process where the rates depend on the initial (rather than final) state ($\alpha = 0$).

(iii) Under the Itô interpretation the standard rules of variable transformation do not apply $\Rightarrow$ Itô calculus, stochastic integration

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4° Diffusion in inhomogeneous media

- For non-interacting particles the positional probability density $P_1(x,t)$ is equivalent to the density $\rho(x,t)$ of a many-particle system

  $\Rightarrow$ FP-eq can be interpreted as a diffusion equation (here: in one spatial dimension)

- On the macroscopic level diffusion processes are governed by Fick's laws, which read (for constant diffusion coefficient D):

(I) $$\frac{\partial \rho}{\partial t} + \frac{\partial j}{\partial x} = 0$$ particle number conservation

(II) $$j = -D \frac{\partial \rho}{\partial x}$$

How is (II) to be generalized when D depends on position, $D = D(x)$?

Two obvious possibilities:

(i) $J = -D(x)\dfrac{\partial\rho}{\partial x}$ (ii) $J = -\dfrac{\partial}{\partial x} D(x)\rho$

Compare to the multiplicative Langevin-equation with $f(x) = 0$:

$$\dot{x} = g(x)\,\xi(t) \qquad \langle \xi(t)\xi(t')\rangle = \delta(t-t')$$

$$\Big\downarrow \text{"interpretation } \alpha\text{"}$$

$$\frac{\partial P_1}{\partial t} = -\frac{\partial}{\partial x}\alpha g' g P_1 + \frac{1}{2}\frac{\partial^2}{\partial x^2} g^2 P_1 =$$

$$= -\frac{\partial}{\partial x}\left[\alpha g' g P_1 - \frac{\partial}{\partial x}\left(\frac{1}{2}g^2\right)P_1\right] =$$

$$= -\frac{\partial}{\partial x}\left[(\alpha - 1) g' g P_1 - \frac{1}{2}g^2\frac{\partial P_1}{\partial x}\right] =$$

$$= -\frac{\partial}{\partial x}\left[(\alpha - 1) D' P_1 - D\frac{\partial P_1}{\partial x}\right]$$

with $D(x) = \frac{1}{2}g(x)^2$.

We conclude that (i) corresponds to $\alpha = 1$, and (ii) to $\alpha = 0$.

In the following we show that the choice of α

- has macroscopically observable consequences
- depends on the microscopic details of the process

a) Macroscopic behavior

Consider the general relation

$$J = -\left[(1-\alpha) D' \rho + D \frac{d\rho}{dx} \right]$$

for different special situations.

- stationary state: $J = 0 \Rightarrow \frac{d\rho_s}{dx} = -(1-\alpha)\frac{D'}{D}\rho_s$

$$\Rightarrow \frac{1}{\rho_s}\frac{d\rho_s}{dx} = -(1-\alpha)\frac{D'}{D} , \quad \frac{d}{dx}\ln\rho = -(1-\alpha)\frac{d}{dx}\ln D$$

$$\Rightarrow \rho_s(x) = C\, D(x)^{-(1-\alpha)}$$

$\alpha = 1$: $\rho_s = \text{const.}$

$\alpha < 1$: Particles accumulate in regions where $D(x)$ is small.

- homogeneous density: $\rho = \text{const.} = \rho_0$

$$\Rightarrow J = -(1-\alpha) D' \rho_0$$

$\alpha = 1$: No current

$\alpha < 1$: Current towards regions where $D(x)$ is small.

- particle drift: Consider the positional probability density $P_1(x,t)$ of a particle with a localized initial condition. The position of the particle at time t is then

$$\langle x \rangle = \int dx \; x \; P_1(x,t)$$

$$\Rightarrow \underline{\frac{d}{dt}\langle x \rangle} = \int dx \; x \frac{\partial P_1}{\partial t} = -\int dx \; x \frac{\partial}{\partial x} J$$

$$= -\int dx \left[(1-\alpha) D' P_1 + D \frac{\partial P_1}{\partial x} \right] =$$

