1. Overview

∘ Statistical Physics

⇒ equilibrium | nonequilibrium

statics dynamics

only partially correct forced / driven systems

energy flux rotational drive

NESS (nonequilibrium steady state)

dynamical problem

⇒ quantum / classical | stochastic modelling

unitary deterministic

random initial data

mesoscopic modelling

P. Krapivsky, S. Redner, E. Ben-Naim

A kinetic view of Stat Phys 2002

Hal Tasaki home page lecture course { fluctuation theorems, large deviations

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⇒ one-particle  | many particles ⟸ my lectures

Bohr atom  since Einstein 1905 Brownian motion ~~stochastic thermodynamics~~

examples ∘ colloidal suspensions

∘ active matter bird flocks

stochastic LG 

continuous time (theory)

discrete ^physical space / local states

nonequilibrium [Glauber dynamics, Kawasaki dynamics

⇒ Markovian evolution ⟸

Monte Carlo simulations discrete time

future past are independent conditioned on now short, necessary

2. Markov jump processes

2.1 General structure

finite state space $\Omega = \{1, \dots, k\}$

$j = 1, \dots, k$

k can be very large

lattice gas $2^{|\Lambda|}$ NO velocities

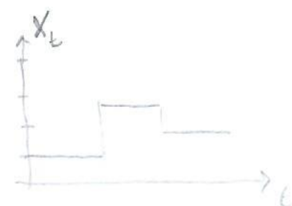
N particles in Λ positions only (overdamped)

$(x_1, \dots, x_N) \in \Lambda^N$ $\quad n = |\Lambda|^N$

jump rates $c_{i \to j} = c_{ij} \geq 0$ $\quad i \neq j$

"hamiltonian" time-independent define the model

Markov evolution



waiting times are random

- $\lambda_i = \sum_{j=1}^{k} c_{ij} > 0$
- wait at i with distribution $\lambda_i e^{-\lambda_i t} \chi(t \geq 0)\, dt$
- jump with probability $\frac{1}{\lambda_i} c_{ij}$ $\qquad \sum_{j=1}^{n} \frac{1}{\lambda_i} c_{ij} = 1$
- random path $t \mapsto x_t \in \Omega$

n jumps

$i_0, \dots, i_n$

start, final

probability $\frac{1}{\cancel{\lambda_{i_0}}} c_{i_0 i_1} \cancel{\lambda_{i_0}} e^{-\lambda_{i_0} t_1} \cdots c_{i_{n-1} i_n} e^{-\lambda_{i_{n-1}} t_{n-1}} \quad dt_1 \dots dt_{n-1}$

normalized to 1 $\qquad$ independent waiting times / jumps $\qquad$ "microscopic"

very detailed information

one is interested in reduced information

- transition probability

$P(i,0\mid j,t)$ average $\delta\left(\sum_{j=0}^{n-1} t_j = t\right)$ fix $i_0 = i,\ i_n = j$ sum over n times

time dependent perturbation theory

matrix L: $L_{ii} = -r_i \qquad L_{ij} = c_{ij},\ i\neq j \qquad i,j = 1,\dots,n$ $\begin{pmatrix} \diagdown & 0 \\ 0 & \diagdown \end{pmatrix}$

$L_0 \begin{pmatrix} \diagdown & 0 \\ 0 & \diagdown \end{pmatrix} \qquad L_1 \begin{pmatrix} 0 & \cdot \\ \cdot & 0 \end{pmatrix}$

$$\left(e^{Lt}\right)_{ij} = \left(e^{L_0 t} + \int_0^t dt_1\, e^{L_0(t-t_1)} L_1 e^{L_0 t_1} + \dots\right)_{ij} \qquad P(i,0\mid j,t) = \left(e^{Lt}\right)_{ij}$$

- L is backward generator $L1 = 0$ observable $f: \Omega \to \mathbb{R}$

$$f(i,t) = \langle f(X_t)\rangle_{X_0 = i} = \sum_{j=1}^{K} P(i,0\mid j,t)\, f(j) = \left(e^{Lt} f\right)_i$$ acts on observables

- L^T is forward generator

probability distribution at t $\quad \rho_j(t) = \sum_{i=1}^{K} \rho_i(0)\, P(i,0\mid j,t) = \rho_j(t)$

