The Smoluchowski-Kramers Approximation: What model describes a Brownian particle?

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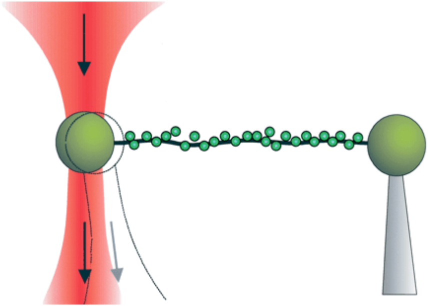
Measuring forces

- Work with Jan Wehr and Giovanni Volpe (experimental physicist).
- Methods for measuring small forces (10^{-15} N).
- Two methods for measurements:
  - **Equilibrium measurements**, needs system to be at or near equilibrium, doesn't need a priori knowledge of force
  - **Drift measurements**, system can be far from equilibrium, does not measure forces from noise.
- Need a model (SDE) to take forces from noise into account.

Application



- DNA stretching (Figure from JCP Issue 26 (2003)).
- See AZDS article Apr. 25 on Prof. Koen Visscher (UA physics dept.) on using optical tweezers for DNA stretching.

Modeling with SDE

- Want to use SDE to model system (e.g. particle displacesment $\mathbf{x}_t \in \mathbb{R}^n$ at time t in viscous fluid)

$$d\mathbf{x}_t = b(\mathbf{x}_t)\ dt + \sigma(\mathbf{x}_t)\ d\mathbf{W}_t, \quad \mathbf{x}_0 = \mathbf{x}.$$

- $\mathbf{W}_t$, m-dim. Wiener Process, b drift σ noise. This assumes zero correlation.

$$\int_0^t \sigma(\mathbf{x}_t)\ d\mathbf{W}_t = \lim_{N\to\infty} \sum_{i=1}^{N} \sigma(\mathbf{x}_{t_i^*}, \omega)(\mathbf{W}_{t_i} - \mathbf{W}_{t_{i-1}}),$$

$$t_i^* = \alpha t_i + (1-\alpha) t_{i-1},$$

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$$t_i^* = \alpha t_i + (1-\alpha) t_{i-1},$$

- Integral varies with α. Special cases $\alpha = 0$ Itô, $\alpha = 1/2$ Stratonovich, $\alpha = 1$ anti-Itô.

$$\int_0^t \mathbf{W}_s\, d_\alpha \mathbf{W}_s, = \frac{1}{2}\mathbf{W}_t^2 - \left(\frac{1}{2} - \alpha\right) t$$

- Physically more realistic to replace $\mathbf{W}_t$ by differentiable process

$$\xi_t^\delta = \frac{1}{\delta} \int k \left(\frac{(t-s)}{\delta} \right) \mathbf{W}_s \, ds,$$

- for smooth kernel k. ξ_t^δ is called **colored noise**.

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Wong, Zakai (1965)

The solution to

$$d\mathbf{x}_t^\delta = b(\mathbf{x}_t^\delta) + \frac{1}{\delta}\sigma(\mathbf{x}_t^\delta)\dot{\xi}_t^\delta \, dt,$$

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- Which model is correct?

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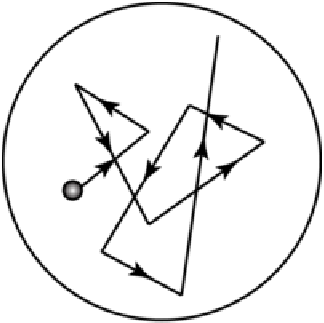
Brownian Motion



Brownian Movement

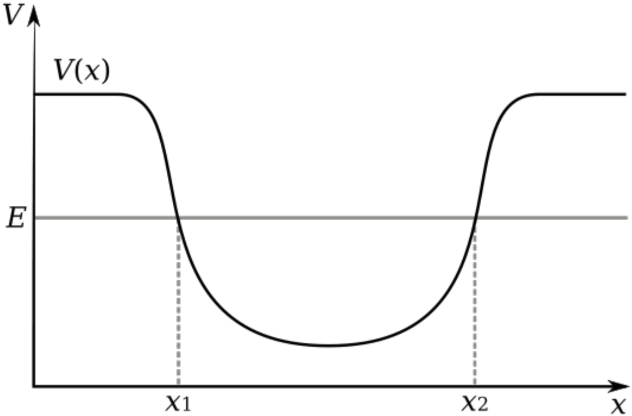
(figure from wiki.one-school.net)

A dynamical theory for Brownian motion

- Einstein and Smoluchowski derived the motion to be diffusive.
- Langevin and later Ornstein and Uhlenbeck (1930s) have dynamical theory.
- Newton's second law

$$\begin{aligned} dx_t^m &= v_t^m dt, \\ m dv_t^m &= F(x_t^m) - \gamma v_t^m dt + \sigma \, dW_t \end{aligned}$$

Kramers



(en.wikipedia.org)

- Hendrick Kramers took $m = 0$ to simplify calculations to chemical reaction rates.

