1 Langevin equation

Although every continuous Markov process has an associated Langevin equation and an associated Fokker-Planck equation, the relation between them is not one to one in more than one dimension, and this brings some subtleties into the mathematical approach. By the same token there isn't a uniform notation to treat the brownian motion on the sphere despite the fact that there is an extensive literature on the theme.

- To design numeric algorithms Langevin equations are easier to handle than the Fokker-Planck equations.
- However, as they represent the same continuous Markov process, and some times (very rare ones!) it's easier to integrate the Fokker-Planck equation, the validity of the solution might be tested comparing the results that come from discrete version of Langevin equations with the analytic solution to the Fokker-Planck equation.

1.1 Langevin equation in $\mathbb{R}^m$

It is well known that if a *process* satisfies simple assumptions about its law of evolution each component of the process will satisfies the multivariate Langevin equation

$$X_k[t+dt] = X_k[t] + A_k[\mathbf{x},t]\,dt + \sum_{j=1}^{m} b_{kj}[\mathbf{x},t]N[0,1]\,(dt)^{1/2} \tag{1}$$

The proof follows from simple arguments from analysis and from the random variable transformation theorem.

1.2 Few remarks for the Langevin equation on the sphere

In this section we are going to obtain in a straightforward manner the Langevin equation for a brownian particle when this is restricted to the surface of a sphere. We simply "map" the physics (fluctuation-dissipation theorem) capture on the Langevin equation

$$m\frac{d}{dt}\dot{\mathbf{x}} = -\gamma\,\dot{\mathbf{x}}(t) + [2KT\gamma]^{1/2}\mathbf{\Gamma}(t), \tag{2}$$

onto the surface of the sphere. We do this using generalized coordinates in order to take into account the forces of constrain. We use this method to deal with the geometric restriction problem, then we interpret the equations obtained as the stochastic law of evolution. This is so because some of the terms, although geometrical correct, are stochastic in nature. Moreover, in this case we must postulate a generalized extremal action principle

$$\delta A \equiv A[\hat{\alpha} + \delta\hat{\alpha}] - A[\hat{\alpha}] = \int_{t_1}^{t_2} \left[\delta L + \delta W^{(d)}\right] \, dt, \tag{3}$$

in order to contemplate the dissipative forces explicit in the Langevin equation. In this generalized principle $W^{(d)}$ represents the dissipated work by the nonconservative forces, and $\hat{\alpha}$ represents the set of geometric parameters necessary to describe a curve in configuration space. From there, we can generate the equations of motion or Lagrange equations

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{q}_k} - \frac{\partial L}{\partial q_k} = Q_k, \quad k = 1, 2, \ldots, 3n - l. \tag{4}$$

In these equations Q_k represents the generalized force, k the number of degrees of freedom, and l is the number of holonomic constrains.

1.2.1 Euler-Lagrange equations for the free particle on $\mathbb{S}^2$

When there are no external forces and no dissipative forces; when we just have the forces of constrain which are normal to the surface, we can write the equations of motion in local coordinates (θ, ϕ). For that purpose, we have to write the Lagrangian of the mechanical system in these generalized coordinates

$$L = \frac{1}{2} m (r^2 \dot{\theta}^2 + r^2 \sin^2\theta \dot{\phi}^2). \tag{5}$$

Using this Lagrangian and plugging it into (4) we get

$$mr^2 \ddot{\theta} - mr^2 \sin\theta \cos\theta \dot{\phi}^2 = 0, \tag{6}$$

for the θ coordinate, and

$$\frac{d}{dt}\left[mr^2 \sin^2\theta \dot{\phi} \right] = 0, \tag{7}$$

for the ϕ coordinate. Naturally these are the two geodesic equations

$$\frac{d^2 x^a}{ds^2} = -\Gamma^a_{b\,c} \frac{dx^b}{ds}\frac{dx^c}{ds}, \quad a = \theta, \phi. \tag{8}$$

when the line element is define through the metric $\mathbf{g} = g_{ab}\, dx^a \otimes dx^b$ and the associated line element $ds^2 = r^2\, d\theta^2 + r^2\, \sin^2\theta\, d\phi^2$ in the surface of a sphere or radius r. This equivalence is due to the fact that we can interpret the inertial tensor as the metric tensor in configuration space.

$$\Gamma^a_{bc} = \frac{1}{2} g^{ak} \left[g_{kb,\,c} + g_{kc,\,b} - g_{bc,\,k} \right] \tag{9}$$

The relevant non-vanishing Christoffel symbols are

$$\begin{aligned}
\Gamma^{\theta}_{r\theta} &= \Gamma^{\theta}_{\theta r} = \frac{1}{r} \\
\Gamma^{\theta}_{\phi\phi} &= -\sin\theta\cos\theta \\
\Gamma^{\phi}_{r\phi} &= \Gamma^{\phi}_{\phi r} = \frac{1}{r} \\
\Gamma^{\phi}_{\theta\phi} &= \Gamma^{\phi}_{\phi\theta} = \cot\theta
\end{aligned} \tag{10}$$

1.2.2 Dissipative force

The dissipated energy by the environment is the result of the particle interaction with the surroundings. Mathematically this stems from or it is capture by the $-\gamma\dot{\mathbf{x}}$ term in Langevin's equation, so we should contemplate a dissipative force with the following structure

$$\mathbf{F}_\gamma = -\gamma(\dot{x}\,\hat{\mathbf{x}} + \dot{y}\,\hat{\mathbf{y}} + \dot{z}\,\hat{\mathbf{z}}). \tag{11}$$

The velocity components in spherical coordinates are given by

$$\dot{x} = \cos\theta\cos\phi\,\dot{\theta} - \sin\theta\sin\phi\,\dot{\phi} \tag{12}$$

$$\dot{y} = \cos\theta\sin\phi\,\dot{\theta} + \sin\theta\cos\phi\,\dot{\phi} \tag{13}$$

$$\dot{z} = -\sin\theta\,\dot{\theta}, \tag{14}$$

then it follows that the generalized force related to the θ coordinate is given by

$$\begin{aligned}
Q_{\gamma_\theta} \equiv \left\langle \mathbf{F}_\gamma, \frac{\partial \mathbf{r}}{\partial\theta} \right\rangle &= -\gamma\left[(\cos^2\theta\{\cos^2\phi + \sin^2\phi\})\,\dot{\theta} - (\sin\theta\cos\theta\sin\phi\cos\phi)\,\dot{\phi} + \right. \\
&\left. + (\sin\theta\cos\theta\sin\phi\cos\phi)\,\dot{\phi} + \sin^2\theta\,\dot{\theta}\right],
\end{aligned}$$

so

$$Q_{\gamma_\theta} = -\gamma\,\dot{\theta}, \tag{15}$$

and the generalized force related to the ϕ coordinate is given by

$$\begin{aligned}
Q_{\gamma_\phi} \equiv \left\langle \mathbf{F}_\gamma, \frac{\partial \mathbf{r}}{\partial\phi} \right\rangle &= -\gamma\left[-(\sin\theta\cos\theta\sin\phi\cos\phi)\,\dot{\theta} + \sin^2\theta\sin^2\phi\,\dot{\phi}\right. \\
&\left. + (\sin\theta\cos\theta\sin\phi\cos\phi)\,\dot{\theta} + \sin^2\theta\cos^2\phi\,\dot{\phi}\right],
\end{aligned}$$

so

$$Q_{\gamma_\phi} = -\gamma\sin^2\theta\,\dot{\phi}. \tag{16}$$

1.2.3 Gaussian white noise

The white noise in three dimensional euclidean space can be seen as the superposition of three mutual independent white noises; one for each dimension

$$\mathbf{\Gamma} = N\left[0, 2KT\gamma/m^2\right]\,\hat{\mathbf{x}} + N\left[0, 2KT\gamma/m^2\right]\,\hat{\mathbf{y}} + N\left[0, 2KT\gamma/m^2\right]\,\hat{\mathbf{z}}. \tag{17}$$

