Stat. Phys. IV: Lecture 5

Spring 2025

Backward Fokker-Planck Equation

Instead of propagating the probability density P forward in time, one can instead look backwards in time, i.e. treat $P\left(x,t|x_0,t_0\right)$ as a function of x_0 and t_0. Reformulating the Chapman-Kolmogorov equation in the following way

$$P\left(x,t|x_0,t_0\right) = \int_{-\infty}^{\infty} d\xi \, P\left(x,t|x_0+\xi,t_0+\Delta t_0\right) P\left(x_0+\xi,t_0+\Delta t_0|x_0,t_0\right)$$

and repeating the Kramers-Moyal expansion with respect to x_0 and t_0 leads to the

Backward Fokker-Planck equation[1]

$$\partial_{t_0} P\left(x,t|x_0,t_0\right) = -A(x_0)\partial_{x_0} P\left(x,t|x_0,t_0\right) - \frac{1}{2} D(x_0)\partial_{x_0}^2 P\left(x,t|x_0,t_0\right)$$

Note that for a homogeneous process $P(x,t|x_0,t_0) = P(x,0|x_0,t_0-t)$ implies $\partial_t P(x,t|x_0,t_0) = \partial_t P(x,0|x_0,t_0-t) = -\partial_{t_0} P(x,t|x_0,t_0)$.

[1] Gillespie, Markov Processes, Chapter 2

Comparison of the forward and backward Fokker-Planck equations

Forward Fokker-Planck equation

$$\partial_t P\left(x,t|x_0,t_0\right) = -\partial_x\left[A(x)P\left(x,t|x_0,t_0\right)\right] + \partial_x^2\left[\frac{1}{2}D(x)P\left(x,t|x_0,t_0\right)\right]$$

Backward Fokker-Planck equation

$$\partial_{t_0} P\left(x,t|x_0,t_0\right) = -A(x_0)\partial_{x_0} P\left(x,t|x_0,t_0\right) - \frac{1}{2}D(x_0)\partial_{x_0}^2 P\left(x,t|x_0,t_0\right)$$

Note that the derivatives act only on P.

Kramers equation[2]

Full Brownian motion gives a bivariate Langevin equation

$$\frac{dv}{dt} = -\gamma v + \frac{F(x)}{m} + \sqrt{\frac{2\gamma}{\beta m}} f(t) \quad \text{and} \quad \frac{dx}{dt} = v$$

with $\beta = 1/k_B T$.

Kramers equation ≡ corresponding Fokker-Planck equation

$$\partial_t P + v\partial_x P + \frac{F(x)}{m}\partial_v P = \gamma \left(\underbrace{\partial_v (vP)}_{\text{Collision kernel}} + \frac{1}{\beta m}\partial_v^2 P \right)$$

Define the density $\rho(x,t) = \int dv\, P(x,v,t)$
and the current $J(x,t) = \int dv\, vP(x,v,t)$
Continuity equation: $\partial_t \rho(x,t) + \partial_x J(x,t) = 0$

[2] See P. Martin's scriptum, 3.4

Stationary solution of the Fokker-Planck equation

$$\frac{d}{dx}\left[a(x,t)P_S(x)\right] - \frac{1}{2}\frac{d^2}{dx^2}\left[b(x)P_S(x)\right] = -\frac{d}{dt}P_S(x) = 0$$

So the current is constant

$$J = a(x)P_S(x) - \frac{1}{2}\frac{d}{dx}\left[b(x)P_S(x)\right] = \text{const}$$

General Stationary solution of Fokker-Planck equation

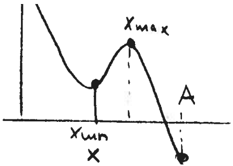
$$P_S(x) = N_0 e^{-\Phi(x)} + J e^{-\Phi(x)} \int^x dx' \, \frac{1}{b(x')} e^{\Phi(x')}$$

with $\Phi(x) = -2\int_0^x \frac{a(x')}{b(x')}\, dx'$

Kramers escape problem[3]

We want the rate of particles escaping from the well.
Taking the derivative of $e^{\beta V(x)} P_S(x)$, we get

$$J = -De^{-\beta V(x)} \frac{d}{dx} \left[e^{\beta V(x)} P_S(x) \right]$$



Integrating
between $x_{\min}$ and A, and assuming $P_S(A) \approx 0$

$$J = De^{\beta V(x_{\min})} P_S(x_{\min}) \left(\int_{x_{\min}}^{A} e^{-\beta V(x)}\, dx \right)$$

