B.1}$$

where v_0 is the speed of the particle and the orientation $\Theta(t)$ randomly switches between a finite set of states $\{\theta_1, \ldots, \theta_n\}$ according to a Markov chain. Mathematically speaking, equation (B.1) is an example of a velocity jump process, see Sect. 10.4. (In one dimension (1D), equation (B.1) reduces to a two state velocity jump process, in which the particle switches between the velocity states $\pm v_0$.) Turning to a 2D model of an ABP, the dynamics evolves according to a stochastic differential equation (SDE) of the form [5]

$$d\mathbf{X}(t) = v_0 \mathbf{n}(\theta(t)) + \sqrt{2\overline{D}}d\overline{\mathbf{W}}(t), \quad d\Theta(t) = \sqrt{2D}dW(t), \tag{B.2}$$

where $\overline{\mathbf{W}}(t) = (\overline{W}_x(t), \overline{W}_y(t))$. The stochastic variables $\overline{W}_x(t), \overline{W}_y(t), W(t)$ are independent Wiener processes, $\overline{D}$ is the translational diffusivity, and D is the rotational diffusivity (with units of inverse time).

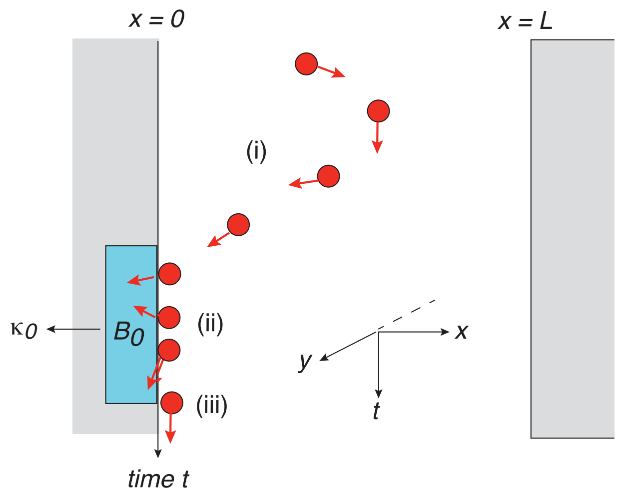

Fig. 13.2: Schematic representation of the time evolution of the position x and the velocity direction (indicated by arrows) of an ABP confined to an infinitely long 2D channel of width L. (i) Motion within the bulk. (ii) The particle hits the impermeable wall at $x = 0$ and remains stuck at the wall (in the bound state B_0) until (iii) rotational diffusion allows it to escape back into the bulk domain. Analogous behavior occurs at the right-hand wall.

Both models exhibit accumulation at the boundaries of a confinement domain, even at the single particle level (see Ref. [3] for an RTP in an interval and Refs. [35, 57, 58, 59] for an ABP in a 2D channel.). This is due to the fact that whenever a particle hits a hard wall, it becomes stuck by pushing on the boundary until a tumble event reverses its direction. At the multi-particle level this results in a pressure being exerted on the confining walls. An equivalent way to formulate the accumulation process is in terms of a sticky boundary condition. That is, whenever the particle collides with a wall, it remains attached to the wall for a random time interval that is determined by the tumbling dynamics. If the escape time back into the bulk is zero then the boundary is totally reflecting, whereas if the particle never escapes then the boundary is totally absorbing. The intermediate case is known as a sticky boundary condition. Sticky boundary conditions also arise within the context of the growth and shrinkage of polymer filaments such as microtubules (Sect. 4.2) and actin-rich cytonemes (Sect. 14.5) in confined 1D domains [62, 41, 10].

Here we consider an ABP confined to a 2D channel $\Omega \subset \mathbb{R}^2$ of width L in the x direction and of infinite extension in the y direction. Let $\mathbf{X}(t) \in \Omega$ and $\Theta(t) \in [0, 2\pi]$ denote the position and orientation of the particle at time t. These stochastic variables are taken to evolve according to the SDE (B.2). For simplicity, we will neglect translational diffusion by setting $\overline{D} = 0$. Let $p(x, y, \theta, t)$ denote the probability density for the triplet $(X(t), Y(t), \Theta(t))$. The density evolves according to the Fokker-Planck (FP) equation

$$\frac{\partial p(\mathbf{x},\theta,t)}{\partial t} = -v_0 \mathbf{n}(\theta)\cdot\nabla p(\mathbf{x},\theta,t) + D\frac{\partial^2 p(\mathbf{x},\theta,t)}{\partial \theta^2}, \quad \mathbf{x}\in\Omega, \quad \theta\in[0,2\pi]. \tag{B.3}$$

Given the translation invariance in the y direction, we assume that p is independent of y so that the FP equation reduces to the quasi-one dimensional form:

$$\frac{\partial p(x,\theta,t)}{\partial t} = -v_0 \cos\theta \frac{\partial p(x,\theta,t)}{\partial x} + D\frac{\partial^2 p(x,\theta,t)}{\partial \theta^2}, \quad x\in(0,L), \quad \theta\in[0,2\pi]. \tag{B.4a}$$

The particle will hit the wall at $x=0$ if it is traveling to the left ($\cos\theta<0$), whereas it will hit the wall at $x=L$ if it is traveling to the right ($\cos\theta>0$). As soon as it hits the wall its linear velocity drops to zero but its orientation will continue to diffuse. The particle remains stuck at the wall until the orientation crosses one of the vertical directions, after which it reenters the bulk domain, see Fig. 13.2. Let $Q_0(\theta,t)$ denote the probability density that the particle is attached to the wall at $x=0$ and has orientation θ ($\cos\theta<0$). Then

$$\frac{\partial Q_0(\theta,t)}{\partial t} = D\frac{\partial^2 Q_0(\theta,t)}{\partial\theta^2} - v_0\cos\theta\, p(0,\theta,t), \quad \theta\in\mathscr{I}_- := (\pi/2, 3\pi/2), \tag{B.4b}$$

which is supplemented by the absorbing boundary conditions $Q_0(\pm\pi/2,t)=0$, which signal the reinsertion of the particle into the bulk domain. The absorbing boundary conditions mean that the net flux between the left-hand wall and the bulk is (for $\cos\theta>0$)