Now we can manipulate this expression to see how this force expresses on the surface of the sphere

$$\begin{aligned}
Q_{\Gamma_\theta} \equiv \left\langle \mathbf{\Gamma}, \frac{\partial \mathbf{r}}{\partial \theta} \right\rangle &= \cos\theta\cos\phi\, N\left[0, 2KT\gamma/m^2\right] + \cos\theta\sin\phi\, N\left[0, 2KT\gamma/m^2\right] - \\
&\quad -\sin\theta\, N\left[0, 2KT\gamma/m^2\right] \\
&= N\left[0, (\cos^2\theta\cos^2\phi)\, 2KT\gamma/m^2\right] + N\left[0, (\cos^2\theta\sin^2\phi)\, 2KT\gamma/m^2\right] + \\
&\quad +N\left[0, (\sin^2\theta)\, 2KT\gamma/m^2\right] \\
&= N\left[0, \{\cos^2\theta(\sin^2\phi + \cos^2\phi) + \sin^2\theta\}\, 2KT\gamma/m^2\right],
\end{aligned}$$

therefore

$$Q_{\Gamma_\theta} = N[0, 2KT\gamma/m^2] = (2KT\gamma/m^2)^{1/2}\, N[0,1]. \tag{18}$$

In the same manner we can obtain

$$\begin{aligned}
Q_{\Gamma_\phi} \equiv \left\langle \mathbf{\Gamma}, \frac{\partial \mathbf{r}}{\partial \phi} \right\rangle &= -\sin\theta\sin\phi\, N\left[0, 2KT\gamma/m^2\right] + \sin\theta\cos\phi\, N\left[0, 2KT\gamma/m^2\right] \\
&= N\left[0, \sin^2\theta(\sin^2\phi + \cos^2\phi) 2KT\gamma/m^2\right] \\
Q_{\Gamma_\phi} &= N\left[0, \sin^2\theta\, 2KT\gamma/m^2\right] = \sin\theta(2KT\gamma/m^2)^{1/2}\, N[0,1]. \qquad (19)
\end{aligned}$$

1.2.4 Lagrange-Langevin equation for the constrained brownian motion

From the above results, we can put an explicit form (in local coordinates) to the Lagrange equations for the brownian motion when this motion is restricted to the surface of a sphere

$$\ddot{\Theta} = \sin\Theta\cos\Theta\,\dot{\Phi}^2 - \frac{\gamma}{m}\,\dot{\Theta} + [2KT\gamma/m^2]^{\frac{1}{2}}\,\Gamma_\Theta \tag{20}$$

$$\ddot{\Phi} = -2\cot\Theta\,\dot{\Theta}\,\dot{\Phi} - \frac{\gamma}{m}\,\dot{\Phi} + [2KT\gamma/m^2]^{\frac{1}{2}}\sin^{-1}\Theta\,\Gamma_\Theta \tag{21}$$

Moreover, we can rewrite this set of two second order equations as a set of four first order equations in the same spirit as in the dynamical systems approach

$$\frac{d}{dt}\begin{bmatrix}\Theta\\ \Phi\\ \dot{\Theta}\\ \dot{\Phi}\end{bmatrix} = \begin{bmatrix}\dot{\Theta}\\ \dot{\Phi}\\ -\frac{\gamma}{m}\,\dot{\Theta} + \sin\Theta\cos\Theta\,\dot{\Phi}^2 + [\frac{2KT\gamma}{m^2}]^{\frac{1}{2}}\,\Gamma_\Theta\\ -\frac{\gamma}{m}\dot{\Phi} - 2\cot\Theta\,\dot{\Theta}\,\dot{\Phi} + [\frac{2KT\gamma}{m^2}]^{\frac{1}{2}}\,\sin^{-1}\Theta\,\Gamma_\Phi\end{bmatrix} \tag{22}$$

in order to be able to read the multivariate Langevin equation explicitly.

1.2.5 Limiting case

As $\gamma \to 0$, we would expect to recover the geodesic equation in (8), which is indeed the case.

2 Fokker-Planck equation

Using the same few principles that obey any continuous Markov process, we can obtain equations that govern the time evolution of the functions that describe these processes, namely Chapman-Kolmogorov equation, Kramers-Moyal equations and from there, using the theorem of the Langevin equation, we can generate the Fokker-Planck equations.

2.1 Fokker-Planck equation in $\mathbb{R}^m$

$$\xi = [\mathbf{x}, \dot{\mathbf{x}}] \in \mathbb{R}^m \tag{23}$$

2.1.1 Forward Fokker-Planck equation

$$\begin{aligned} \frac{\partial}{\partial t} P(\xi, t|\xi_0, t_0) &= -\sum_{k=1}^{m} \frac{\partial}{\partial \xi_k} \{A_k[\xi, t] P(\xi, t|\xi_0, t_0)\} + \\ &+ \frac{1}{2} \sum_{k=1}^{m} \frac{\partial^2}{\partial \xi_k^2} \{D_k[\xi, t] P(\xi, t|\xi_0, t_0)\} + \\ &+ \sum_{i<j}^{m} \frac{\partial^2}{\partial \xi_i \partial \xi_j} \{C_{ij}[\xi, t] P(\xi, t|\xi_0, t_0)\} . \end{aligned} \tag{24}$$

therein

$$D_k[\xi, t] = \sum_{s=1}^{m} b_{ks}^2[\xi, t]. \tag{25}$$

$$C_{ij}[\xi, t] = \sum_{s=1}^{m} b_{is}[\xi, t] b_{js}[\xi, t]. \tag{26}$$

2.1.2 Backward Fokker-Planck equation

$$
\begin{aligned}
-\frac{\partial}{\partial t_0} P(\xi, t|\xi_0, t_0) &= \sum_{k=1}^{m} A_k[\xi_{\mathbf{0}}, t_0] \frac{\partial}{\partial \xi_{0k}} \{P(\xi, t|\xi_0, t_0)\} + \\
&+ \frac{1}{2} \sum_{k=1}^{m} D_k[\xi_{\mathbf{0}}, t_0] \frac{\partial^2}{\partial \xi_{0k}^2} \{P(\xi, t|\xi_0, t_0)\} + \\
&+ \sum_{i<j}^{m} C_{ij}[\xi_{\mathbf{0}}, t_0] \frac{\partial^2}{\partial \xi_{0i} \partial \xi_{0j}} \{P(\xi, t|\xi_0, t_0)\}.
\end{aligned}
\tag{27}
$$

therein

$$
D_k[\xi_0, t_0] = \sum_{s=1}^{m} b_{ks}^2[\xi_0, t_0]. \tag{28}
$$

$$
C_{ij}[\xi_0, t_0] = \sum_{s=1}^{m} b_{is}[\xi_0, t_0] b_{js}[\xi_0, t_0]. \tag{29}
$$

2.2 Smoluchowski equation in $\mathbb{R}^m$

2.3 Fokker-Planck equation in $\mathbf{T}\mathbb{S}^2$

$$
\eta = [r = 1, \theta, \phi, \dot{r} = 0, \dot{\theta}, \dot{\phi}] = [\theta, \phi, \dot{\theta}, \dot{\phi}] \in \mathrm{T}\mathbb{S}^2 \tag{30}
$$

