Livi & Politi

1. Brownian motion, Langevin, Fokker-Planck

(→ escape time from an energy barrier
→ Arrhenius equation)

Markov chains, master equation, detailed balance

2. Linear Response Theory and Transport phenomena

- Kubo relation
Green-Kubo relation $D = \lim_{t \to \infty} \int_0^t d\tau \langle v_x(t) v_x(0) \rangle$
- Kramers-Kronig relations → $\boxed{\text{FLUCTUATION DISSIPATION THEOREM}}$

- Onsager Theory → regression relation
- entropy production, thermodynamic fluxes & forces
- applications → thermoelectric effects
Seebeck, Peltier effect

3. Out-of-equilibrium phase transitions

NESS (Non Equilibrium Steady State)

→ phase transitions with absorbing state

- Directed Percolation universality class

→ (scaling, meanfield, critical exponents

- TASEP (driven systems)
- Bridge model (non equilibrium symmetry breaking)

Mezard & Montanari

- Intro to information theory:
  Shannon entropy, mutual information
  → data compression, channel transmission
- Random Energy Model (analytical computation with replica trick)
  → spin glasses
- Channel transmission → Random code ensemble

Fluctuation Theorems: Jarzinski; Gallavotti - Cohen

equilibrium free energy difference

→ application to single molecule experiments

$$\exp\left(-\frac{\Delta F}{k_B T}\right) = \left\langle \exp\left(-W/_{k_B T}\right)\right\rangle$$

work dissipated

average over out-of-equilibr. trajectories

Wang-Landau method ← • Generalized ensemble methods (simulations) → sampling of rare events

- Large deviation theory → rate functions

Random Walk $\quad \vec{x}_i = l_i \hat{x}_i \quad l_i$ from $p(l)$ ← normalized PDF

$$\vec{X} = \sum_1^N i \, \vec{x}_i$$

$$X^2 = \vec{X} \cdot \vec{X} = \sum_{ij} \vec{x}_i \cdot \vec{x}_j = \sum_1^N i \, x_i^2 + \sum_{i \neq j} \vec{x}_i \cdot \vec{x}_j$$

average over different realizations

step direction is chosen randomly (independently from previous steps)

$$\vec{x}_i \cdot \vec{x}_j = l_i l_j \cos(\vartheta_{ij})$$

angle $\vec{x}_j, \vec{x}_i$; ϑ_{ij}

$$\langle X^2 \rangle = \sum_1^N i \langle x_i^2 \rangle + \underbrace{\sum_{i \neq j} \langle x_i \cdot x_j \rangle}_{= 0}$$

$$= \sum_1^N i \langle l_i^2 \rangle = N \langle l^2 \rangle$$

$$p(l) = \frac{1}{\lambda} \exp(-l/\lambda)$$

Poisson distribution

λ = mean free path

$$\langle l \rangle = \lambda \; ; \; \langle l^2 \rangle = 2\lambda^2$$

$$\langle X^2 \rangle = 2N\lambda^2 = 2\lambda \langle v \rangle t$$

$$= 2dDt \leftarrow \text{diffusion}$$

total length traveled by the walker

$$\langle L \rangle = \lambda N = \langle v \rangle t$$

diffusion coefficient $\underbrace{D = \lambda \langle v \rangle}$ 1

d = space dimension

average velocity

$(T = 20°C)$ air molecule

$\lambda = \langle v \rangle \tau = \frac{1}{\sqrt{2}\, n\, \sigma}$

$\langle v \rangle = \sqrt{\frac{8T}{\pi m}} \approx 450\ m/s$

$(k_B = 1)$

(from Kinetic theory)

n = density

$\lambda \sim 60\ nm$

$\boxed{\tau \sim \mathcal{O}(10^{-11}\ s)}$ collision time

$\sigma = 4\pi r^2$

collision cross section

(r molecule size)

$$D \sim 9\ mm^2/s$$

- Brownian Motion → mesoscopic particle

size $R \sim 1 \div 10\ \mu m$

macroscopic object → dissipation using Stokes's law

$$\vec{F} = m \frac{d\vec{v}}{dt} = -\tilde{\gamma}\, \vec{v} = -6\pi\eta R \vec{v}$$

$$\frac{d\vec{v}}{dt} = -\frac{\tilde{\gamma}}{m}\vec{v}$$

friction coefficient ($\tilde{\gamma}$)

viscosity (η)

$t_d = m/\tilde{\gamma}$ dissipation time scale

$$t_d = \frac{m}{6\pi\eta R} \sim \mathcal{O}(10^{-7}\ s)$$

$\boxed{t_d \gg \tau}$

$t \gg t_d$ diffusive regime

$t \ll t_d$ ballistic regime