Random transitions described by the stochastic Smoluchowski-Poisson system and by the stochastic Keller-Segel model

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We study random transitions between two metastable states that appear below a critical temperature in a one dimensional self-gravitating Brownian gas with a modified Poisson equation experiencing a second order phase transition from a homogeneous phase to an inhomogeneous phase [P.H. Chavanis and L. Delfini, Phys. Rev. E 81, 051103 (2010)]. We numerically solve the N-body Langevin equations and the stochastic Smoluchowski-Poisson system which takes fluctuations (finite N effects) into account. The system switches back and forth between the two metastable states (bistability) and the particles accumulate successively at the center or at the boundary of the domain. We explicitly show that these random transitions exhibit the phenomenology of the ordinary Kramers problem for a Brownian particle in a double-well potential. The distribution of the residence time is Poissonian and the average lifetime of a metastable state is given by the Arrhenius law, i.e. it is proportional to the exponential of the barrier of free energy $\Delta F$ divided by the energy of thermal excitation $k_B T$. Since the free energy is proportional to the number of particles $N$ for a system with long-range interactions, the lifetime of metastable states scales as $e^N$ and is considerable for $N \gg 1$. As a result, in many applications, metastable states of systems with long-range interactions can be considered as stable states. However, for moderate values of $N$, or close to a critical point, the lifetime of the metastable states is reduced since the barrier of free energy decreases. In that case, the fluctuations become important and the mean field approximation is no more valid. This is the situation considered in this paper. By an appropriate change of notations, our results also apply to bacterial populations experiencing chemotaxis in biology. Their dynamics can be described by a stochastic Keller-Segel model that takes fluctuations into account and goes beyond the usual mean field approximation.

I. INTRODUCTION

The theory of Brownian motion is an important topic in physics [1]. In most studies, the Brownian particles do not interact, or have short-range interactions. When an overdamped Brownian particle evolves in a double-well potential $V(x)$ (i.e. a potential with two minima and a maximum), it undergoes random transitions between the minima of the potential (metastable states). The position $x(t)$ of the particle switches back and forth between the location of the minima and presents a phenomenon of bistability. The distribution $P(x, t)$ of the position of the particle is governed by a Fokker-Planck equation called the Smoluchowski equation. At equilibrium, we get the Boltzmann distribution $P(x) = Z(\beta)^{-1} e^{-\beta V(x)}$ which is bimodal. The transition probability between the two minima, or the escape time, has been determined by Kramers in a famous paper [2, 5]. It is given by the Arrhenius law $e^{\Delta V/k_B T}$ where $\Delta V = V_{\text{max}} - V_{\text{min}}$ is the difference of potential between the metastable state (minimum) and the unstable state (maximum). Furthermore, the distribution of the residence time of the system in the metastable states is Poissonian.

The study of Brownian particles with long-range interactions (corresponding to the canonical ensemble) is a challenging problem [2, 5]. A system of fundamental interest is the self-gravitating Brownian gas model studied in [9]. This model may be relevant to describe the dynamics of dust particles in the solar nebula (where the particles experience a friction with the gas and a stochastic force due to small-scale turbulence) and the formation of planetesimals by gravitational collapse [10]. In the strong friction limit $\xi \rightarrow +\infty$, and in the thermodynamic limit $N \rightarrow +\infty$, the evolution of the density of the self-gravitating Brownian gas is described by the Smoluchowski equation coupled to the Poisson equation. In a space of dimension $d \geq 2$, these equations display a phenomenon of isothermal collapse [9] below a critical temperature $T_c$ leading to the formation of a Dirac peak [11]. By contrast, in $d = 1$, there is no collapse and the density always reaches a stable steady state [9].

Interestingly, the Smoluchowski-Poisson (SP) system is closely related to the Keller-Segel (KS) model that describes the chemotaxis of bacterial populations in biology [12]. In this model, the bacteria undergo Brownian motion (diffusion) but they also secrete a chemical substance (a sort of pheromone) and are collectively attracted by it. It turns out that this long-range interaction is similar to the gravitational interaction in astrophysics [13, 14]. As a result, the KS model displays a phenomenon of chemotactic collapse in $d \geq 2$ leading to Dirac peaks. Actually, the KS model is more general than the SP system because the Poisson equation is replaced by a reaction-diffusion equation. In certain approximations (no degradation and large diffusivity of the secreted chemical) the reaction-diffusion equation can be reduced to a modified Poisson equation that includes a sort of “neutralizing background” (similar to the Jellium model of a plasma). As a result, a spatially homogeneous distribution of particles is always a steady state of the KS.
model, which is not the case for the ordinary SP system. This analogy prompts us to consider a model of self-gravitating Brownian particles with a modified Poisson equation \[10\]. By an appropriate change of notations, this "gravitational" model can be mapped onto a "chemotactic" model. In that model, a spatially homogeneous phase exists at any temperature but it becomes unstable below a critical temperature \(T^*_c\) where it is replaced by an inhomogeneous (clustered) phase. This second order phase transition exists in any dimension of space including the dimension \(d = 1\). This is interesting because the usual SP system does not present any phase transition in \(d = 1\) \[9\]. In \(d \geq 2\), this second order phase transition at \(T^*_c\) adds to the isothermal collapse at \(T_c\) described above. A detailed study of phase transitions in this model has been performed in \[16\] in various dimensions of space.

The inhomogeneous (clustered) phase that appears below \(T^*_c\) is degenerate. The particles may accumulate either at the center of the domain \((r = 0)\) or at the boundary of the domain \((r = R)\). These two configurations correspond to local minima of the mean field free energy \(F[\rho]\) at fixed mass, where \(\rho(r)\) is the density field. Since the phase transition is second order, these two minima are at the same height. On the other hand, the unstable homogeneous phase \(\rho = M/V\) corresponds to a saddle point of free energy. In the \(N \rightarrow +\infty\) limit, the evolution of the system is described by the deterministic SP system (with the modified Poisson equation). For \(T < T^*_c\) this equation relaxes towards one of the two metastable states (the choice depends on the initial condition and on a notion of basin of attraction) and remains in that state for ever. However, if we take finite \(N\) effects into account, there are fluctuations, and the system undergoes random transitions between the two metastable states. These fluctuations are particularly important close to the critical point \(T^*_c\) where the barrier of free energy \(\Delta F\) to overcome is small.\(^2\)

In this paper, we study these random transitions by numerically solving the \(N\)-body Langevin equations and the stochastic SP system in \(d = 1\) (with the modified Poisson equation). The stochastic SP system takes fluctuations into account by including a noise term whose strength is proportional to \(1/\sqrt{N}\). We investigate the random transitions between the two metastable states and show that they follow the phenomenology of the Kramers problem for a Brownian particle in a double-well potential. The equilibrium distribution of the density is \(P[\rho] = Z(\beta)^{-1}e^{-\beta F[\rho]}\) which is bimodal. The system switches back and forth between the two metastable states (bistability) and the particles accumulate successively at the center or at the boundary of the domain. The difference with the Kramers problem is that our stochastic variable is a density field \(\rho(x, t)\) instead of the position \(x(t)\) of a particle. Furthermore, in our problem, the \(N\) particles interact collectively and create their own free energy landscape while in the usual Kramers problem a unique particle (or a set of non-interacting particles) moves in an externally imposed potential \(V(x)\). These analogies and differences with the Kramers problem make the present model interesting to study. We show that the distribution of the residence time \(P(\tau)\) is Poissonian and that the average time \(\langle \tau \rangle\) spent by the system in a metastable state is given by the Arrhenius law \(e^{\Delta F/k_B T}\) where \(\Delta F = F_{\text{saddle}} - F_{\text{meta}}\) is the difference of free energy between the metastable state (minimum) and the unstable state (saddle point). Since the free energy \(F\) scales as \(N\) for systems with long-range interactions, this implies that the lifetime of the metastable states generally scales as \(e^N\) because close to a critical point where the barrier of free energy \(\Delta F\) is small (this result was previously reported in \[21\]–\[23\]). Therefore, when \(N \gg 1\) the metastable states have considerably long lifetimes and they may be considered as stable states in practice.\(^3\) The probability to pass from one metastable state to the other is a rare event since it scales as \(e^{-N}\). Random transitions between metastable states can be seen only close to the critical point, for moderate values of \(N\), and for sufficiently long times. This result also implies that the limits \(N \rightarrow +\infty\) and \(T \rightarrow T^*_c\) do not commute. Indeed, since there is no homogeneous phase in that case \[20\]. In \(d \geq 3\), the system develops a gravothermal catastrophe below a critical energy \(E_c\) leading to a binary star surrounded by a hot halo. In \(d = 1\) and \(d = 2\) there is no collapse and the system reaches an inhomogeneous statistical equilibrium state.

\(^1\) In astrophysics, when we consider the dynamical stability of an infinite homogeneous self-gravitating system, we have to do the so-called "Jeans swindle" \[15\]. There is no such swindle in the context of chemotaxis \[13\].

\(^2\) We expect similar results in the microcanonical ensemble for isolated self-gravitating systems with a modified Poisson equation. In that case, two degenerate metastable states appear below a critical energy \(E^*_c\) \[10\]. The system undergoes random transitions between these metastable states that are controlled by the barrier of entropy \(\Delta S\) instead of the barrier of free energy \(\Delta F\). For Hamiltonian self-gravitating systems the noise is due only to finite \(N\) effects while for self-gravitating Brownian particles it is due both to the stochastic force and to finite \(N\) effects. Furthermore, before reaching the statistical equilibrium state (and undergoing random transitions), isolated self-gravitating systems may be stuck in non-Boltzmannian quasi stationary states (QSSs) \[17\]–\[19\] while self-gravitating Brownian particles in the overdamped limit directly relax towards the Boltzmann statistical equilibrium state (and undergo random transitions) without forming QSSs. Finally, the dynamical behavior of isolated self-gravitating systems with the usual Poisson equation is very different from their evolution with the modified Poisson equation.

\(^3\) This result has important consequences in astrophysics where the number of stars in a globular cluster may be as large as \(10^6\) \[15\], resulting in a lifetime of the metastable states of the order of \(\epsilon t_{\text{dyn}}\) where \(t_{\text{dyn}}\) is the dynamical time. The probability to cross the barrier of entropy is exponentially small since it requires very particular correlations. As a result, self-gravitating systems may be found in long-lived metastable states (local entropy maxima) although there is no statistical equilibrium state (global entropy maximum) in a strict sense (see \[20\]–\[23\] for more detail). In reality, the lifetime of globular clusters is ultimately controlled by the processes of evaporation and core collapse \[13\].
close to the critical point, the fluctuations become important and the mean field approximation is no more valid (or requires a larger and larger number of particles as $T \to T_\ast^\ast$).

The paper is organized as follows. In Sec. II we review the basic equations describing a gas of Brownian particles with long-range interactions in the overdamped limit. The equation of main interest is the stochastic Smoluchowski equation \([50]\) that takes fluctuations (finite $N$ effects) into account. In the $N \to +\infty$ limit, the fluctuations become negligible and we recover the mean field Smoluchowski equation \([40]\). In Sec. III we apply these equations to self-gravitating Brownian particles and bacterial populations with a modified Poisson equation. In Sec. IV we specifically consider the dimension $d = 1$ where a second order phase transition between a homogeneous phase and an inhomogeneous (clustered phase) appears below a critical temperature $T_c^\ast$. We numerically solve the modified stochastic Smoluchowski-Poisson system \([66]-[67]\) and describe random changes between the two metastable states below $T_c^\ast$. We characterize these transitions and show that they display a phenomenology similar to the standard Kramers problem. We also present results from direct $N$-body simulations.