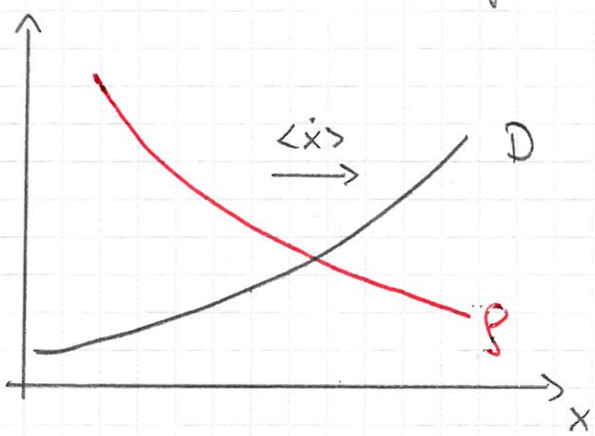
$$= \int dx \left(\alpha D' P_1 - \frac{\partial}{\partial x} D P_1 \right) = \alpha \int dx \; D' P_1$$

$$\simeq \underline{\alpha D'(\langle x \rangle)}$$ if $D(x)$ is slowly varying.

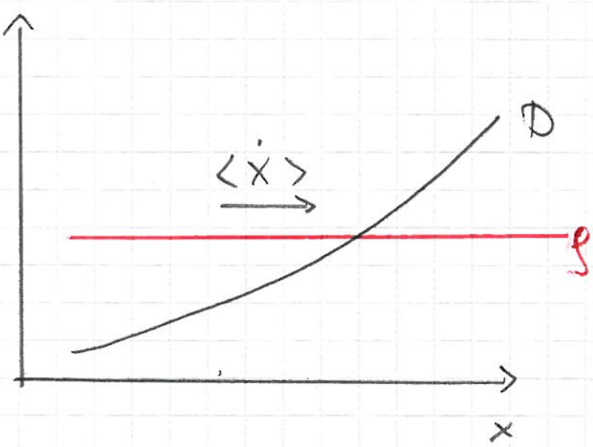
$\underline{\alpha = 0}$: No drift

$\underline{\alpha > 0}$: Drift towards regions where $D(x)$ is large

This implies "drift without flux" in the stationary case and "drift against the flux" in the case of homogeneous density



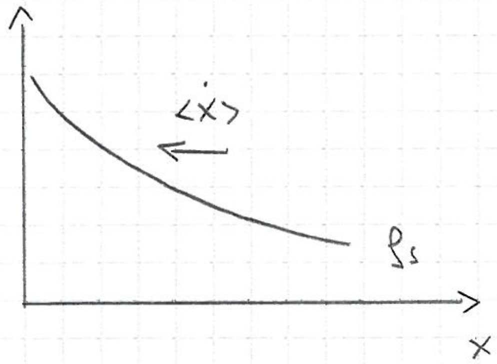
$J = 0$



$\rho = $ const.

Analogy: Diffusion in an external force field (e.g., gravity)

$$\left.\begin{aligned} \dot{x} = -F + \xi(t) \quad \Rightarrow \quad & \langle \dot{x} \rangle = -F \\ & \rho_s(x) \sim e^{-Fx} \end{aligned}\right\}$$



$\Rightarrow$ density gradient compensates the drift such that $j = 0$ in the stationary state.

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b) Microscopic model (Lançon et al., 2001)

Consider a random walk in discrete time and continuous one-dimensional space.

- Jumps occur at discrete times $t_n = n\,\Delta t$ with equal probability to the left or right
- Jump length depends on position through

$$\left.\begin{aligned} & \underbrace{x(t+\Delta t) - x(t)}_{\Delta x} = \pm\sqrt{2\tilde{D}(x(t),\Delta x)\cdot\Delta t} \\ & \tilde{D}(x,\Delta x) = D(x + \alpha\,\Delta x) \end{aligned}\right\}$$

$$\left.\begin{aligned} & \alpha = 0: \ D \text{ evaluated at initial position} \\ & \alpha = 1: \ D \text{ evaluated at final position} \end{aligned}\right\}$$

