3. Dissipative systems in physical space

In the strong friction limit $\xi \to +\infty$, we can formally neglect the inertial term $d\mathbf{v}_i/dt$ in Eq. (16) and we obtain the overdamped Langevin equations

$$\xi \frac{d\mathbf{r}_i}{dt} = -\frac{1}{m}\frac{\partial H}{\partial \mathbf{r}_i} + \sqrt{2D}\mathbf{R}_i(t). \tag{23}$$

The statistical equilibrium state of this system (described by the canonical ensemble [9]) is obtained by solving the minimization problem

$$\min_{\rho} \{F[\rho]\,|\,M[\rho]=M\}, \tag{24}$$

with

$$F = \frac{1}{2}\int \rho(\mathbf{r},t)u(\mathbf{r},\mathbf{r}')\rho(\mathbf{r}',t)\,d\mathbf{r}d\mathbf{r}' + \int \rho V\,d\mathbf{r} + k_B T\int \frac{\rho}{m}\ln\frac{\rho}{m}\,d\mathbf{r}. \tag{25}$$

Writing the variational principle as

$$\delta F + \alpha T\delta M = 0, \tag{26}$$

we obtain the mean field Boltzmann distribution (11). This critical point is a (local) minimum of free energy at fixed mass iff

$$\delta^2 F = \frac{1}{2}\int \delta\rho\delta\Phi\,d\mathbf{r} + \frac{k_B T}{m}\int \frac{(\delta\rho)^2}{2\rho}\,d\mathbf{r} \geq 0, \tag{27}$$

for all perturbations $\delta\rho$ that conserves mass.

In the mean field approximation, the evolution of the density profile $\rho(\mathbf{r},t)$ is governed by a kinetic equation of the form

$$\frac{\partial\rho}{\partial t} = \nabla\cdot\left[\frac{1}{\xi}\left(\frac{k_B T}{m}\nabla\rho + \rho\nabla\Phi\right)\right], \tag{28}$$

coupled to the mean field equation (14). This is called the mean field Smoluchowski equation. The mean field Smoluchowski equation (28) conserves mass and satisfies an H-theorem for the Boltzmann free energy (25), i.e. $\dot{F} \leq 0$ with an equality iff ρ is the Boltzmann distribution (11). Furthermore, the Boltzmann distribution is dynamically stable iff it is a (local) minimum of free energy at fixed mass. Therefore, the kinetic equation (28) is consistent with the minimization problem (24) describing the statistical equilibrium state of the system in CE.

Remark 1: the Smoluchowski equation (28) can also be deduced from the Kramers equation (21) in the strong friction limit [46]. For $\xi, D \to +\infty$ and $\beta = \xi/Dm$ finite, the time-dependent distribution function $f(\mathbf{r},\mathbf{v},t)$ is Maxwellian

$$f(\mathbf{r},\mathbf{v},t) = \left(\frac{\beta m}{2\pi}\right)^{d/2}\rho(\mathbf{r},t)e^{-\beta m\frac{v^2}{2}} + O(1/\xi), \tag{29}$$

and the time-dependent density $\rho(\mathbf{r},t)$ is solution of the Smoluchowski equation (28). Using Eq. (29), we can express the free energy (18) as a functional of the density and we obtain the free energy (25) up to some unimportant constants.

Remark 2: it is shown in Appendix A that the maximization problems (17) and (24) are equivalent in the sense that $f(\mathbf{r},\mathbf{v})$ is solution of (17) iff $\rho(\mathbf{r})$ is solution of (24). Thus, we have

$$(17) \Leftrightarrow (24). \tag{30}$$

As a consequence, the Maxwell-Boltzmann distribution $f(\mathbf{r},\mathbf{v})$ is dynamically stable with respect to the mean field Kramers equation (21) iff the corresponding Boltzmann distribution $\rho(\mathbf{r})$ is dynamically stable with respect to the mean field Smoluchowski equation (28). On the other hand, according to the implication (22), the Maxwell-Boltzmann distribution $f(\mathbf{r},\mathbf{v})$ is dynamically stable with respect to the kinetic equation (13) if it is stable with respect to the mean field Kramers equation (21), but the reciprocal is wrong in case of ensembles inequivalence.

4. The Keller-Segel model of chemotaxis

The Keller-Segel model [3] describing the chemotaxis of biological populations can be written as

$$\frac{\partial\rho}{\partial t} = \nabla\cdot(D\nabla\rho - \chi\rho\nabla c), \tag{31}$$

$$\frac{1}{D'}\frac{\partial c}{\partial t} = \Delta c - k^2 c + \lambda\rho, \tag{32}$$

where ρ is the concentration of the biological species (e.g. bacteria) and c is the concentration of the secreted chemical. The bacteria diffuse with a diffusion coefficient D and undergo a chemotactic drift with strength χ along the gradient of chemical. The chemical is produced by the bacteria at a rate $D'\lambda$, is degraded at a rate $D'k^2$ and diffuses with a diffusion coefficient D'. We adopt Neumann boundary conditions [3]:

$$\nabla c\cdot\mathbf{n} = 0, \qquad \nabla\rho\cdot\mathbf{n} = 0, \tag{33}$$

where $\mathbf{n}$ is a unit vector normal to the boundary of the domain. The drift-diffusion equation (31) is similar to the mean field Smoluchowski equation (28) where the concentration of chemical $-c(\mathbf{r},t)$ plays the role of the potential $\Phi(\mathbf{r},t)$. Therefore, there exists many analogies between chemotaxis and Brownian particles in interaction [6]. In particular, the effective statistical ensemble associated with the Keller-Segel model is the canonical ensemble. The steady states of the Keller-Segel model are of the form

$$\rho = Ae^{\frac{\chi}{D}c}, \tag{34}$$