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$$dx_t = \frac{F(x_t)}{\gamma} dt + \frac{\sigma}{\gamma} \, dW_t.$$

- Called **Smoluchoski-Kramers** approximation.
- Since σ and σ/γ constant, the integral is the same for all interpretations.

General Model

$$
\begin{aligned}
dx_t^m &= v_t^m \, dt \\
dv_t^m &= \left(\frac{F(x_t^m)}{m} - \frac{\gamma(x_t^m)}{m} v_t^m \right) \, dt + \frac{\sigma(x_t^m)}{m} \, dW_t.
\end{aligned}
$$

- For σ, γ positive and Lipschitz, then use property of stochastic integral:
- For f smooth $(E[|f(s,\omega) - f(t,\omega)|^2] \leq k|s-t|^{1+\epsilon})$,

$$\int_0^t f(s,\omega) \, d_\alpha W_s = \int_0^t f(s,\omega) \, dW_s, \qquad \text{for all } \alpha.$$

- Approximated by the Smoluchowski-Kramers approximation as $m \to 0$,

$$dx_t = \frac{F(x_t)}{\gamma(x_t)}\, dt + \frac{\sigma(x_t)}{\gamma(x_t)}\, d_\alpha W_t,$$

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$$dx_t = \left[\frac{F(x_t)}{\gamma(x_t)} + \alpha \frac{\sigma(x_t)}{\gamma(x_t)} \frac{d}{dx_t}\left(\frac{\sigma(x_t)}{\gamma(x_t)}\right)\right] dt + \frac{\sigma(x_t)}{\gamma(x_t)}\, dW_t,$$

- The second drift term is called spurious (or noise induced) drift. *Crucial to drift measurements.*
- **What is** α?

Results

Nelson (1965)

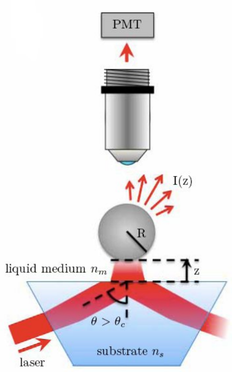
For γ and σ constant, $x_t^m \to x_t$ a.s.

Freidlin (2004)

(1) For γ constant and $\sigma(x_t)$, $x_t^m \to x_t$ in probability for $\alpha = 0$.
(2) For γ constant, $\sigma(x_t)$ and colored noise, $x_t^{m,\delta} \to x_t$ in probability for $\alpha = 1/2$ ($m \to 0$ then $\delta \to 0$).

- What about $\gamma(x_t)$?
- Is this case relevant?

Experiment



(courtesy Giovanni Volpe)
Measure the drift forces

Model of experiment

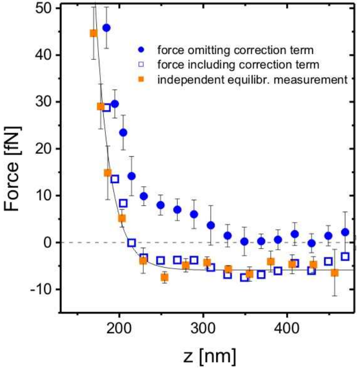
$$
\begin{aligned}
dx_t &= v_t \; dt \\
m dv_t &= F(x_t) - \frac{k_B T}{D_\perp(x_t)} v_t \; dt + \frac{k_B T\sqrt{2}}{\sqrt{D_\perp(x_t)}} \; dW_t
\end{aligned}
$$

- $D_\perp(x_t) \to 0$ as $x_t \to 0$, and $D_\perp(x_t) \approx D_\infty$ for $x_t > 0$.
- Model satisfies the Fluctuation-Dissipation relation $\gamma = c\sigma^2$.
- As $m \to 0$, approximate

$$dx_t = \frac{F(x_t)D_\perp(x_t)}{k_B T} \; dt + \sqrt{2D_\perp(x_t)} \; d_\alpha W_t.$$

- What value of α gives the dynamics of x_t?

Results of Experiment



- Difference between Itô and anti-Itô is a change in sign of force.
- Correction to drift corresponds to anti-Itô stochastic integral ($\alpha = 1$).

