Review of Classical Mechanics

1 1

1.1

Given a phase space with coordinates $\mu = (\boldsymbol{q}, \boldsymbol{p})$ where $\boldsymbol{q} = (q^1, ..., q^N)$ and $\boldsymbol{p} = (p^1, ..., p^N)$. Given a volume in such phase space, denotes the initial condition as $\mathcal{R}(0) = \{\mu(0) \mid \mu(0) \in \mathcal{R}_0\} \overset{\text{time evolution}}{\rightarrow} \mathcal{R}(t) = \{\mu(t) \mid \mu(0) \in \mathcal{R}\}$. For a instance time $t \to t + \varepsilon$, we has:

$$\begin{aligned} d\mu_{t+\varepsilon} &= \det\left(\frac{\partial \mu_{t+\varepsilon}}{\partial \mu_t}\right) d\mu_t \\ &= \det\left(\delta_{ij} + \varepsilon \frac{\partial \dot{\mu}_{ti}}{\partial \mu_{tj}} + O(t^2)\right) d\mu_t \\ &= \left(1 + \varepsilon \mathrm{Tr}\left(\frac{\partial \dot{\mu}_t}{\partial \mu_t}\right)_i + O(t^2)\right) d\mu_t \quad (\log\det M = \mathrm{Tr}\log M) \end{aligned} \tag{1.1}$$

We haven' t introduce the dynamic equation yet, if it satisfy the canonical form:

$$\mathrm{Tr}(...) = \left(\frac{\partial \dot{q}_{ti}}{\partial q_{ti}} + (q \to p)\right) = \left(\frac{\partial}{\partial q_{ti}} \frac{\partial H}{\partial p_{ti}} - \frac{\partial}{\partial p_{ti}} \frac{\partial H}{\partial q_{ti}}\right) = 0 \tag{1.2}$$

Which is just a reframe of the basic Hamiltonian equation, because we just integrate phase point solely.

That' s, given a distribution $\rho(\mu, t)$:

$$\begin{aligned} \rho(\mu, t) &= \rho(\boldsymbol{p}, \boldsymbol{q}, t) \\ \frac{d\rho}{dt} &= \frac{\partial \rho}{\partial t} + \{\rho, H\} = 0 \end{aligned} \tag{1.3}$$

Above called *Liouville' s equation*.

A famous theorem is *Poincaré recurrence theorem*, which states that for a system with finite energy, the system will return to a state arbitrarily close to the initial state after a sufficiently long time. This is a consequence of the conservation of phase space volume and the deterministic nature of Hamiltonian dynamics.

Given a distribution $\delta(E - H(\boldsymbol{q}, \boldsymbol{p}))$, one has the possible phase space volume as the total volume T the initial condition can transverse, for example $\frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 = H(x, p) = E$. Then we can apply a continuous transformation to the phase space volume, due to **finite energy/volume**, the union space. We clarify such transformation as g_τ with given τ as time parameter or any parameter you want, then we has:

$$\mathrm{T} = \bigcup_{k=0}^{\infty} g_\tau^k \mathcal{R}_0 \quad \mathcal{R}_0 \text{ is initial condition phase volume} \tag{1.4}$$

Thus we must have intersection of possible transverse like k to $k + l$ finitely, otherwise T would be infinite due to infinite disjoint sets.

$$g_\tau^k \mathcal{R}_0 \cap g_\tau^{k+l} \mathcal{R}_0 \neq \emptyset \overset{g \text{ is reversible}}{\rightarrow} \mathcal{R}_0 \cap g_\tau^l \mathcal{R}_0 \neq \emptyset \tag{1.5}$$

Which prove the theorem. It said that for a non-dissipative or closed(**invertible + volume preservation**), **finite** system, the system will emerge recurrence. However, this theorem is not collide with macro equilibrium.