Moreover, the probability to be in the well is given
by

$$P = \int_{x_1}^{x_2} P_S(t) \approx P_S(x_{\min}) e^{\beta V(x_{\min})} \int_{x_1} x_2 e^{-\beta V(x)}\, dx$$

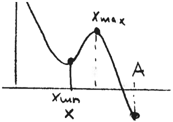
[3]See H. Risken, The Fokker-Planck Equation, 5.10

Kramers escape rate

Escape rate: $r = \frac{J}{P}$ so that

Kramers escape rate

$$\frac{1}{r} \approx 2\pi e^{\beta(V(x_{\max})-V(x_{\min}))} \frac{m\gamma}{\sqrt{V''(x_{\min})V''(x_{\max})}}$$



Where we used asymptotic approximations to evaluate the integrals.
Applications: Laser trapping of particles [4], chemical reaction rates [5] ...

[4] Neuman, Keir C., and Steven M. Block. "Optical trapping." Review of scientific instruments 75.9 (2004): 2787-2809.

[5] Hänggi, Peter, Peter Talkner, and Michal Borkovec. "Reaction-rate theory: fifty years after Kramers." Reviews of modern physics 62.2 (1990): 251.

Kramers escape: first passage time[6]

Probability to stay between a and b until time t

$$G(x,t) = \int_a^b P(x',t|x,0)\,dx'$$

same as probability that escape time (or first passage) $T > t$.
This means that the probability distribution for T is

$$P_T(T) = -\frac{\partial G(x,t)}{\partial t}$$

so using integration by part, we find:

$$T(x) \equiv \langle T \rangle = -\int_0^\infty t\frac{\partial G(x,t)}{\partial t}\,dt = \int_0^\infty G(x,t)\,dt$$

[6] See Gardiner, Stochastic Methods, 5.2.7

Kramers escape: first passage time

Using the backward Fokker-Planck equation, we can derive a differential equation for G and then for $T(x)$

Differential equation for time of first passage

$$A(x)\partial_x T(x) + \frac{1}{2}B(x)\partial_x^2 T(x) = -1$$

Solving with appropriate boundary condition, one gets
$T(x) = \int_x^b \frac{dy}{\Psi(y)} \int_a^y \frac{\Psi(z)}{B(z)} dz$ with $\Psi(x) = \exp(\int_0^x dx' 2\frac{A(x')}{B(x')})$

Kramers escape: first passage time

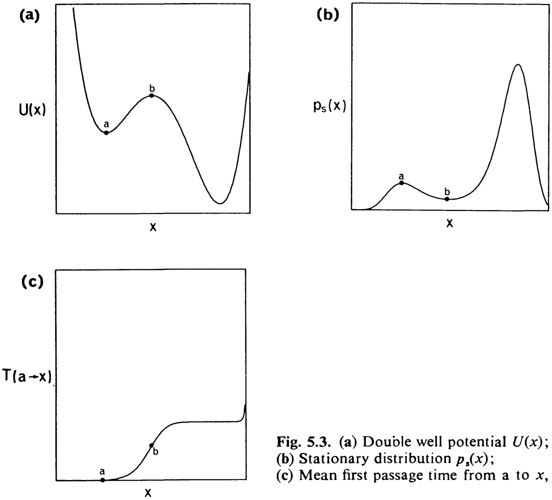


Fig. 5.3. **(a)** Double well potential $U(x)$;
(b) Stationary distribution $p_s(x)$;
(c) Mean first passage time from a to x, $T(a \to x_0)$