II. OVERDAMPED BROWNIAN PARTICLES WITH LONG-RANGE INTERACTIONS

A. The Langevin equations

We consider a system of $N$ Brownian particles in interaction. The dynamics of these particles is governed by the coupled stochastic Langevin equations

\[
\frac{d\mathbf{r}_i}{dt} = \mathbf{v}_i, \\
\frac{d\mathbf{v}_i}{dt} = -\frac{1}{m} \nabla_i U(\mathbf{r}_1, ..., \mathbf{r}_N) - \xi \mathbf{v}_i + \sqrt{2D} \mathbf{R}_i(t). \tag{1}
\]

The particles interact through the potential $U(\mathbf{r}_1, ..., \mathbf{r}_N) = \sum_{i < j} m v_i^2/2 + U(\mathbf{r}_1, ..., \mathbf{r}_N)$. $\mathbf{R}_i(t)$ is a Gaussian white noise satisfying $\langle \mathbf{R}_i(t) \rangle = 0$ and $\langle R_i^\alpha(t) R_j^\beta(t') \rangle = \delta_{ij} \delta_{\alpha\beta} \delta(t - t')$ where $i = 1, ..., N$ label the particles and $\alpha = 1, ..., d$ the coordinates of space. $D$ and $\xi$ are respectively the diffusion and friction coefficients. The former measures the strength of the noise, whereas the latter quantifies the dissipation to the external environment. We assume that these two effects have the same physical origin, like when the system interacts with a heat bath. In particular, we suppose that the diffusion and friction coefficients satisfy the Einstein relation

\[
D = \frac{\xi k_B T}{m}, \tag{2}
\]

where $T$ is the temperature of the bath. The temperature measures the strength of the stochastic force (for a given friction coefficient). For $\xi = D = 0$, we recover the Hamiltonian equations of particles in interaction which conserve the energy $E = H$.

B. The strong friction limit

In the strong friction limit $\xi \to +\infty$, the inertia of the particles can be neglected. This corresponds to the overdamped Brownian model. In this paper, we restrict ourselves to this model.\(^4\) The stochastic Langevin equations \((1)\) reduce to

\[
\frac{d\mathbf{r}_i}{dt} = -\mu \nabla_i U(\mathbf{r}_1, ..., \mathbf{r}_N) + \sqrt{2D} \mathbf{R}_i(t), \tag{3}
\]

where $\mu = 1/(\xi m)$ is the mobility and $D_\ast = D/\xi$ is the diffusion coefficient in physical space. The Einstein relation \((2)\) may be rewritten as

\[
D_\ast = \frac{k_B T}{\xi m} = \mu k_B T. \tag{4}
\]

The temperature measures the strength of the stochastic force (for a given mobility).

C. The $N$-body Smoluchowski equation

The evolution of the $N$-body distribution function $P_N(\mathbf{r}_1, ..., \mathbf{r}_N, t)$ is governed by the $N$-body Fokker-Planck equation \([5]\):

\[
\frac{\partial P_N}{\partial t} = \sum_{i=1}^{N} \frac{\partial}{\partial \mathbf{r}_i} \left[ D_\ast \frac{\partial P_N}{\partial \mathbf{r}_i} + \mu P_N \frac{\partial}{\partial \mathbf{r}_i} U(\mathbf{r}_1, ..., \mathbf{r}_N) \right]. \tag{5}
\]

This is the so-called $N$-body Smoluchowski equation. It can be derived directly from the stochastic equations \([3]\). The $N$-body Smoluchowski equation satisfies an H-theorem for the free energy

\[
F[P_N] = \int P_N U d\mathbf{r}_1 ... d\mathbf{r}_N + k_B T \int P_N \ln P_N d\mathbf{r}_1 ... d\mathbf{r}_N \\
- \frac{d}{2} N k_B T \ln \left( \frac{2\pi k_B T}{m} \right). \tag{6}
\]

A simple calculation gives

\[
\hat{F} = -\sum_{i=1}^{N} \int \frac{m}{\xi P_N} \left( \frac{k_B T}{m} \frac{\partial P_N}{\partial \mathbf{r}_i} + \frac{1}{m} P_N \frac{\partial U}{\partial \mathbf{r}_i} \right)^2 d\mathbf{r}_1 ... d\mathbf{r}_N. \tag{7}
\]

Therefore, $\hat{F} \leq 0$ and $\hat{F} = 0$ if, and only if, $P_N$ is the canonical distribution in physical space defined by

\(^4\) The inertial Brownian model, and its connection to the overdamped Brownian model, is further discussed in \([8]\).
Eq. (10) below. Because of the $H$-theorem, the system converges towards the canonical distribution (10) for $t \to +\infty$.

We note that the free energy may be written as $F[P_N] = E[P_N] - TS[P_N]$ where

$$E[P_N] = \frac{d}{2}Nk_BT + \int P_N U \, dr_1...dr_N, \quad (8)$$

$$S[P_N] = -k_B \int P_N \ln P_N \, dr_1...dr_N$$

are the energy and the entropy [8].

D. The canonical distribution

The statistical equilibrium state of the Brownian particles in interaction is described by the canonical distribution [8]:

$$P_N(r_1, ..., r_N) = \frac{1}{Z(\beta)} \left( \frac{2\pi}{\beta m} \right)^{dN/2} e^{-\beta U(r_1, ..., r_N)}, \quad (10)$$

where

$$Z(\beta) = \left( \frac{2\pi}{\beta m} \right)^{dN/2} \int e^{-\beta U(r_1, ..., r_N)} \, dr_1...dr_N \quad (11)$$

is the partition function determined by the normalization condition $\int P_N \, dr_1,...,dr_N = 1$. The canonical distribution (10) is the steady state of the $N$-body Smoluchowski equation [4] provided that the Einstein relation [4] is satisfied. It gives the probability density of the microstate $\{r_1, ..., r_N\}$. The free energy is defined by $F(T) = -k_BT \ln Z(T)$. We note that the canonical distribution (10) is the minimum of $F[P_N]$ respecting the normalization condition. At equilibrium, we have $F[P_N] = -k_BT \ln Z(T) = F(T)$.

E. The Yvon-Born-Green (YBG) hierarchy

We introduce the reduced probability distributions

$$P_j(r_1, ..., r_j) = \int P_N(r_1, ..., r_N) \, dr_{j+1}...dr_N. \quad (12)$$

Differentiating the defining relation (12) for $P_j$ and using Eq. (10), we obtain the YBG hierarchy of equations [4] [24]:

$$\frac{\partial P_j}{\partial r_1}(r_1, ..., r_j) = -\beta m^2 P_j(r_1, ..., r_j) \sum_{i=2}^j \frac{\partial u_{1,i}}{\partial r_1}$$

$$-\beta m^2 (N-j) \int P_{j+1}(r_1, ..., r_{j+1}) \frac{\partial u_{1,j+1}}{\partial r_1} \, dr_{j+1}; \quad (13)$$

where we have noted $u_{i,j}$ for $u(|r_i - r_j|)$. The first equation of the YBG hierarchy is

$$\frac{\partial P_1}{\partial r_1}(r_1) = -\beta m^2 (N-1) \int P_2(r_1, r_2) \frac{\partial u_{1,2}}{\partial r_1} \, dr_2, \quad (14)$$

where $P_1(r_1)$ is the one-body distribution function and $P_2(r_1, r_2)$ is the two-body distribution function. This equation is exact but it is not closed.

We now consider a system with long-range interactions. The proper thermodynamic limit $N \to +\infty$ amounts to writing the Hamiltonian in the rescaled form

$$H = \frac{1}{2} \sum_{i} \frac{1}{2} m v_i^2 + \frac{1}{N} \sum_{i<j} m^2 \hat{u}_{ij} \quad (15)$$

with $r \sim t \sim v \sim m \sim \hat{u} \sim 1$. The factor $1/N$ in front of the potential energy corresponds to the Kac scaling [25]. With this scaling $E \sim N$, $T \sim 1$, $S \sim N$, and $F \sim N$. The energy is extensive but it remains fundamentally non-additive. For $N \to +\infty$ we can neglect the correlations between the particles [26]. Therefore, the mean field approximation is exact and the $N$-body distribution function can be factorized in a product of $N$ one-body distribution functions

$$P_N(r_1, ..., r_N) = P_1(r_1)...P_1(r_N). \quad (16)$$

In particular, $P_2(r_1, r_2) = P_1(r_1) P_1(r_2)$. In that case, the first equation of the YBG hierarchy reduces to

$$\frac{\partial P_1}{\partial r_1}(r_1) = -\beta m^2 N P_1(r_1) \int P_1(r_2) \frac{\partial u_{1,2}}{\partial r_1} \, dr_2. \quad (17)$$

Introducing the average density $\rho(r) = \langle \sum_i m \delta(r-r_i) \rangle = N m P_1(r)$, we get

$$\frac{k_BT}{m} \nabla \rho(r) = -\rho(r) \int \rho(r') \nabla u(|r-r'|) \, dr', \quad (18)$$

where we used the fact that the particles are identical. Integrating this equation, we obtain the integral equation

$$\rho(r) = A e^{-\beta m \Phi(r)}, \quad (19)$$

determining the equilibrium density profile. It can be rewritten as a mean field Boltzmann distribution

$$\rho(r) = A e^{-\beta m \Phi(r)}, \quad (20)$$

where $\Phi(r)$ is the self-consistent mean field potential given by

$$\Phi(r) = \int u(|r-r'|) \rho(r') \, dr'. \quad (21)$$

The constant of integration $A$ is determined by the normalization condition $\int P_1(r_1) \, dr_1 = 1$ or equivalently by the mass constraint

$$M[\rho] = \int \rho \, dr. \quad (22)$$

We also note that, in the mean field approximation, the average potential energy is given by

$$W[\rho] = \frac{1}{2} \int \rho \Phi \, dr. \quad (23)$$
F. The distribution of the smooth density

We wish to determine the equilibrium distribution of the smooth (coarse-grained) density \( \rho(\mathbf{r}) \) in position space.\(^5\) A microstate is defined by the specification of the exact positions \( \{ \mathbf{r}_i \} \) of the \( N \) particles. A macrostate is defined by the specification of the density \( \rho(\mathbf{r}) \) of particles in each cell \( [\mathbf{r}, \mathbf{r} + d\mathbf{r}] \) irrespectively of their precise position in the cell. Let us call \( \Omega[\rho] \) the unconditional number of microstates \( \{ \mathbf{r}_i \} \) corresponding to the macrostate \( \rho(\mathbf{r}) \). The unconditional entropy of the macrostate \( \rho(\mathbf{r}) \) is defined by the Boltzmann formula

\[
S_0[\rho] = k_B \ln \Omega[\rho]. \tag{24}
\]

The unconditional probability density of the density \( \rho(\mathbf{r}) \) is therefore \( P_0[\rho] \propto \Omega[\rho] \propto e^{S_0[\rho]/k_B} \). The number of complexities \( \Omega[\rho] \) can be obtained by a standard combinatorial analysis. For \( N \gg 1 \), when there is no microscopic constraints, using the Stirling formula, we find that the Boltzmann entropy is given by

\[
S_0[\rho] = -k_B \int \frac{d\rho}{m} \ln \left( \frac{\rho}{Nm} \right) \, d\mathbf{r}. \tag{25}
\]

This is the same expression as in a perfect gas since the interaction between particles does not appear at that stage.