- master equations

$$\frac{d}{dt} f = L f \quad , \quad \frac{d}{dt}\rho(t) = L^T \rho(t) \quad \Big| \quad \frac{d}{dt}\rho_i = \sum_{j=1}^{K} \Big(\underbrace{c(j,i)\,\rho_j}_{\text{gain}} - \underbrace{c(i,j)\,\rho_i}_{\text{loss}}\Big)$$

for many body computations L is preferred

simple observables sum over initial

$$(Lf)_i = \sum_{j=1}^{K} c(i,j)\,\big(\underbrace{f(j)}_{\text{after}} - \underbrace{f(i)}_{\text{before}}\big)$$

$\Omega_\ell \quad \ell = 1,\dots,m$

- long time limit

Ω_ℓ are the connected components

in each component there is a unique steady state

(much simpler than hamiltonian)

2.2 Equilibrium

Ω connected, unique steady state ρ

- detailed balance $\Leftrightarrow$ time reversibility

$$\mathbb{P}(\{x_t, 0 \le t \le T\}) = \mathbb{P}(x_{T-t}, 0 \le t \le T)$$

trajectory reversed

$\simeq$ detailed balance

stationary $\rho_j = e^{-\varepsilon_j}$ "energies" $j \in \Omega$

$\rho_j \, c_{ji} = \rho_i \, c_{ij}$ detailed balance

$c_{ij} = e^{-(\varepsilon_j - \varepsilon_i)} \, c_{ji}$ implies that $(L^T \rho)_j = 0$

- L is a symmetric matrix in the weighted space

flat $\Leftrightarrow$ weighted

$\langle , \rangle$ $\langle \cdot, \cdot \rangle_\rho$

$$\langle f, g \rangle_\rho = \sum_{j=1}^{k} \rho_j f_j g_j$$

$\langle f, Lg \rangle_\rho = \langle Lf, g \rangle_\rho$ $\rho_i L_{ij} = \rho_j L_{ji}$

eigenvalues

left / right

$L 1 = 0$ always $\quad$ $L^T \rho = 0$ detailed balance

exponential relaxation

- equilibrium time correlations

$$\langle g(x_0) f(x_t) \rangle_\rho = \langle g, e^{Lt} f \rangle_\rho = \sum_\alpha \langle \rho g | \psi_\alpha \rangle \langle \tilde{\psi}_\alpha | f \rangle e^{\lambda_\alpha t}$$

flat $\quad$ eigenvalues ψ_α $\tilde{\psi}_\alpha$ eigenvectors

$$= \langle g \rangle_\rho \langle f \rangle_\rho + \sum_{\alpha \ne 0} e^{\lambda_\alpha t} \langle \rho g | \psi_\alpha \rangle \langle \tilde{\psi}_\alpha | f \rangle$$

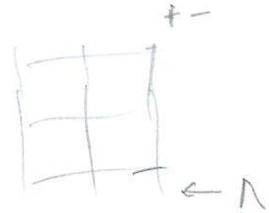
$\to 0$

operators are similar to those in QM

interpretation is very different !!

3. Voter model

many-particle system nonequilibrium



Ising state space Λ finite box $\Lambda \subset \mathbb{Z}^d$

$\sigma_x = \pm 1$, $x \in \Lambda$, $\sigma = \{\sigma_x \mid x \in \Lambda\}$ configuration $|\Omega| = 2^{|\Lambda|}$

"Glauber" flip rate $\sigma_x \rightsquigarrow -\sigma_x$

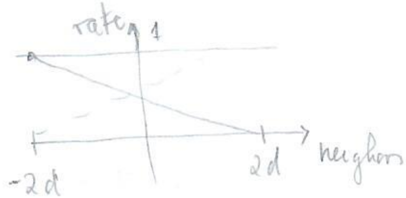
notation $\sigma \to \sigma^x$

$$L f(\sigma) = \sum_{x \in \Lambda} c_x(\sigma)\,(f(\sigma^x) - f(\sigma))$$

many-spin

HERE <u>voter model</u> $\pm$ are opinions, follow your neighbor

flip rate $\sigma_x = +1$



$\rightsquigarrow \quad c_x(\sigma) = 1 - \gamma \frac{1}{2d} \sum_{|e|=1} \sigma_x \sigma_e$

$\gamma = 0$ independent flips randomize uniform

<u>problem</u>: initial Bernoulli $\langle \sigma_x \rangle = m$ $|m| \leq 1$ independent

$t \to \infty$ NESS What are its properties?