2.3.1 Forward Fokker-Planck equation (Kramer's equation)

$$
\begin{aligned}
\frac{\partial}{\partial t} P(\xi, t|\xi_0, t_0) &= -\sum_{k=1} \left[\sum_{s=1} \frac{\partial}{\partial \eta_s} \{A_k[\xi, t] P(\xi, t|\xi_0, t_0)\} \frac{\partial \eta_s}{\partial \xi_k} \right] + \\
&+ \frac{1}{2} \sum_{k=1} \left[\sum_{r} \sum_{s} \frac{\partial^2}{\partial \eta_r \eta_s} \{D_k[\xi, t] P(\xi, t|\xi_0, t_0)\} \left(\frac{\partial \eta_s}{\partial \xi_k} \right) \left(\frac{\partial \eta_r}{\partial \xi_k} \right) + \right. \\
&\left. + \sum_{s} \frac{\partial}{\partial \eta_s} \{D_k[\xi, t] P(\xi, t|\xi_0, t_0)\} \frac{\partial^2 \eta_s}{\partial \xi_k^2} \right] + \\
&+ \sum_{i<j} \left[\sum_{r} \sum_{s} \frac{\partial^2}{\partial \eta_r \partial \eta_s} \{C_{ij}[\xi, t] P(\xi, t|\xi_0, t_0)\} \left(\frac{\partial \eta_s}{\partial \xi_i} \right) \left(\frac{\partial \eta_r}{\partial \xi_j} \right) + \right. \\
&\left. + \sum_{s} \frac{\partial}{\partial \eta_s} \{C_{ij}[\xi, t] P(\xi, t|\xi_0, t_0)\} \frac{\partial^2 \eta_s}{\partial \xi_i \partial \xi_j} \right].
\end{aligned}
$$

2.3.2 Backward Fokker-Planck equation

$$\begin{aligned}
-\frac{\partial}{\partial t_0} P(\xi, t|\xi_0, t_0) &= \sum_{k=1} A_k[\xi_0, t_0] \left[\sum_{s=1} \frac{\partial}{\partial \eta_{0s}} \{P(\xi, t|\xi_0, t_0)\} \frac{\partial \eta_{0s}}{\partial \xi_{0k}} \right] + \\
&+ \frac{1}{2} \sum_{k=1} D_k[\xi_0, t_0] \left[\sum_r \sum_s \frac{\partial^2}{\partial \eta_{0r} \eta_{0s}} \{P(\xi, t|\xi_0, t_0)\} \left(\frac{\partial \eta_{0s}}{\partial \xi_{0k}} \right) \left(\frac{\partial \eta_{0r}}{\partial \xi_{0k}} \right) + \right. \\
&\left. + \sum_s \frac{\partial}{\partial \eta_{0s}} \{P(\xi, t|\xi_0, t_0)\} \frac{\partial^2 \eta_{0s}}{\partial \xi_{0k}^2} \right] + \\
&+ \sum_{i<j} C_{ij}[\xi_0, t_0] \left[\sum_r \sum_s \frac{\partial^2}{\partial \eta_{0r} \partial \eta_{0s}} \{P(\xi, t|\xi_0, t_0)\} \left(\frac{\partial \eta_{0s}}{\partial \xi_{0i}} \right) \left(\frac{\partial \eta_{0r}}{\partial \xi_{0j}} \right) + \right. \\
&\left. + \sum_s \frac{\partial}{\partial \eta_{0s}} \{P(\xi, t|\xi_0, t_0)\} \frac{\partial^2 \eta_{0s}}{\partial \xi_{0i} \partial \xi_{0j}} \right].
\end{aligned}$$

2.4 Smoluchowski equation in $\mathbb{S}^2$

2.4.1 Position $\mathbf{X}(t)$ as a Wiener Process in $\mathbb{R}^3$

$$\xi = (x, y, z, \dot{x}, \dot{y}, \dot{z}) \tag{31}$$

$$\frac{d}{dt} \begin{bmatrix} x \\ y \\ z \\ \dot{x} \\ \dot{y} \\ \dot{z} \end{bmatrix} = \begin{bmatrix} \dot{x} \\ \dot{y} \\ \dot{z} \\ -\frac{\gamma}{m}\dot{x} + [2KT\gamma/m^2]^{1/2}\Gamma_x(t) \\ -\frac{\gamma}{m}\dot{y} + [2KT\gamma/m^2]^{1/2}\Gamma_y(t) \\ -\frac{\gamma}{m}\dot{z} + [2KT\gamma/m^2]^{1/2}\Gamma_z(t) \end{bmatrix} \tag{32}$$

Suppose $\frac{m}{\gamma} \ll 1$ but at the same time $[2KT/\gamma]^{1/2} = [2D]^{1/2} \approx O(1)$, then

$$\frac{d}{dt} \begin{bmatrix} x \\ y \\ z \\ \dot{x} \\ \dot{y} \\ \dot{z} \end{bmatrix} \approx \begin{bmatrix} [2KT/\gamma]^{1/2}\Gamma_x(t) \\ [2KT/\gamma]^{1/2}\Gamma_y(t) \\ [2KT/\gamma]^{1/2}\Gamma_z(t) \\ 0 \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} [2D]^{1/2}\Gamma_x(t) \\ [2D]^{1/2}\Gamma_y(t) \\ [2D]^{1/2}\Gamma_z(t) \\ 0 \\ 0 \\ 0 \end{bmatrix} \tag{33}$$

$$D_k[\xi, t] = 2D, \quad k = 1, 2, 3. \tag{34}$$

2.4.2 Position (Θ, Φ) as a Wiener Process in $\mathbb{S}^2$

$$\frac{d}{dt}\begin{bmatrix}\Theta\\ \Phi\\ \dot\Theta\\ \dot\Phi\end{bmatrix} = \begin{bmatrix}\dot\Theta\\ \dot\Phi\\ -\frac{\gamma}{m}\,\dot\Theta + \sin\Theta\cos\Theta\,\dot\Phi^2 + [\frac{2KT\gamma}{m^2}]^{\frac{1}{2}}\,\Gamma_\Theta\\ -\frac{\gamma}{m}\dot\Phi - 2\cot\Theta\,\dot\Theta\,\dot\Phi + [\frac{2KT\gamma}{m^2}]^{\frac{1}{2}}\,\sin^{-1}\Theta\,\Gamma_\Phi\end{bmatrix} \tag{35}$$

Suppose $\frac{m}{\gamma} \ll 1$ but at the same time $[2KT/\gamma]^{1/2} = [2D]^{1/2} \approx O(1)$, then

$$\frac{d}{dt}\begin{bmatrix}\Theta\\ \Phi\\ \dot\Theta\\ \dot\Phi\end{bmatrix} \approx \begin{bmatrix}[2D]^{\frac{1}{2}}\,\Gamma_\Theta\\ [2D]^{\frac{1}{2}}\,\sin^{-1}\Theta\,\Gamma_\Phi\\ 0\\ 0\end{bmatrix} \tag{36}$$

$$D_k[\eta, t] = \begin{cases}2D\,r^{-2} & \text{if } k = \theta\\ 2D\,r^{-2}\sin^{-1}\theta & \text{if } k = \phi\end{cases} \tag{37}$$

$$\xi = (x, y, z) \tag{38}$$

$$\eta = (r = 1, \theta, \phi) \tag{39}$$

It's associated Fokker-Planck equation, in this case, ought to be

$$\begin{aligned}\frac{\partial}{\partial t}P(\xi, t|\xi_0, t_0) \;&=\; +\frac{1}{2}\sum_{k=1}\Bigg[\sum_r\sum_s \frac{\partial^2}{\partial\eta_r\eta_s}\{D_k[\xi,t]P(\xi,t|\xi_0,t_0)\}\left(\frac{\partial\eta_s}{\partial\xi_k}\right)\left(\frac{\partial\eta_r}{\partial\xi_k}\right) +\\ &\quad + \sum_s \frac{\partial}{\partial\eta_s}\{D_k[\xi,t]P(\xi,t|\xi_0,t_0)\}\frac{\partial^2\eta_s}{\partial\xi_k^2}\Bigg]\end{aligned}$$