To evaluate the partition function \([11]\), instead of integrating over the microstates \( \{ \mathbf{r}_i \} \), we can integrate over the macrostates \( \rho(\mathbf{r}) \). If we consider a system with long-range interactions so that a mean field approximation applies at the thermodynamic limit \( N \to +\infty \), introducing the unconditional number of microstates \( \Omega[\rho] \) corresponding to the macrostate \( \rho \) [see Eqs. (24) and (25)], and the potential energy \( W[\rho] \) of the macrostate \( \rho \) [see Eq. (23)], we obtain for \( N \gg 1 \):

\[
Z(\beta) \simeq e^{\frac{\beta}{2} \ln(\frac{\beta m}{\pi})} \int e^{-\beta \rho W[\rho]} \Omega[\rho] \delta(M[\rho] - M) \, d\rho
\]

\[
\simeq e^{\frac{\beta}{2} \ln(\frac{\beta m}{\pi})} \int e^{S_0[\rho]/k_B - \beta W[\rho]} \Omega[\rho] \delta(M[\rho] - M) \, d\rho
\]

\[
\simeq \int e^{-\beta F[\rho]} \delta(M[\rho] - M) \, d\rho, \tag{26}
\]

where the free energy \( F[\rho] \) is given by

\[
F[\rho] = \frac{1}{2} \int \rho \Phi \, d\mathbf{r} + k_B T \int \frac{\rho}{m} \ln \left( \frac{\rho}{Nm} \right) \, d\mathbf{r}
\]

\[
- \frac{dN}{2} k_B T \ln \left( \frac{2\pi k_B T}{m} \right). \tag{27}
\]

The canonical probability density of the distribution \( \rho \) is therefore

\[
P[\rho] = \frac{1}{Z(\beta)} e^{-\beta F[\rho]} \delta(M[\rho] - M). \tag{28}
\]

G. The most probable macrostate

For systems with long-range interactions, for which the mean field approximation is exact in the proper thermodynamic limit \( N \to +\infty \), we have the extensive scaling \( F \sim N \). Accordingly, writing \( F[\rho] = N f[\rho] \) where \( f \sim 1 \), the partition function \([20]\) may be written as

\[
Z(\beta) = \int e^{-\beta N f[\rho]} \delta(M[\rho] - M) \, d\rho. \tag{29}
\]

For \( N \to +\infty \), we can make the saddle point approximation. We obtain

\[
Z(\beta) = e^{-\beta F(\beta)} \simeq e^{-\beta N f[\rho_*]}, \tag{30}
\]

i.e.

\[
\lim_{N \to +\infty} \frac{1}{N} F(\beta) = f[\rho_*], \tag{31}
\]

where \( \rho_* \) is the global minimum of free energy \( F[\rho] \) at fixed mass. This corresponds to the most probable macrostate. We are led therefore to solving the minimization problem

\[
F(T) = \min_{\rho} \{ F[\rho] \mid M[\rho] = M \}. \tag{32}
\]

The previous results assume that there is a single global minimum of free energy at fixed mass. More generally, we shall be interested by possible local minima of free energy at fixed mass, which correspond to metastable states (the importance of these metastable states will be stressed in the sequel). The critical points of free energy at fixed mass are determined by the condition

\[
\delta F + k_B T \alpha \delta M = 0, \tag{33}
\]

where \( \alpha \) is a Lagrange multiplier associated with the conservation of mass. Performing the variations, we obtain the mean field Boltzmann distribution \([20]\) where \( A = Nme^{-\alpha m} \). A critical point of free energy at fixed mass is a (local) minimum if, and only if,

\[
\delta^2 F = k_B T \left( \int \frac{(\delta \rho)^2}{2\rho m} \, d\mathbf{r} + \frac{1}{2} \int \delta \rho \delta \Phi \, d\mathbf{r} \right) > 0 \tag{34}
\]

for all perturbations \( \delta \rho \) that conserve mass: \( \delta M = 0 \).

H. The mean field Smoluchowski equation

We now derive kinetic equations governing the evolution of the average density \( \rho(\mathbf{r}, t) \) of the Brownian gas in interaction. From the \( N \)-body Smoluchowski equation \([5]\), we can obtain the equivalent of the BBGKY hierarchy \([5]\):

\[
\frac{\partial P_j}{\partial t} = \sum_{i=1}^{j} \frac{\partial}{\partial \mathbf{r}_i} \left[ D_\ast \frac{\partial P_j}{\partial \mathbf{r}_i} + \mu m^2 P_j \sum_{k=1, k \neq i}^{j} \frac{\partial u_{i,k}}{\partial \mathbf{r}_i} \right] + (N - j) \mu m^2 \int P_{j+1} \frac{\partial u_{i,j+1}}{\partial \mathbf{r}_i} \, d\mathbf{r}_{j+1}. \tag{35}
\]

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\(^5\) The coarse-grained density should be noted \( \overline{\rho}(\mathbf{r}) \) \([6]\) \([7]\) but in order to simplify the notations we shall omit the bar.
The stationary solutions of these equations coincide with the equations (13) of the YBG hierarchy. The first equation of this hierarchy is

$$\frac{\partial P_1}{\partial t} = \frac{\partial}{\partial r_1} \left[ D_s \frac{\partial P_1}{\partial r_1} + \mu m^2 (N - 1) \int \frac{\partial \mu_{12}}{\partial r_1} P_2 \, dr_2 \right].$$

(36)

This equation is exact but it is not closed.

For systems with long-range interactions, we can neglect the correlations between the particles in the proper thermodynamic limit $N \to +\infty$ described previously [28]. Therefore, the mean field approximation is exact and the $N$-body distribution function can be factorized, at any time $t$, in a product of $N$ one-body distribution functions:

$$P_N(r_1, ..., r_N, t) = P_1(r_1, t)...P_1(r_N, t).$$

(37)

In particular, $P_2(r_1, r_2, t) = P_1(r_1, t)P_1(r_2, t)$. In that case, the first equation of the BBGKY hierarchy reduces to

$$\frac{\partial P_1}{\partial t} = \frac{\partial}{\partial r_1} \left[ D_s \frac{\partial P_1}{\partial r_1} + N \mu m^2 P_1(r_1, t) \int \frac{\partial \mu_{12}}{\partial r_1} P_2 \, dr_2 \right].$$

(38)

Therefore, the evolution of the average density $\rho(r, t) = \langle \sum_i m \delta(r - r_i(t)) \rangle = N \rho P_1(r, t)$ is governed by the integro-differential equation

$$\frac{\partial \rho}{\partial t} = D_s \rho + \mu m \nabla \cdot \left[ \rho \nabla \int u(|r - r'|) \rho(r', t) \, dr' \right].$$

(39)

In can be rewritten as a mean field Smoluchowski equation [5]:

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

(40)

where the self-consistent mean field potential $\Phi(r, t)$ is given by

$$\Phi(r, t) = \int u(|r - r'|) \rho(r', t) \, dr'.$$

(41)

The mean field Smoluchowski equation (40) satisfies an $H$-theorem for the mean field free energy (26) which can be obtained from Eq. (6) by using the mean field approximation (16). In terms of the free energy, the mean field Smoluchowski equation (40) can be written as a gradient flow

$$\frac{\partial \rho}{\partial t} = \nabla \cdot \left[ \frac{1}{\xi} \nabla \left( \frac{\delta F}{\delta \rho} \right) \right].$$

(42)

A simple calculation gives

$$\dot{F} = - \int \rho \left[ \nabla \left( \frac{\delta F}{\delta \rho} \right) \right] \, dr$$

$$= - \int \frac{1}{\xi \rho} \left( \frac{k_B T}{m} \nabla \rho + \rho \nabla \Phi \right)^2 \, dr.$$

(43)

Therefore, $\dot{F} \leq 0$ and $\dot{\hat{F}} = 0$ if, and only if, $\rho$ is the mean field Boltzmann distribution (20) with the temperature of the bath $T$. Because of the $H$-theorem, the system converges, for $t \to +\infty$, towards a mean-field Boltzmann distribution that is a (local) minimum of free energy at fixed mass. If several minima exist at the same temperature, the selection depends on a notion of basin of attraction.

We note that the mean field free energy (27) may be written as $F[\rho] = E[\rho] - TS[\rho]$ where

$$E[\rho] = \frac{d}{2} N k_B T + \frac{1}{2} \int \rho \Phi \, dr,$$

(44)

$$S[\rho] = -k_B \int \frac{\rho}{m} \ln \left( \frac{\rho}{N m} \right) \, dr$$

$$+ \frac{d}{2} N k_B \ln \left( \frac{2 \pi k_B T}{m} \right) + \frac{d}{2} N k_B$$

(45)

are the energy and the entropy [8].

I. The stochastic Smoluchowski equation

In the preceding section we have considered the mean field limit $N \to +\infty$ which amounts to neglecting the fluctuations. If the free energy $F[\rho]$ has several minima (metastable states), and if $N$ is finite, the system undergoes random transitions between the different metastable states due to fluctuations. It explores the whole free energy landscape and the distribution of the smooth (coarse-grained) density at equilibrium is given by Eq. (28). It is therefore important to describe the fluctuations (finite $N$ effects) giving rise to these random transitions.

Dean [28] has shown that the discrete density $\rho_d(r, t) = \sum_i m \delta(r - r_i(t))$ satisfies the stochastic equation

$$\frac{\partial \rho_d}{\partial t} = D_s \rho_d(r, t)$$

$$+ \mu m \nabla \cdot \left[ \rho_d(r, t) \nabla \int \rho_d(r', t) u(|r - r'|) \, dr' \right]$$

$$+ \nabla \cdot \left[ \sqrt{2D_s \rho_d(r, t) \mathbf{R}(r, t)} \right],$$

(46)

where $\mathbf{R}(r, t)$ is a Gaussian white noise such that $\langle \mathbf{R}(r, t) \rangle = 0$ and $\langle \mathbf{R}^\alpha(r, t) \mathbf{R}^\beta(r', t') \rangle = \delta_{\alpha\beta} \delta(r - r') \delta(t - t').$

6 The steady states of the mean field Smoluchowski equation are the critical points (minima, maxima, saddle points) of the free energy $F[\rho]$ at fixed mass. It can be shown [27] that a critical point of free energy is dynamically stable with respect to the mean field Smoluchowski equation if, and only if, it is a (local) minimum. Maxima are unstable for all perturbations so they cannot be reached by the system. Saddle points are unstable only for certain perturbations so they can be reached if the system does not spontaneously generate these dangerous perturbations.
This equation is exact and bears the same information as the \( N \)-body Langevin equations [3] or as the \( N \)-body Smoluchowski equation [5]. In this sense, it contains too much information. Furthermore, \( \rho_d(r,t) \) is a sum of Dirac \( \delta \)-functions which is not easy to handle in practice. If we take the ensemble average of Eq. (46) we obtain

\[
\frac{\partial \rho}{\partial t} = D, \Delta \rho + \mu m \nabla \cdot \int \langle \rho_d(r,t) \rho_d(r',t) \rangle \nabla u(|r-r'|) \, dr'.
\]

Using the identity

\[
\langle \rho_d(r,t) \rho_d(r',t) \rangle = N m^2 P_1(r,t) \delta(r-r') + N(N-1)m^2 P_2(r,r,t),
\]

we see that this equation is equivalent to the first equation (36) of the BBGKY hierarchy. However, these equations are not closed and they do not account for random transitions between metastable states since they have been averaged.

