

Ising model

Relevant microstates are 'spin configurations'

$$(s_1, s_2, \dots, s_N)$$

$$s_i \in \{-1, 1\}$$

$$H\{s\} = -J \sum_{\langle i, j \rangle} s_i s_j - B \sum_{i=1}^N s_i$$

summation over nearest neighbours on the d -dim lattice

We treat in detail the case $d=1$

Interested in free energy per spin in the limit $N \rightarrow \infty$

$$f(\beta) = - \lim_{N \rightarrow \infty} \frac{1}{\beta N} \log Z(\beta)$$

Useful method to calculate

$f(\beta)$ is the so-called

transfer matrix method / sum

- 47 -

general powerful method, but
here illustrated for a special
example, the 1-d Ising model)

$$Z_N = \sum_{s_1, \dots, s_N} \exp \left(\beta J \sum_{j=1}^N s_j s_{j+1} + \beta B \sum_{j=1}^N s_j \right)$$

periodic boundary conditions

$$s_{N+1} = s_1$$

Define factors $v(s, s')$

$$v(s, s') = \exp \left[\beta J s s' + \frac{1}{2} \beta B (s + s') \right]$$

$\Rightarrow$

$$Z_N = \sum_{s_1, \dots, s_N} v(s_1, s_2) v(s_2, s_3) \dots v(s_{N-1}, s_N) \cdot v(s_N, s_1)$$

The transfer matrix is

$$V = \begin{pmatrix} v(+1, +1) & v(+1, -1) \\ v(-1, +1) & v(-1, -1) \end{pmatrix} \\ = \begin{pmatrix} e^{\beta(J+B)} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta(J-B)} \end{pmatrix}$$

Summation over $s_2, \dots, s_N$ is equivalent to matrix multiplication of N matrices V . Summation over s_1 is taking the trace of V^N .

$$\Rightarrow Z_N = \text{trace } V^N$$

V is symmetric

$\Rightarrow$ we can find linearly independent eigenvectors x_1, x_2 s.t.

$$V \cdot x_j = \lambda_j x_j \quad j=1,2$$

Trace is invariant under equivalence transformations of a matrix

$$\Rightarrow Z_N = \text{trace} \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix}^N = \lambda_1^N + \lambda_2^N$$

$$\lambda_1 > \lambda_2$$

$$F(\beta) = - \lim_{N \rightarrow \infty} \frac{1}{\beta N} \log Z_N$$

$$= - \lim_{N \rightarrow \infty} \frac{1}{\beta N} \log \left\{ \lambda_1^N \left(1 + \underbrace{\left(\frac{\lambda_2}{\lambda_1} \right)^N}_{\rightarrow 0} \right) \right\}$$

Hence

$$\begin{aligned} F(\beta) &= - \lim_{N \rightarrow \infty} \frac{1}{\beta} \frac{1}{N} N \log \lambda_1 \\ &= - \frac{1}{\beta} \log \lambda_1 \end{aligned}$$

Very general result:

Free energy given by
log of largest eigenvalue
of transfer operator

Non equilibrium systems

Stochastic process $Y(t)$

$$Y \in \mathbb{R}^n$$

Look at n -point functions

$$P_n(y_1, t_1; y_2, t_2; \dots, y_n, t_n)$$

$$= P_{n-1}(y_1, t_1; \dots, y_{n-1}, t_{n-1}) \cdot P_{1|n-1}(y_n, t_n | y_1, t_1, \dots, y_{n-1}, t_{n-1})$$

Need all n -point functions for $n=1, 2, 3, \dots$ to fully characterize stoch. process

Important subclasses of stoch. processes

Markov process

$$P_{1|n-1}(y_n, t_n | y_1, t_1; \dots, y_{n-1}, t_{n-1}) = P_{1|1}(y_n, t_n | y_{n-1}, t_{n-1})$$

Wiener process $W(t)$

$$P_1(y, t) = \frac{1}{\sqrt{2\pi t}} \exp \left\{ -\frac{y^2}{2t} \right\} \quad \text{A} \rightarrow \text{~}$$

$$P_{1|1}(y_2, t_2 | y_1, t_1) = \frac{1}{\sqrt{2\pi(t_2 - t_1)}} \exp \left\{ -\frac{(y_2 - y_1)^2}{2(t_2 - t_1)} \right\}$$

Stochastic Differential eq.

$$\dot{Y} = G(X, Y, Z, \dots)$$

Solving the stoch. diff. eq. means finding the stochastic process $Y(t)$ that satisfies it.