- method of moments
  hierarchy of correlations

σ_x is regarded as function

$$\frac{d}{dt}\sigma_x = L\sigma_x = \sum_{y \in \Lambda} c_y(\sigma)\,((\sigma_x)^y - \sigma_x) \qquad 1 \to 1$$

$$= \frac{1}{d} \sum_{|e|=1} (\gamma \sigma_{x+e} - \sigma_x)$$

$\frac{d}{dt}\sigma_x\sigma_y$

$$= L\sigma_x\sigma_y = \frac{1}{d} \sum_{|e|=1} \big((\gamma\sigma_{x+e} - \sigma_x)\sigma_y + \sigma_x(\gamma\sigma_{y+e} - \sigma_y) \big) \qquad x \neq y$$

$2 \to 2$
$\to 0$

$\frac{d}{dt}\sigma_x\sigma_x = 0 \qquad x = y$

$0 \le \gamma < 1$ decay as $e^{-(1-\gamma)t}$ $t \to \infty$ $\langle \prod_{j=1}^{n} \sigma_{x_j} \rangle \to 0$

distinct

randomizes Bernoulli $\frac{1}{2}$

|| interesting case $\gamma = 1$ ||

$+$ $+ \; (+) \; +$ $+$ stabilized

trapping state $t+1$

1 particle random walk

2 particles random walk with annihilation

disappear

b.c.

initial $\langle \prod_{j=1}^{n} \underbrace{\sigma_{x_j}}_{\text{distinct}} \rangle = m^n$

time t

$$\langle \prod_{j=1}^{n} \sigma_{x_j}(t) \rangle = \mathbb{E}\left(m^{\overset{\text{random walk}}{n(t)}} \right)$$

$n(t) = \#$ walkers at time t

limit $t \to \infty$

- $d = 1, 2$ walkers annihilate with probability 1

$n(t) \to 0$ $n(t) \to 1$

limit state $\langle \prod_{j=1}^{n} \sigma_{x_j} \rangle_{ss} = 1$ (even) $\langle \prod_{j=1}^{n} \sigma_{x_j} \rangle = m$ (odd)

in other words ground states all $+$ probability $\frac{1}{2}(1+m)$

all $-$ " $\frac{1}{2}(1-m)$

agreement is reached

[geometry of clusters is interesting and
has be studied, spinodal decomposition with 0 surface tension]

$d \geq 3$ $\quad Z_1(0) = x,\ Z_2(0) = y,\ x \neq y$ $\quad$ Prob ($Z_1(t), Z_2(t)$ meet at some time) $= Q(x-y)$ $\quad$ RW

$Q < 1$

$Q(x) \simeq |x|^{-d+2}$ $\qquad |x|^{-1}$ in $d=3$

steady state

$\langle (\sigma_x - m)(\sigma_y - m) \rangle_{ss} = (1-m^2)\, Q(x-y)$

one-parameter family of NESS

non-trivial statistics, slow decay of correlations, critical

in fact, on large scales Gaussian mass less field

covariance $(-\Delta)^{-1}$

4. Stochastic lattice gases

- conservation law HERE density only (kawasaki)

1D for simplicity, exclusion, occupation variable $\eta_x = 0, 1$

unlabeled particles

as exchange rate between x and y

$c_{xy}(\eta) \geq 0 \qquad \eta \to \eta^{xy}$

$$Lf(\eta) = \sum_{x,y} c_{xy}(\eta)\left(f(\eta^{xy}) - f(\eta)\right)$$

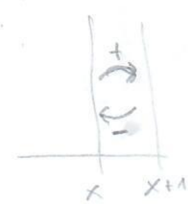
translation invariance

nearest neighbor jumps only $\quad c_{x,x+1} \geq 0$

$c_{xy} = 0$ otherwise $y \neq x+1$

$N = \sum_{x \in \Lambda} \eta_x$ # of particles (random)

state space decomposes as $n = 0, 1, \ldots, |\Lambda|$



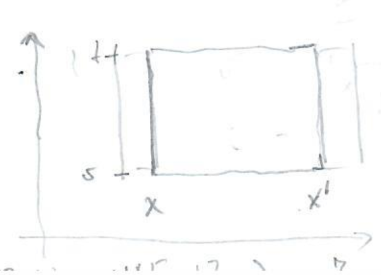
Λ interval, for each n there is a unique invariant measure