In previous papers [6, 7], we have argued that for systems with long-range interactions, the evolution of the smooth (coarse-grained) density \( \rho(r,t) \) is governed by the stochastic Smoluchowski equation

\[
\frac{\partial \rho}{\partial t} = D, \Delta \rho + \mu m \nabla \cdot \left[ \rho(r,t) \nabla \left( \nabla \cdot \int \rho(r',t) u(|r-r'|) \, dr' \right) \right] + \nabla \cdot \left[ \sqrt{2D, m \rho(r,t)} \mathbf{R}(r,t) \right].
\]

This equation can be obtained from the theory of fluctuating hydrodynamics (see Appendix B of [6]). Although it has a similar mathematical form as Eq. (46), this equation is fundamentally different from Eq. (46) since it applies to a smooth density \( \rho(r,t) \), not to a sum of \( \delta \)-functions. It is also different from Eqs. (36) and (47) since it is closed and not fully averaged. In a sense, it describes the evolution of the system at a mesoscopic level, intermediate between Eqs. (46) and (47) [6, 7].

Introducing the mean potential [11], the stochastic Smoluchowski equation takes the form

\[
\frac{\partial \rho}{\partial t} = \nabla \cdot \left[ \frac{1}{\xi} \left( \frac{k_B T}{m} \nabla \rho + \rho \nabla \Phi \right) \right] + \nabla \cdot \left( \frac{\sqrt{2k_B T \rho}}{\xi} \mathbf{R} \right).
\]

In terms of the mean field free energy (27), it can be rewritten as

\[
\frac{\partial \rho}{\partial t} = \nabla \cdot \left[ \rho \nabla \left( \frac{\delta F}{\delta \rho} \right) \right] + \nabla \cdot \left( \frac{2k_B T \rho}{\xi} \mathbf{R} \right).
\]

Eq. (51) may be interpreted as a stochastic Langevin equation for the field \( \rho(r,t) \). The corresponding Fokker-Planck equation for the probability density \( P[\rho, t] \) of the density profile \( \rho(r,t) \) at time \( t \) is

\[
\xi \frac{\partial P}{\partial t}[\rho, t] = -\int \frac{\delta}{\delta \rho(r,t)} \left\{ \nabla \cdot \rho \nabla \left[ k_B T \frac{\delta}{\delta \rho} + \frac{\delta F}{\delta \rho} \right] P[\rho, t] \right\} \, dr.
\]

Its stationary solution returns the canonical distribution [28] which shows the consistency of our approach. Actually, the form of the noise in Eq. (51) may be determined precisely in order to recover the distribution [28] at equilibrium. We note that the noise is multiplicative since it depends on \( \rho(r,t) \) (it vanishes in regions devoid of particles).

Using a proper scaling as in Eq. (15), it can be shown that the noise term in Eq. (50) is of order \( 1/\sqrt{N} \) so that it disappears in the \( N \to +\infty \) limit. In that case, Eq. (50) reduces to the mean field Smoluchowski equation (40). If the free energy \( F[\rho] \) has a single minimum, the mean field Smoluchowski equation relaxation towards this minimum (this corresponds to the most probable macrostate). If the free energy \( F[\rho] \) has several (local) minima, the mean field Smoluchowski equation relaxes towards one of these minima and stays there for ever. However, when \( N \) is finite, we must take fluctuations into account and use the stochastic Smoluchowski equation (50). This equation describes random transitions between the metastable states, establishing thecanonical distribution [25]. In this paper, we solve the stochastic Smoluchowski equation (50) for a system of self-gravitating Brownian particles with a modified Poisson equation. This system displays a second order phase transition below a critical temperature \( T_c^* \) so that the free energy \( F[\rho] \) has a double-well structure and the particles undergo random transitions between the two minima of this “potential”. This leads to a “barrier crossing problem” similar to the Kramers problem for the diffusion of an overdamped particle in a double well potential.

Remark: the stochastic Smoluchowski equation (51) is
different from the stochastic Ginzburg-Landau equation
\[
\frac{\partial \rho}{\partial t} = -\Gamma \frac{\delta F}{\delta \rho} + \sqrt{2\Gamma k_B T} \zeta(r, t),
\] (53)
where \(\zeta(r, t)\) is a Gaussian white noise, used to describe the time-dependent fluctuations about equilibrium. Eq. (53) is a phenomenological equation because, in general, it is an impossible task to derive the true equation for the macroscopic variables directly from the dynamics of the microscopic variables of the system [29]. However, for Brownian particles with long-range interactions, this task is realizable and leads to the stochastic Smoluchowski equation [51] instead of Eq. (53).

J. The lifetime of metastable states

The lifetime of a metastable state can be estimated by using an adaptation of the Kramers formula [1]. Let us assume that below \(T^*_c\) the free energy \(F[\rho]\) has two local minima \(F_{\text{meta}}\) at the same height (metastable states) separated by a saddle point \(F_{\text{saddle}}\) (unstable). This is the case for second order phase transitions. In order to pass from a metastable state to the other the system has to cross a barrier of free energy played by the saddle point. The distribution of the smooth (coarse-grained) density \(\rho(r)\) at a fixed temperature \(T\) is given by Eq. (28). For a system initially prepared in a metastable state \(\rho_{\text{meta}}(r)\) corresponding to the saddle point of free energy, it can then switch to the other metastable state. Therefore, the lifetime of a metastable state may be estimated by \(t_{\text{life}} \sim 1/F[\rho_{\text{saddle}}]\), i.e. \(t_{\text{life}} \sim e^{\Delta F}\) where \(\Delta F = F_{\text{saddle}} - F_{\text{meta}}\) is the barrier of free energy between the metastable state and the saddle point. For systems with long-range interactions, in the proper thermodynamic limit \(N \to +\infty\), the free energy is proportional to \(N\) so we can write \(F[\rho] = N f[\rho]\) where \(f[\rho] \sim 1\). Therefore, we obtain the estimate \(t_{\text{life}} \sim e^{N\beta \Delta f}\). (54)

Except in the vicinity of the critical point \(T^*_c\) where \(\Delta f \to 0\), the lifetime of a metastable state increases exponentially rapidly with the number of particles, as \(e^N\), and becomes infinite in the thermodynamic limit \(N \to +\infty\) [21–23]. Therefore, for systems with long-range interactions, metastable states have considerable lifetimes and they can be regarded as stable states in practice. The probability to pass from one metastable state to the other is a rare event even since it scales as \(e^{-N}\). Random transitions between the two metastable states will be seen only close to the critical point and/or for a sufficiently small number of particles (provided that we wait long enough).

Remark: of course, these results can be generalized if the free energy has a local minimum (metastable state) and a global minimum of free energy (stable state) separated by a saddle point. This is the case for first order phase transitions. The lifetime of the metastable and stable states are still given by Eq. (54). However, since the barrier of free energy between the saddle point and the stable state is larger than the barrier of free energy between the saddle point and the metastable state, the system will remain longer in the stable state than in the metastable state.

III. SELF-GRAVITATING BROWNIAN PARTICLES AND BACTERIAL POPULATIONS WITH A MODIFIED POISSON EQUATION

A. The Smoluchowski-Poisson system

We consider a system of self-gravitating Brownian particles in a space of dimension \(d\). In the \(N \to +\infty\) limit, we can ignore fluctuations. In that case, the evolution of the density of particles is governed by the Smoluchowski-Poisson system

\[
\xi \frac{\partial \rho}{\partial t} = \nabla \cdot \left( \frac{k_B T}{m} \nabla \rho + \rho \nabla \Phi \right),
\] (55)

\[
\Delta \Phi = S_d G \rho,
\] (56)

where \(S_d\) is the surface of a unit sphere in \(d\) dimensions. Its steady states are determined by the Boltzmann-Poisson equation

\[
\Delta \Phi = S_d G a e^{-\beta m \Phi}.
\] (57)

These equations have been studied in [9]. When the system is enclosed within a spherical box of radius \(R\) in order to prevent evaporation, the following results are found. In \(d = 3\), there is no global minimum of free energy. However, there exist a local minimum of free energy (metastable state) for \(T > T_c\) where \(T_c = GMm/(2.52 R k_B)\). For \(T < T_c\) there is no critical point of free energy and the system undergoes an isothermal collapse leading to a Dirac peak. In \(d = 2\), there exist a global minimum of free energy for \(T > T_c\) where
$T_c = GMm/(4k_B)$. For $T < T_c$ there is no critical point of free energy and the system undergoes an isothermal collapse leading to a Dirac peak. In $d = 1$, there exist a global minimum of free energy for any $T > 0$. We note that the equilibrium states of Eqs. (55)-(56) are spatially inhomogeneous. A homogeneous distribution is not a steady state of the ordinary SP system.

Following [16], we consider a slightly different model of gravitational dynamics where the Poisson equation (56) is replaced by the modified Poisson equation

$$\Delta \Phi = \rho - \bar{\rho},$$

(58)

where $\bar{\rho} = M/V$ is the mean density. The steady states of the modified Smoluchowski-Poisson system defined by Eqs. (55) and (58) are determined by the modified Boltzmann-Poisson equation

$$\Delta \Phi = \bar{\rho} (\rho - \bar{\rho}).$$

(59)

In that case, the uniform distribution $\rho = M/V$ and $\Phi = 0$ is a steady state of the modified SP system for all temperatures. However, this uniform distribution is stable only for $T > T_c^x(d)$, where $T_c^x(d)$ is a critical temperature depending on the dimension of space (see Sec. V of [16]). For $T < T_c^x(d)$ the system displays a second order phase transition from homogeneous to inhomogeneous states. In $d > 1$, this second order phase transition adds to the ordinary isothermal collapse below $T_c$ mentioned above. In $d = 1$, the modified SP system exhibits a second order phase transition while the usual SP system does not. These phase transitions have been discussed in detail in [16].

If we take fluctuations (finite $N$ effects) into account, the evolution of the density of particles is governed by the stochastic Smoluchowski equation

$$\xi \frac{\partial \rho}{\partial t} = \nabla \cdot \left( \frac{k_B T}{m} \nabla \rho + \rho \nabla \Phi \right) + \nabla \cdot \left( \sqrt{2\xi k_B T} \rho \mathbf{R} \right),$$

(60)

coupled to the Poisson equation (56) or to the modified Poisson equation (58). For $N \to +\infty$, we can ignore the last term in Eq. (60) and we recover the deterministic Smoluchowski equation (55). However, the stochastic Smoluchowski equation will be particularly relevant close to the critical points $T_c$ and $T_c^x$ where the mean field approximation is not valid due to the enhancement of fluctuations.