(i) Particle drift: If $D(x)$ is slowly varying

$$D(x + \alpha \Delta x) \simeq D(x) + \alpha \Delta x \, D'(x)$$

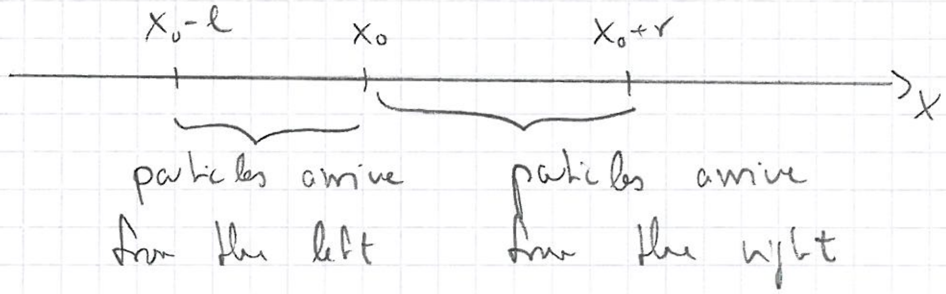
$$\Rightarrow \quad (\Delta x)^2 = 2 D(x + \alpha \Delta x) \cdot \Delta t \simeq$$

$$\simeq 2D(x) \Delta t + 2D'(x) \alpha \Delta x \, \Delta t$$

$$\Rightarrow \quad \Delta x = \alpha D'(x) \Delta t \pm \frac{1}{2} \sqrt{8 D \Delta t + 4 \alpha^2 D'^2 \Delta t^2}$$

$$\Rightarrow \quad \Delta x = \alpha D'(x) \Delta t$$

(ii) Particle current in a homogeneous system:



$$\Rightarrow \quad j = \frac{1}{2} \rho (l - r)$$

Particles jumping from $x_0 - l$ to x_0 satisfy

$$l = \sqrt{2D(x_0 - l + \alpha l) \Delta t}$$

$$\Rightarrow \quad l^2 \cong 2D(x_0) - 2(1-\alpha) \, l \, D'(x_0) \Delta t$$

$$\left.\begin{aligned} \Rightarrow \quad l &\cong -(1-\alpha) D'(x_0) \Delta t + \sqrt{2D(x_0) \Delta t} \\ r &= (1-\alpha) D'(x_0) \Delta t + \sqrt{2D(x_0) \Delta t} \end{aligned}\right\}$$

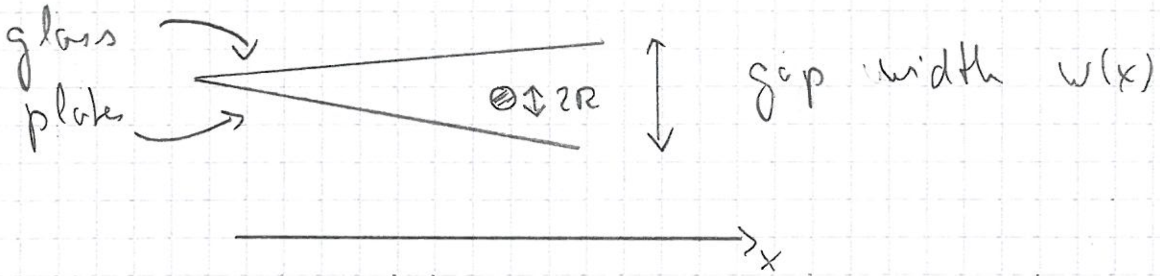
$$\Rightarrow \quad J = -\rho(1-\alpha)\, D'(x)$$

in precise agreement with the macroscopic model.

c) Applications

(i) Brownian motion in confined geometry

(Lançon et al., 2001)