Connection to PDE

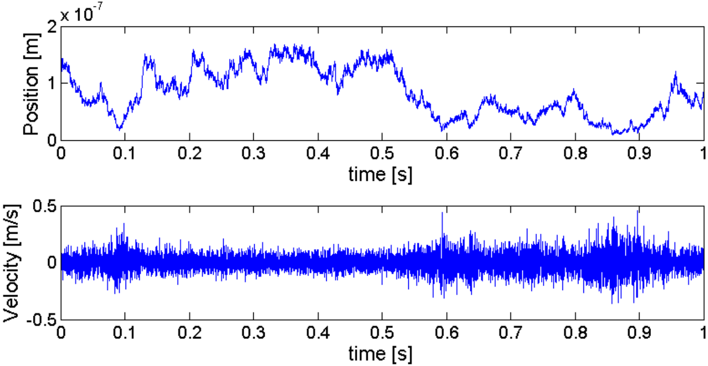
$$\begin{aligned} dx_t^m &= v_t^m \; dt \\ m dv_t^m &= F(x_t^m) - \gamma(x_t^m) v_t \; dt + \sigma(x_t^m) \; dW_t, \end{aligned}$$

Density $p_m(x', v', t' | x, v, t)$ satisfies the *Backward Kolmogorov* equation

$$\begin{aligned} \frac{\partial p_m}{\partial t} &= \frac{\sigma(x)^2}{2m} \frac{\partial^2 p_m}{\partial v^2} + v \frac{\partial p_m}{\partial x} + \left(\frac{(F(x) - \gamma(x) v)}{m} \right) \frac{\partial p_m}{\partial v} \\ &= L_{x,v} p_m, \end{aligned}$$

Also, for all $(x', v') \in \mathbb{R}^2$, p_m satisfies the *forward Kolmogorov* (or Fokker-Planck) equation

$$\frac{\partial p_m}{\partial t'} = L^*_{x',v'} p_m.$$


x 10^-7
2
1
0
Position [m]
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
time [s]
0.5
0
-0.5
Velocity [m/s]
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
time [s]

Homogenization

- Normalize velocity, $u_t = \sqrt{m} v_t$.
- Infinitesimal operator written as

$$\frac{\partial p_m}{\partial t} = L_{x,u} p_m = \left(\frac{1}{m} L_1 + \frac{1}{\sqrt{m}} L_2 \right) p_m.$$

- Assume, p_m the solution to the backward Kolmogorov equation,

$$p_m = p_0 + \sqrt{m} p_1 + m p_2 + \ldots$$

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- Solve the system for p_0

$$L_1 p_0 = \left(\frac{\sigma(x)^2}{2} \frac{\partial^2}{\partial u^2} - \gamma(x) u \frac{\partial}{\partial u} \right) p_0 = 0,$$

$$L_1 p_1 = -L_2 p_0 = -\left(u \frac{\partial}{\partial x} + F(x) \frac{\partial}{\partial u} \right) p_0,$$

$$\frac{\partial p_0}{\partial t} = L_1 p_2 + L_2 p_1,$$

- For Fredholm alternative arg. need solution to,

$$L_1^*\rho(u;x) = \frac{\sigma(x)^2}{2}\frac{\partial^2\rho}{\partial u^2} - \gamma(x)\frac{\partial(u\rho)}{\partial u} = 0.$$

- Need σ, γ independent of u.
- Stationary Fokker-Planck for OU process (in u).
- Solution is a Gaussian density.

$$\rho(u;x) = C(x)\exp\left\{\frac{-\gamma(x)u^2}{\sigma(x)^2}\right\}.$$

- the BK equation satisfied by p_0.

$$\frac{\sigma(x)^2}{2\gamma(x)^2}\frac{\partial^2 p_0}{\partial x^2} + \left(\frac{F(x)}{\gamma(x)} - \frac{\sigma(x)^2}{2\gamma(x)^3}\frac{d(\gamma(x))}{dx}\right)\frac{\partial p_0}{\partial x} = \frac{\partial p_0}{\partial t}.$$

- Compare to the PDE of SK

$$\frac{\sigma(x)^2}{2\gamma(x)^2}\frac{\partial^2 p}{\partial x^2}+\left(\frac{F(x)}{\gamma(x)} + \alpha\left[-\frac{\sigma(x)}{\gamma(x)^3}\gamma'(x) - \frac{\sigma(x)^2}{\gamma(x)^2}\sigma'(x)\right]\right)\frac{\partial p}{\partial x} = \frac{\partial p}{\partial t}.$$