B. The Keller-Segel model

As discussed in [16], the Smoluchowski-Poisson system is connected to the Keller-Segel model describing the chemotaxis of bacterial populations in biology [12]. In general, the fluctuations are neglected leading to the deterministic Keller-Segel model

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

(61)

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

(62)

where $\rho(\mathbf{r}, t)$ is the density of bacteria and $c(\mathbf{r}, t)$ is the concentration of the secreted chemical (pheromone). The bacteria diffuse with a diffusion coefficient $D$ and they also experience a chemotactic drift with strength $\chi$ along the gradient of the 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 $D'$. In the limit of large diffusivity of the chemical ($D' \to +\infty$) and in the absence of degradation ($k = 0$), the reaction-diffusion equation (62) takes the form of a modified Poisson equation

$$\Delta c = -\lambda (\rho - \bar{\rho}).$$

(63)

Therefore, this equation emerges naturally and rigorously in the biological problem in a well-defined limit. Furthermore, the “box” is justified in the biological problem since the bacteria are usually enclosed in a container. In that case, the Keller-Segel model (61) and (63) becomes isomorphic to the modified Smoluchowski-Poisson system (55) and (58) provided that we make the correspondences

$$\Phi = -c, \quad \chi = \frac{1}{\xi}, \quad D = \frac{k_BT}{\xi m}, \quad \lambda = S_d G.$$  

(64)

In particular, the concentration $-c(\mathbf{r}, t)$ of the secreted chemical in chemotaxis plays the same role as the gravitational potential $\Phi(\mathbf{r}, t)$ in astrophysics. We can therefore map the SP system with a modified Poisson equation into the KS model.

The ordinary KS model (61)-(62) ignores fluctuations. In a previous paper [20], we have proposed to describe them with an equation of the form

$$\frac{\partial \rho}{\partial t} = \nabla \cdot \left( D \nabla \rho - \chi \rho \nabla c \right) + \nabla \cdot \left( \sqrt{2D \rho m} \mathbf{R} \right),$$

(65)

equivalent to the stochastic Smoluchowski equation (60).

Remark: Since the modified Poisson equation (63) is justified in biology, but not in astrophysics, it would seem more logical to present the following results with the notations of biology. However, in order to make contact with previous works on self-gravitating systems, it is preferable to use the notations of astrophysics. These notations are also identical to those used in thermodynamics and in the theory of Brownian motion while the notations used in biology for the chemotactic problem are not directly related to thermodynamics.\( ^9 \) Of course, our results can be immediately transposed to the problem of chemotaxis by using the correspondences in Eq. (64).

\( ^9 \) The interpretation of the Keller-Segel model in terms of thermodynamics is given in [24].
IV. THE STOCHASTIC SMOLUCHOWSKI-POISSON SYSTEM

A. The equation for the density

We consider a gas of self-gravitating Brownian particles with the modified Poisson equation \[ \frac{\partial \rho}{\partial t} = \nabla \cdot \left( k_B T \frac{\nabla \rho}{m} + \rho \nabla \Phi \right) + \nabla \cdot \left( \sqrt{2 \xi k_B T \rho R} \right), \tag{66} \]

\[ \Delta \Phi = S_d G(\rho - \bar{\rho}), \tag{67} \]

where \( \bar{\rho} = M/V \) is the mean density. It is convenient to work with dimensionless variables. As shown in Appendix A Eqs. (66) and (67) can be rewritten in dimensionless form as

\[ \frac{\partial \rho}{\partial t} = \nabla \cdot \left( T \nabla \rho + \rho \nabla \Phi \right) + \frac{1}{\sqrt{N}} \nabla \cdot \left( \sqrt{2T \rho R} \right), \tag{68} \]

\[ \Delta \Phi = S_d (\rho - \bar{\rho}), \tag{69} \]

where now \( R = 1 \) and the density is normalized such that \( \int \rho \, dx = 1 \). Therefore, \( \bar{\rho} = d/S_d \). These equations can be obtained from the original ones by setting \( R = m = \xi = k_B = 1 \) and \( G = 1/N \), and by rescaling the density by \( N \) (i.e. we write \( \rho = N \tilde{\rho} \) and finally note \( \rho \) instead of \( \tilde{\rho} \) ). This corresponds to the Kac scaling. In the thermodynamic limit \( N \to +\infty \), we have \( E \sim N \), \( T \sim 1 \), \( S \sim N \) and \( F \sim N \).

In this paper, we consider a one dimensional system and we make it symmetric with respect to the origin by imposing \( R(-x,t) = -R(x,t) \). In that case, the foregoing equations reduce to

\[ \frac{\partial \rho}{\partial t} = \frac{\partial}{\partial x} \left( T \frac{\partial \rho}{\partial x} + \rho \frac{\partial \Phi}{\partial x} \right) + \frac{1}{\sqrt{N}} \frac{\partial}{\partial x} \left( \sqrt{2T \rho R} \right), \tag{70} \]

\[ \frac{\partial^2 \Phi}{\partial x^2} = 2(\rho - \bar{\rho}), \tag{71} \]

where \( \bar{\rho} = 1/2 \). These equations can be solved in the domain \([0, 1]\) with the Neumann boundary conditions \( \rho'(0, t) = \rho'(1, t) = 0 \) and \( \Phi'(0, t) = \Phi'(1, t) = 0 \). The normalization condition is \( 2 \int_0^1 \rho(x, t) \, dx = 1 \).

B. The equation for the mass profile

We can reduce the two coupled equations (70) and (71) into a single equation for the mass profile (or integrated density) defined by

\[ M(x, t) = 2 \int_0^x \rho(x', t) \, dx'. \tag{72} \]

We clearly have

\[ \frac{\partial M}{\partial t} = 2 \rho, \quad \frac{\partial \Phi}{\partial x} = M(x, t) - x. \tag{73} \]

Integrating the stochastic Smoluchowski equation (70) between 0 and \( x \), and using Eq. (73), we find that the evolution of the mass profile is given by

\[ \frac{\partial M}{\partial t} = T \frac{\partial^2 M}{\partial x^2} + (M - x) \frac{\partial M}{\partial x} + 2 \sqrt{\frac{T}{N} \frac{\partial M}{\partial x}} R(x, t). \tag{74} \]

This stochastic partial differential equation (SPDE) has to be solved with the boundary conditions \( M(0, t) = 0 \) and \( M(1, t) = 1 \).

Remark: For the usual SP system where \( M - x \) is replaced by \( M \), we note that Eq. (74) is similar to a noisy Burgers equation for a fluid with velocity \( u(x, t) = -M(x, t) \) and viscosity \( \nu = T \). This analogy is only valid in \( d = 1 \).

C. The equations of the N-body problem

We may also directly solve the N-body dynamics. For the modified gravitational force in one dimension, the stochastic Langevin equations of motion of the N Brownian particles are given by

\[ \frac{dx_i}{dt} = \frac{1}{\xi} F(x_i) + \sqrt{\frac{2k_B T}{m \xi}} R_i(t), \tag{75} \]

with

\[ F(x_i) = Gm \sum_{x_j \in S_+} \text{sgn}(x_j - x_i) + G\bar{\rho}(2x_i - R). \tag{76} \]

We consider only particles in the interval \( S_+ = [0, 1] \). The expression (76) of the gravitational force is derived in Appendix C. Using the scaling defined previously (see also Appendix B), these equations can be rewritten in dimensionless form as

\[ \frac{dx_i}{dt} = \frac{1}{N} \sum_j \text{sgn}(x_j - x_i) + \frac{1}{2} (2x_i - 1) + \sqrt{2T} R_i(t). \tag{77} \]
D. Second order phase transitions in $d = 1$

The equilibrium states of the modified Smoluchowski-Poisson system [Eqs. (55) and (58)] are determined by the modified Boltzmann-Poisson equation (59). They have been studied in detail in [16]. In $d = 1$, the caloric curve $E(T)$ giving the energy as a function of the temperature is represented in Figs. 1 and 2. It displays a second order phase transition at the critical temperature $T_c^* = 1/\pi^2$ marked by the discontinuity of $dE/dT$. For $T > T_c^*$ the system is in the homogeneous phase which is the global minimum of free energy at fixed mass (see Fig. 3). For $T < T_c^*$ the homogeneous phase is unstable and is replaced by an inhomogeneous phase corresponding to the bifurcated branch $n = 1$ in Figs. 1 and 2 (as shown in Fig. 4 there exist other bifurcated branches with $n$ clusters but they are unstable [16]: only the branch with $n = 1$ cluster that we are considering is stable). Actually, this branch is degenerate. For $T < T_c^*$, the free energy has two local minima (metastable states) at the same height (metastable states) and a local maximum (unstable state). The local maximum corresponds to the homogeneous phase ($\lambda = 1$). The minima correspond to the inhomogeneous states concentrated near $x = 0$ (specifically $\lambda = 0.69$) or near $x = 1$ (specifically $\lambda = 1.54$).

FIG. 1: Caloric curve giving the energy per particle $-E/N$ as a function of the inverse temperature $1/T$. The left branch corresponds to the homogeneous phase. It is stable (S) for $T > T_c^* = 1/\pi^2$ and unstable (U) for $T < T_c^*$. In that case, it is replaced by an inhomogeneous phase which is stable. This corresponds to the right branch denoted $n = 1$. This branch is parameterized by the density contrast $\lambda = \bar{\rho}/\rho_0$. It is degenerate in the sense that, for a given temperature $T < T_c^*$, there exist two inhomogeneous states with the same energy but a different density contrast.

FIG. 2: Zoom of Fig. 1 near the critical point $T_c^* = 1/\pi^2 \approx 0.101$. We have indicated by a dashed line the temperature $T = 0.1 < T_c^*$ that will be considered in the section devoted to numerical simulations.

FIG. 3: Free energy $F(\lambda) = E(\lambda) - TS(\lambda)$ versus $\lambda$ for $T = 1/9 \approx 0.111 > T_c^*$. It presents a single minimum (stable state) corresponding to the homogeneous phase ($\lambda = 1$).

FIG. 4: Free energy $F(\lambda) = E(\lambda) - TS(\lambda)$ versus $\lambda$ for $T = 0.1 < T_c^*$. It has a double-well structure with two minima at the same height (metastable states) and a local maximum (unstable state). The local maximum corresponds to the homogeneous phase ($\lambda = 1$). The minima correspond to the inhomogeneous states concentrated near $x = 0$ (specifically $\lambda = 0.69$) or near $x = 1$ (specifically $\lambda = 1.54$).
two states have the same energy (see Figs. 4 and 6) and the same free energy (see Figs. 4 and 6). The homogeneous phase ($\lambda = 1$) corresponds to a saddle point of free energy (unstable). The barrier of free energy $\Delta F/Nk_B T$ between the saddle point and the minima is represented as a function of the temperature in Fig. 7.

For $N \to +\infty$, the evolution of the density $\rho(x,t)$ is described by the Smoluchowski equation (55) coupled to the modified Poisson equation (58). This corresponds to the mean field approximation. For $T > T^*_c$, this equation converges towards the homogeneous phase which is the unique minimum of free energy at fixed mass (stable state). For $T < T^*_c$, this equation converges towards one of the inhomogeneous states which is a local minimum of free energy at fixed mass (metastable state). The choice of the metastable state depends on the initial condition and on a notion of basin of attraction. For $N \to +\infty$, the system remains in that state for ever. For “small” values of $N$, or for $T$ close to the critical point $T^*_c$, the fluctuations become important. For $T < T^*_c$ they induce random transitions between the two metastable states discussed above. Such transitions can be described by the modified stochastic Smoluchowski-Poisson system (70)-(71) or, equivalently, by the stochastic partial differential equation (74) for the mass profile.