Which after some not so lengthy though very tidy "algebra", simplify to

$$\begin{aligned}\frac{\partial P(\theta, t|\theta_0, t_0)}{\partial t} \;&=\; \frac{D}{r^2}\left\{\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left[\sin\theta\frac{\partial}{\partial\theta}\left[P(\theta,t|\theta_0,t_0)\right]\right]\right\} +\\ &\quad + \frac{\partial^2}{\partial\phi^2}\left[\frac{D}{r^2\sin^2\theta}P(\theta,t|\theta_0,t_0)\right]\end{aligned} \tag{40}$$

From this expression we can appreciate how the geometry of the surface expresses different diffusion functions $D_k[\xi, t]$ from the ones of the 3 dimensional euclidean space, equation (34). When we have this particular symmetry, we may take them as defined by

$$D_k[\eta, t] = \begin{cases}r^{-2}\,D & \text{if } k = \theta\\ r^{-2}\sin^{-2}\theta\,D & \text{if } k = \phi\end{cases} \tag{41}$$

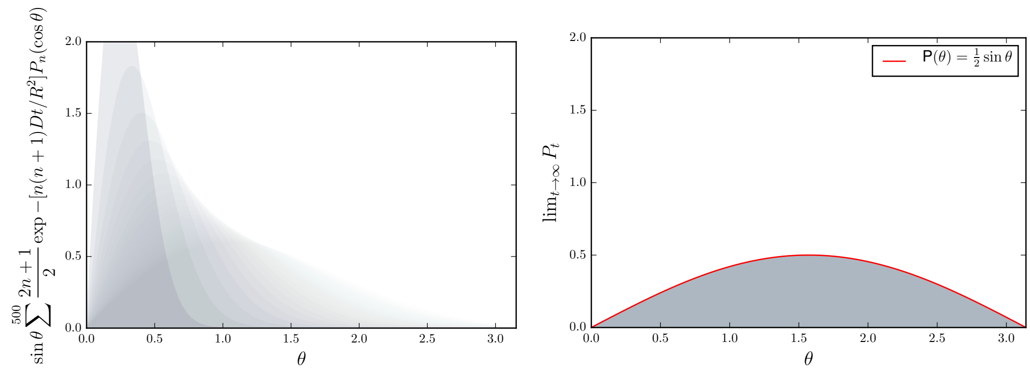


Figure 1: Time evolution of the marginal distribution to the solution of the Fokker-Planck equation (40) $\mathrm{P}(\theta, t|0,0) = \int_0^{2\pi} \mathrm{P}(\theta,\phi|0,0)\sin\theta\, d\phi$. The right side is the stationary state $1/2\sin\theta$ in which it transforms.

which at the same time coincides with the expressions in Langevin equation for the diffusion functions (37), as should be. The solution to this (parabolic) partial differential equation subject to the initial condition $P(\theta_2, t_2 = t_1|\theta_1, t_1) = \delta(\theta_2 - \theta_1)$, is well known because appears in many different branches of physics, and is given by

$$\begin{aligned} P(\theta_2, t_2|\theta_1, t_1) &= \sum_{n=0}^{\infty} Y_n^0(\theta_2,\phi_2) Y_n^{0*}(\theta_1,\phi_1) \exp\left[-\frac{n(n+1)\,D\,(t_2-t_1)}{r^2}\right] \\ &= \sum_{n=0}^{\infty} P_n(\cos\theta_2) P_n(\cos\theta_1) \exp\left[-\frac{n(n+1)\,D\,(t_2-t_1)}{r^2}\right] \end{aligned} \tag{42}$$

In particular, if $\theta_1 = 0$ and $t_1 = 0$, that is if $P(\theta, t|0,0) = \delta(\theta)$, then

$$P(\theta, t|0,0) = \sum_{n=0}^{\infty} \frac{2n+1}{4\pi r^2} P_n(\cos\theta) \exp\left[-\frac{n(n+1)\,D\,t}{r^2}\right] \tag{43}$$

To get this last expression it has been used the spherical harmonic addition theorem[1]

2.4.3 Numeric estimation of D in these contexts

$$\langle P_1(\theta(t))|0,0\rangle = \langle\cos\theta(t)|0,0\rangle = \int_0^{2\pi}\int_0^{\pi} \cos\theta\, P(\theta,t|0,0)\, r^2\, d\Omega \tag{44}$$

$$\int_0^{\pi} P_n(\cos\theta)\, P_m(\cos\theta) \sin\theta\, d\theta = \frac{2}{2n+1}\delta_{n,m}, \tag{45}$$

[1]The spherical harmonic addition theorem [**?**], in this context, implies $P_n(\cos\theta_1)\, P_n(\cos\theta_2) = \frac{2n+1}{4\pi r^2} P_n(\cos\gamma)$, where γ is the angle between the vectors with coordinates (θ_1, ϕ_1) and (θ_2, ϕ_2) respectively, however, if $\theta_1 \equiv 0$ so $\theta_2 = \gamma$, then we may take γ as the polar angle θ.

$$
\begin{aligned}
\langle \cos\theta(t)|0,0\rangle &= \int_0^{2\pi}\int_0^{\pi} \cos\theta \left[\sum_{n=0}^{\infty} \frac{2n+1}{4\pi r^2} P_n(\cos\theta) \exp\left[-n(n+1)Dt/r^2\right]\right] r^2\, d\Omega \\
&= \sum_{n=0}^{\infty} \frac{2n+1}{2} \exp\left[-n(n+1)Dt/r^2\right] \int_0^{\pi} P_1(\cos\theta) P_n(\cos\theta) \sin\theta\, d\theta \\
&= \sum_{n=0}^{\infty} \frac{2n+1}{2} \exp\left[-n(n+1)Dt/r^2\right] \frac{2}{2n+1} \delta_{n,1},
\end{aligned}
$$

from where it follows that

$$\langle \cos\theta(t)|0,0\rangle^2 = \exp\left[-4Dt/r^2\right]. \tag{46}$$

$$\log \langle \cos\theta(t)|0,0\rangle^2 = -\frac{4D}{r^2}\, t, \tag{47}$$

In conclusion, we obtain a linear relation in time which depends on the diffusion coefficient D and can be calculated directly from the numerical simulations because it is related to an average quantity of the ensamble $\langle \cdots \rangle$.