1.2 Kac Ring Model

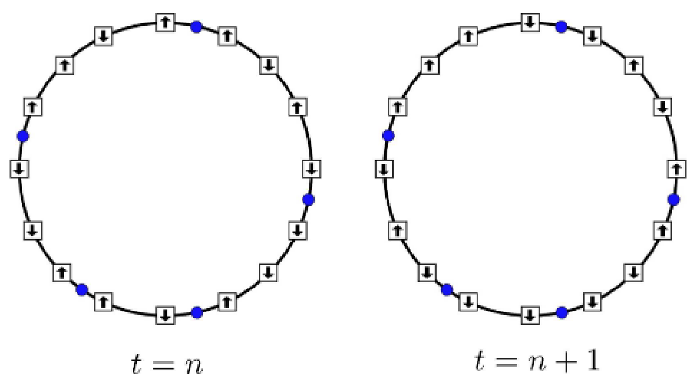

Figure 1. Left: A configuration of the Kac ring with $N = 16$ sites and $F = 4$ flippers. The flippers, which live on the links, are represented by blue dots. Right: The ring system after one time step. Evolution proceeds by clockwise rotation. Spins passing through flippers are flipped. "

Above picture shows a simple model, N sites is a instance with spin up and down, then we also have F flippers on the link between sites, which can flip spin instance. The evolution is just rotate the ring clockwise one step and the spin instance would be flipped if it pass through the flipper. Thus, it' s deterministic and invertible with finite state. It must has **recurrence**.[1]

Now suppose $s(0) = (s_i(0))$ is the initial state, we has a general probability relation:

$$\begin{gathered}\sum_i s_i^+(n) + \sum_i s_i^-(n) = N \\ \sum_i s_i^+(n+1) = \frac{N-F}{N} \sum_i s_i^+(n) + \frac{F}{N} \sum_i s_i^-(n)\end{gathered} \tag{1.6}$$

$$\begin{gathered}N^+ + N^- = N \\ p^+(n+1) = (1-\eta)p^+(n) + \eta(1 - p^+(n)) \quad \eta = \frac{F}{N} \\ p^+(n+1) = (1-2\eta)p^+(n) + \eta\end{gathered} \tag{1.7}$$

Thus one should have:

$$\begin{gathered}p^+(n) = a + b(1-2\eta)^n \\ p^+(0) = a + b \\ p^+(\infty) = \frac{1}{2} = a \\ p^+(n) = \frac{1}{2} + \left(p^+(0) - \frac{1}{2}\right)(1-2\eta)^n\end{gathered} \tag{1.8}$$

[1]You may wonder why we can apply recurrence to a system without canonical Hamiltonian equation. The reason is that the theorem is not about Hamiltonian system, but about the finite state system with invertible and volume preservation.

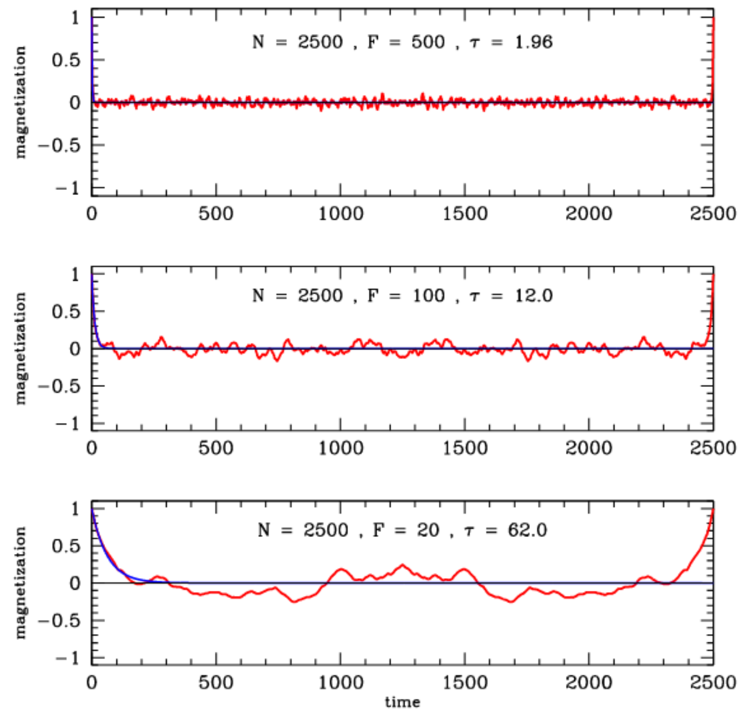

Figure 2. Three simulations of the Kac ring model with $N = 2500$ sites and three different concentrations of flippers. The red line shows the magnetization as a function of time, starting from an initial configuration in which 100% of the spins are up. The blue line shows the prediction of the Stosszahlansatz, which yields an exponentially decaying magnetization with time constant τ.