E. Numerical simulations of the modified stochastic SP system

We numerically solve Eq. (74) using the finite differences method described in (52). We work in the interval $[0,1]$. The boundary conditions are $M(0,t) = 0$ and $M(1,t) = 1$. We start from a uniform distribution $M(x,0) = x$. We solve Eq. (74) for $N = 8000$, 10000, and 12000 particles. We choose the time step $\Delta t = 0.0001$ to make the integration scheme stable, and we run each realization up to a time of order $10^6 - 10^7$ in our units. Performing this analysis for several values of $T$ and $N$ results in very long simulations taking several months of CPU time. This is necessary to have a good statistics and obtain clean results.

Fig. 8 shows the temporal evolution of the normalized central density $\rho(0,t)/\bar{\rho} = 1/\lambda(t)$ for $T = 0.1 < T^*_c$ and $N = 10000$. The system undergoes random transitions between the metastable state $\lambda = 0.69$ and the metastable state $\lambda = 1.54$. In the first case, the density profile is concentrated around $x = 0$ while in the second case it is concentrated around $x = 1$. The homogeneous phase ($\lambda = 1$) is unstable. Since the phase transition is second order, the two metastable states have the same free energy and, consequently, the average time spent by the system in each metastable state is the same. For $N \to +\infty$ the duration of the plateau becomes infinite and the system remains in only one of these states.

Fig. 9 shows the spatio-temporal evolution of the density profile $\rho(x,t)$. We clearly see the random displacement of the particles from the center of the domain ($x = 0$) to the boundary ($x = 1$) and vice versa.

In Fig. 10 we plot the density profiles of the two metastable states at $T = 0.1$. The numerical profiles
FIG. 8: Normalized central density $\rho(0, t)/\rho = 1/\lambda(t)$ as a function of time for $T = 0.1$ and $N = 10000$. One observes clear signatures of bistability. The system switches back and forth between two stable inhomogeneous states around $\lambda = 0.69$ (red) and $\lambda = 1.54$ (blue). The homogeneous phase is unstable. Since the two stable configurations have the same value of free energy, the average duration spent by the system in these two states is the same.

FIG. 9: Evolution of the density profile $\rho(x, t)$ as a function of time in a spatio-temporal diagram $(x, t)$. High densities correspond to red color and low densities to blue color. (green curves) are obtained by solving the stochastic partial differential equation (74) with $N = 10000$ and averaging the density in each phase ($\lambda < 1$ or $\lambda > 1$) over an ensemble of very long simulations. They are compared with the mean field profiles (red and blue curves) calculated in [16] showing a very good agreement. We have also plotted the numerical profiles (black curves) obtained by directly solving the $N$-body equations (77) with $N = 500$. The agreement is also good. The small differences are probably due to finite $N$ effects.

In Fig. 10 we have plotted the density profiles of the two metastable states for $T = 0.1$ obtained by solving the stochastic partial differential equation (74) with $N = 10000$ (green curves) or by solving the stochastic $N$-body equations (77) with $N = 500$ (black curves). They are compared with the mean field equilibrium distributions obtained in [16] for $N \to +\infty$ (red and blue curves).

FIG. 10: Distribution of the residence time $\tau$ for $T = 0.1$ and $N = 10000$. The distribution is Poissonian indicating that the random transitions from one metastable state to the other are statistically independent.

FIG. 11: Density profiles of the two metastable states for $T = 0.1$ obtained by solving the stochastic partial differential equation (74) with $N = 10000$ (green curves) or by solving the stochastic $N$-body equations (77) with $N = 500$ (black curves). They are compared with the mean field equilibrium distributions obtained in [16] for $N \to +\infty$ (red and blue curves).

In Fig. 11 we have plotted the distribution of the residence time $\tau$ for $T = 0.1$ and $N = 10000$. The distribution is Poissonian indicating that the random transitions from one metastable state to the other are statistically independent. The small differences are probably due to finite $N$ effects.

In Fig. 11 we have plotted the distribution of the residence time $\tau$ of the system in the metastable states. This is the time spent by the system in a metastable state before switching to the other ($\tau$ is also called the “first passage time” from one state to the other). If two successive transitions are statistically independent of one another, the distribution of the residence time should be described by a Poisson process

$$P(\tau) = \frac{1}{\langle \tau \rangle} e^{-\tau/\langle \tau \rangle},$$

where $\langle \tau \rangle^{-1}$ gives the transition probability (per unit time) to switch from one state to the other. The average time spent by the system in a metastable state is $\langle \tau \rangle$. The Poissonian distribution of the residence time is confirmed by our numerical simulations. As mentioned before, we need to run the simulations for a very long time (especially for large $N$) in order to obtain a large number of transitions between the two metastable states.
Obtaining Fig. 11 requires several months of CPU time in order to obtain a good statistics for the residence time.

Since the system is at equilibrium with the thermal bath, we expect that the average time \( \langle \tau \rangle \) spent by the system in a metastable state is given by the Arrhenius law

\[
\langle \tau \rangle \propto e^{\Delta F/k_BT},
\]

where \( \Delta F = F_{\text{saddle}} - F_{\text{meta}} \) is the barrier of free energy between the metastable state (inhomogeneous phase) and the unstable state (homogeneous phase). This is similar to an activation process in chemical reactions. For a Brownian particle in a double-well potential this formula has been established by Kramers [2]. Here, the problem is more complicated because the role of the particle \( x(t) \) is played a field \( \rho(x, t) \) but the phenomenology remains the same. In the thermodynamic limit \( N \to +\infty \), the barrier of free energy scales as \( N \) and the dependence of the barrier of free energy per particle \( \Delta F/Nk_BT \) on the temperature \( T \) is represented in Fig. 7, using the results of [14]. To test the law

\[
\langle \tau \rangle \propto e^{N\Delta f/k_BT},
\]

we first fix \( N \) and plot \( \langle \tau \rangle \) as a function of \( \Delta f/k_BT \) in semi-logarithmic coordinates by changing the temperature (see Fig. 12). We find a nice linear relationship confirming the exponential dependence of \( \langle \tau \rangle \) with \( \Delta f/k_BT \) for fixed \( N \). According to this result, if we are close (resp. far) from the critical point \( T_c \) the barrier of free energy is small (resp. large) and the system remains in a metastable state for a short (resp. long) time. This is essentially the meaning of the usual Kramers law.

We have also investigated the dependence of the coefficients with the number of particles \( N \). To that purpose, we have written Eq. (80) in the more general form

\[
\langle \tau \rangle = e^{b(N)\Delta f/k_BT+c(N)}.
\]

The functions \( b(N) \) and \( c(N) \) obtained numerically are plotted in Figs. 13 and 14. We find that \( b(N) \) varies linearly with \( N \) while \( c(N) \) does not change appreciably. We note, however, that \( b(N) \) differs from the relation \( b(N) = N \) expected from Eq. (80). We find \( b(N) = 0.38N \) or \( b(N) = 0.40N - 278 \) depending on the fit. The reason of this difference with the expected result \( b(N) = N \) is not known. This may be a finite \( N \) effect.\(^{11}\) It would

\(^{11}\) The validity of Eq. (80) requires \( N \gg 1 \). First, this is necessary in order to have \( \Delta F \sim N \). Actually, even if we impose this scaling for all \( N \) (for example by solving Eq. (68) for any \( N \) although it is valid only for \( N \gg 1 \)) we still need \( N \gg 1 \) in order to justify the Kramers formula (79). Indeed, as shown in Appendix D this formula is valid only in the weak noise limit which in our case corresponds to \( N \gg 1 \). Therefore, \( b(N) = N \) is valid only for \( N \gg 1 \) and \( N = 10000 \) may not be large enough. The observed relation \( b(N) \approx 0.4N \) may be a non-asymptotic result. It is also possible that the Kramers formula only gives \( \ln(\tau) \propto \).
be interesting to redo the analysis for larger values of $N$ but this would require very long simulations in order to achieve a good statistics.

According to the Arrhenius law \( \text{(79)} \) and the fact that the free energy scales as $N$ for systems with long-range interactions, we conclude that the lifetime of a metastable state scales as

\[
\langle \tau \rangle \sim e^{N},
\]

except close to a critical point where the barrier of free energy $\Delta f$ is small. As a result, for $N \gg 1$ (which is the norm for systems with long-range interactions), metastable states have very long lifetimes and, in practice, they can be considered as stable states. In other words, metastable states (local minima of free energy) are as much, or sometimes even more, relevant than fully stable states (global minima of free energy) for systems with long-range interactions (see \[20\] [23] for an application of these considerations in astrophysics). This exponential dependence of the lifetime of the metastable states with the number of particles for systems with long-range interactions \[21\] [23] is a new result as compared to the usual Kramers problem where there is only one particle.

**F. Numerical simulations of the N-body equations**

We have also performed direct numerical simulations of the stochastic $N$-body dynamics defined by Eq. \[77\]. Fig. 15 shows the spatio-temporal evolution of the particles for $T = 1/12$ and $N = 100$. We clearly see the random collective displacements of the particles between the center of the domain and the boundary. In Fig. 16 we plot the time evolution of the symmetrized mass $\chi(t)$ as a function of time obtained by solving the stochastic $N$-body equations \[77\] with $N = 100$ and $1/T = 12$.

**V. CONCLUSION**

We have studied a one dimensional model of self-gravitating Brownian particles with a modified Poisson equation \[16\]. This model also describes the chemotaxis of bacterial populations in the limit of high diffusivity of the chemical and in the absence of degradation. It presents a second order phase transition from a homogeneous phase to an inhomogeneous phase below a critical temperature $T^*_c$. For $T < T^*_c$, it displays a bistable behavior. The particles switch back and forth between the center of the domain and the boundary. These two configurations correspond to metastable states that are local minima of the mean field free energy $F[\rho]$ at fixed mass. This leads to a “barrier crossing problem” similar to the Kramers problem for the diffusion of an overdamped particle in a double well potential. We have shown with theoretical arguments and numerical simulations that the phenomenology of these random transitions is similar to that of the usual Kramers problem. In particular, the mean lifetime of the system in a metastable state is proportional to the exponential of the barrier of free energy $\Delta F$ divided by $k_B T$. However, a specificity of systems with long-range interactions (with respect to the Kramers problem) is that the barrier of free energy is proportional to $N$ so that the typical lifetime of a metastable state is considerable since it scales as $e^{N}$ (except close to a critical point). Therefore, metastable states are stable states in practice \[21\] [23]. The probability to pass from one metastable state to the other is a rare event since it scales as $e^{-N}$. Random transitions between metastable states

\[ N \Delta f/k_B T \] but does not determine the coefficient because of non trivial prefactors.
can be seen only close to the critical point, for moderate values of \( N \), and for sufficiently long times. This is the situation investigated in this paper.