- empirical current $\mathcal{J}_{(x,x+1)}([s,t])$ = # signed jumps between $x, x+1$

bond

single history

conservation law



microscopic conservation law

5. Hydrodynamic limit (reversible)

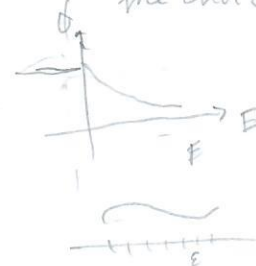
5.1 Local conservation law

- equilibrium $H(\eta)$, $\Delta_{xy} H(\eta) = H(\eta^{xy}) - H(\eta)$

$$c_{xy}(\eta) = c_{xy}(\eta^{xy})\, e^{-\beta \Delta_{xy} H(\eta)} \qquad c_{xy}(\eta) = \phi(\Delta_{xy} H(\eta))$$

$$\phi(E) = \underbrace{\phi(-E)}_{\text{free choice}} e^{-\beta E}$$

for each sector n $e^{-\beta H(\eta)}$ is stationary



grand canonical

$$e^{-\beta H(\eta) + \mu N} \qquad \mu \leftrightarrow \rho$$

- space dependent μ slow variation $\mu(\varepsilon x)$

hydrodynamics governs the motion of μ, i.e. ρ

$$\frac{d}{dt}\eta_x = L\eta_x = \sum_j c_{j,j+1}(\eta)\,(\eta_x^{j,j+1} - \eta_x)$$

$$= \underbrace{c_{x-1\,x}(\eta_{x-1} - \eta_x)}_{j_{x-1,x}} + \underbrace{c_{x,x+1}(\eta_{x+1} - \eta_x)}_{-\,j_{x,x+1}}$$

$j_{x\,x+1}(\eta)$ is the current function . $j_{x,x+1}(\eta)\,dt = \langle \mathfrak{J}_{x,x+1}(dt)\rangle_\eta$

$$\rightsquigarrow \frac{d}{dt}\langle \eta_x \rangle_t + \partial_x \langle j_{x,x+1}\rangle_t = 0 \qquad \partial_x f = f(x+1) - f(x)$$

$x \sim t$ ballistic times $\varepsilon^{-1}\tau$

assume local equilibrium $\leftarrow$ hydrodynamics!!

ε, x, q macroscop

- equilibrium average

$$\sum_\eta e^{-\beta H(\eta)+\mu N} c_{01}(\eta)(\eta_0-\eta_1)$$ detailed balance

$$= \sum_\eta e^{-\beta H(\eta^{01})+\mu N} c_{01}(\eta^{01})(\eta_0-\eta_1)$$ resum

$$= \sum_\eta e^{-\beta H(\eta)+\mu N} c_{01}(\eta)(\eta_1-\eta_1)$$

$\leadsto \langle j_{01}\rangle_\mu = 0$.

nonequilibrium $\langle j_{01}\rangle \neq 0$
(overdamped
compare with fluids)

5.2 Green-Kubo formula

first order correction — diffusivity

$$j(q) = -D(\rho(q))\,\partial_q \rho(q)$$

$\leadsto \partial_t \rho = \partial_q D(\rho)\,\partial_q \rho$ nonlinear diffusion equation

What is D

simple example $c_{x,x+1}(\eta) = (\eta_x - \eta_{x+1})^2$ SSEP

$$j_{x,x+1} = \eta_{x+1}-\eta_x$$

$$\frac{d}{dt}\eta_x = \Delta \eta_x \qquad \Delta f_x = f_{x+1} - 2f_x + f_{x-1}$$

$\leadsto D = 1$ hierarchy decouples

general case

equilibrium $\quad e^{-\beta H + \mu N} \quad , \quad \langle \eta_x \rangle_{eq} = \rho$

perturb at $x = 0$, record at x , structure function

$$S(x,t) = \langle \eta_x(t)\, \eta_0(0) \rangle_{eq} - \rho^2$$

normalization $\quad \sum_x S(x,t) = \sum_x (\langle \eta_x \eta_0 \rangle - \rho^2) = \chi \quad$ static susceptibility

$$S(x,t) \cong \chi \frac{1}{\sqrt{4\pi D t}}\, e^{-\frac{1}{4Dt} x^2} \qquad D = D(\rho)$$

$$D(\rho) = \lim_{t \to \infty} \frac{1}{t} \frac{1}{2\chi} \underbrace{\sum_x x^2 \left(S(x,t) - S(x,0)\right)}_{(*)}$$

conservation law

$$\eta_t(x) = \mathcal{J}_{(x-1,x)}([0,t]) - \mathcal{J}_{(x,x+1)}([0,t])$$

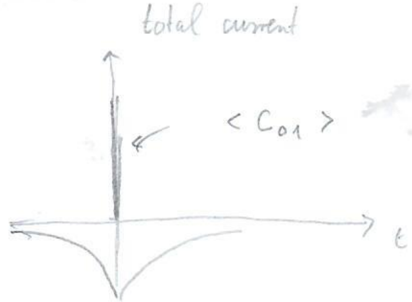
$$\leadsto \quad * = \int_0^t ds \int_0^t ds' \sum_x \langle \mathcal{J}_{x,x+1}(ds)\, \mathcal{J}_{0,1}(ds') \rangle_\rho$$