Application of the Kramers escape rate: Optical tweezers

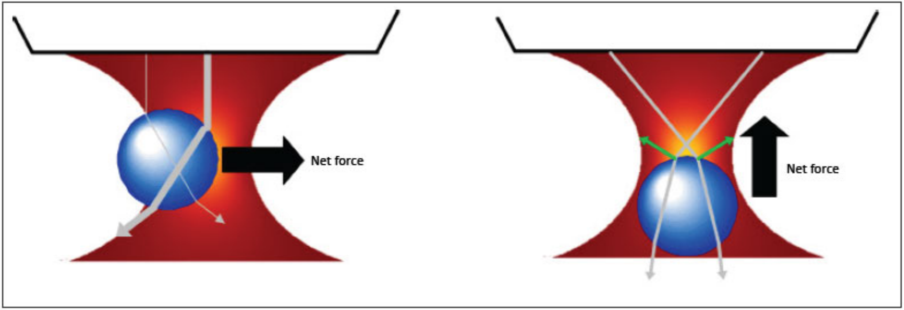
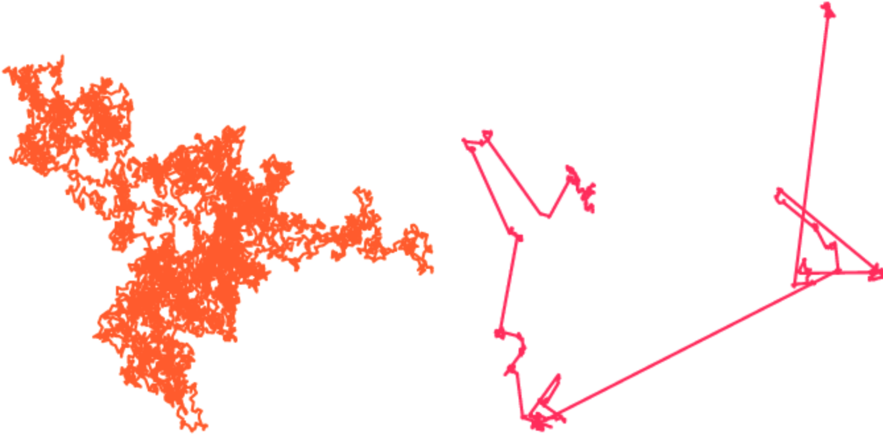


FIGURE 1: The refracted rays (grey) produce corresponding forces on the bead, resulting in a net force toward the most intense region of the beam. In the axial direction, the gradient force must be greater than the scattering force to obtain three-dimensional trapping.

$$F_{\text{grad}} = \frac{1}{2} n_{\text{m}} \alpha \nabla |E|^2 = \frac{n_{\text{m}}^3 \left(\frac{d}{2}\right)^3}{2} \left(\frac{n_{\text{p}}^2 - n_{\text{m}}^2}{n_{\text{p}}^2 + 2n_{\text{m}}^2} \right)^2 \nabla |E|^2,$$

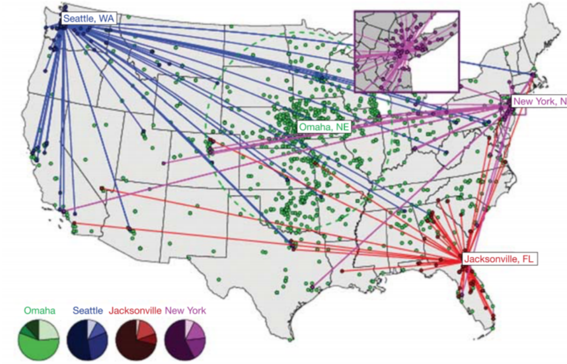
Svoboda, Karel, et al. "Direct observation of kinesin stepping by optical trapping interferometry." Nature 365.6448 (1993): 721.

Lévy flight versus Brownian motion[7]



[7] **brockmann˙scaling˙2006**.

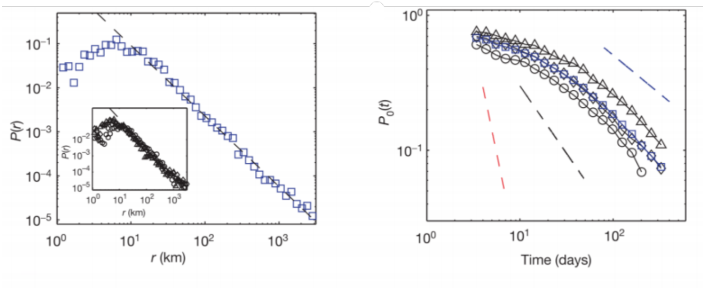
The scaling laws of human travel [8]



Dispersal of bank notes and humans on geographical scales and Trajectories of bank notes originating from four different places.

[8]Vespignani, Alessandro. "Predicting the behavior of techno-social systems." Science 325.5939 (2009): 425-428.

The scaling laws of human travel



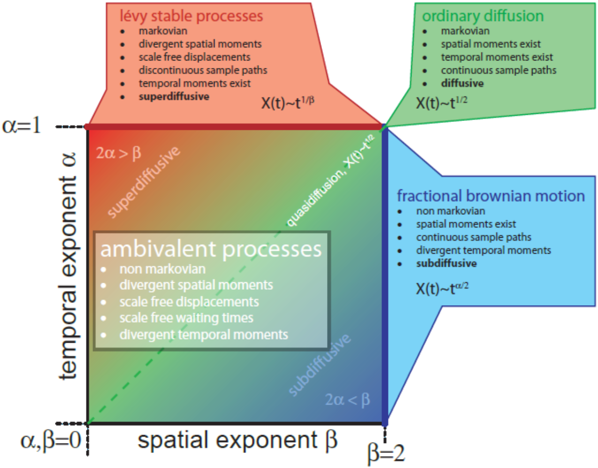
Dispersal of bank notes and humans on geographical scales. c, The short-time dispersal kernel. The measured probability density function $P(r)$ of traversing a distance r in less than $T = 4$ days is depicted in blue symbols. d, The relative proportion $P_0(t)$ of secondary reports within a short radius $(r_0 = 20\mathrm{km})$ of the initial entry location as a function of time. Blue squares show $P_0(t)$ averaged over 25,375 initial entry locations.

