MAE 545

Special Topics - Lessons from Biology for Engineering Tiny Devices

Lectures:
T, Th 1:30-2:50 PM,
Friend Center 003

Office hours:
W 1:30-3:00 PM,
EQUAD D414

Andrej Košmrlj
andrej@princeton.edu
Lecture Notes

- text books: none
- lecture slides will be posted on Blackboard

http://blackboard.princeton.edu

course: MAE545_F2015

Assignments

- presentation of research paper in class
- final paper (final project)
Random walks

Brownian motion

Swimming of E. coli

Polymer random coils

Protein search for a binding site on DNA
Protein filaments

Actin filament

Microtubule

Cargo transport

Segregation of chromosomes during cell division

Crawling of cells
Viruses

assembly of viral capsids

packing of viral DNA inside the capsid

infection of cells
Structural colors


H. Cao, Yale
Structure and form of organs and plants

Brain

Gut

Plantain Lily leaf

Bauhinia seed pods
DNA Origami

C. E. Castro et al., Nature methods (2011)
Elastic metamaterials

phononic crystals

buckliball

swelling of patterned gels

- Elastic metamaterials
- Phononic crystals
- Buckliball
- Swelling of patterned gels
Lecture 1 (9/17)
Brownian motion of small particles

History

1827 Robert Brown: observed irregular motion of small pollen grains suspended in water

1905-06 Albert Einstein, Marian Smoluchowski: microscopic description of Brownian motion and relation to diffusion equation
Random walk on a 1D lattice

At each step particle jumps left or right with probability 1/2.

What is the probability $p(x,N)$ that we find particle at position $x$ after $N$ jumps?

Probability that particle makes $k$ jumps to the right and $N-k$ jumps to the left obeys the binomial distribution

$$\binom{N}{k} 2^{-N}$$

This corresponds to particle position

$$x = k\ell - (N - k)\ell = (2k - N)\ell$$

Therefore

$$p\left(x = (2k - N)\ell, N\right) = \binom{N}{k} 2^{-N}$$
Random walk on a 1D lattice

Gaussian approximation for $p(x,N)$

Position $x$ after $N$ jumps can be expressed as the sum of individual jumps $x_i$

$$x = \sum_{i=1}^{N} x_i$$

Mean value averaged over all possible random walks

$$\langle x \rangle = N \langle x_1 \rangle = N \left( \frac{1}{2} \ell - \frac{1}{2} \ell \right) = 0$$

Variance averaged over all possible random walks

$$\sigma^2 = \langle x^2 \rangle - \langle x \rangle^2 = N \langle x_1^2 \rangle = N \ell^2$$

$$\sigma^2 \equiv 2DN$$

effective diffusion constant

$$D = \ell^2 / 2$$

According to the central limit theorem $p(x,N)$ approaches gaussian distribution for large $N$

$$p(x,N) \approx \frac{1}{\sqrt{2\pi\sigma^2}} e^{-x^2/2\sigma^2}$$
Random walk on a 1D lattice

Exact distribution

\[ p\left(x = (2k - N)\ell, N\right) = \binom{N}{k} 2^{-N} \]

Gaussian approximation

\[ p(x, N) \approx \frac{1}{\sqrt{2\pi N\ell^2}} e^{-x^2/2N\ell^2} \]

Note: exact discrete distribution has been made continuous by replacing discrete peaks with boxes whose area corresponds to the same probability.
Master equation and diffusion equation

Master equation provides recursive relation for the evolution of probability distribution, where $\Pi(x, y)$ describes probability for a jump from $y$ to $x$. 

$$p(x, N + 1) = \sum_y \Pi(x, y)p(y, N)$$

For our example master equation reads

$$p(x, N + 1) = \frac{1}{2}p(x - \ell, N) + \frac{1}{2}p(x + \ell, N)$$

Initial condition: $p(x, N = 0) = \delta(x)$

In the limit of large number of jumps $N$ and small step size $\ell$, we can Taylor expand master equation to derive an approximate diffusion equation

$$\frac{\partial p(x, N)}{\partial N} = D \frac{\partial^2 p(x, N)}{\partial x^2}$$

$D = \ell^2 / 2$
Fokker-Planck equation

In general the probability distribution $\Pi$ of jump lengths $s$ can depend on the particle position $x$. $\Pi(s|x)$

Assume that jumps occur in regular small time intervals $\Delta t$

Generalized master equation

$\frac{\partial p(x, t)}{\partial t} = \sum_s \Pi(s|x - s)p(x - s, t)$

Again Taylor expand master equation above to derive the Fokker-Planck equation

$$
\frac{\partial p(x, t)}{\partial t} = -\frac{\partial}{\partial x} \left[ v(x)p(x, t) \right] + \frac{\partial^2}{\partial x^2} \left[ D(x)p(x, t) \right]
$$

$\text{drift velocity}$

(external fluid flow, external potential)

$v(x) = \sum_s \frac{s}{\Delta t} \Pi(s|x) = \frac{\langle s(x) \rangle}{\Delta t}$

$\text{diffusion coefficient}$

(e.g. position dependent temperature)

$D(x) = \sum_s \frac{s^2}{2\Delta t} \Pi(s|x) = \frac{\langle s^2(x) \rangle}{2\Delta t}$
**Probability current**

