An introduction to statistical physics with simple examples

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17 April 2012

Presentation and computer code for the simulations at
http://www.maths.qmul.ac.uk/~ht/talks/

Outline

1. What is statistical physics?
2. Basic concepts
3. Applications

Statistical physics

- Study of physical systems using probabilities and statistics
- Study of systems having many components / particles / molecules
  - Gases, liquids, solids
  - Classical or quantum systems
  - Molecules, polymers, etc.
- Study of physical systems having random components / behavior
  - Weather system
  - Turbulent fluids
  - Electron diffusion
  - ...

Ingredients

- Many particles or components ($\sim 10^{23}$)
- Randomness (vs determinism)
- No exact prediction
- Prediction on average or with some probability

Basic concepts

Random variable

Variable X taking one of several values x at random

Examples:

- Coin: $X = \text{head}$ or $X = \text{tail}$, $P(\text{head}) = P(\text{tail}) = 0.5$
- Dice: $X \in \{1, 2, 3, 4, 5, 6\}$
- Gas molecule: $(X, V) = (\text{position}, \text{velocity})$

Probability distribution

Probabilities for the different values of a random variable:

$$P(x) = \text{Prob}(X = x)$$

- $0 < P(x) < 1$
- $\sum_x P(x) = 1$

Basic concepts (cont'd)

Examples

- Dice:

$$P(x) = \frac{1}{6}, \quad x = 1, 2, 3, 4, 5, \text{ or } 6$$

- Gas molecule: $P(x, y, z, v_x, v_y, v_z)$

Mean, average or expectation

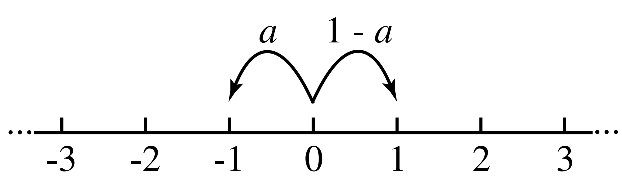
$$E[X] = \sum_x x\, P(x)$$

Variance

$$\mathrm{var}(X) = E[X^2] - E[X]^2 = \sum_x x^2\, P(x) - \left(\sum_x x\, P(x)\right)^2 > 0$$

The bigger the variance, the more random a random variable is.

Application 1: Basic random walk



- Start at 0
- Move left or right with probability

$$P(-1) = a, \quad P(+1) = 1 - a$$

- Repeat N times
- Displacement:

$$S_N = \sum_{i=1}^{N} X_i$$

- $X_i = \pm 1$: Displacement at ith jump
- See computer simulations

Basic random walk (cont'd)

- Mean displacement:

$$E[S_N] = E[\sum_{i=1}^{N} X_i] = \sum_{i=1}^{N} E[X_i] = N(1-2a)$$

  - $a = \frac{1}{2}$: unbiased random walk
  - $a > \frac{1}{2}$: left bias
  - $a < \frac{1}{2}$: right bias

- Variance:

$$\mathrm{var}(S_N) = E[S_N^2] - E[S_N]^2 = N(2a - 2a^2) \sim N$$

- Random walk spreads $\sim \sqrt{\mathrm{var}} \sim \sqrt{N}$
- See computer simulations

Basic random walk (cont'd)

- Probability distribution ($a = 1/2$):

steps	-5	-4	-3	-2	-1	0	1	2	3	4	5
0						1					
1					$\frac{1}{2}$	0	$\frac{1}{2}$				
2				$\frac{1}{4}$	0	$\frac{2}{4}$	0	$\frac{1}{4}$			
3			$\frac{1}{8}$	0	$\frac{3}{8}$	0	$\frac{3}{8}$	0	$\frac{1}{8}$		
4		$\frac{1}{16}$	0	$\frac{4}{16}$	0	$\frac{6}{16}$	0	$\frac{4}{16}$	0	$\frac{1}{16}$	
5	$\frac{1}{32}$	0	$\frac{5}{32}$	0	$\frac{10}{32}$	0	$\frac{10}{32}$	0	$\frac{5}{32}$	0	$\frac{1}{32}$

- See computer graphs
- Random walk in 2D or 3D
- See computer simulations

Application 2: Brownian motion

- Jump by any amount $\Delta x \in \mathbb{R}$
- Jump after a time Δt
- Probability density for the jumps:

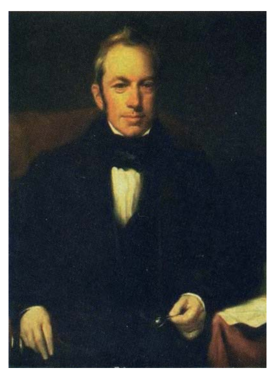
$$P(\Delta x) = \frac{1}{\sqrt{2\pi\sigma^2\Delta t}} e^{-\Delta x^2/(2\sigma^2\Delta t)}$$

  - Mean 0
  - Variance $\sigma^2\Delta t$
- Position at time t:

$$X(t) = \sum_{i=1}^{t/\Delta t} \Delta x_i$$

- $\mathrm{var}(X(t)) \sim t$
- See computer simulations

Brownian motion (cont'd)