We have to compute the total current - current correlation.

$$\sum_x \langle \mathcal{J}_{x,x+1}(ds)\, \mathcal{J}_{0,1}(ds') \rangle_\rho = \langle c_{0,1} \rangle_{eq}\, \delta(s-s') - \sum_x \langle j_{x,x+1}\, e^{L|s-s'|}\, j_{0,1} \rangle_\rho$$

$\leadsto$ Green - Kubo formula

$$D = \frac{1}{2\chi} \left(\langle c(0,1) \rangle_{eq} - 2 \int_0^\infty dt \sum_x \langle j_{x\,x+1}\, e^{Lt}\, j_{0,1} \rangle_\rho \right)$$



L has real eigenvalues, spectral weight

$$\sum_x \langle j_{x,x+1}\, e^{L|t|}\, j_{0,1} \rangle = \int_0^\infty \mu(d\lambda)\, e^{-\lambda t}$$

decay?, higher dimensions, at criticality?

5.3 Einstein relation, linear response

driving field F

potential

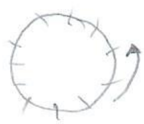
$$H_F = H - F \sum_x x \eta_x$$

local detailed balance

$$c^F_{x,x+1}(\eta) = c_{x,x+1}(\eta^{x,x+1})\, e^{-\Delta_{x,x+1} H(\eta) + F(\eta_x - \eta_{x+1})}$$

in interval

inhomogeneous equilibrium state



on ring NESS (we do not know well)

nonequilibrium

no good perturbation expansion

because dynamics is diffusive

average current $\langle c^F_{01}(\eta_0 - \eta_1) \rangle_{\rho, F}$

NESS

there is no run away

linear response

expand in F $\quad \langle c^F_{01} (\eta_0 - \eta_1) \rangle_{\rho, F} \hat{=} \sigma F$

(1) yields $\langle c_{01} \rangle$!

(2) yields $\int dt$ as in Green Kubo

$f(\mu)$
$f' = \rho$
$f'' = \chi$

$\sigma = \chi D$ Einstein relation

Onsager $\partial_t \rho + \partial_q j = 0$ $\quad j = -D \partial_q \rho = -\sigma \partial_q \mu(\rho)$

$= -\sigma \frac{1}{\chi'} \partial_q \rho$

example SSEP $\quad \chi = \sum_x \langle \eta_x \eta_0 \rangle - \rho^2 = \rho - \rho^2 = \rho(1-\rho)$

Green-Kubo $\quad \langle c_{01} \rangle = \langle (\eta_0 - \eta_1)^2 \rangle = \langle \eta_0 \rangle + \langle \eta_1 \rangle - 2 \langle \eta_0 \rangle \langle \eta_1 \rangle$

$= 2\rho(1-\rho)$

$D = 1$ as shown before

hydrodynamics show its own limits

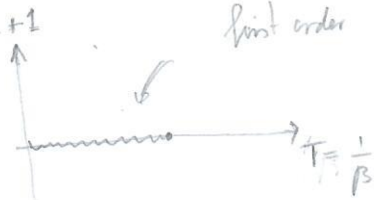
5.4 bulk diffusivity at low temperatures

spin exchange
Kawasaki

symmetry $0 \leftrightarrow 1$

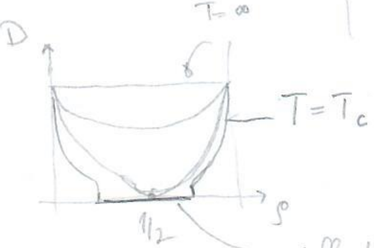
a) attractive lattice gas

$$H = - \sum_{|x-y|=1} \eta_x \eta_y$$



phase diagram

$$D = \frac{\sigma}{\chi}$$



different physics beyond hydrodynamics
|| important feature
theory exhibits its own limitations

claim: $\sigma > 0$ even at low temperatures.