2.5 Approximated solution when $t \ll 1$ and $\theta \approx 0$

In this section we close the synergies cycle recovering the solution to the diffusion in 2 dimensional euclidean space, analyzing the specific form the operator (the Laplace-Beltrami operator) asumes. The problem with the specific form that this operator takes in these particular coordinates is that it is singular in the poles. In order to understand the behavior of these singular points

$$\frac{\partial p}{\partial t} = D\left[\frac{\partial^2 p}{\partial \theta^2} - \cot\theta\, \frac{\partial p}{\partial \theta} + \frac{1}{\sin^2\theta}\, p\right] \tag{48}$$

subject to initial condition $p(\theta, t=0) = \delta(\theta)$, we have to expand the operator defining functions in their Laurent series, retaining just the first non-vanishing term

$$\frac{\partial \rho}{\partial t} = D\left[\frac{\partial^2 \rho}{\partial \theta^2} - \frac{1}{\theta}\frac{\partial \rho}{\partial \theta} + \frac{1}{\theta^2}\, \rho\right] \tag{49}$$

with $\rho(\theta, t=0) = \delta(\theta)$. This equation admits the following group of scale transformations

$$t^* = \beta^2 t, \quad \theta^* = \beta\theta, \quad \rho^* = \beta^{-1} \tag{50}$$

Therefore, it follows that ρ in (49) satisfies the relation

$$\beta^{-1}\, \rho(\theta, t) = \rho(\beta\,\theta, \beta^2 t) \tag{51}$$

In particular, we can take $\beta = t^{-1/2}$, and this expression would rather say

$$\rho(\theta, t) = t^{-1/2}\,\rho(t^{1/2}\,\theta, 1) \tag{52}$$

If we define $\rho(\theta, 1) = G(\theta)$, then

$$\rho(\theta, t) = t^{-1/2}\,G(t^{-1/2}\,\theta) \tag{53}$$

Now we can obtain an equation for G using the equation (49)

$$G'' + \left[\theta - \frac{1}{\theta}\right] G' + \left[1 + \frac{1}{\theta^2}\right] G = 0 \tag{54}$$

with the restriction $\int_0^\pi G(\theta)\,d\theta = 1$. This equation has unique solution $G(\theta) = \theta\,\exp -[\theta^2/2]$, and therefore the solution to (49) is given by

$$P(\theta, t|0, 0) \approx \frac{\theta}{4\pi Dt\,\sin\theta}\,\exp -[\theta^2/4Dt] \tag{55}$$

The relation between the arc length s and the angle θ is $s = r\,\theta$, and in our considerations $r = 1$, and using the well known fact that $\lim_{s\to 0}\sin s/s = 1$, then

$$P(\theta, t|0, 0) \approx \frac{1}{4\pi Dt}\,\exp -[s^2/4Dt] \tag{56}$$

which is the solution to the $\mathbb{R}^2$ diffusion problem as should be.

3 A bistable potential as an example

$$U(x, y, z) = 1 - \frac{2z^2}{x^2 + y^2 + z^2} \tag{57}$$

$$A_1[\mathbf{x}, t] = -\frac{\partial}{\partial x}U(x, y, z) = -\frac{4xz^2}{(x^2 + y^2 + z^2)^2} = -\frac{4\sin\theta\cos^2\theta\cos\phi}{r} \tag{58}$$

$$A_2[\mathbf{x}, t] = -\frac{\partial}{\partial y}U(x, y, z) = -\frac{4yz^2}{(x^2 + y^2 + z^2)^2} = -\frac{4\sin\theta\cos^2\theta\sin\phi}{r} \tag{59}$$

$$A_3[\mathbf{x}, t] = -\frac{\partial}{\partial z}U(x, y, z) = \frac{4z(x^2 + y^2)}{(x^2 + y^2 + z^2)^2} = \frac{4\sin^2\theta\cos\theta}{r} \tag{60}$$

$$U(r, \theta, \phi) = -\cos 2\theta \tag{61}$$

3.1 Lagrange-Langevin Equation for bistable potential

$$\frac{d}{dt}\begin{bmatrix}\Theta\\ \Phi\\ \dot{\Theta}\\ \dot{\Phi}\end{bmatrix} = \begin{bmatrix}\dot{\Theta}\\ \dot{\Phi}\\ -\frac{\gamma}{m}\,\dot{\Theta} + \sin\Theta\cos\Theta\,\dot{\Phi}^2 + \frac{1}{m}\frac{\partial}{\partial\theta}\,(\cos 2\Theta) + [\frac{2KT\gamma}{m^2}]^{\frac{1}{2}}\,\Gamma_\Theta\\ -\frac{\gamma}{m}\dot{\Phi} - 2\cot\Theta\,\dot{\Theta}\,\dot{\Phi} + [\frac{2KT\gamma}{m^2}]^{\frac{1}{2}}\,\sin^{-1}\Theta\,\Gamma_\Phi\end{bmatrix} \tag{62}$$

Suppose $\frac{m}{\gamma} \ll 1$ but at the same time $[2KT/\gamma]^{1/2} = [2D]^{1/2} \approx O(1)$, then

$$\frac{d}{dt}\begin{bmatrix}\Theta\\ \Phi\\ \dot{\Theta}\\ \dot{\Phi}\end{bmatrix} \approx \begin{bmatrix}\frac{1}{\gamma}\frac{\partial}{\partial\theta}\,(\cos 2\Theta) + [2D]^{\frac{1}{2}}\,\Gamma_\Theta\\ [2D]^{\frac{1}{2}}\,\sin^{-1}\Theta\,\Gamma_\Phi\\ 0\\ 0\end{bmatrix} \tag{63}$$

3.2 Fokker-Planck (Smoluchowski) Equation for bistable potential

$$\begin{aligned}\frac{\partial}{\partial t}P(\eta,t|\eta_0,t_0) \;=\;& -\sum_{k=1}^{3}\left\{\frac{\partial}{\partial\theta}\{A_k[\eta,t]P(\eta,t|\eta_0,t_0)\}\frac{\partial\theta}{\partial x_k}+\right.\\ &\left.+\frac{\partial}{\partial\phi}\{A_k[\eta,t]P(\eta,t|\eta_0,t_0)\}\frac{\partial\phi}{\partial x_k}\right\}+\\ &+\frac{1}{2}\sum_{k=1}^{3}\left[\sum_r\sum_s\frac{\partial^2}{\partial\eta_r\eta_s}\{D_k[\eta,t]P(\xi,t|\eta_0,t_0)\}\left(\frac{\partial\eta_s}{\partial x_k}\right)\left(\frac{\partial\eta_r}{\partial x_k}\right)+\right.\\ &\left.+\sum_s\frac{\partial}{\partial\eta_s}\{D_k[\eta,t]P(\eta,t|\eta_0,t_0)\}\frac{\partial^2\eta_s}{\partial x_k^2}\right]\end{aligned}$$

When $D_k[\eta,t]$ is defined as the constant value $2D$, then the last sum over k reduce naturally to the well known laplacian in spherical coordinates, or Laplace-Beltrami as is known in the orthodox mathematical context.