$$\begin{aligned} v_0\cos\theta\, p(0,\theta,t) = D&\frac{\partial Q_0(\pi/2,t)}{\partial\theta}\delta(\theta-\pi/2+\varepsilon) \\ &-D\frac{\partial Q_0(-\pi/2,t)}{\partial\theta}\delta(\theta+\pi/2-\varepsilon), \end{aligned} \tag{B.4c}$$

where $0<\varepsilon\ll 1$. The small parameter ε is introduced to avoid the singularities at $\pm\theta=\pi/2$. However, the resulting solution is well defined in the limit $\varepsilon\to 0$. Similarly, the probability density $Q_L(\theta,t)$ that the particle is attached to the wall at $x=L$ and has orientation θ ($\cos\theta>0$) evolves according to the equation

$$\frac{\partial Q_L(\theta,t)}{\partial t} = D\frac{\partial^2 Q_L(\theta,t)}{\partial\theta^2} + v_0\cos\theta\, p(L,\theta,t), \quad \theta\in\mathscr{I}_+ := (-\pi/2, \pi/2), \tag{B.4d}$$

with $Q_L(\pm\pi/2,t)=0$ and (for $\cos\theta<0$)

$$\begin{aligned} v_0\cos\theta\, p(L,\theta,t) = -D&\frac{\partial Q_L(\pi/2,t)}{\partial\theta}\delta(\theta-\pi/2-\varepsilon) \\ &+D\frac{\partial Q_L(-\pi/2,t)}{\partial\theta}\delta(\theta+\pi/2+\varepsilon). \end{aligned} \tag{B.4e}$$

B.2 Steady-state analysis and two-way diffusion

In the case of an ABP confined to a 2D channel, the resulting boundary value problem (BVP) for the steady-state is non-trivial, since the boundary conditions at the channel walls are only defined on the orientation half spaces $\theta \in \mathscr{I}_- := (\pi/2, 3\pi/2)$ and $\theta \in \mathscr{I}_+ := (-\pi/2, \pi/2)$. That is, the BVP is an example of a so-called two-way diffusion problem for which classical spectral methods do not apply [28, 6, 7], We will describe a hybrid analytical/numerical method recently developed to solve the two-way diffusion problem for the steady-state density [35, 57, 58, 59]. The steady-state equations take the form

$$D\frac{\partial^2 p(x,\theta)}{\partial \theta^2} = v_0 \cos\theta \frac{\partial p(x,\theta)}{\partial x}, \quad x \in (0,L), \quad \theta \in [-\pi,\pi], \tag{B.5a}$$

$$D\frac{d^2 Q_0(\theta)}{d\theta^2} = v_0 \cos\theta\, p(0,\theta), \quad \theta \in \mathscr{I}_-, \tag{B.5b}$$

$$D\frac{d^2 Q_L(\theta)}{d\theta^2} = -v_0 \cos\theta\, p(L,\theta), \quad \theta \in \mathscr{I}_+, \tag{B.5c}$$

$$v_0 \cos\theta\, p(0,\theta) = D\frac{dQ_0(\pi/2)}{d\theta}\delta(\theta - \pi/2 + \varepsilon) - D\frac{dQ_0(-\pi/2)}{d\theta}\delta(\theta + \pi/2 - \varepsilon), \quad \text{for } \cos\theta > 0 \tag{B.5d}$$

$$v_0 \cos\theta\, p(L,\theta) = -D\frac{dQ_L(\pi/2)}{d\theta}\delta(\theta - \pi/2 - \varepsilon) + D\frac{dQ_L(-\pi/2)}{d\theta}\delta(\theta + \pi/2 + \varepsilon), \quad \text{for } \cos\theta < 0. \tag{B.5e}$$

The first step is to introduce the separable solution $p(x,\theta) = X(x)\Theta(\theta)$ into equation (B.5a), which yields the pair of ODEs

$$\frac{dX}{dx} = \lambda X/\ell, \quad \ell = \frac{v_0}{D}, \tag{B.6a}$$

$$\frac{d^2\Theta}{d\theta^2} - \lambda \cos\theta\Theta = 0, \quad \Theta(\theta) = \Theta(\theta + 2\pi). \tag{B.6b}$$

(The separable functions $X(x)$ and $\Theta(\theta)$ should be distinguished from the stochastic variables $X(t)$ and $\Theta(t)$.) The first equation has the solution $\mathrm{e}^{\lambda X/\ell}$ for a given λ. The second equation is related to Mathieu's equation. Since $\cos\theta$ is an even function of θ, the eigenfunctions can be partitioned into odd and even subsets. If $\Theta(\theta)$ is an eigenfunction corresponding to an eigenvalue λ, then $\overline{\Theta}(\theta) \equiv \Theta(\theta + \pi)$ is an eigenfunction whose eigenvalue is $-\lambda$. The proof is straightforward:

$$\frac{d^2\overline{\Theta}(\theta)}{d^2\theta} = \frac{d^2\Theta(\theta+\pi)}{d^2\theta} = \lambda\cos(\theta+\pi)\Theta(\theta+\pi) = -\lambda\cos\theta\overline{\Theta}(\theta).$$

It can also be proven that the non-zero eigenvalues are non-degenerate [28], which motivates the following ordering of the non-zero eigenvalues: $\ldots < \lambda_2 < \lambda_1 < 0 < \lambda_{-1} < \lambda_{-2} < \ldots$ with $\lambda_k = -\lambda_{-k}$. The eigenfunctions $\Theta_k(\theta)$ satisfy the orthogonality relation

$$\int_{-\pi}^{\pi} \Theta_j(\theta)\Theta_k(\theta)\cos\theta d\theta = \delta_{i,j}\mathrm{sgn}(k), \quad jk \neq 0. \tag{B.7}$$

In order to establish equation (B.7), consider two distinct eigenvalues λ_k and λ_l with $l \neq k$. Multiply the eigenvalue equation for Θ_k by Θ_j and multiply the eigenvalue equation for Θ_j by Θ_k. Subtracting the pair of equations gives

$$\Theta_j(\theta)\frac{d^2\Theta_k(\theta)}{d\theta^2} - \Theta_k(\theta)\frac{d^2\Theta_j(\theta)}{d\theta^2} = (\lambda_k - \lambda_j)\cos\theta\Theta_j(\theta)\Theta_k(\theta). \tag{B.8}$$

Integrating both sides with respect to θ using integration by parts and periodicity of the eigenfunctions yields equations (B.7) for $k \neq j$. This is supplemented by the normalization $\int_{-\pi}^{\pi}\Theta_k^2(\theta)\cos\theta d\theta = \mathrm{sgn}(k)$.