$$\chi(\rho) = |\rho - \tfrac{1}{2}|^{1-\delta}$$

d	2	3	4 $\to$
δ	15	4.8	3 $\to$

mean field

$$\partial_t \rho = \nabla_q D(\rho) \nabla_q \rho \qquad \text{initial condition} \quad \rho_0 = \tfrac{1}{2} + u(q), \quad u \geq 0$$

porous medium equation

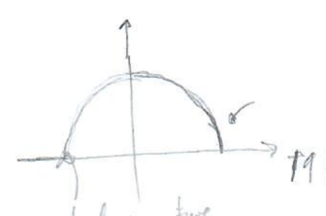
$$\partial_t u = \Delta u^m \qquad m > 0$$

mass conservation

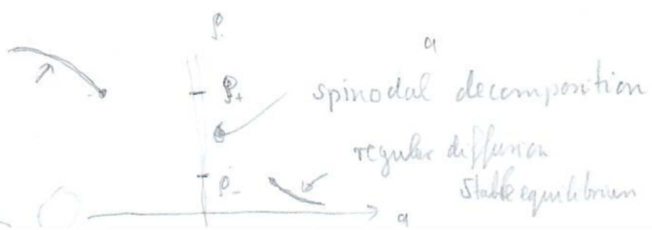
free boundary value

solution is of scaling form $\quad u(q,t) = t^{-\alpha d}\, \Phi(q\, t^{-\alpha})$

Φ has compact support $\qquad \alpha = \dfrac{1}{2 + d(\delta - 1)}$



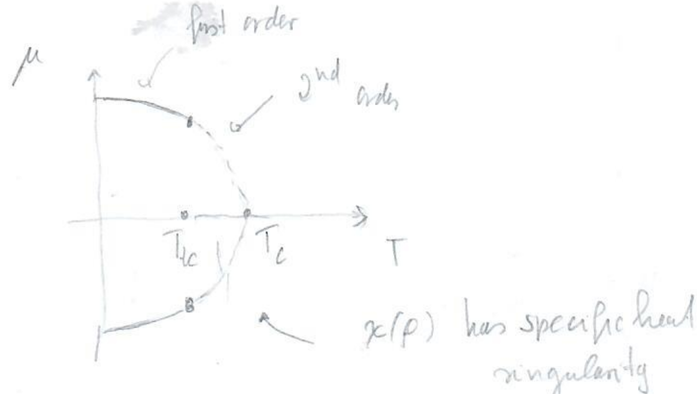
below T_c

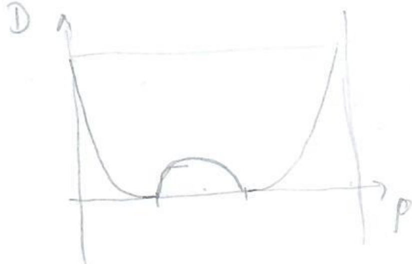


omit

f) repulsive case

$$H = + \sum_{|x-y|=1} \eta_x \eta_y$$





$T_{tc} < T < T_c$

the order parameter is not conserved

local equilibrium $\begin{matrix} + - + - \\ - + - + \end{matrix}$ + reversed

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5.3 ~~Einstein relation, linear response~~

biased jump , local detailed balance

$$H_F = H_1 - F \sum_x x \eta_x$$

$$c^F_{x x+1}(\eta) = c^F_{x,x+1}(\eta^{x,x+1})\, e^{-\Delta_{x x+1} H(\eta) + F(\eta_x - \eta_{x+1})}$$

closed interval . equilibrium state

 ring steady state current is well defined

ring, allows for current, nonequilibrium

runaway in mechanical systems

average current $\langle \overset{①}{c^F_{x\,x+1}} \underset{②}{(\eta_x - \eta_{x+1})} \rangle_{\rho, F}$ two terms ① yields $\delta(t)$ ② yields $\int dt$

so

$$\langle j_{x,x+1} \rangle = F \cdot \sigma \quad \text{in linear response}$$

Einstein

$$\sigma = \chi D$$

Onsager formulation $j = - D \partial_q \rho = -\underbrace{\sigma}_{\text{mobility}} \times \underbrace{\partial_q \mu(\rho)}_{\text{driving force}}$

since $\mu' = \frac{1}{\chi}$

$f(\mu)$ $f' = \rho$

$f'' = \rho' = \chi$