$$
\begin{aligned}
\frac{\partial}{\partial t}P(\eta,t|\eta_0,t_0) &= -\frac{4}{r^2}\left\{\frac{\partial}{\partial\theta}\left[-\sin\theta\cos^2\theta\cos\phi\,P(\eta,t|\eta_0,t_0)\right]\cos\theta\cos\phi+\right.\\
&+\frac{\partial}{\partial\theta}\left[-\sin\theta\cos^2\theta\sin\phi\,P(\eta,t|\eta_0,t_0)\right]\cos\theta\sin\phi+\\
&+\frac{\partial}{\partial\theta}\left[\sin^2\theta\cos\theta\,P(\eta,t|\eta_0,t_0)\right](-\sin\theta)+\\
&+\frac{\partial}{\partial\phi}\left[\sin\theta\cos^2\theta\cos\phi\,P(\eta,t|\eta_0,t_0)\right](-\frac{\sin\phi}{\sin\theta})+\\
&\left.+\frac{\partial}{\partial\phi}\left[\sin\theta\cos^2\theta\sin\phi\,P(\eta,t|\eta_0,t_0)\right](\frac{\cos\phi}{\sin\theta})\right\}+\\
&+\frac{D}{\sin\theta}\frac{\partial}{\partial\theta}\left[\sin\theta\frac{\partial}{\partial\theta}\left[P(\eta,t|\eta_0,t_0)\right]\right]+\frac{D}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\left[P(\eta,t|\eta_0,t_0)\right]
\end{aligned}
$$

$$
\begin{aligned}
\frac{\partial}{\partial t}P(\eta,t|\eta_0,t_0) &= -\frac{4}{r^2}\left\{\frac{\partial}{\partial\theta}\left[-\sin\theta\cos^2\theta\cos\phi\,P(\eta,t|\eta_0,t_0)\right]\cos\theta\cos\phi+\right.\\
&+\frac{\partial}{\partial\theta}\left[-\sin\theta\cos^2\theta\sin\phi\,P(\eta,t|\eta_0,t_0)\right]\cos\theta\sin\phi+\\
&\left.+\frac{\partial}{\partial\theta}\left[\sin^2\theta\cos\theta\,P(\eta,t|\eta_0,t_0)\right](-\sin\theta)\right\}+\\
&+\frac{D}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left[\sin\theta\frac{\partial}{\partial\theta}\left[P(\eta,t|\eta_0,t_0)\right]\right]+\frac{D}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\left[P(\eta,t|\eta_0,t_0)\right]
\end{aligned} \tag{64}
$$

$$
\begin{aligned}
\frac{\partial}{\partial t}P(\eta,t|\eta_0,t_0) &= -\frac{4}{r^2}\left\{-\frac{\partial}{\partial\theta}\left[\sin\theta\cos^2\theta\,P(\eta,t|\eta_0,t_0)\right]\cos\theta-\right.\\
&\left.-\frac{\partial}{\partial\theta}\left[\sin^2\theta\cos\theta\,P(\eta,t|\eta_0,t_0)\right]\sin\theta\right\}+\\
&+\frac{D}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left[\sin\theta\frac{\partial}{\partial\theta}\left[P(\eta,t|\eta_0,t_0)\right]\right]+\frac{D}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\left[P(\eta,t|\eta_0,t_0)\right]
\end{aligned}
$$

Isotropy demands that P cannot depend explicitly on ϕ

$$
\begin{aligned}
\frac{\partial}{\partial t}P(\theta,t|\theta_0,t_0) &= -\frac{4}{r^2}\left\{-\frac{\partial}{\partial\theta}\left[\sin\theta\cos^2\theta\,P(\theta,t|\theta_0,t_0)\right]\cos\theta-\right.\\
&\left.-\frac{\partial}{\partial\theta}\left[\sin^2\theta\cos\theta\,P(\theta,t|\theta_0,t_0)\right]\sin\theta\right\}+\\
&+\frac{D}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left[\sin\theta\frac{\partial}{\partial\theta}\left[P(\theta,t|\theta_0,t_0)\right]\right]
\end{aligned}
$$

$$
\begin{aligned}
\frac{\partial}{\partial t}P(\theta,t|\theta_0,t_0) &= \frac{1}{r^2}\frac{\partial}{\partial\theta}\Big[2\sin(2\theta)\,P(\theta,t|\theta_0,t_0)\Big] + \\
&\quad +\frac{D}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left[\sin\theta\frac{\partial}{\partial\theta}\left[P(\theta,t|\theta_0,t_0)\right]\right]
\end{aligned}
$$

$$
\begin{aligned}
\frac{\partial}{\partial t}P(\theta,t|\theta_0,t_0) &= -\frac{1}{r^2}\frac{\partial}{\partial\theta}\Big[-2\sin(2\theta)\,P(\theta,t|\theta_0,t_0)\Big] + \\
&\quad +\frac{D}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left[\sin\theta\frac{\partial}{\partial\theta}\left[P(\theta,t|\theta_0,t_0)\right]\right]
\end{aligned}
$$

$$
\begin{aligned}
\frac{\partial}{\partial t}P(\theta,t|\theta_0,t_0) &= -\frac{1}{r^2}\frac{\partial}{\partial\theta}\Big[-\frac{\partial}{\partial\theta}\left[-\cos(2\theta)\right]\,P(\theta,t|\theta_0,t_0)\Big] + \\
&\quad +\frac{D}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left[\sin\theta\frac{\partial}{\partial\theta}\left[P(\theta,t|\theta_0,t_0)\right]\right]
\end{aligned}
$$

$$
\begin{aligned}
\frac{\partial}{\partial t}P(\theta,t|\theta_0,t_0) &= -\frac{1}{r^2}\frac{\partial}{\partial\theta}\Big[-\frac{\partial}{\partial\theta}\left[U(\theta)\right]\,P(\theta,t|\theta_0,t_0)\Big] + \\
&\quad +\frac{D}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left[\sin\theta\frac{\partial}{\partial\theta}\left[P(\theta,t|\theta_0,t_0)\right]\right]
\end{aligned}
$$

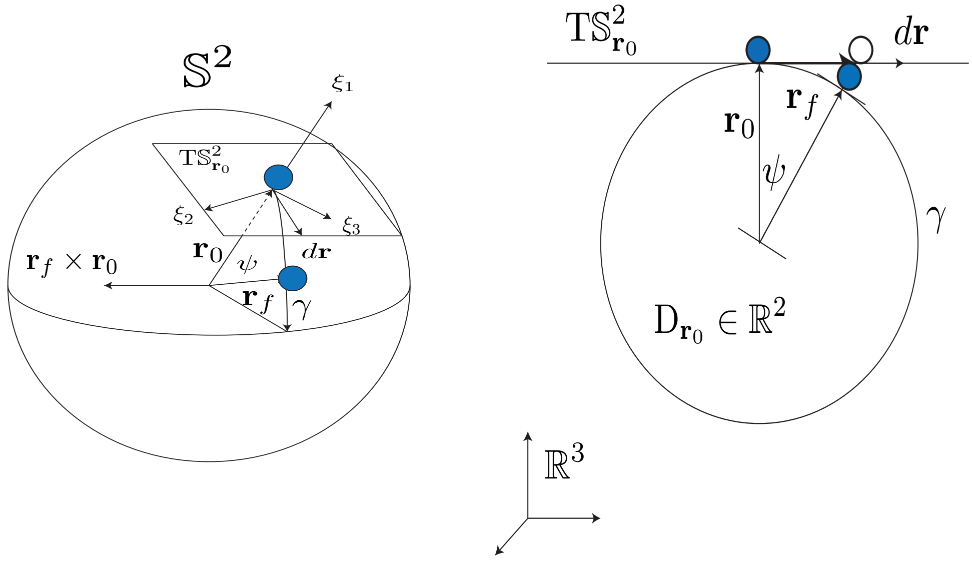
$$
U(\theta) \equiv -\cos(2\theta) \tag{65}
$$

$$
A_\theta[\theta,\phi,t] \equiv -\frac{\partial}{\partial\theta}\left[-\cos 2\theta\right] = -2\sin 2\theta \tag{66}
$$

$$
\begin{aligned}
\frac{\partial}{\partial t}P(\theta,t|\theta_0,t_0) &= -\frac{1}{r^2}\frac{\partial}{\partial\theta}\Big[A_\theta[\theta]\,P(\theta,t|\theta_0,t_0)\Big] + \\
&\quad +\frac{D}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left[\sin\theta\frac{\partial}{\partial\theta}\left[P(\theta,t|\theta_0,t_0)\right]\right]
\end{aligned}
$$