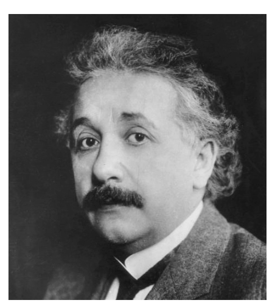
- Observed by Brown (1827)
- Studied by Einstein (1905)
- Probability density:

$$P(x) = \frac{1}{\sqrt{2\pi\sigma_t^2}} e^{-x^2/(2\sigma_t^2)}$$

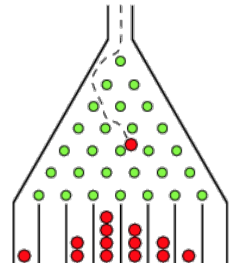
- Variance:

$$\sigma_t^2 = E[X(t)] = \frac{2k_B T}{3\pi\eta a} t$$

  - Viscosity: η
  - Particle radius: a
- See video [http://www.youtube.com/watch?v=cDcprgWiQEY]



Application 3: Galton board



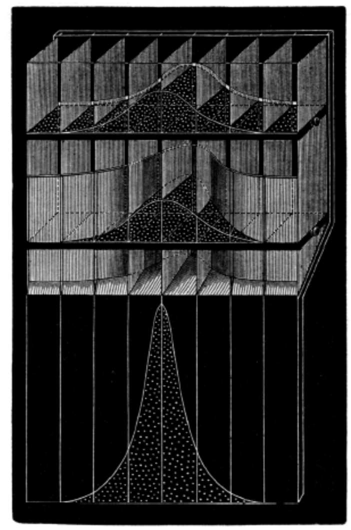
- See video
  [http://www.youtube.com/watch?v=J7AGOptcR1E]
- Displacement at ith peg:

$$P(X_i = -1) = P(X_i = 1) = \frac{1}{2}$$

- Final position after N pegs:

$$S_N = \sum_{i=1}^{N} X_i$$

- That's our 1D random walk
- Convergence to Gaussian distribution
- See computer graphs



Application 4: Maxwell's distribution

- Gas of N particles
- Velocity of particle i: $\mathbf{v}_i = (v_{x,i}, v_{y,i}, v_{z,i})$
- Velocity distribution:

$$P(v_x, v_y, v_z) = \left(\frac{m}{2\pi k_B T}\right)^{3/2} \exp\left[-\frac{m(v_x^2 + v_y^2 + v_z^2)}{2k_B T}\right]$$

- Variance $= \frac{k_B T}{m}$
- Speed: $v = \sqrt{v_x^2 + v_y^2 + v_z^2}$
- Speed distribution:

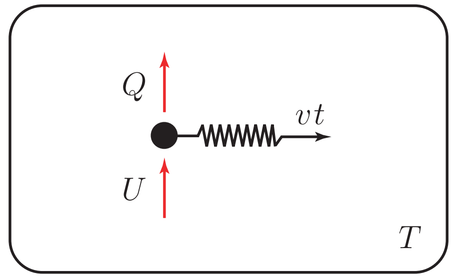
$$P(v) = \sqrt{\frac{2}{\pi}\left(\frac{m}{k_B T}\right)^3}\, v^2 \exp\left(-\frac{mv^2}{2k_B T}\right)$$

- Typical speed: $v \sim \sqrt{2k_B T/m} \approx 422$ m/s for N_2 at room temp
- See applet
  [http://www.chm.davidson.edu/vce/kineticmoleculartheory/Maxwell.html]

Application 5: Pulled Brownian particle

- Langevin dynamics:

$$m\ddot{x}(t) = \underbrace{-\alpha\dot{x}}_{\text{drag}} \underbrace{-k[x(t) - vt]}_{\text{spring force}} + \underbrace{\xi(t)}_{\text{noise}}$$



- Work = force × displacement
- Work per unit time:

$$W_\tau = \frac{1}{\tau}\int_0^\tau F(t)\, v\, dt = \underbrace{\Delta U}_{\text{potential}} + \underbrace{Q_\tau}_{\text{heat}}$$

- Work probability distribution:

$$P(W_\tau = w) \approx \sqrt{\frac{\tau}{4\pi c}} \exp\left[-\frac{\tau(w-c)}{4c}\right], \quad c = v^2$$

- $\text{var}(W_\tau) \sim 1/\tau$

Other applications

- Equilibrium systems
  - Isolated system with fixed energy (microcanonical ensemble)
  - System with fixed temperature (canonical ensemble)
- Diffusion
  - Ions in liquids, liquids in liquids
  - Electron diffusion
  - Percolation in porous solids
- Chemical reations (rates of reactions)
- Nonequilibrium systems
  - Forced steady states
- Biophysics
  - Properties of ADN
  - ATP "burning" in muscles
- Nanophysics
  - Small engines (e.g., ratchets)
- Finance (times series)
- Many more...

General property

Random sums

$$S_N = \frac{1}{N}\sum_{i=1}^{N} X_i, \qquad P(S_N = s) \approx e^{-NI(s)}$$

Long-time stochastic processes

$$W_\tau = \frac{1}{\tau}\int_0^\tau f(t)dt \qquad P(W_\tau = w) \approx e^{-\tau I(w)}$$

Fixed-temperature systems

$$U_N = \frac{\text{total energy}}{\text{no. particles}}, \qquad P(U_N = u) \approx e^{-NI(u)}$$

- Large deviation theory
- Applicable to many systems
- Foundations of equilibrium statistical mechanics

Further reading

Wikipedia
- Random walk
- Brownian motion
- Galton board
- Statistical mechanics

David Chandler
Introduction to Modern Statistical Mechanics
Oxford University Press, 1987

http://stp.clarku.edu/books/
List of other useful books on statistical physics

H. Touchette
A basic introduction to large deviations:
Theory, applications, simulations
http://arxiv.org/abs/1106.4146

Presentation and computer code for the simulations at
http://www.maths.qmul.ac.uk/~ht/talks/