**Fokker-Planck equation**

\[
\frac{\partial p(x, t)}{\partial t} = -\frac{\partial}{\partial x} \left[ v(x) p(x, t) \right] + \frac{\partial^2}{\partial x^2} \left[ D(x) p(x, t) \right]
\]

**Conservation law of probability**
(no particles created/removed)

\[
\frac{\partial p(x, t)}{\partial t} = -\frac{\partial J(x, t)}{\partial x}
\]

By comparing equations above we can define probability current

\[
J(x, t) = v(x) p(x, t) - \frac{\partial}{\partial x} \left[ D(x) p(x, t) \right]
\]

Note that for the steady state distribution, where \( \frac{\partial p^*(x, t)}{\partial t} \equiv 0 \) the steady state current is constant and independent on \( x \)

\[
J^* \equiv v(x) p^*(x) - \frac{\partial}{\partial x} \left[ D(x) p^*(x) \right] = \text{const}
\]

If we don’t create/remove particles at boundaries then \( J^*=0 \)

\[
p^*(x) \propto \frac{1}{D(x)} \exp \left[ \int_{-\infty}^{x} dy \frac{v(y)}{D(y)} \right]
\]
Spherical particle suspended in fluid in external potential

Newton’s law

\[ m \frac{\partial^2 x}{\partial t^2} = -\lambda v(x) - \frac{\partial U(x)}{\partial x} + F_r \]

- fluid drag
- external potential force
- random Brownian force

For simplicity assume overdamped regime and ignore inertial term on the left hand side. This produces average drift velocity

\[ \langle v(x) \rangle = -\frac{1}{\lambda} \frac{\partial U(x)}{\partial x} \]

Equilibrium probability distribution

\[ p^*(x) = Ce^{-U(x)/\lambda D} = Ce^{-U(x)/k_BT} \]

(see previous slide) (equilibrium physics)

Einstein - Stokes equation

\[ D = \frac{k_BT}{\lambda} = \frac{k_BT}{6\pi \eta R} \]
Example of Einstein-Stokes equation

\[ D = \frac{k_B T}{\lambda} = \frac{k_B T}{6\pi\eta R} \]

Spherical particle suspended in water at room temperature

- Water viscosity \( \eta \approx 10^{-3} \text{kg m/s} \)
- Temperature \( T = 300 \text{K} \)
- Boltzmann constant \( k_B = 1.38 \times 10^{-23} \text{J/K} \)

**Particle radius**

- \( R = 1 \mu\text{m} \)
- \( R = 1 \text{mm} \)

**Diffusion constant**

- \( D \approx 0.2 \mu\text{m}^2/\text{s} \)
- \( D \approx 2 \times 10^{-4} \mu\text{m}^2/\text{s} \)

**Diffusion important**

- Small diffusion
Random walk with absorbing boundaries

What is the probability $P_B(x)$ that particle that starts at position $x$ gets absorbed at site B?

$$P_B(x) = \sum_s \Pi(s|x) P_B(x + s)$$

$$0 = v(x) \frac{dP_B(x)}{dx} + D(x) \frac{d^2P_B(x)}{dx^2}$$

Boundary conditions

$$P_B(x = b) = 1$$
$$P_B(x = a) = 0$$

Example

$v = 0, D = \text{const}$

$$P_B(x) = \frac{x - a}{b - a}$$

$v, D = \text{const}$

$$P_B(x) = \frac{(1 - e^{-v(x-a)/D})}{(1 - e^{-v(b-a)/D})}$$
Random walk with absorbing boundaries

What is the mean time $T(x)$ that particle that starts at position $x$ gets absorbed at either site?

$$T(x) = \sum_s \Pi(s|x)T(x + s) + \Delta t$$

boundary conditions

$$T(x = a) = 0$$
$$T(x = b) = 0$$

Example

$v = 0, D = \text{const}$

$$T(x) = \frac{(x - a)(b - x)}{2D}$$
What is the average time $T_{\text{esc}}$ it takes for a particle to escape over a barrier?

Once particle crosses the peak it quickly descends into the global minimum. Therefore estimate the escape time, by placing reflecting boundary at $x=\text{a}$ and absorbing boundary at $x=\text{b}$.

\[
-1 = v(x)\frac{dT(x)}{dx} + D(x)\frac{d^2T(x)}{dx^2}
\]

boundary conditions
\[
\begin{align*}
\frac{dT}{dx}(x=a) &= 0 \\
T(x=b) &= 0
\end{align*}
\]

**Arrhenious Law**

\[
T_{\text{esc}} = T(a) \approx \frac{\pi \lambda}{\sqrt{U''(a)U''(b)}} e^{[U(b)-U(a)]/k_BT}
\]
Fick’s laws

N noninteracting Brownian particles

Local concentration \( c(x, t) = Np(x, t) \)

Fick’s laws below directly follow from Fokker-Plank equations

**First Fick’s law**

Concentration flux \( J = vc - \frac{\partial}{\partial x} \left[ Dc \right] \)

**Second Fick’s law**

Diffusion of concentration

\[
\frac{\partial c}{\partial t} = -\frac{\partial}{\partial x} \left[ vc \right] + \frac{\partial^2}{\partial x^2} \left[ Dc \right]
\]

Generalization to higher dimensions

\[
\vec{J} = \vec{v}c - \vec{\nabla}(Dc)
\]

\[
\frac{\partial c}{\partial t} = -\vec{\nabla} \cdot (\vec{v}c) + \vec{\nabla}^2(Dc)
\]
Further reading