One subtle point is that the set of eigenfunctions $\{\Theta_k(\theta), k \neq 0\}$ with corresponding non-zero eigenvalues λ_k do not form a complete basis set. This is a consequence of the fact that the eigenfunctions $\Theta_k(\theta)$ satisfy the additional orthogonality relations

$$\int_{-\pi}^{\pi} \Theta_k(\theta)\cos\theta d\theta = 0, \quad \int_{-\pi}^{\pi} \Theta_k(\theta)\cos^2\theta d\theta = 0, \quad k \neq 0. \tag{B.9}$$

Equations (B.9) follow directly from integrating equation (B.6b). However, there exists a doubly degenerate zero eigenvalue whose eigenspace is spanned by the functions $u_0 = \alpha$ and $\widehat{u}_0 = \beta(x/\ell - \cos\theta)$, where α, β are constants. The latter eigenfunction is non-separable and is known as the diffusion solution. Inclusion of this additional pair of eigenfunctions generates a complete basis set, leading to a general solution of the form

$$p(x,\theta) = \alpha + \beta(x/\ell - \cos\theta) + \sum_{k>0} a_k \mathrm{e}^{\lambda_k x/\ell}\Theta_k(\theta) + \sum_{k<0} a_k \mathrm{e}^{\lambda_k [x-L]/\ell}\Theta_k(\theta). \tag{B.10}$$

Soluition of two-sided BVP

The next step is to determine the coefficients α, β, a_k by imposing the boundary conditions at the walls. In order to summarize the theory of [57, 58], we. first consider the simplified boundary conditions

$$p(0,\theta) = v_+(\theta) \text{ for } \cos\theta > 0, \quad p(L,\theta) = v_-(\theta) \text{ for } \cos\theta < 0. \tag{B.11}$$

Let us define the function

$$v(\theta) = \begin{cases} v_+(\theta) - \alpha_0 + \beta_0\cos\theta, & \cos\theta > 0 \\ v_-(\theta) - \alpha_0 - \beta_0(L - \cos\theta), & \cos\theta < 0 \end{cases}. \tag{B.12}$$

The coefficients α_0, β_0 are chosen so that $\int_{-\pi}^{\pi} v(\theta)\cos\theta d\theta = 0 = \int_{-\pi}^{\pi} v(\theta)\cos^2\theta d\theta$. We can then expand $v(\theta)$ as

$$v(\theta) = \sum_{k\neq 0} a_k^0 \Theta_k(\theta), \quad a_k^0 = \mathrm{sgn}(k) \int_{-\pi}^{\pi} v(\theta)\Theta_k(\theta)\cos\theta d\theta. \tag{B.13}$$

Introduce the approximate solution

$$p_0(x,\theta) = \alpha_0 + \beta_0(x/\ell - \cos\theta) + \sum_{k>0} a_k^0 \mathrm{e}^{\lambda_k x/\ell}\Theta_k(\theta) + \sum_{k<0} a_k^0 \mathrm{e}^{\lambda_k [x-L]/\ell}\Theta_k(\theta). \tag{B.14}$$

At $x=0$ we have

$$\begin{aligned} p_0(0,\theta) &= \alpha_0 - \beta_0\cos\theta + \sum_{k>0} a_k\Theta_k(\theta) + \sum_{k<0} a_k \mathrm{e}^{-\lambda_k L/\ell}\Theta_k(\theta) \\ &= v(\theta) - \sum_{k<0} a_k^0 \left(1 - \mathrm{e}^{-\lambda_k L/\ell}\right)\Theta_k(\theta) \text{ for } \cos\theta > 0, \end{aligned} \tag{B.15a}$$

Similarly, at $x=L$ we have

$$\begin{aligned} p_0(L,\theta) &= \alpha_0 - \beta_0[L - \cos\theta] + \sum_{k>0} a_k \mathrm{e}^{\lambda_k L/\ell}\Theta_k(\theta) + \sum_{k<0} a_k\Theta_k(\theta) \\ &= v(\theta) - \sum_{k>0} a_k^0 \left(1 - \mathrm{e}^{\lambda_k L/\ell}\right)\Theta_k(\theta) \ \text{ for } \cos\theta < 0. \end{aligned} \tag{B.15b}$$

Thus the leading order approximation p_0 satisfies equation (B.5a) but does not exactly match the boundary conditions.

At the next iteration we consider the error $\Delta p^{(1)}(x,\theta) = p(x,\theta) - p_0(x,\theta)$, which satisfies equation (B.5a) together with the boundary conditions

$$\Delta p^{(1)}(0,\theta) = v_{1,+}(\theta) \equiv \sum_{k<0} a_k^0 \left(1 - \mathrm{e}^{-\lambda_k L/\ell}\right)\Theta_k(\theta) \text{ for } \cos\theta > 0, \tag{B.16a}$$

$$\Delta p^{(1)}(L,\theta) = v_{1,-}(\theta) \equiv \sum_{k>0} a_k^0 \left(1 - \mathrm{e}^{\lambda_k L/\ell}\right)\Theta_k(\theta) \ \text{ for } \cos\theta < 0. \tag{B.16b}$$

We then define the function

$$v_1(\theta) = \begin{cases} v_{1,+}(\theta) - \alpha_1 + \beta_1\cos\theta, & \cos\theta > 0 \\ v_{1,-}(\theta) - \alpha_1 - \beta_1(L - \cos\theta), & \cos\theta < 0 \end{cases}, \tag{B.17}$$

and find new coefficients α_1, β_1, a_k^1. The error Δp is then approximated by p_1 with

$$p_1(x,\theta) = \alpha_1 + \beta_1(x/\ell - \cos\theta) + \sum_{k>0} a_k^1 \mathrm{e}^{\lambda_k x/\ell}\Theta_k(\theta) + \sum_{k<0} a_k^1 \mathrm{e}^{\lambda_k [x-L]/\ell}\Theta_k(\theta). \tag{B.18}$$

The new error function is $\Delta p^{(2)} = p - p_0 - p_1$, which is approximated along the same lines etc.