In $\mathbb{S}^2$

$$
\begin{aligned}
\frac{\partial}{\partial t}P(\theta,t|\theta_0,t_0) &= -\frac{\partial}{\partial\theta}\Big[A_\theta[\theta]\,P(\theta,t|\theta_0,t_0)\Big] + \\
&\quad +\frac{D}{\sin\theta}\frac{\partial}{\partial\theta}\left[\sin\theta\frac{\partial}{\partial\theta}\left[P(\theta,t|\theta_0,t_0)\right]\right]
\end{aligned}
$$



(a) Tangent plane to $\mathbb{S}^2$

(b) Plane containing the geodesic γ

Figure 2: $(\hat{\xi}_1, \hat{\xi}_2, \hat{\xi}_3)$ is an orthonormal base ($\langle \hat{\xi}_a, \hat{\xi}_b \rangle = \delta_{a,b}$) in $\mathbb{R}^3$, and $(\hat{\xi}_2, \hat{\xi}_3)$ a base in the tangent space $\mathrm{T}_{\mathbf{r}_0}\mathbb{S}^2$ to the unit sphere $\mathbb{S}^2$, in the point $\mathbf{r}_0 \in \mathbb{S}^2$. In this image $\mathbf{r}_f$ is the final vector position final after the displacement over a geodesic.

4 Appendix

4.1 The numerical algorithm

$$d\mathbf{r} = \cos\psi\,\hat{\xi}_2 + \sin\psi\,\hat{\xi}_3 \tag{67}$$

$$\Psi = U[0, 2\pi] = \begin{cases} \frac{1}{2\pi} & \text{if } \psi \in [0, 2\pi] \\ 0 & \text{otherwise} \end{cases} \tag{68}$$

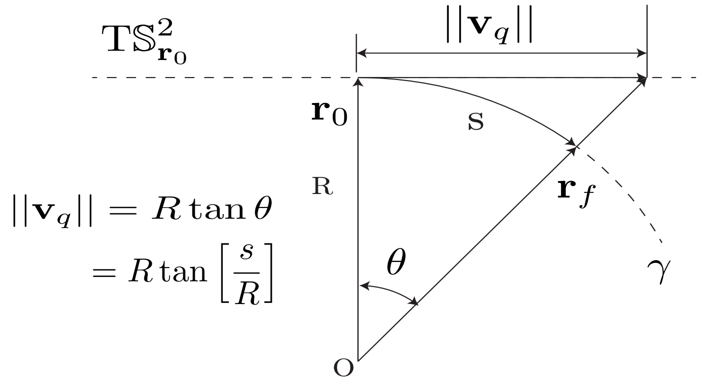
4.1.1 Ansatz

$$\mathbf{v}_q = \frac{R}{\Delta t} \cdot \tan\left[\frac{N(0, 4D\Delta t)}{R}\right] \cdot \left[\cos\Psi\,\hat{\xi}_2 + \sin\Psi\,\hat{\xi}_3\right] \tag{69}$$

4.2 External Field

If besides the effects that arise because of the interaction with the fluid particles, the particle is subject to an external field, which at the same time might be described as the derivative of a coordinate function

$$F_{\text{ext}} = -U'(x) \tag{70}$$



$$\mathbf{v}_q = \frac{R}{\Delta t}\cdot\tan\left[\frac{N(0,4D\Delta t)}{R}\right]\cdot\left[\cos\Psi\,\hat{\xi_2}+\sin\Psi\,\hat{\xi_3}\right]$$

Figure 3: In this figure we show the scale problem and the procedure to solve it. In it, it has been shown the plane which contains the geodesic curve γ of the trajectory that connects the initial position $\mathbf{r}_0$ with the final position $\mathbf{r}_f$.

it would be logical to relate the following law of evolution to the process

$$\begin{cases} \frac{dV(t)}{dt} = -\frac{\gamma}{m}V(t) - \frac{1}{m}U'(X) + (\frac{2KT\gamma}{m^2})^{1/2}\Gamma(t) \\ \frac{dX(t)}{dt} = V(t) \end{cases} \tag{71}$$

Neither the process $X(t)$ nor $V(t)$ are markovian, however they constitute a bivariate continuous Markov process (V, X).

4.3 Kramers' equation

The associated Fokker-Planck equation for the bivariate continuous Markov process in 71 is

$$\begin{aligned}\frac{\partial}{\partial t}P(x,v,t|x_0,v_0,t_0) &= \frac{\partial}{\partial v}\left\{\frac{\gamma v+U'(x)}{m}\cdot P(x,v,t|x_0,v_0,t_0)\right\} - \\ &\quad -v\,\frac{\partial}{\partial x}P(x,v,t|x_0,v_0,t_0) + \frac{KT\gamma}{m^2}\frac{\partial^2}{\partial v^2}P(x,v,t|x_0,v_0,t_0)\end{aligned}$$

and according to Gillespie it has been coined "the Kramer's equation" by Gardiner.

The stationary solution to the above partial differential equation is given by

$$\lim_{t_0\to-\infty} P(x,v,t|x_0,v_0,t_0) =: P^*(x,v|x_0,v_0,t_0) = C\exp\left[-(\frac{1}{2}mv^2+U(x))/KT\right] \tag{72}$$

which can be verified by direct substitution and correspond to the limit of statistical mechanics. The Kramer's equation govern the way in which the process $(\mathbf{x}, \mathbf{v})$ approximate to this stationary state.

4.4 Smoluchowski equation

In cases where the velocity changes are negligible $dV(t)/dt \approx 0$, then we might considere that $X(t)$ is (approximately) a continuous Markov process described by the equation

$$\frac{d}{dt}X(t) \approx -\frac{1}{\gamma}U'(x) + (2D)^{1/2}\Gamma(t) \tag{73}$$

At the same time it will have an associated Fokker-Planck equation

$$\frac{\partial}{\partial t}P_X(x,t|x_0,t_0) \approx \frac{1}{\gamma}\frac{\partial}{\partial x}[U'(x)P_X(x,t|x_0,t_0)] + D\frac{\partial^2}{\partial x^2}P_X(x,t|x_0,t_0). \tag{74}$$

This equation is known as the Smoluchowski equation and its approximated character is usually forgotten.