Einstein relation: $D = \dfrac{k_B T}{6\pi \eta R}$

- glass plates increase friction

  $\Rightarrow \eta(x)$ with $\eta' < 0$

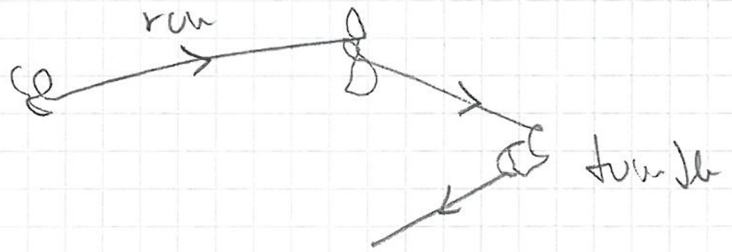
- thermal equilibrium $\Rightarrow T = \text{const.}$

$$\Rightarrow \left.\begin{array}{l} D' > 0, \\ \rho_s = \text{const.} \Rightarrow \alpha = 1 \ (\text{"isothermal"}) \end{array}\right\}$$

$$\Rightarrow \langle \dot{x} \rangle = \alpha D' > 0$$

(ii) Chemotaxis of bacteria

E. coli move by a sequence of straight runs and random tumbles:



- length of runs T_{run} ~ step length of RW

$$\Rightarrow \quad D \sim T_{run}^2 \sim \frac{1}{\text{tumbling rate}^2}$$

- T_{run} depends on nutrient concentration

  $\Rightarrow$ how to adjust this dependence in order to move towards increasing nutrient concentration?

- Bacterial drift $\langle \dot{x} \rangle = \alpha D'$

  $\Rightarrow$ D and T_{run} should increase, tumbling rate decrease with nutrient concentration

- Mechanism works only if $\alpha > 0$

  $\Rightarrow$ evaluating nutrient concentration at one position is not sufficient.

5° Fokker-Planck and Schrödinger operators

Fokker-Planck operator for systems with additive noise:

$$\mathcal{L} = -\frac{\partial}{\partial y} f(y) + \frac{1}{2} A \frac{\partial^2}{\partial y^2}$$

$\Rightarrow$ stationary distribution

$$P_s(y) = C\, e^{-\frac{2}{A} V(y)} \quad , \quad V(y) = -\int_0^y dy'\, f(y')$$

$$=: C\, e^{-\Phi(y)}$$

P_s is a right eigenfunction of $\mathcal{L}$ with eigenvalue 0.

What can we say about other eigenfunctions?

a) Eigenfunction expansion of the FP-operator

Goal: Transform $\mathcal{L}$ into a symmetric ("Hermitian") differential operator.

To this end we note that, for any φ,

$$\frac{1}{2} A \frac{\partial}{\partial y} e^{-\Phi} \frac{\partial}{\partial y} e^{\Phi} \varphi(y) =$$

$$= \frac{1}{2} A \frac{\partial}{\partial y} \left\{ \Phi' + \frac{\partial}{\partial y} \right\} \varphi(y) =$$

$$= \frac{1}{2} A \frac{\partial}{\partial y} \left\{ -\frac{2}{A} f(y) + \frac{\partial}{\partial y} \right\} \varphi(y) = \mathcal{L}\, \varphi(y)$$

$$\Rightarrow \quad \mathcal{L} = \frac{1}{2} A \frac{\partial}{\partial y} e^{-\Phi} \frac{\partial}{\partial y} e^{\Phi}$$

Now introduce the (symmetrized) operator

$$\tilde{\mathcal{L}} := e^{\Phi/2} \mathcal{L} e^{-\Phi/2} =$$

$$= \frac{1}{2} A e^{\Phi/2} \frac{\partial}{\partial y} e^{-\Phi} \frac{\partial}{\partial y} e^{\Phi/2}$$

which we claim is symmetric with respect to the standard scalar product:

$$\frac{2}{A} \langle \varphi \mid \tilde{\mathcal{L}} \psi \rangle = \frac{2}{A} \int dy\, \varphi(y)\, \tilde{\mathcal{L}}\, \psi(y) =$$

$$= \int dy\, \underbrace{\varphi(y)\, e^{\Phi/2}}_{\tilde{\varphi}(y)} \frac{\partial}{\partial y} e^{-\Phi} \frac{\partial}{\partial y} \underbrace{e^{\Phi/2} \psi(y)}_{\tilde{\psi}(y)} = \text{(part. int.)}$$

$$= - \int dy\, e^{-\Phi} \left(\frac{\partial}{\partial y} \tilde{\varphi}\right)\left(\frac{\partial}{\partial y} \tilde{\psi}\right) = \text{(part. int.)}$$

$$= \int dy\, \tilde{\psi} \frac{\partial}{\partial y} e^{-\Phi} \frac{\partial}{\partial y} \tilde{\varphi} = \frac{2}{A} \langle \psi \mid \tilde{\mathcal{L}} \varphi \rangle \quad \square$$