Solution of full BVP

So far the analysis has neglected the tumbling dynamics and absorption at the walls, as determined by the bound state probability densities $Q_0(\theta)$ and $Q_L(\theta)$. If the latter were known explicitly then one could determine the functions $v_{\pm}(\theta)$ from the boundary conditions (B.5d) and (B.5e):

$$v_+(\theta) = \frac{A_0}{\ell\cos\theta}\delta(\theta - \pi/2 + \varepsilon) + \frac{B_0}{\ell\cos\theta}\delta(\theta + \pi/2 - \varepsilon), \tag{B.19a}$$

$$v_-(\theta) = -\frac{A_L}{\ell\cos\theta}\delta(\theta - \pi/2 - \varepsilon) - \frac{B_L}{\ell\cos\theta}\delta(\theta + \pi/2 + \varepsilon), \tag{B.19b}$$

where

$$A_{0,L} := \frac{\partial Q_{0,L}(\pi/2)}{\partial\theta},\ B_{0,L} := -\frac{\partial Q_{0,L}(-\pi/2)}{\partial\theta}. \tag{B.20}$$

In principle, we now have to deal with the fact that the probability densities $Q_0(\theta)$ and $Q_L(\theta)$ are only defined implicitly, since the remaining pair of boundary conditions (B.5b) and (B.5c) depend on $p(0,\theta)$ and $p(L,\theta)$. Hence, the unknown coefficients $A_{0,L}$ and $B_{0,L}$ have to be determined self-consistently. However, the symmetry of the problem implies that $A_0 = A_L = B_0 = B_L \equiv \mathcal{N}$ as there is a balance of fluxes at both ends [57]. Hence, one can treat $\mathcal{N}$ as a global factor that simply acts as a normalization. In Ref. [57], the hybrid numerical/analytical scheme is compared with direct simulations and found to be in good agreement. Example density profiles are sketched in Fig. **??**.

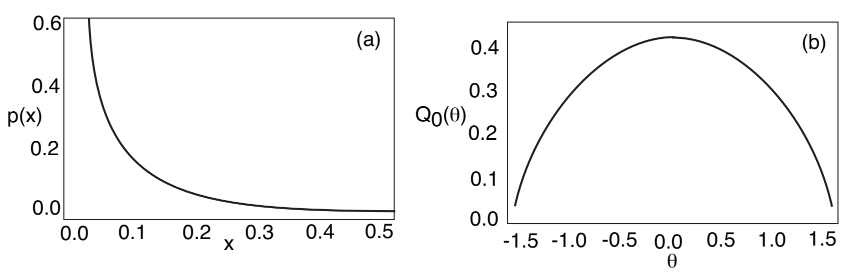

Fig. 13.3: Sketch of marginal density $p(x) = \int_{-\pi}^{\pi} p(x,\theta)d\theta$ as a function of distance x from the left wall. We take $\ell_p = 1$ and $L = 7$. One finds that the enhancement of the bulk density occurs in a boundary layer of thickness $\ell_p/2$. (b) Sketch of orientational density $Q_0(\theta)$ at the left-hand wall for $L = 20$.

Convergence of series solution

A more mathematically rigorous formulation of the solution to a two-sided diffusion problem can also be developed [58]. In order to avoid the additional complications of the doubly degenerate zero eigenvalue, consider the slightly modified BVP

$$D\frac{\partial^2 p(x,\theta)}{\partial\theta^2} - \kappa_0 p(x,\theta) = v_0\cos\theta\frac{\partial p(x,\theta)}{\partial x}, \quad x\in(0,L), \quad \theta\in[-\pi,\pi], \tag{B.21a}$$

$$p(0,\theta) = v_+(\theta) \text{ for } \cos\theta>0, \quad p(L,\theta)=v_-(\theta) \text{ for } \cos\theta<0. \tag{B.21b}$$

Here κ_0 could represent the rate of degradation in the bulk. Introduce the space $\mathscr{H}$ of continuous piecewise, twice-differentiable functions of θ and definie $v(\cdot,s), f(\cdot,s)\in\mathscr{H}$ with

$$v(\theta) = \begin{cases} v_+(\theta), \ \cos\theta>0 \\ v_-(\theta), \ \cos\theta<0 \end{cases}, \quad f(\theta,s) = \begin{cases} f_+(\theta)\equiv p(0,\theta), \ \cos\theta>0 \\ f_-(\theta)\equiv p(L,\theta), \ \cos\theta<0 \end{cases}. \tag{B.22}$$

The boundary condition can then be written in the more compact form $f(\theta)=v(\theta)$ for all $\theta\in(-\pi,\pi)$. The eigenfunctions $\{\Theta_k(\theta,s), k\neq 0\}$ with

$$\frac{d^2\Theta}{d\theta^2} - [\lambda\cos\theta+\kappa_0]\Theta = 0, \quad \Theta(\theta)=\Theta(\theta+2\pi). \tag{B.23}$$

form a complete orthonormal basis set for $\mathscr{H}$ when $\kappa_0>0$. (They are now related to Hill functions [36] rather than Mathieu functions.) This means that we can set $v(\theta)=\sum_{k\neq 0} v_k^{(0)}\Theta_k(\theta)$ with

$$v_k^{(0)} \equiv \text{sgn}(k)\int_{-\pi}^{\pi} v(\theta)\Theta_k(\theta)\cos\theta d\theta. \tag{B.24}$$

Moreover, the general solution to the above BVP can be written as

$$p(x,\theta) = \sum_{k>0} c_k \mathrm{e}^{\lambda_k x/\ell}\Theta_k(\theta) + \sum_{k<0} c_k \mathrm{e}^{\lambda_k[x-L]/\ell}\Theta_k(\theta). \tag{B.25}$$