4.4.1 Fuck...ng Algebra

$$r = \sqrt{x^2+y^2+z^2} \tag{75}$$

$$\theta = \arccos\left[\frac{z}{\sqrt{x^2+y^2+z^2}}\right] \tag{76}$$

$$\phi = \arctan\left[\frac{y}{x}\right] \tag{77}$$

$$\dot{r} = 0 \tag{78}$$

$$\dot{\theta} = -\frac{\dot{z}}{\sqrt{x^2+y^2}} \tag{79}$$

$$\dot{\phi} = \pm\left[\frac{||v||^2}{x^2+y^2} - \frac{(x^2+y^2+z^2)}{(x^2+y^2)^2}\dot{z}\right]^{1/2} \tag{80}$$

$$\frac{\partial\theta}{\partial x} = \frac{xz}{\sqrt{x^2+y^2}}\frac{1}{x^2+y^2+z^2} = \frac{\cos\theta\cos\phi}{r} \tag{81}$$

$$\frac{\partial\theta}{\partial y} = \frac{yz}{\sqrt{x^2+y^2}}\frac{1}{x^2+y^2+z^2} = \frac{\cos\theta\sin\phi}{r} \tag{82}$$

$$\frac{\partial\theta}{\partial z} = \frac{-\sqrt{x^2+y2}}{x^2+y^2+z^2} = \frac{-\sin\theta}{r} \tag{83}$$

$$\frac{\partial\phi}{\partial x} = -\frac{y}{x^2+y^2} = -\frac{\sin\phi}{r\sin\theta} \tag{84}$$

$$\frac{\partial\phi}{\partial y} = \frac{x}{x^2+y^2} = \frac{\cos\phi}{r\sin\theta} \tag{85}$$

$$\frac{\partial\phi}{\partial z} = 0 \tag{86}$$

$$(d\theta, d\theta) = \sum_{k=1}^{3}\left[\frac{\partial\theta}{\partial\xi_k}\right]^2 = \left[\frac{\partial\theta}{\partial x}\right]^2 + \left[\frac{\partial\theta}{\partial y}\right]^2 + \left[\frac{\partial\theta}{\partial z}\right]^2 = \frac{1}{r^2} \tag{87}$$

$$(d\phi, d\phi) = \sum_{k=1}^{3}\left[\frac{\partial\phi}{\partial\xi_k}\right]^2 = \left[\frac{\partial\phi}{\partial x}\right]^2 + \left[\frac{\partial\phi}{\partial y}\right]^2 + \left[\frac{\partial\phi}{\partial z}\right]^2 = \frac{1}{r^2\sin^2\theta} \tag{88}$$

$$\frac{\partial^2\theta}{\partial x^2} = \frac{z}{\sqrt{x^2+y^2}(x^2+y^2+z^2)}\left\{\frac{y^2}{x^2+y^2} - \frac{x^2}{x^2+y^2+z^2}\right\} \tag{89}$$

$$\frac{\partial^2\theta}{\partial y^2} = \frac{z}{\sqrt{x^2+y^2}(x^2+y^2+z^2)}\left\{\frac{x^2}{x^2+y^2} - \frac{y^2}{x^2+y^2+z^2}\right\} \tag{90}$$

$$\frac{\partial^2\theta}{\partial z^2} = \sum_{k=1}^{3}\frac{\partial^2\theta}{\partial\xi_k^2} = \frac{z}{\sqrt{x^2+y^2}(x^2+y^2+z^2)}\left\{\frac{x^2+y^2}{x^2+y^2+z^2}\right\} \tag{91}$$

$$\frac{\partial^2\phi}{\partial x^2} = \frac{2yx}{(x^2+y^2)^2} = \frac{2\sin\phi\cos\phi}{r^2\sin^2\theta} \tag{92}$$

$$\frac{\partial^2\phi}{\partial y^2} = -\frac{2xy}{(x^2+y^2)^2} = -\frac{2\sin\phi\cos\phi}{r^2\sin^2\theta} \tag{93}$$

$$\frac{\partial^2\phi}{\partial z^2} = 0 \tag{94}$$

Then

$$\nabla^2_{\mathbf{x}}\theta = \sum_{k=1}^{3}\frac{\partial^2\theta}{\partial\xi_k^2} = \frac{\partial^2\theta}{\partial x^2} + \frac{\partial^2\theta}{\partial y^2} + \frac{\partial^2\theta}{\partial z^2} = \frac{z}{\sqrt{x^2+y^2}(x^2+y^2+z^2)} = \frac{\cot\theta}{r^2} \tag{95}$$

$$\nabla^2_{\mathbf{x}}\phi = \sum_{k=1}^{3}\frac{\partial^2\phi}{\partial\xi_k^2} = \frac{\partial^2\phi}{\partial x^2} + \frac{\partial^2\phi}{\partial y^2} + \frac{\partial^2\phi}{\partial z^2} = 0 \tag{96}$$

$$\frac{\partial \dot{\theta}}{\partial x} = -\frac{x\dot{z}}{(x^2+y^2)^{3/2}} = \frac{\cos\phi}{r}\dot{\theta} \tag{97}$$

$$\frac{\partial \dot{\theta}}{\partial y} = -\frac{y\dot{z}}{(x^2+y^2)^{3/2}} = \frac{\sin\phi}{r}\dot{\theta} \tag{98}$$

$$\frac{\partial \dot{\theta}}{\partial z} = 0 \tag{99}$$

$$\frac{\partial \dot{\theta}}{\partial \dot{x}} = 0 \tag{100}$$

$$\frac{\partial \dot{\theta}}{\partial \dot{y}} = 0 \tag{101}$$

$$\frac{\partial \dot{\theta}}{\partial \dot{z}} = -\frac{1}{(x^2+y^2)^{1/2}} = -\frac{1}{r\sin\theta} \tag{102}$$

$$\frac{\partial \dot{\phi}}{\partial x} = \mp x\left[\frac{||v||^2}{x^2+y^2} - \frac{(x^2+y^2+z^2)}{(x^2+y^2)^2}\dot{z}\right]^{-1/2}\left\{\frac{||v||^2}{(x^2+y^2)^2}+\right. \tag{103}$$

$$\left. + \dot{z}\left[\frac{1}{(x^2+y^2)^2} - \frac{2(x^2+y^2+z^2)}{(x^2+y^2)^3}\right]\right\} \tag{104}$$

$$\frac{\partial \dot{\phi}}{\partial y} = \mp y\left[\frac{||v||^2}{x^2+y^2} - \frac{(x^2+y^2+z^2)}{(x^2+y^2)^2}\dot{z}\right]^{-1/2}\left\{\frac{||v||^2}{(x^2+y^2)^2}+\right. \tag{105}$$

$$\left. + \dot{z}\left[\frac{1}{(x^2+y^2)^2} - \frac{2(x^2+y^2+z^2)}{(x^2+y^2)^3}\right]\right\} \tag{106}$$

$$\frac{\partial \dot{\phi}}{\partial z} = \mp\left[\frac{||v||^2}{x^2+y^2} - \frac{(x^2+y^2+z^2)}{(x^2+y^2)^2}\dot{z}\right]^{-1/2}\left\{\frac{z\,\dot{z}}{(x^2+y^2)^2}\right\} \tag{107}$$

$$\frac{\partial \dot{\phi}}{\partial \dot{x}} = \pm\left[\frac{||v||^2}{x^2+y^2} - \frac{(x^2+y^2+z^2)}{(x^2+y^2)^2}\dot{z}\right]^{-1/2}\left\{\frac{\dot{x}}{(x^2+y^2)}\right\} \tag{108}$$

$$\frac{\partial \dot{\phi}}{\partial \dot{y}} = \pm\left[\frac{||v||^2}{x^2+y^2} - \frac{(x^2+y^2+z^2)}{(x^2+y^2)^2}\dot{z}\right]^{-1/2}\left\{\frac{\dot{y}}{(x^2+y^2)}\right\} \tag{109}$$

$$\frac{\partial \dot{\phi}}{\partial \dot{z}} = \pm\left[\frac{||v||^2}{x^2+y^2} - \frac{(x^2+y^2+z^2)}{(x^2+y^2)^2}\dot{z}\right]^{-1/2}\left\{\frac{2\dot{z}}{(x^2+y^2)} - \frac{(x^2+y^2+z^2)}{(x^2+y^2)^2}\dot{z}\right\} \tag{110}$$