25.9.2014

Statistical Physics Tutorial

1) Detailed Balance

(Lecture last week)

Setup: N atoms in z different microstates

Aim: Find time evolution (master equation) and steady-state solution of the system

Assumptions: Probability (for each unit/atom independently) to switch from microstate ν to ν' (in Δt): $p_{\nu\nu'}$

↳ transition rate $\Gamma_{\nu\nu'} = \frac{p_{\nu\nu'}}{\Delta t}$

⇒ time evolution (discrete timesteps t_n)

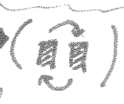
$$N_\nu(t_{n+1}) = N_\nu(t_n) \underbrace{- \Delta t \sum_{\nu'\neq\nu} \Gamma_{\nu\nu'} N_\nu(t_n)}_{\text{leaving state } \nu} \underbrace{+ \Delta t \sum_{\nu'\neq\nu} \Gamma_{\nu'\nu} N_{\nu'}(t_n)}_{\text{entering state } \nu}$$

- statistical equation
  - approximation, good for large N
  - inherent "irreversibility" through transition probabilities
- evolution towards fixed point $N_\nu(t_{n+1}) = N_\nu(t_n)$, which satisfies

$$0 = \sum_{\nu'\neq\nu} \Gamma_{\nu\nu'} N_\nu(t_n) - \sum_{\nu'\neq\nu} \Gamma_{\nu'\nu} N_{\nu'}(t_n) \quad \forall \nu \qquad (a)$$

⇒ Solution:

- further assumption: $\{\Gamma_{\nu\nu'} = \Gamma_{\nu'\nu}\}$ or $\{R_{\nu\nu'} = \Gamma_{\nu\nu'}\chi_\nu = \Gamma_{\nu'\nu}\chi_{\nu'} = R_{\nu'\nu}$ with $N_\nu = \chi_\nu \phi_\nu\}$

leads to 

leads to (more generally) 

(NOTE: not ) ← (will lead to)

Detailed balance condition

$$\Gamma_{\nu\nu'} N_\nu - \Gamma_{\nu'\nu} N_{\nu'} = 0$$

$$\Rightarrow N_\nu = N_{\nu'} = \frac{N}{z}$$

N ← total numbers of atoms

z ← microstates

Proof:

(a) translates to $0 = \sum_{\nu'} (R_{\nu\nu'}\phi_\nu - R_{\nu'\nu}\phi_{\nu'}) = \sum_{\nu'} R_{\nu\nu'}(\phi_\nu - \phi_{\nu'})$ (b)

Now suppose $\phi_1 = \phi_2 = \ldots = \phi_{\nu_1} > \phi_{\nu_1+1} = \phi_{\nu_1+2} = \ldots = \phi_{\nu_2} > \phi_{\nu_2+1} = \ldots > \ldots = \phi_z > 0$.

Then pick $\nu \leq \nu_1$ and we get

$$\sum_{\nu'} R_{\nu\nu'}(\phi_\nu - \phi_{\nu'}) = \sum_{\nu' > \nu_1} R_{\nu\nu'}(\phi_\nu - \phi_{\nu'}) > 0$$

which contradicts (b) ↯

Hence $\phi_\nu = \phi = \text{const}\ \forall \nu$. Hence $0 = R_{\nu\nu'}(\phi_\nu - \phi_{\nu'}) = \Gamma_{\nu\nu'} N_\nu - \Gamma_{\nu'\nu} N_{\nu'}$. ■

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2) Stirling approximation

often relevant!

$$\boxed{\ln N! = N \ln N - N + \frac{1}{2}\ln(2\pi N) + \text{l.o.}}$$

More precisely:

differ by only a constant!

$$\sqrt{2\pi N}\left(\frac{N}{e}\right)^N \leq N! \leq e\, N^{N+\frac{1}{2}} e^{-N}$$

with $\displaystyle\lim_{N\to\infty} \frac{N!}{\sqrt{2\pi N}\left(\frac{N}{e}\right)^N} = 1$

Derivation:

(a) Up to $O(N)$: an easy approximation:

$$\ln(N!) = \sum_{j=1}^{N} \ln(j) \approx \int_1^N \ln(x)\,dx = \Big[x\ln x - x\Big]_1^N = \underline{N\ln N - N} + 1$$

CHECK integration by parts

substitution: $y = \frac{x}{N}$

(b)
$$N! \overset{\text{integration by parts}}{=} \int_0^\infty x^N e^{-x}\,dx = \int_0^\infty e^{N\ln x - x}\,dx = N e^{N\ln N} \underbrace{\int_0^\infty e^{N(\ln y - y)}\,dy}_{\substack{\text{approximate with Laplace} \\ \sim \sqrt{\frac{2\pi}{N}}\,e^{-N}}}$$

$$\approx e^{\ln N - N}\sqrt{2\pi N} \quad (\hat{=}\ \text{Stirling})$$

Applications:

① Interpretation of the H-function: (see 1.22 in lecture notes)

to show: $N H(t) \approx \ln W(\{N_\nu\})$

number of available configurations for the set $\{N_\nu\}$

(H function increases with time $\hat{=}$ system moves towards state with most configurations)