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- Effective SDE for x_t,

$$dx_t = \left(\frac{F(x_t)}{\gamma(x_t)} - \frac{\sigma(x_t)^2}{2\gamma(x_t)^3}\gamma'(x_t)\right) dt + \frac{\sigma(x_t)}{\gamma(x_t)}\, d\tilde{W}_t, \qquad (1)$$

- $\tilde{W}_t$ is an arbitrary Wiener process. (From studying the inf. operator)

Equation for α

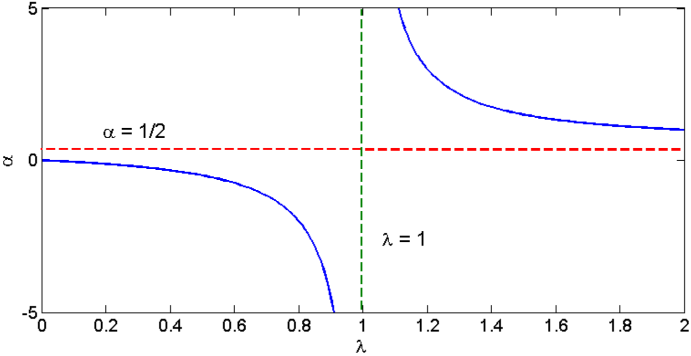
$$\alpha = \alpha(x) = \frac{\gamma'(x)\sigma(x)}{2(\gamma'(x)\sigma(x) - \gamma(x)\sigma'(x))}.$$

α constant iff $\gamma(x) = c\sigma(x)^\lambda$.

$$\alpha = \frac{\lambda}{2(\lambda - 1)}$$
$$\lambda = \frac{\alpha}{\alpha - \frac{1}{2}}$$

This coincides with Freidlin ($\lambda = 0 \implies \alpha = 0$) and Wehr/Volpe ($\lambda = 2 \implies \alpha = 1$).

α vs λ



$\lambda = 1$

- For $\gamma(x) = c\sigma(x)$ ($\lambda = 1$), then α doesn't have interpretation.
- Effective equation for x_t,

$$dx_t = \left(\frac{F(x_t)}{c\sigma(x_t)} - \frac{\sigma'(x_t)}{2c^2\sigma(x_t)} \right) dt + \frac{1}{c} d\tilde{W}_t.$$

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- "Noise" induced drift, with no position dependent noise.
- Application for Brownian particle in temp. gradient.

$$\gamma(x) = \frac{k_B T(x)}{D} \quad \sigma(x) = \frac{k_B T(x)\sqrt{2}}{\sqrt{D}}$$

Color Noise

- After computed approximation, found source (Pavliotis and Stuart (2008)).
- Systems with color noise of the form,

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$$\eta_t = \sqrt{\frac{2a}{\delta^2}}\int_0^t \exp\left\{\frac{a}{\delta^2}(s-t)\right\}\,dW_s$$

- Mean zero Gaussian random variable with covariance

$$E[\eta_{t_1}\eta_{t_2}] = \exp\left\{-\frac{a}{\delta^2}|t_1 - t_2|\right\}.$$

Pav Stuart Results

- Refine Freidlin Results ($\gamma = 1$ const $\sigma(x_t)$ varying, for simplicity external force $F = 0$),

$$\begin{aligned} dx_t &= v_t \; dt \\ m dv_t &= (-v_t + \sigma(x_t)\eta_t) \; dt, \\ d\eta_t &= -\frac{a\eta_t}{\delta^2} \; dt + \sqrt{\frac{2b}{\delta^2}} dW_t, \end{aligned}$$

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\end{aligned}
$$

- For $m = \tau\delta^2$, apply same asymptotic analysis for the Backward Kolmogorov equation. Need to solve,

$$
L_1^* \rho(u, \eta; x) = -\frac{\partial}{\partial u}\left[\left(-\frac{1}{\tau}u + \frac{\sigma(x)}{\sqrt{\tau}}\eta\right)\rho\right] + \alpha\frac{\partial}{\partial \eta}(\eta\rho) + \lambda\frac{\partial^2 \rho}{\partial \eta^2} = 0.
$$

- Again F-P of 2-dim OU process in η, u.

Future work

- $\tau \to 0$ gives Stratonovich ($\alpha = 1/2$) and $\tau \to \infty$ gives Itô ($\alpha = 0$).

$$dx_t = \frac{b}{a^2(1+\tau a)}\sigma(x_t)\sigma'(x_t)\,dt + \sqrt{\frac{2b}{a^2}}\sigma(x_t)\,d\tilde{W}_t.$$

- Does OU colored noise give interpolation of $\alpha = 1/2$ and correct α for power law?
- Can you get convergence of SDEs in general case instead of inf. gens?
- Multi-dimensional case.
- Questions?