Most important stoch. Diff. eq. in statistical physics is the Langevin eq.

$$dY = A(Y)dt + \sigma dW$$

$$\Leftrightarrow \dot{Y} = A(Y) + \sigma L(t)$$

$$A: \mathbb{R}^n \rightarrow \mathbb{R}^n$$

$$L(t) = \frac{dW}{dt}$$

↑
Gaussian white noise

$$\langle L(t) \rangle = 0$$

↑
expectation

$$\langle L(t_1) L(t_2) \rangle = \delta(t_1 - t_2)$$

$L(t)$ is a rapidly fluctuating random force.

Example

Brownian particle

$$A(y) = -\gamma y$$

γ : velocity of the Brownian particle
 γ : friction constant

$$\dot{Y} = -\gamma Y + \sigma L(t)$$

Solution of this stochastic diff. eq.
 is the Ornstein-Uhlenbeck process

$$P_1(y, t) = \left(\frac{\pi \sigma^2}{\gamma} \right)^{-\frac{1}{2}} \exp \left\{ -\frac{\gamma}{\sigma^2} y^2 \right\}$$

$$P_{12}(y_2, t_2 | y_1, t_1)$$

$$\beta = \frac{\gamma}{2\sigma^2} \quad E_{kin} = \frac{1}{2} \gamma^2$$

$$= \left(\frac{\pi \sigma^2}{\gamma} (1 - e^{-2\gamma\tau}) \right)^{-\frac{1}{2}} \exp \left\{ -\frac{\gamma}{\sigma^2} \frac{(y_2 - y_1 e^{-\gamma\tau})^2}{(1 - e^{-2\gamma\tau})} \right\}$$

$$\tau := t_2 - t_1$$

Theorem

The general solution of the
 Langevin eq. for general $A(y)$
 is a Markov process whose
 1-point function

and transition prob. $P_{12}(y_2, t_2 | y_1, t_1)$

satisfy the Fokker-Planck eq. -47

$$\frac{\partial P}{\partial t} = -\nabla(A P) + \frac{1}{2} \sigma^2 \Delta P$$

$$A(Y) : \mathbb{R}^n \rightarrow \mathbb{R}^n \quad Y = \begin{pmatrix} y_1 \\ \vdots \\ y_n \end{pmatrix}$$

$$\nabla = \begin{pmatrix} \frac{\partial}{\partial y_1} \\ \vdots \\ \frac{\partial}{\partial y_n} \end{pmatrix}$$

$$\Delta = \nabla^2 = \frac{\partial^2}{\partial y_1^2} + \dots + \frac{\partial^2}{\partial y_n^2}$$

$$P = P_n(y, t)$$

(if P is P_{n+1} , then $t = t_c$)

Stationary solution of the Fokker-Planck eq.

$$\frac{\partial P}{\partial t} = 0$$

$$\Rightarrow 0 = -\nabla(A P) + \frac{1}{2} \sigma^2 \underbrace{\Delta}_{\nabla^2} P$$

$$0 =: \text{const} = -A P + \frac{1}{2} \sigma^2 \nabla P$$

$$\boxed{\nabla P = \frac{2}{\sigma^2} A P}$$

$$\frac{\partial}{\partial y_1} P = \frac{2}{\sigma^2} A(y) P$$

$\vdots$

$$\frac{\partial}{\partial y_n} P = \frac{2}{\sigma^2} A(y) P$$

Claim solution is given by

$$P(\gamma, \gamma) = \text{const} \exp \left\{ -\frac{2}{\sigma^2} V(\gamma) \right\}$$

where

$$A(\gamma) = -\nabla V(\gamma)$$

Proof

↑ non-equilibrium potential

$$\begin{aligned} \nabla P(\gamma) &= \text{const} \cdot \exp \left\{ -\frac{2}{\sigma^2} V(\gamma) \right\} \\ &\quad \cdot \left(-\frac{2}{\sigma^2} \right) \nabla V(\gamma) \\ &= P(\gamma) \cdot \frac{2}{\sigma^2} A(\gamma) \quad \text{q.e.d.} \end{aligned}$$