Following Ref. [58], we now introduce two sets of projection operators. The first pair $\mathcal{Q}_\pm$ projects an element $u\in\mathscr{H}$ onto functions restricted to the domains $\theta\in\mathscr{I}_\pm$:

$$\mathcal{Q}_+u(\theta) = \begin{cases} u_+(\theta), \ \cos\theta>0 \\ \quad 0 \quad\ \cos\theta<0 \end{cases}, \quad \mathcal{Q}_-u(\theta) = \begin{cases} \quad 0, \quad \cos\theta>0 \\ u_-(\theta) \ \ \cos\theta<0 \end{cases}. \tag{B.26}$$

In order to define the second pair of projection operators $\mathcal{P}_\pm$, we expand an arbitrary element $u\in\mathscr{H}$ as $u(\theta)=\sum_{k\neq 0} u_k\Theta_k(\theta)$ and set

$$\mathcal{P}_+u(\theta) = \sum_{k>0} u_k\Theta_k(\theta), \quad \mathcal{P}_-u(\theta) = \sum_{k<0} u_k\Theta_k(\theta). \tag{B.27}$$

We now note that the functions $f_\pm(\theta)$ can be rewritten as

$$f_+(\theta) = [\mathcal{P}_+ + \mathcal{P}_-\mathscr{M}_L]F(\theta), \quad f_-(\theta) = [\mathcal{P}_+\mathscr{M}_L + \mathcal{P}_-]F(\theta), \tag{B.28}$$

where

$$F(\theta) := \sum_{k\neq 0} c_k\Theta_k(\theta), \quad \mathscr{M}_L F(\theta) := \sum_{k\neq 0} c_k \mathrm{e}^{-|\lambda_k|L/\gamma}\Theta_k(\theta). \tag{B.29}$$

It follows that the boundary condition becomes

$$\begin{aligned} v(\theta) &= \mathcal{Q}_+ f_+(\theta) + \mathcal{Q}_- f_-(\theta) \\ &= \{\mathcal{Q}_+[\mathcal{P}_+ + \mathcal{P}_-\mathscr{M}_L] + \mathcal{Q}_-[\mathcal{P}_+\mathscr{M}_L + \mathcal{P}_-]\}F(\theta) \\ &= \mathscr{V}F(\theta,s) + \mathscr{W}\mathscr{M}_L F(\theta), \end{aligned} \tag{B.30}$$

where $\mathscr{V} = \mathcal{Q}_+\mathcal{P}_+ + \mathcal{Q}_-\mathcal{P}_-$, $\quad \mathscr{W} = \mathcal{Q}_+\mathcal{P}_- + \mathcal{Q}_-\mathcal{P}_+$. Using the operator identity $\mathscr{V} + \mathscr{W} = (\mathcal{Q}_+ + \mathcal{Q}_-)(\mathcal{P}_+ + \mathcal{P}_-) = I$, we obtain the result

$$v(\theta) = (I - \mathscr{W}_L)F(\theta), \quad \mathscr{W}_L = \mathscr{W} - \mathscr{W}\mathscr{M}_L, \tag{B.31}$$

which can beformally inverted in terms of a Neumann series [58]

$$F(\theta) = \sum_{n=0}^{\infty} \mathscr{W}_L^n v(\theta). \tag{B.32}$$

A non-trivial issue is whether or not the infinite series representation of $F(\theta)$ converges. In terms of the L^2 inner product, this is equivalent to the condition $\|\mathscr{W}_L\| < 1$. As discussed by Wagner *et al.* [58], the norm of $\mathscr{W}_L$ is difficult to estimate. However, in practice, one can establish convergence numerically by restricting the Hilbert space $\mathscr{H}$ to the space $\mathscr{H}_N = \mathrm{span}\{\Theta_k, |k \leq N\}$, that is, the space spanned by the first $2N$ eigenfunctions ordered by the magnitude of their corresponding eigenvalues. Modifying the definitions of the projection operators accordingly, one finds that $\|\mathscr{W}_N\| < 1$ for values of N up to $O(10^3)$ with an asymptote suggesting that $\lim_{N\to\infty}\|\mathscr{W}_N\| < 1$ (see Fig. 1 of Wagner *et al.* [58]). It remains to justify approximating solutions by restricting to the space $\mathscr{H}_N$. This is valid provided that the BVP defined by equations (B.6a), (B.6b) and (B.11) has solutions that are sufficiently smooth and slowly varying. Since eigenfunctions with larger eigenvalues are faster varying, it follows that they do not contribute significantly. Assuming that the Neumann series (B.32) is convergent, one can generate a sequence of approximate analytic solutions along analogous lines to Wagner *et al.* [58]. Let $F^{(n)}(\theta)$ denote the approximation obtained by truncating the series solution at the nth term. It immediately follows that the zeroth order solution is $F^{(0)}(\theta) = \sum_{k\neq 0} v_k^{(0)}\Theta_k(\theta)$. At the next level of approximation, the contribution on the right-hand side of equation (B.32) is

$$\mathscr{W}_L v(\theta) = [\mathcal{Q}_+\mathcal{P}_- + \mathcal{Q}_-\mathcal{P}_+]v(\theta) = \begin{cases} \sum_{k<0} v_k^{(0)} \Theta_k(\theta), \, \cos\theta > 0 \\ \sum_{k>0} v_k^{(0)} \Theta_k(\theta), \, \cos\theta < 0 \end{cases}. \tag{B.33}$$

Note that that the eigenfunctions $\{\Theta_k(\theta), k<0\}$ span the set of functions restricted to the domain $\cos\theta > 0$ and the subset $\{\Theta_k(\theta), k>0\}$ span the set of functions restricted to the domain $\cos\theta < 0$; this is known as the half-range completeness property [28, 6, 7]. Rewriting $\mathscr{W}_L v(\theta)$ as

$$\mathscr{W}_L v(\theta) = \sum_{k\neq 0} v_k^{(1)} \Theta_k(\theta), \quad \theta \in [0, 2\pi]; \quad v_k^{(1)}(r) = \int_{-\pi}^{\pi} \mathscr{W}_L \Theta_k(\theta) \cos\theta d\theta \tag{B.34}$$

leads to the next level approximation $F^{(1)}(\theta) = \sum_{k\neq 0}[v_k^{(0)} + v_k^{(1)}]\Theta_k(\theta)$. Iterating the procedure generates an approximation to arbitrary order n with $c_k \approx \sum_{j=0}^{n} v_k^{(j)}$.