It follows that $\tilde{\mathcal{L}}$ has orthogonal eigenfunctions ψ_n with real eigenvalues λ_n:

$$\tilde{\mathcal{L}} \psi_n = \lambda_n \psi_n , \qquad \langle \psi_n \mid \psi_m \rangle = \delta_{nm} .$$

from which eigenfunctions of $\mathcal{L}$ can be constructed:

$$\mathcal{L}\big(\underbrace{e^{-\Phi/2}\psi_n}_{\phi_n}\big) = e^{-\Phi/2}\tilde{\mathcal{L}}\psi_n = \lambda_n \underbrace{e^{-\Phi/2}\psi_n}_{\phi_n}$$

In particular, the stationary distribution $\phi_0 \sim e^{-\Phi}$ correspond to the "ground state" $\psi_0 \sim e^{-\Phi/2}$ with eigenvalue $\lambda_0 = 0.$

We next show that all eigenvalues are negative or zero:

$$\lambda_n = \int dy\, \psi_n \tilde{\mathcal{L}} \psi_n = \int dy\, e^{\Phi/2}\phi_n\, e^{\Phi/2}\mathcal{L}\phi_n$$

$$= \frac{1}{2}A \int dy\, e^{\Phi}\phi_n \frac{\partial}{\partial y} e^{-\Phi} \frac{\partial}{\partial y} e^{\Phi}\phi_n = (\text{p.i.})$$

$$= -\frac{1}{2}A\int dy\, e^{-\Phi}\left(\frac{\partial}{\partial y} e^{-\Phi}\phi_n\right)^2 \leq 0.$$

$$\Rightarrow \underline{0 = \lambda_0 \geq \lambda_1 \geq \lambda_2 \geq \ldots}$$

Provided $\lambda_1 < 0$, the convergence of an arbitrary initial condition to the stationary distribution occurs at rate λ_1:

$$P_1(y,t) = \sum_n c_n \phi_n(y)\, e^{-\lambda_n t} \longrightarrow c_0\phi_0(y)$$

b) Mapping to a Schrödinger problem

Consider the application of $\tilde{\mathcal{L}}$ to a function φ:

$$\frac{2}{A}\tilde{\mathcal{L}}\varphi = e^{\Phi/2}\frac{\partial}{\partial y}e^{-\Phi}\frac{\partial}{\partial y}e^{\Phi/2}\varphi =$$

$$= e^{\Phi/2}\frac{\partial}{\partial y}e^{-\Phi/2}\left(\frac{1}{2}\Phi'\varphi + \varphi'\right) =$$

$$= \cancel{e^{\Phi/2}}\left\{-\frac{\Phi'}{2}\left(\frac{1}{2}\Phi'\varphi + \cancel{\varphi'}\right)\cancel{e^{-\Phi/2}} + \right.$$

$$\left. + \cancel{e^{-\Phi/2}}\left(\frac{1}{2}\Phi''\varphi + \frac{1}{2}\cancel{\Phi'\varphi'} + \varphi''\right)\right\}$$

$$= \varphi'' + \left(\frac{1}{2}\Phi'' - \frac{1}{4}(\Phi')^2\right)\varphi$$

$\Rightarrow$ $\tilde{\mathcal{L}} = -\mathcal{H}$ with the Schrödinger operator

$$\mathcal{H} = -\frac{A}{2}\frac{\partial^2}{\partial y^2} + V_s(y)$$

$$V_s(y) = \frac{1}{4}A\left[\frac{1}{2}(\Phi')^2 - \Phi''\right] =$$

$$= \frac{1}{4}A\left[\frac{1}{2}\left(\frac{2}{A}f(y)\right)^2 + \frac{2}{A}f'(y)\right] =$$

$$= \frac{1}{2}\left(f(y)^2/A + f'(y)\right)$$