1.3 Ergodicity

A stronger statement is *ergodicity*, it means given all possible phase volume T, the distribution of phase point in a longer enough time would transverse all possible phase point in T, in $t \to \infty$:

$$\begin{aligned} \langle \rho(\mu) \rangle_t &= \lim_{T\to\infty} \left(\frac{1}{T}\right) \int_0^T d\mu \rho(\mu t) \\ &= \int d\mu \rho(\mu) \delta(E - H(\mu)) / \int d\mu \delta(E - H(\mu)) \\ &= \langle \rho(\mu) \rangle_E \end{aligned} \tag{1.9}$$

Usually, denoted as the hyper-surface as:

$$D(E) = \int d\mu \delta(E - H(\mu)) = \int_{S_E} d\Sigma_E \tag{1.10}$$

However, the integral inspection doesn' t ensure the stability of the distribution, clearly, we can have a distribution with oscillation in time and with a suitable boundary condition, which make cause equality, but the oscillation property of the distribution won' t disappear in time.

$$\begin{aligned} f(q, p) &= \sum_{m,n} \hat{f}_{m,n} e^{imq+inp} \\ \langle f(q, p) \rangle_t &= \hat{f}_{0,0} = \langle f(q, p) \rangle_E \end{aligned} \tag{1.11}$$

$$S(p_i, \lambda_a) = -\sum_i p_i \log p_i + \sum_a \lambda_a \left(\sum_i X_i^a p_i - X^a \right) \tag{1.12}$$

With λ_a the Lagrange multiplier, $\sum_i X_i^a = X^a$ the summation constraint. We has such extreme point:

$$\begin{aligned} \frac{\partial S}{\partial p_i} &= -\log p_i - 1 + \sum_a \lambda_a X_i^a = 0 \\ \frac{\partial S}{\partial \lambda_a} &= \sum_i X_i^a p_i - X^a = 0 \end{aligned} \tag{1.13}$$

Thus we have the distribution:

$$p_i = \exp\left(\sum_a \lambda_a X_i^a - 1 \right) = \frac{1}{Z} \exp\left(\sum_a \lambda_a X_i^a \right) \tag{1.14}$$

We can extend such in continuous case by the generalized Lebesgue integral, therefore a example can be shown that:

$$\int d\mu(x) P(x) = 1 \quad \int d\mu(x) x P(x) = \langle x \rangle \quad \int d\mu(x) P(x) x^2 = \langle x^2 \rangle \tag{1.15}$$

$$\begin{aligned} P(x) &= C e^{\lambda_1 x + \lambda_2 x^2} \\ &= C \exp\left(\frac{\lambda_1^2}{4\lambda_2} \right) \exp\left(-\lambda_2 \left(x + \frac{\lambda_1}{2\lambda_2} \right)^2 \right) \\ &= A \exp(...) \end{aligned} \tag{1.16}$$