B.3 Steady-state analysis of a confined active Ornstein-Uhlenbeck particle (AOUP)

Let $\mathbf{X}(t) \in \mathbb{R}^d$ denote the position of a freely moving AOUP at time t. In the absence of an external potential, the corresponding over-damped Langevin equation takes the form

$$\frac{d\mathbf{X}(t)}{dt} = \mathbf{V}(t) + \sqrt{2D}\boldsymbol{\xi}(t), \tag{B.35}$$

where $\boldsymbol{\xi}(t)$ is a vector of d independent Gaussian white noise processes with first and second moments

$$\langle \xi_a(t) \rangle = 0, \quad \langle \xi_a(t)\xi_b(t') \rangle = \delta_{a,b}\delta(t-t'), \tag{B.36}$$

D is the passive diffusivity for translational motion and $\mathbf{V}$ is a random persistent velocity that evolves according to the OU process

$$\tau \frac{d\mathbf{V}(t)}{dt} = -\mathbf{V}(t) + \sqrt{2K}\boldsymbol{\eta}(t). \tag{B.37}$$

Here $\boldsymbol{\eta}(t)$ is a vector of Gaussian white noise process,

$$\langle \eta_a(t) \rangle = 0, \quad \langle \eta_a(t)\eta_b(t') \rangle = \delta_{a,b}\delta(t-t'), \tag{B.38}$$

whose components are uncorrelated with $\boldsymbol{\xi}(t)$, τ is a persistence time, and K is an active diffusivity with $K = v_0^2\tau/d$ for some characteristic speed v_0. It follows that

$$\langle V_a(t) \rangle = 0, \quad \langle V_a(t)V_b(t') \rangle = \delta_{a,b}\frac{v_0^2}{d}\mathrm{e}^{-|t-t'|/\tau}, \tag{B.39}$$

and

$$\langle \mathbf{X}^2(t)\rangle = 2dDt + 2v_0^2\tau^2\left[\frac{t}{\tau} - 1 + \mathrm{e}^{-t/\tau}\right]. \tag{B.40}$$

In particular, for $t \gg \tau$, the ballistic contribution approximately averages to zero and we have an effective diffusivity $D_{\rm eff} = D + K$ with $\langle \mathbf{X}^2(t)\rangle \approx 2dD_{\rm eff}t$.

Now suppose that the particle is restricted to a bounded domain $\Omega \subset \mathbb{R}^d$ with a reflecting boundary $\partial\Omega$. Let $p(\mathbf{x},\mathbf{v},t)$ denote the probability density at time t. The density evolves according to the Fokker-Planck (FP) equation

$$\frac{\partial p}{\partial t} = D\boldsymbol{\nabla}_{\mathbf{x}}^2 p - \mathbf{v}\cdot\boldsymbol{\nabla}_{\mathbf{x}}p + \frac{K}{\tau^2}\boldsymbol{\nabla}_{\mathbf{v}}^2 p + \frac{1}{\tau}\boldsymbol{\nabla}_{\mathbf{v}}\cdot\mathbf{v}p, \quad (\mathbf{x},\mathbf{v})\in\Omega\times\mathbb{R}^d \tag{B.41}$$

for a given initial condition $p(\mathbf{x},\mathbf{v},0) = p_0(\mathbf{x},\mathbf{v})$ and normalization

$$\int_\Omega d\mathbf{x}\int_{\mathbb{R}^d} d\mathbf{v}\, p(\mathbf{x},v,t) = 1. \tag{B.42}$$

Introducing the probability fluxes

$$\mathbf{J}_{\mathbf{x}}(\mathbf{x},\mathbf{v},t) = \mathbf{v}p(\mathbf{x},\mathbf{v},t) - D\boldsymbol{\nabla}_{\mathbf{x}}p(\mathbf{x},\mathbf{v},t), \tag{B.43}$$

$$\mathbf{J}_{\mathbf{v}}(\mathbf{x},\mathbf{v},t) = -\frac{\mathbf{v}}{\tau}p(\mathbf{x},\mathbf{v},t) - \frac{K}{\tau^2}\boldsymbol{\nabla}_{\mathbf{v}}p(\mathbf{x},\mathbf{v},t). \tag{B.44}$$

we can express the reflecting boundary condition as

$$J_{\mathbf{x}}(\mathbf{x},\mathbf{v},t) = 0, \quad (\mathbf{x},\mathbf{v})\in\partial\Omega\times\mathbb{R}^d, \tag{B.45}$$

and rewrite the FP equation as a conservation equation of the form

$$\frac{\partial p}{\partial t} = -\boldsymbol{\nabla}_{\mathbf{x}}\cdot\mathbf{J}_{\mathbf{x}} - \boldsymbol{\nabla}_{\mathbf{v}}\cdot\mathbf{J}_{\mathbf{v}}. \tag{B.46}$$

Integrating equation (B.46) with respect to $\mathbf{x}\in\Omega$ using the reflecting boundary condition and setting $\rho(\mathbf{v},t) = \int_\Omega p(\mathbf{x},\mathbf{v},t)d\mathbf{x}$ shows that ρ satisfies the reduced FP equation

$$\frac{\partial\rho}{\partial t} = \frac{K}{\tau^2}\boldsymbol{\nabla}_{\mathbf{v}}^2\rho + \frac{1}{\tau}\boldsymbol{\nabla}_{\mathbf{v}}\cdot\mathbf{v}\rho, \quad \mathbf{v}\in\mathbb{R}^d. \tag{B.47}$$

The steady-state solution of the latter is the Gaussian distribution

$$\rho(\mathbf{v}) = \frac{1}{\sqrt{2\pi v_0^2/d}}\exp\left(-\frac{\mathbf{v}^2}{2v_0^2/d}\right). \tag{B.48}$$