Proof:

$$\ln W(\{N_\nu\}) = \ln\left(\frac{N!}{N_1!\,N_2!\ldots N_z!}\right) \approx N\ln N - N - \left(\sum_\nu N_\nu \ln N_\nu - N_\nu\right) + O(\ln N$$

$$= N\cancel{\ln N} \cancel{- N} - N\left(\sum_\nu \frac{N_\nu}{N}\ln\frac{N_\nu}{N} + \cancel{\frac{N_\nu}{N}\ln N}\right) \cancel{+ N}$$

$$= -N\sum_\nu \omega_\nu \ln \omega_\nu = N H(t).$$

$$\omega_\nu = \frac{N_\nu}{N}$$

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② Number of configurations in z-level system, close to maximum/peak

(see 1.29 & 1.30 in lecture notes)

(Lecture last week: 2-level system)

N units with magnetic moments with microstates

$$m_i = \begin{cases} +1 & \nu = 1 \\ -1 & \nu = 2 \end{cases}$$

Simple time evolution

given transition probability

generated random number between 0 and 1

$$m_i(t_{n+1}) = \begin{cases} m_i(t_n) & \text{if } p < R < 1 \\ -m_i(t_n) & \text{if } 0 \leq R \leq p \end{cases}$$

Average magnetization per unit

$$M(t) = \frac{1}{N} \sum_{i=1}^{N} m_i(t)$$

$\Rightarrow$ fixed point : $N_1 = N_2 = \frac{N}{2}$

# of units with magnetic moment +1   # of units with magn. moment −1

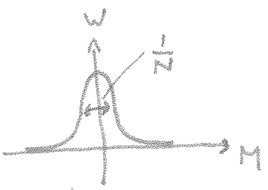
Number of realizations

$$W = \frac{N!}{\{(N/2)!\}^2} \approx 2^N \sqrt{\frac{2}{\pi N}} \quad \text{for large } N.$$

Around the fixed point, for $N_1 = \frac{N}{2}(1+M)$ & $N_2 = \frac{N}{2}(1-M)$,

$$W(\{N_\nu\}) = W(M) \approx 2^N \sqrt{\frac{2}{\pi N}}\, e^{-M^2 N/2} \quad \text{(Gaussian!)}$$

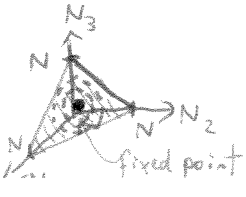
uniquely determines the set $\{N_\nu\}$ in the 2-level system



centered around $M=0$ with $\sigma^2 = \frac{1}{N}$.

Derivation of $W(\{N_\nu\})$ for general z-state system around fixed point distribution:

- still Gaussian, but now no longer one parameter "magnetization" that uniquely determines the set $\{N_\nu\}$
- use $N_\nu = \frac{N}{z}(1+s_\nu)$ with constraint $\sum_\nu s_\nu = 0$ ($\leftarrow \sum_\nu N_\nu = N$ fixed)
- e.g. $z=3$:



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$W(\{N_\nu\})$ for general z-state system

Stirling: this time $O(\ln N)$ needed!

$$\ln W(\{N_\nu\}) = \ln\left(\frac{N!}{N_1!\,N_2!\cdots N_z!}\right) \approx N\ln N - N + \frac{1}{2}\ln(2\pi N) - \left(\sum_\nu N_\nu \ln N_\nu - N_\nu + \frac{1}{2}\ln(2\pi N_\nu)\right)$$

$N_\nu = \frac{N}{z}(1+s_\nu)$

$$= N\ln N - N + \frac{1}{2}\ln(2\pi N) - \Big(\sum_\nu \frac{N}{z}(1+\underbrace{s_\nu}_{\sum_\nu s_\nu = 0})\ln\frac{N}{z} + \frac{N}{z}(1+s_\nu)\ln(1+s_\nu) - \frac{N}{z}(1+\underbrace{s_\nu}_{\sum_\nu s_\nu=0}) + \frac{1}{2}\ln\left(2\pi\frac{N}{z}\right) + \underbrace{\frac{1}{2}\ln(1+s_\nu)}_{\substack{<O(\ln N)\\ \text{and } O(z),\\ \text{small constant}}}\Big)$$

$\ln(1+x) \approx x - \frac{1}{2}x^2 + \ldots$

$$= \frac{1}{2}\ln(2\pi N) + N\ln z - \frac{N}{z}\left(\sum_\nu \ln(1+s_\nu) + s_\nu\ln(1+s_\nu)\right) - \frac{z}{2}\ln\left(2\pi\frac{N}{z}\right)$$

$$\approx \left(\frac{1}{2} - \frac{z}{2}\right)\ln(2\pi N) + \left(N + \frac{z}{2}\right)\ln z - \frac{N}{z}\Big(\underbrace{\sum_\nu s_\nu}_{=0} - \frac{1}{2}s_\nu^2 + s_\nu^2 - \underbrace{\frac{1}{2}s_\nu^3}_{\text{neglect}}\Big)$$

$$\approx \frac{1}{2}(1-z)\ln(2\pi N) + \left(N + \frac{z}{2}\right)\ln z - \frac{N}{2z}\sum_\nu s_\nu^2$$

$$\Rightarrow W(\{N_\nu\}) = \sqrt{2\pi N}\, z^N \left(\frac{2\pi N}{z}\right)^{-\frac{z}{2}} e^{-\frac{N}{2z}\sum_\nu s_\nu^2}$$

$\Rightarrow$ Gaussian ("z-dim.") with variance $\sigma^2 = \frac{z}{N}$.