The present results have been obtained for a particular model but they are expected to be valid for any system with long-range interactions presenting second order phase transitions. Another example is the Brownian mean field (BMF) model \([34]\). Below a critical temperature \( T_c = 1/2 \) it undergoes random transitions between two states with magnetization \( M_x = 1 \) and \( M_x = -1 \) if we enforce a symmetry with respect to the \( x \)-axis (i.e. if we impose \( M_y = 0 \)). Similar results should also be obtained for systems with long-range interactions presenting first order phase transitions. In that case, the system exhibits random transitions between a stable state (global minimum of free energy) and a metastable state (local minimum of free energy). The switches between these two states are asymmetric and the system remains longer in the stable state that corresponds to the global minimum of free energy. Apart from that asymmetry, the phenomenology is similar to the one reported in this paper. An example of systems with long-range interactions presenting first order phase transitions is provided by a 3D self-gravitating gas in a box with a small-scale exclusion constraint \([20, 33]\).

In the present work, and in the other examples quoted above, the system is at equilibrium with a thermal bath. The case of systems with long-range interactions that are maintained out-of-equilibrium by an external forcing is also interesting \([35, 36]\). These systems present a similar phenomenology except that the equivalent of the external potential \( V(x) \) in the usual Kramers problem, or the mean field free energy \( F[\rho] \) in the present problem, is not obvious at first sight and requires a specific treatment.

A domain of physical interest where random transitions between different attractors occur concerns two-dimensional fluid flows \([37]\). Different types of phase transitions have been evidenced in that context. For example, phase transitions in a flow with zero circulation and low energy enclosed in a rectangular domain have been investigated in \([38]\). In a domain of aspect ratio \( \sqrt{\rho} = 1/\tau \) with long-range interactions presenting second order model but they are expected to be valid for any system investigated in this paper.

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**Appendix A: The dimensionless stochastic Smoluchowski-Poisson system**

The dimensional stochastic Smoluchowski-Poisson system is given by Eqs. \([66, 67]\). It conserves the total mass \( M = Nm = \int \rho dV \). If we introduce dimensionless variables \( n, x, \phi, \eta = 1/\theta, \tau \) and \( Q \) through the relations

\[
\frac{\partial n}{\partial \tau} = \nabla \cdot (\theta \nabla n + n \nabla \phi) + \frac{1}{\sqrt{N}} \nabla \cdot \left( \sqrt{2n} \eta \right), \quad (A2)
\]

\[
\Delta \phi = S_\theta (n - \bar{n}), \quad (A3)
\]

where \( \bar{n} = d/S_\theta \) is the mean density of a sphere of unit mass and unit radius. The conservation of mass is expressed by \( \int n \, d\tau = 1 \). On the other hand, \( Q(x, \tau) \) is a Gaussian white noise satisfying \( \langle Q(x, \tau) \rangle = 0 \) and \( \langle Q_i(x, \tau) Q_j(x', \tau') \rangle = \delta_{ij} \delta(x - x') \delta(\tau - \tau') \). We see that the only control parameters are the dimensionless temperature \( \eta = 1/\theta \) and the number of particles \( N \). In the thermodynamic limit \( N \to +\infty \) with fixed \( \theta \), the noise term disappears and we recover the deterministic Smoluchowski-Poisson system.

**Appendix B: The dimensionless stochastic equations of motion**

If we introduce the dimensionless variables \( X, \eta = 1/\theta, \tau \) and \( q \) through the relations

\[
x = RX, \quad \eta = \beta GMmR = \frac{1}{\theta}, \quad \tau = \frac{\xi R}{GM}, \quad R = \sqrt{\frac{GM}{\xi R}}, \quad (B1)
\]

\[
t = \frac{\xi R}{GM}, \quad \eta = \beta GMmR = \frac{1}{\theta}, \quad \tau = \frac{\xi R}{GM}, \quad R = \sqrt{\frac{GM}{\xi R}}, \quad (B2)
\]
we find that Eqs. (75) and (76) may be rewritten as
\[
\frac{dX_i}{d\tau} = \frac{1}{N} \sum_j \text{sgn}(X_j - X_i) + \frac{1}{2}(2X_i - 1) + \sqrt{2\delta q_i(\tau)},
\]
(B2)
where \(q_i(\tau)\) is a Gaussian white noise satisfying \(\langle q_i(\tau) \rangle = 0\) and \(\langle q_i(\tau)q_j(\tau') \rangle = \delta_{ij}\delta(\tau - \tau')\).

Appendix C: The gravitational force corresponding to the modified Newtonian model in \(d = 1\)

In \(d = 1\), the modified Poisson equation (57) takes the form
\[
\frac{\partial^2 \Phi}{\partial x^2} = 2G(\rho - \bar{\rho}),
\]
(C1)
where \(\bar{\rho} = M/(2R)\). Integrating this equation from 0 to \(x\) and using the boundary condition \(\Phi'(0) = 0\), we get
\[
\frac{\partial \Phi}{\partial x} = 2G \int_0^x (\rho(x') - \bar{\rho}) \, dx'.
\]
(C2)
Similarly, integrating the modified Poisson equation (C1) from \(x\) to \(R\) and using the boundary condition \(\Phi'(R) = 0\), we get
\[
-\frac{\partial \Phi}{\partial x} = 2G \int_x^R (\rho(x') - \bar{\rho}) \, dx'.
\]
(C3)
Subtracting these two expressions, we obtain
\[
\frac{\partial \Phi}{\partial x} = G \int_0^x (\rho(x') - \bar{\rho}) \, dx' - G \int_x^R (\rho(x') - \bar{\rho}) \, dx'.
\]
(C4)
This equation can be rewritten as
\[
\frac{\partial \Phi}{\partial x} = G \int_0^R (\rho(x') - \bar{\rho}) \, dx' \text{sgn}(x - x') \, dx',
\]
(C5)
where \(\text{sgn}(x) = 1\) if \(x > 0\) and \(\text{sgn}(x) = -1\) if \(x < 0\). Therefore, the gravitational field \(F = -\Phi'\) at \(x\) is
\[
F(x) = G \int_0^R (\rho(x') - \bar{\rho}) \, \text{sgn}(x' - x) \, dx'.
\]
(C6)
It can be rewritten as
\[
F(x) = G \int_0^R \rho(x') \, \text{sgn}(x' - x) \, dx' + G\bar{\rho}(2x - R).
\]
(C7)
Finally, using \(\rho(x) = \sum_j m_0 \delta(x - x_j)\), the force by unit of mass experienced by the \(i\)-th particle due to the interaction with the other particles and with the background density \(\bar{\rho}\) is
\[
F(x_i) = Gm \sum_{x_j \in S_+} \text{sgn}(x_j - x_i) + G\bar{\rho}(2x_i - R),
\]
(C8)
where \(S_+\) denotes the interval \([0, R]\). We note that the first term is equal to the mass situated on the right of the \(i\)-th particle \(x_j > x_i\) minus the mass situated on its left \(x_j < x_i\). This is a striking property of the gravitational force in one dimension. On the other hand, the background density \(\bar{\rho}\) creates a force directed towards the wall \(x = R\) when \(x_i > R/2\) and towards the center of the domain \(x = 0\) when \(x_i < R/2\).

Appendix D: Derivation of the Kramers formula from the instanton theory

In this Appendix, we calculate the escape rate \(\Gamma\) of a system of Brownian particles with long-range interactions across a barrier of free energy by using the instanton theory. This provides a justification of the Kramers formula (54), giving the typical lifetime of a metastable state.

We first consider an overdamped particle moving in one dimension in a bistable potential \(V(x)\) subject to a Gaussian white noise \(\dot{R}(t)\). The Langevin equation is \(\dot{x} = -V'(x)/\xi_m + \sqrt{2k_B T/\xi_m} \dot{R}(t)\). When \(T = 0\) (no noise), the evolution is deterministic and the particle relaxes to one of the minima of the potential since \(dV/dt = -(1/\xi_m)V'(x)^2 \leq 0\). When \(T > 0\), the particle switches back and forth between the two minima (attractors). For \(T \to 0\), the transition between the two metastable states is a rare event. One important problem is to determine the rate \(\Gamma\) for the particle, initially located in a metastable state, to cross the potential barrier and reach the other metastable state. The most probable path for the stochastic process \(x(t)\) between \((x_1, t_1)\) and \((x_2, t_2)\), was first determined by Onsager and Machlup (10). The probability of the path \(x(t)\) is \(P[x(t)] \propto e^{-S[x]/k_B T}\) where \(S[x] = \langle (\xi_m/4) \int dt \dot{x} + V'(x)/\xi_m \rangle^2\) is the Onsager-Machlup functional. The probability to pass from \((x_1, t_1)\) to \((x_2, t_2)\) is \(P[x_1, t_1, x_2, t_2] = \int Dxe^{-S[x]/k_B T}\). The functional \(S[x]\) may be called an action by analogy with the path-integrals formulation of quantum mechanics (the temperature \(T\) plays the role of the Planck constant \(\hbar\) in quantum mechanics) (11). The most probable path \(x_c(t)\) connecting two states is called an “instanton” (12). It is obtained by minimizing the Onsager-Machlup functional. In the weak noise limit \(T \to 0\), the transition probability from one state to the other is dominated by

\[\text{This observation may help interpreting the results of (10). The modified Boltzmann-Poisson equation (59) with the boundary conditions \(\Phi'(0) = 0\) and \(\Phi'(R) = 0\) admits an infinite number of solutions, presenting \(n\) clusters (oscillations). However, the solutions with \(n \geq 2\) are unstable. Only the solution \(n = 1\), corresponding to the density profiles shown in Fig. (10) is stable. In that case, the particles are concentrated at \(x = 0\) or \(x = R\). The solution in which the particles are concentrated at \(x = R/2\), corresponding to \(n = 2\), is unstable. Physically, this is due to the effect of the background density \(\bar{\rho}\) in the modified Poisson equation (C1) that “pushes” the particles either towards \(x = 0\) or \(x = R\) according to the expression of the force (C8).}\]
the most probable path: $P[x_2,t_2|x_1,t_1] \propto e^{-S[x_c]/k_BT}$.

Therefore, the action of the most probable path between two metastable states determines the escape rate $\Gamma \sim \exp(-S[x_c]/k_BT)$ of the particle over the potential barrier. One finds $\dot{x}_c = +V'(x_c)/\xi m$ for the uphill path and $\dot{x}_c = -V'(x_c)/\xi m$ for the downhill path so that $S[x_c] = \Delta V$ where $\Delta V = V_{\text{max}} - V_{\text{meta}}$ is the barrier of potential energy. This yields the Arrhenius law $\Gamma \sim \exp(-\Delta V/k_BT)$ stating that the transition rate is inversely proportional to the exponential of the potential barrier. A general path-integrals formalism determining the escape rate of a particle in the weak noise limit has been developed by Bray et al. Their theory accounts for white noises for which $S[x_c] \neq \Delta V$.