Determining the $\mathbf{x}$-dependence of the steady-state solution $p(\mathbf{x},\mathbf{v})$ in the bounded domain Ω is non-trivial. One way to proceed is to perform a perturbation and eigenfunction series expansion along the lines of Ref. [60]. The first step is to non-dimensionalize the FP equation (B.41) by performing the scalings

$$\widetilde{t} = \frac{t}{\tau}, \quad \widetilde{\mathbf{x}} = \frac{\mathbf{x}}{\lambda}, \quad \widetilde{\mathbf{v}} = \frac{\mathbf{v}}{\sigma}, \quad \widetilde{p}(\widetilde{\mathbf{x}},\widetilde{\mathbf{v}},t) = p(\lambda\widetilde{x},\sigma\widetilde{\mathbf{v}},t)(\lambda\sigma)^d,$$

where

$$\lambda = \sqrt{2D\tau}, \quad \sigma = \sqrt{2K/\tau} = \sqrt{2v_0^2/d}. \tag{B.49}$$

In particular, λ is the typical distance a passive particle diffuses over the persistence time τ. After dropping the tildes, the FP equation away from boundary takes the form

$$\frac{\partial p}{\partial t} = \boldsymbol{\nabla}_{\mathbf{x}}^2 p + \boldsymbol{\nabla}_{\mathbf{v}}^2 p + 2\boldsymbol{\nabla}_{\mathbf{v}} \cdot \mathbf{v} p - 2\varepsilon \mathbf{v} \cdot \boldsymbol{\nabla}_{\mathbf{x}} p, \tag{B.50}$$

where

$$\varepsilon = \sqrt{\frac{v_0^2 \tau}{dD}} \equiv \sqrt{\mathrm{Pe}}, \tag{B.51}$$

and Pe is the Péclet number. The latter is the ratio of the rates of active and passive transport, and characterizes how active the particle is. The next step is to consider a regular perturbation series expansion of the steady-state solution in the weakly active regime (small ε):

$$p(\mathbf{x}, \mathbf{v}) = \sum_{n=0}^{\infty} \varepsilon^n p^{(n)}(\mathbf{x}, \mathbf{v}). \tag{B.52}$$

Substituting into the time-independent version of the dimensionless FP equation (B.50) gives

$$\boldsymbol{\nabla}_{\mathbf{x}}^2 p^{(n)} + \boldsymbol{\nabla}_{\mathbf{v}}^2 p^{(n)} + 2\boldsymbol{\nabla}_{\mathbf{v}} \cdot \mathbf{v} p^{(n)} = 2\mathbf{v} \cdot \boldsymbol{\nabla}_{\mathbf{x}} p^{(n-1)}, \quad n \geq 1. \tag{B.53}$$

Note that $p^{(0)}$ satisfies the closed equation

$$\boldsymbol{\nabla}_{\mathbf{x}}^2 p^{(0)} + \boldsymbol{\nabla}_{\mathbf{v}}^2 p^{(0)} + 2\boldsymbol{\nabla}_{\mathbf{v}} \cdot \mathbf{v} p^{(0)} = 0, \tag{B.54}$$

which we assume can be solved explicitly. Further simplification is obtained by performing an eigenfunction expansion with respect to Hermite polynomials H_m, $m \geq 0$. This follows from the observation that the differential operator $\mathbb{L}_v \equiv \boldsymbol{\nabla}_{\mathbf{v}}^2 + 2\boldsymbol{\nabla}_{\mathbf{v}} \cdot \mathbf{v}$ appearing in equations (B.50) and (B.53) can be mapped to the corresponding operator of the FP equation for a particle in a harmonic potential. More specifically, we set (see appendix B of Ref. [60])

$$p^{(n)}(\mathbf{x}, \mathbf{v}) = \sum_{m_1=0}^{\infty} \cdots \sum_{m_d=0}^{\infty} C_{\mathbf{m}}^{(n)}(\mathbf{x}) \mathrm{e}^{-\mathbf{v}^2} \prod_{i=1}^{d} H_{m_i}(v_i), \tag{B.55}$$

where $\mathbf{m} = (m_1, \ldots, m_d)$. The solution of the steady-state boundary-value problem (BVP) for the full density $p(\mathbf{x}, \mathbf{v})$, $\mathbf{x} \in \Omega$, then reduces to solving a recursive BVP for the coefficients $C_{\mathbf{m}}^{(n)}(\mathbf{x})$.

AOUP on a finite interval.

First consider the 1D example of an AOUP on the finite interval $x \in [-L, L]$ with a reflecting boundary at $x = \pm L$. (In unscaled units the length is $L\sqrt{2D\tau}$.) Equation (B.55) becomes

$$p^{(n)}(x,v) = \sum_{m=0}^{\infty} C_m^{(n)}(x) \mathrm{e}^{-v^2} H_m(v), \quad x \in [0, L], \tag{B.56}$$

with H_m satisfying the Hermite equation

$$\frac{d^2 H_m}{dv^2} - 2v \frac{d}{dv}(H_m) = -2m H_m. \tag{B.57}$$

It follows that the function $F_m(v) = \mathrm{e}^{-v^2} H_m(v)$ satisfies the eigenvalue equation

$$\mathbb{L}_v F_m \equiv \frac{d^2 F_m}{dv^2} + 2\frac{d}{dv}(v F_m) = -2m F_m, \tag{B.58}$$

The leading-order Hermite polynomials are

$$H_0(v) = 1, \quad H_1(v) = 2v, \quad H_2(v) = 4v^2 - 2, \quad H_3(v) = 8v^3 - 12v. \tag{B.59}$$

Moreover, they satisfy the orthogonality condition

$$\int_{-\infty}^{\infty} H_n(v) H_m(v) \mathrm{e}^{-v^2} dv = \sqrt{\pi} 2^n n! \delta_{n,m}, \tag{B.60}$$

and the recursion relations

$$2v H_m(v) = H_{m+1}(v) + 2m H_{m-1}(v), \quad H_m'(v) = 2m H_{m-1}(v). \tag{B.61}$$

Substituting the eigenfunction expansion (B.56) into the 1D version of equation (B.53), one obtains a differential equation for the coefficients of the form

$$\frac{d^2 C_m^{(n)}}{dx^2} - 2m C_m^{(n)} = \frac{d}{dx}\left[C_{m-1}^{(n-1)} + 2(m+1) C_{m+1}^{(n-1)}\right]. \tag{B.62}$$