Now we try to deduce coefficients λ_1 and λ_2 by the constraint:

$$\begin{aligned} x &\to x + \frac{\lambda_1}{2\lambda_2} = y \\ \int_{-\infty}^{\infty} P(x) dx &= A\sqrt{\frac{\pi}{\lambda_2}} = 1 \\ A\int_{-\infty}^{\infty}\left(y - \frac{\lambda_1}{2\lambda_2}\right) e^{-\lambda_2 y^2} dy &= -A\frac{\lambda_1}{2\lambda_2}\sqrt{\frac{\pi}{\lambda_2}} = \langle x \rangle \\ A\int_{-\infty}^{\infty}\left(y - \frac{\lambda_1}{2\lambda_2}\right)^2 e^{-\lambda_2 y^2} dy &= \frac{1}{2\lambda_2} + \frac{\lambda_1^2}{4\lambda_2^2} = \langle x^2 \rangle \end{aligned} \tag{1.17}$$

$$\begin{aligned} \frac{\lambda_1}{\lambda_2} &= -2\langle x \rangle \\ \frac{1}{2\lambda_2} &= \langle x^2 \rangle - \langle x \rangle^2 \end{aligned} \tag{1.18}$$

$$\begin{aligned} \langle x \rangle = \alpha \quad \langle x^2 \rangle - \langle x \rangle^2 &= \beta^2 \\ P(x) = A\exp&\left(\frac{(x-\alpha)^2}{2\beta^2}\right) \end{aligned} \tag{1.19}$$

Is the final answer, which is a Gaussian distribution with mean α and variance β^2.

$$\begin{aligned} P(\mu) = \frac{1}{Z} e^{\lambda H(\mu)} \quad Z &= \int d\mu e^{\lambda H(\mu)} \\ \int_S d\mu H(\mu) P(\mu) &= \langle H(\mu) \rangle = E \\ \frac{1}{Z}\int_S d\mu H(\mu) e^{\lambda H(\mu)} &= E \\ \frac{1}{Z}\frac{\partial Z}{\partial \lambda} = \frac{\partial \ln Z}{\partial \lambda} &= E \end{aligned} \tag{1.20}$$

$$\begin{aligned} P(\mu) &= \frac{1}{Z}\exp\left(\sum_a \lambda_a X^a(\mu)\right) \\ \frac{\partial \ln Z}{\partial \lambda_a} &= \langle X^a(\mu) \rangle \end{aligned} \tag{1.21}$$

Inspect that, the equilibrium is formulated by:

$$
\begin{aligned}
S[P(\mu)]|_{\text{extreme}} &= \int d\mu P(\mu) \log P(\mu)|_{\text{extreme}} \\
&= \int d\mu P(\mu)(\lambda H(\mu) - \log Z) \\
&= \lambda E - \log Z
\end{aligned} \tag{1.22}
$$

$$
\lambda^{-1} \log Z = E - \lambda^{-1} S[P(\mu)]|_{\text{extreme}} \rightsquigarrow F = \lambda^{-1} \log Z = E - TS \tag{1.23}
$$

Given a exchange ensemble with particle number N and volume V, we has:

$$
\begin{aligned}
P(\mu, N) &= \frac{1}{Z} \exp(\lambda_1 H(\mu) + \lambda_2 N(\mu)) \\
\frac{\partial \ln Z}{\partial \lambda_1} &= E \\
\frac{\partial \ln Z}{\partial \lambda_2} &= \langle N(\mu) \rangle = N
\end{aligned} \tag{1.24}
$$

$$
\begin{aligned}
\lambda_1 &= \lambda_{1'} \text{ in equalibrium} \\
\lambda_2 &= \lambda_{2'} \text{ in equalibrium} \\
&\rightsquigarrow \frac{\lambda_1}{\lambda_2} = \frac{\lambda_{1'}}{\lambda_{2'}}
\end{aligned} \tag{1.25}
$$

$$
\begin{gathered}
S[P(\mu)]|_{\text{extreme}} = \lambda_1 E + \lambda_2 N - \log Z \\
\lambda_1^{-1} \log Z = E + \lambda_2 \lambda_1^{-1} N - \lambda^{-1} S[P(\mu)]|_{\text{extreme}} \rightsquigarrow G = E - uN - TS
\end{gathered} \tag{1.26}
$$

$$
\lambda_1 \frac{\partial \lambda_1^{-1} \ln Z}{\partial \lambda_2} = N \tag{1.27}
$$

Given general parameters, we have general exchange system or grand canonical system:

$$
\lambda_1 d \log Z = \overline{X_a} d\lambda_a \tag{1.28}
$$