We apply it here to the case of Brownian particles with long-range interactions described by the stochastic Smoluchowski equation [44]. In order to apply the formalism of instanton theory in a simple setting, it is convenient to consider spherically symmetric distributions. If we ignore the noise in a first step, the mean field Smoluchowski-Poisson system is equivalent to a single partial differential equation for $M(r,t)$ [9]. The free energy [27] can be written as a functional of $M(r,t)$ of the form

$$F[M] = \frac{1}{2} \int \frac{\partial M}{\partial r} \Phi dr + \frac{k_BT}{m} \int \frac{\partial M}{\partial r} \ln \left( \frac{1}{NmS[d-r^d-1]} \right) dr - \frac{dN}{2} k_BT \ln \left( \frac{2\pi k_BT}{m} \right).$$

(D2)

Since

$$\frac{\delta F}{\delta M} = -\frac{\partial \Phi}{\partial r} - \frac{k_BT}{m} \frac{1}{\partial r} \left( \frac{\partial^2 M}{\partial r^2} - \frac{d - 1}{r} \frac{\partial M}{\partial r} \right)$$

we can rewrite Eq. (D1) as

$$\xi \frac{\partial M}{\partial t} = -\frac{\partial M}{\partial r} \frac{\delta F}{\delta M}. \quad \text{(D4)}$$

The $H$-theorem writes

$$\dot{F} = -\frac{1}{\xi} \int_0^{\infty} \frac{\partial M}{\partial r} \left( \frac{\delta F}{\delta M} \right)^2 dr \leq 0. \quad \text{(D5)}$$

We can now introduce the noise in order to recover the canonical Boltzmann distribution at equilibrium (see the remark following Eq. (52)). This leads to the stochastic partial differential equation

$$\xi \frac{\partial M}{\partial t} = -\frac{\partial M}{\partial r} \frac{\delta F}{\delta M} + \sqrt{2k_BT \frac{\partial M}{\partial r}} R(r,t), \quad \text{(D6)}$$

where $R(r,t)$ is a Gaussian white noise satisfying $\langle R(r,t) \rangle = 0$ and $\langle R(r,t)R(r',t') \rangle = \delta(r-r')\delta(t-t')$.

Since the noise breaks the spherical symmetry in the stochastic Smoluchowski equation (50), this result is valid only in an average sense (it is, however, exact for one-dimensional systems). A direct derivation of Eq. (66) starting from the stochastic Smoluchowski equation (50) is given in [48]. We note that Eq. (66) looks similar to the stochastic Ginzburg-Landau equation (53) with a mobility $\Gamma$ proportional to $\partial M/\partial r(r,t)$. The corresponding Fokker-Planck equation for the probability density $P[M,t]$ of the profile $M(r,t)$ at time $t$ is

$$\xi \frac{\partial P}{\partial r}[M,t] = \int_0^{+\infty} \delta \frac{\partial M}{\partial r} \left[ k_BT \frac{\delta}{\delta M} + \frac{\delta F}{\delta M} \right] P[M,t] dr. \quad \text{(D7)}$$

We can check that it relaxes towards the canonical distribution

$$P[M] = \frac{1}{Z(\beta)} e^{-\beta F[M]}, \quad \text{(D8)}$$

Since the distribution of the Gaussian white noise $R(r,t)$ is

$$P[R(r,t)] \propto e^{-\frac{1}{2} \int_0^{+\infty} R^2 dr}, \quad \text{(D9)}$$

the probability to observe the path $M(r,t)$ between $(M_1(r),t_1)$ and $(M_2(r),t_2)$ is given by

$$P[M(r,t)] \propto e^{-\frac{1}{2\xi} \int_0^{t_2} dt \int_0^{+\infty} dr \frac{d}{\partial r} \left( \frac{\partial M}{\partial t} + \frac{\partial M}{\partial r} \frac{\delta F}{\delta M} \right)^2}. \quad \text{(D10)}$$

This is the proper generalization of the Onsager-Machlup functional for our problem. It can be written as $S = \int L dt$ where $L$ is the Lagrangian. The probability density to find the system with the profile $M_2(r)$ at time $t_2$ given that it had the profile $M_1(r)$ at time $t_1$ is

$$P[M_2,t_2|M_1,t_1] \propto \int dM e^{-S[M]/k_BT}, \quad \text{(D12)}$$

where the integral runs over all paths satisfying $M(r,t_1) = M_1(r)$ and $M(r,t_2) = M_2(r)$. For $N \to +\infty$,
using the scaling of Sec. [11E] the noise is weak so that the typical paths explored by the system are concentrated close to the most probable path. In that case, a steepest-descent evaluation of the path integrals is possible. We thus have to determine the most probable path, i.e. the one that minimizes the action \( S[M] \). The equation for the most probable path (instanton) between two metastable states (attractors) is obtained by canceling the first order variations of the action: \( \delta S = 0 \). Actually, it is preferable to remark that, since the Lagrangian does not explicitly depend on time, the Hamiltonian

\[
H = \int_0^{+\infty} \dot{M} \frac{\delta L}{\delta M} dr - L \tag{D13}
\]

is conserved (we have noted \( \dot{M} = \partial M/\partial t \)). Using Eq. (D11), we get

\[
H = \frac{1}{4\xi} \int_0^{+\infty} dr \frac{1}{\xi M} \left( \frac{\partial M}{\partial t} + \frac{\partial M}{\partial r} \frac{\delta F}{\delta M} \right) \times \left( \frac{\partial M}{\partial t} - \frac{\partial M}{\partial r} \frac{\delta F}{\delta M} \right). \tag{D14}
\]

Since the attractors satisfy \( \partial M/\partial t = 0 \) and \( \delta F/\delta M = 0 \), the constant \( H \) is equal to zero. Then, we find that the instanton satisfies

\[
\xi \frac{\partial M}{\partial t} = \mp \frac{\partial M}{\partial r} \frac{\delta F}{\delta M} \tag{D15}
\]

with the boundary conditions \( M(r, t_1) = M_1(r) \) and \( M(r, t_2) = M_2(r) \). Coming back to the original model written in terms of the density, the instanton equation is

\[
\frac{\partial \rho}{\partial t} = \pm \nabla \cdot \left[ \frac{\rho}{\xi} \frac{\delta F}{\delta \rho} \right]. \tag{D16}
\]

We note that the most probable path corresponds to the gradient driven dynamics \([12]\) with a sign \( \pm \), similarly to the one dimensional problem recalled above \([40, 43]\). The physical interpretation of this result is given below. For \( N \to +\infty \) (weak noise), the main contribution to the path integral in Eq. (D12) corresponds to the path that minimizes the action. This leads to the large deviation result

\[
P[M_2, t_2|M_1, t_1] \propto e^{-N s_s[M_1]/\kappa_B T}, \tag{D17}
\]

where we have written \( S = N s \) with \( s \sim 1 \). We note the analogies between Eqs. (D10), (D12), (D17) and Eqs. (28), (29), (30).

In the limit of weak noise, and for a stochastic process that obeys a fluctuation-dissipation relation, the most probable path between two metastable states must necessarily pass through the saddle point \([43, 48, 50]\). Once the system reaches the saddle point it may either return to the initial metastable state or reach the other metastable state. In the latter case, it has crossed the barrier of free energy. The physical interpretation of Eq. (D16) is the following. Starting from a metastable state, the most probable path follows the time-reversed dynamics against the free energy gradient up to the saddle point; beyond the saddle point, it follows the forward-time dynamics down to the metastable state. According to Eqs. (D11) and (D15), the action of the most probable path corresponding to the transition from the saddle point to a metastable state (downhill solution corresponding to Eq. (D15) with the sign \( - \)) is zero while the action of the most probable path corresponding to the transition from a metastable state to the saddle point (uphill solution corresponding to Eq. (D15) with the sign \( + \)) is non zero. This is expected since the descent from the saddle point to a metastable state is a “free” descent that does not require external noise; it thus gives the smallest possible value of zero of the action. By contrast, the rise from a metastable state to the saddle point requires external noise. The action for the uphill solution is

\[
S[M^+] = \int dt \int_0^{+\infty} dr \frac{\partial M}{\partial t} \frac{\delta F}{\delta M} = \int_0^{+\infty} dr \int_{M_{meta}}^{M_{saddle}} \frac{\delta F}{\delta M} dM = \Delta F \tag{D18}
\]

or, equivalently,

\[
S[M^+] = \frac{1}{\xi} \int dt \int_0^{+\infty} dr \frac{\partial M}{\partial r} \left( \frac{\delta F}{\delta M} \right)^2 = \int dt \int_0^{+\infty} dr \frac{\partial M}{\partial r} \frac{\delta F}{\delta M} = \int dt \dot{F} = \Delta F, \tag{D19}
\]

where \( \Delta F = F(M_{saddle}) - F(M_{meta}) \). The total action for the most probable path connecting the metastable states is \( S_c = S[M^+] + S[M^-] = \Delta F + 0 = \Delta F \). It is determined solely by the uphill path. The instanton solution gives the dominant contribution to the transition rate for a weak noise. Therefore, the rate for the system to pass from one metastable state to the other (escape rate) is

\[
\Gamma \sim e^{-\Delta F/k_B T}. \tag{D20}
\]

The typical lifetime of a metastable state is \( \sim \Gamma^{-1} \) returning the Arrhenius-Kramers formula \([54]\) stating that the transition rate is inversely proportional to the exponential of the barrier of free energy.

It may also be interesting to discuss the link with the principle of maximum dissipation of free energy \([51]\). We introduce the dissipation functions

\[
E_d = \frac{1}{2} \int_0^{+\infty} dr \left( \frac{\partial M}{\partial t} \right)^2, \tag{D21}
\]

\[
E_d^s = \frac{1}{2\xi} \int_0^{+\infty} \frac{\partial M}{\partial r} \left( \frac{\delta F}{\delta M} \right)^2 dr. \tag{D22}
\]

This type of functionals first appeared in the works of Lord Rayleigh \([52]\) and Onsager \([51]\). We also recall that

\[
\dot{F} = \int_0^{+\infty} \frac{\delta F}{\delta M} \frac{\partial M}{\partial t} dr. \tag{D23}
\]
First, we note that the mean field Smoluchowski equation (D4) can be obtained by minimizing the functional $\tilde{F} + E_d$ with respect to the variable $M$. This is the principle of maximum dissipation (in absolute value) of free energy [51] (see also [53] and Sec. 2.10.3 of [27]). Actually, in the present context, the validity of this “principle” can be proven rigorously since the mean field Smoluchowski equation can be derived from the $N$-body dynamics of the Brownian particles when $N \to +\infty$. The first variations $\delta(F + E_d) = 0$ return Eq. (D4). This corresponds to a true minimum since $\delta^2(F + E_d) = \frac{1}{2} \xi \int_0^{\infty} (\delta M)^2 / (\partial M / \partial r) \, dr \geq 0$. Then, we find that $\tilde{F} = -2E_d - 2E_*^{\tau}$.

Using Eqs. (D21)–(D23), the action (D11) can be expanded as

$$S[M] = \frac{1}{2} \int (E_d + E_*^{\tau} + \tilde{F}) \, dt. \quad (D4)$$

This is the counterpart of Eq. (4-18) of Onsager and Machlup [40]. The minimization of $S$ for variations with respect to $M$ is equivalent to the minimization of $\tilde{F} + E_d$ which returns the principle of maximum dissipation of free energy and the mean field Smoluchowski equation (D4). This corresponds to the downhill instanton solution for which we have $\tilde{F} = -2E_d = -2E_*^{\tau}$ and $S = 0$. On the other hand, for the uphill instanton solution corresponding to the mean field Smoluchowski equation (D4) with the opposite sign, we have $\tilde{F} = 2E_d = 2E_*^{\tau}$ and $S = \int \tilde{F} \, dt = \Delta F$. Therefore, the probability for the system to pass from a metastable state to a state $M(r)$ is $P[M] \propto e^{-\beta S} \propto e^{-\beta(\tilde{F}[M] - F_{meta})}$. This is in agreement with the heuristic arguments of Sec. IVJ that are now justified from the instanton theory.

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