This is supplemented by boundary conditions at $x = \pm L$, which are obtained by expressing the spatial component of the steady-state flux as

$$J_x(x,v) = \sum_{n=0}^{\infty} \varepsilon^n \sum_{m \geq 0} \left[C_{m-1}^{(n-1)}(x) + 2(m+1) C_{m+1}^{(n-1)}(x) - \frac{dC_m^{(n)}(x)}{dx}\right] \mathrm{e}^{-v^2} H_m(v) \tag{B.63}$$

Setting $J_x(x,v) = 0$ at $x = \pm L$ and using the orthogonality condition (B.60) implies that

$$\left\{C_{m-1}^{(n-1)}(x)+2(m+1)C_{m+1}^{(n-1)}(x)-\frac{dC_m^{(n)}(x)}{dx}\right\}\Big|_{x=\pm L}=0. \tag{B.64}$$

with $C_{-1}^{(n-1)}\equiv 0$. Finally, note that the coefficients $C_m^{(0)}$ are obtained by solving the zeroth-order equation

$$\frac{\partial^2 p^{(0)}}{\partial x^2}+\frac{\partial^2 p^{(0)}}{\partial v^2}+2\frac{\partial}{\partial v}(vp^{(0)})=0, \quad x>0 \tag{B.65a}$$

$$\left.\frac{\partial p^{(0)}(x,v)}{\partial x}\right|_{x=\pm L}=0. \tag{B.65b}$$

It follows that

$$C_m^{(0)}(x)=N\delta_{m,0}, \quad N=\frac{1}{2L\sqrt{\pi}}. \tag{B.66}$$

Setting $n=1$ in equation (B.62) implies that $C_m^{(1)}(x)=C^{(1)}(x)\delta_{m,1}$ with

$$\frac{d^2C^{(1)}(x)}{dx^2}-2C^{(1)}(x)=0, \quad \left.\frac{dC^{(1)}(x)}{dx}\right|_{x=\pm L}=N. \tag{B.67}$$

Hence,

$$C_m^{(1)}(x)=\frac{N\sqrt{2}\sinh(\sqrt{2}x)}{2\cosh(\sqrt{2}L)}\delta_{m,1}. \tag{B.68}$$

In order to determine the coefficients $n\geq 2$ we have to impose the conservation conditions

$$\int_0^L C_m^{(n)}(x)dx=0. \tag{B.69}$$

This gives, for example,

$$C_0^{(2)}(x)=N\left[\frac{\cosh(\sqrt{2}x)}{\cosh(\sqrt{2}L)}-\frac{\tanh(\sqrt{2}x)}{\sqrt{2}L}\right]. \tag{B.70}$$

Combining the various results yields the leading order approximation

$$p(x,v)\approx\frac{e^{-v^2}}{2L\sqrt{\pi}}\left[1+\varepsilon H_1(v)\frac{\sqrt{2}\sinh(\sqrt{2}x)}{2\cosh(\sqrt{2}L)}\right.$$
$$\left.+\varepsilon^2\left[\frac{\cosh(\sqrt{2}x)}{\cosh(\sqrt{2}L)}-\frac{\tanh(\sqrt{2}x)}{\sqrt{2}L}+C_2^{(2)}H_2(v)\right]\right], \quad x\in[0,L], \tag{B.71}$$

Finally, integrating with respect to v gives the marginal density

$$p(x)\approx\frac{1}{2L}\left[1+\varepsilon^2\left[\frac{\cosh(\sqrt{2}x)}{\cosh(\sqrt{2}L)}-\frac{\tanh(\sqrt{2}x)}{\sqrt{2}L}\right]\right], \quad x\in[0,L], \tag{B.72}$$

The resulting density profile consists of an enhancement of the density at either wall combined with a depletion at the center of the domain.

Higher spatial dimensions

Analogous results hold for $d > 1$ [60]. For example, the function defined by $F_{\mathbf{m}}(\mathbf{v}) = \mathrm{e}^{-\mathbf{v}^2}\prod_{i=1}^d H_{m_i}(v_i)$ satisfies the higher-dimensional eigenvalue equation

$$\mathbb{L}_{\mathbf{v}}F_{\mathbf{m}} = \nabla_{\mathbf{v}}^2 F_{\mathbf{m}} + 2\nabla_{\mathbf{v}}\cdot(\mathbf{v}F_{\mathbf{m}}) = -2(m_1+\ldots m_d)F_{\mathbf{m}}. \tag{B.73}$$

Moreover, the coefficients $C_{\mathbf{m}}^{(n)}$ satisfy a Helmholtz-type equation of the form

$$\nabla_{\mathbf{x}}^2 C_{\mathbf{m}}^{(n)} - 2\left(\sum_{i=1}^d m_i\right)C_{\mathbf{m}}^{(n)} = \nabla_{\mathbf{x}}\cdot\mathbf{w}, \tag{B.74}$$

with

$$w_j = C_{\mathbf{m};m_{j-1}}^{(n-1)} + 2(m_j+1)C_{\mathbf{m};m_{j+1}}^{(n-1)}, \tag{B.75}$$

and

$$C_{\mathbf{m};m_{j\pm1}}^{(n-1)} = C_{m_1,\ldots,m_j\pm1,\ldots,m_d}^{(n-1)}. \tag{B.76}$$

The corresponding boundary conditions for the coefficients $C_{\mathbf{m}}^{(n)}(\mathbf{x})$ are determined by setting $J(\mathbf{x},\mathbf{v}) = 0$ for all $\mathbf{x}\in\partial\Omega$ with

$$J_{\mathbf{x}}(\mathbf{x},\mathbf{v}) = \sum_{n=0}^{\infty}\varepsilon^n\sum_{\mathbf{m}}[\mathbf{w}-\nabla_{\mathbf{x}}C_m^{(n)}(\mathbf{x})]\mathrm{e}^{-\mathbf{v}^2}\prod_{i=1}^d H_{m_i}(v_i), \tag{B.77}$$

and using the orthogonality condition (B.60).

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