Continuous time random walks

Consider processes for which $P(y, \Delta t) = f(y)\Phi(\Delta t)$ where both $f$and Φ are probability density distributions.

Process	f	Φ	$P(x, \Delta t)$	Scaling
Ordinary diffusion	gaussian	exponential	$\frac{e^{-x^2/Dt}}{\sqrt{t}}$	$t^{1/2}$
Levy flight	$\frac{1}{y^{\beta+1}}$	*	$\frac{L_\beta(x/t^{1/\beta})}{t^{1/\beta}}$	$t^{1/\beta}$
Fractional brownian motion	gaussian	$\frac{1}{(\Delta t)^{\alpha+1}}$	$\frac{L_\beta(x/t^{\alpha/2})}{t^{\alpha/2}}$	$t^{\alpha/2}$
Ambivalent process	$\frac{1}{y^{\beta+1}}$	$\frac{1}{(\Delta t)^{\alpha+1}}$		$t^{\alpha/2\beta}$

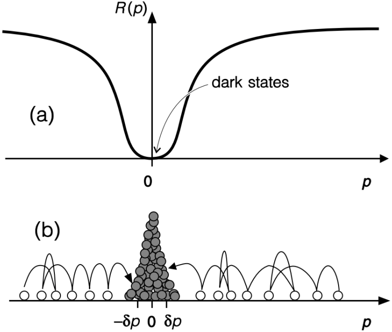
Asymptotic Universality Classes of CTRWs[9]



[9]**brockmann˙scaling˙2006**.

Application: sub-recoil laser cooling

- During the interaction time with the laser field, an atom will be trapped for some time intervals τ_i and will be in the recycling region for some other intervals $\hat{\tau}_i$
- The sums formed by summing the trapping times, i.e. $\tau_N = \sum_{i=1}^{N} \tau_i$ are Lévy sums
- Main idea: construct a momentum dependent fluorescence rate $R(p)$ in the trapping region such that $R(p) \approx 0$ around $p \approx 0$



Application: sub-recoil laser cooling

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Subrecoil Laser Cooling and Lévy Flights

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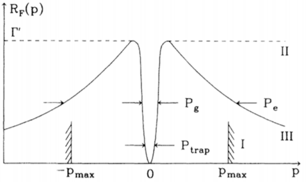

FIG. 2. Variations with p of the fluorescence rate $R_F(p)$ (see text). The narrow dip around $p=0$, with a width p_g, is due to VSCPT. The trapping zone is defined by $|p|<p_{\text{trap}}$. Three different models are taken for the variations of $R_F(p)$ at large p. Model I: walls confining the atomic momentum to $|p| \leq p_{\max}$. Model II: constant fluorescence rate equal to Γ' out of the dip (interrupted line). Model III (corresponding to actual experiments, full line): decrease of the fluorescence rate for $|p|>p_e$, due to a Doppler detuning from the optical resonance.

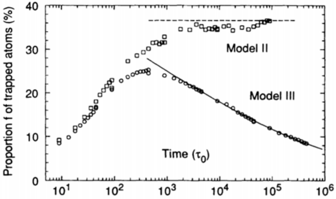

FIG. 3. Variations with the interaction time θ of the proportion f of trapped atoms ($|p|<p_{\text{trap}}$), calculated from N Monte Carlo runs for the models II and III of Fig. 2. Model II (squares): $N=4000$, $p_g=0.5\hbar k$, $p_{\text{trap}}=0.08\hbar k$; the interrupted line represents the asymptotic theoretical prediction $f=0.365$ corresponding to $E_R/\hbar\Gamma'=0.59$. Model III (circles): $N=16000$, $p_g=0.5\hbar k$, $p_{\text{trap}}=0.08\hbar k$, $p_e=9.4\hbar k$; the full line represents the best fit for the asymptotic theoretical prediction (see text). Model II requires more computer time than model III. This is why N is smaller and the statistical uncertainty larger.