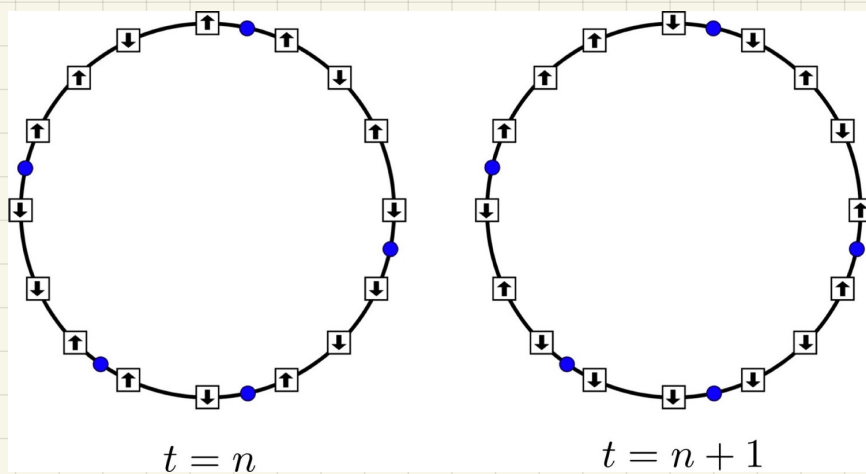


- $g_T$  not invertible: Let  $g: \mathbb{R} \rightarrow [0, 1)$  with  $g(x) = \text{frac}(x)$ , the fractional part of  $x$ . Acting on sets of volume (length) less than one, this map is volume preserving, but obviously  $g$  is not invertible, so the proof fails.
- $\Gamma$  not finite: Let  $g: \mathbb{R} \rightarrow \mathbb{R}$  with  $g(x) = x + a$ . Clearly this is invertible and volume-preserving, but not recurrent.

## - Kac ring model Lecture 14 (Nov. 18)

Can a system exhibit both equilibration and recurrence? Formally no, but practically yes. We noted how for the case of the open perfume bottle, the recurrence time could be vastly longer than age of the universe.

A nice example due to Mark Kac shows how both equilibration and recurrence can be present, on different but accessible time scales. Consider  $N$  spins  $\uparrow$  or  $\downarrow$  on



a ring which evolve by rotating clockwise. There are thus  $N$  sites and  $N$  links. Along  $F$  of these links are

flippers which flip each spin from  $\uparrow$  to  $\downarrow$  or from  $\downarrow$  to  $\uparrow$  as it passes by. The configuration of flippers is frozen in from the start ("quenched randomness"). See the above figure. The number of possible spin configurations is finite and given by  $\text{vol}(\Gamma) = 2^N$ .

Consider the evolution of a single spin, and let  $p_n$  be the probability the spin is up at time  $n$  (units of  $\tau$ ). Let  $x = F/N$  be the fraction of flippers. If the flippers were to move about randomly, we would write

$$p_{n+1} = (1-x)p_n + x(1-p_n) \quad \text{"Stosszahlansatz"}$$

probability up at time  $n$  and did not pass flipper  $\nearrow$

$\nwarrow$  probability down at time  $n$  and passed by a flipper

We can solve this easily:  $u_n \equiv p_n - \frac{1}{2}$ ;  $u_{n+1} = (1-2x)u_n = (1-2x)^n u_1$

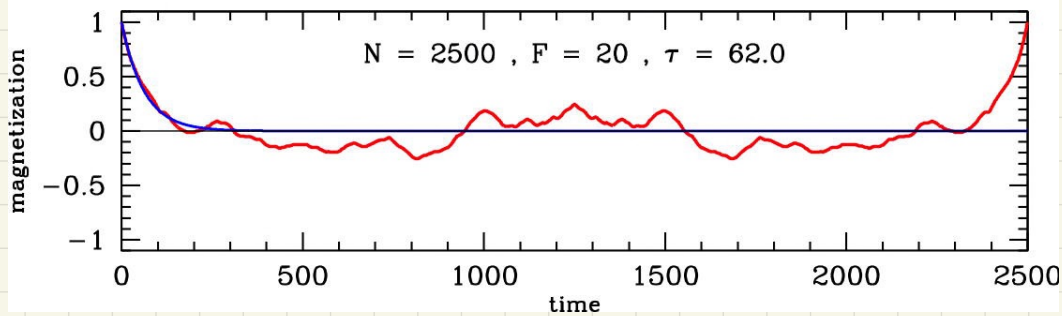
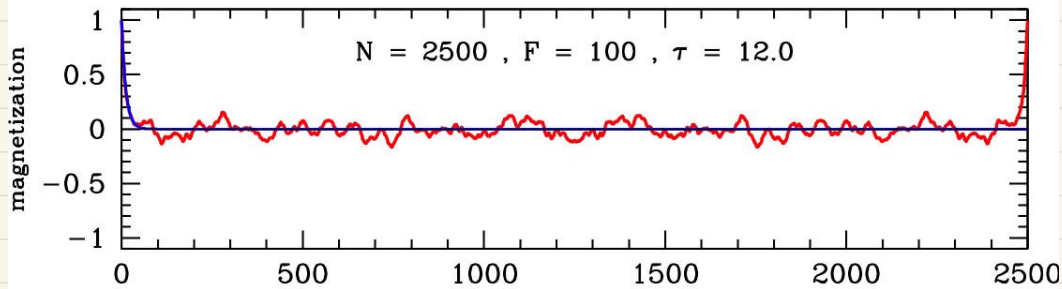
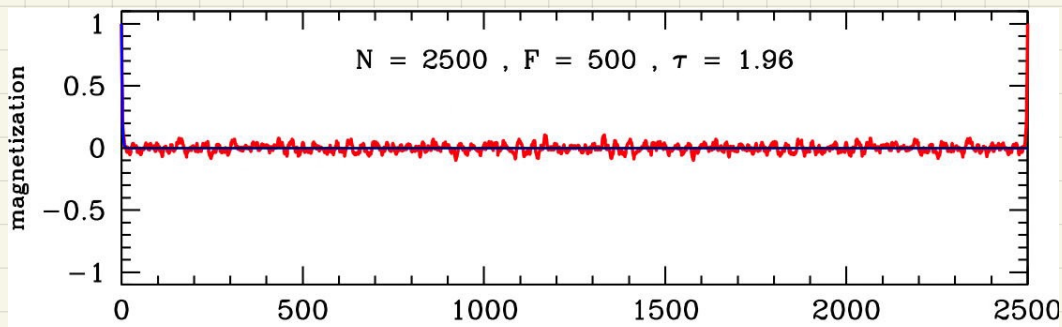
$$p_{n+1} - \frac{1}{2} = (1-2x)(p_n - \frac{1}{2}) \Rightarrow p_n = \frac{1}{2} + (1-2x)^n (p_0 - \frac{1}{2})$$

Thus there is exponential convergence to the equilibrium state  $p_{n \rightarrow \infty} = \frac{1}{2}$  on a time scale  $\tau^* = -1/\ln|1-2x|$ .

Note  $\tau^*(0) = \tau^*(1) = 0$  while  $\tau^*(1/2) = \infty$ . We identify  $\tau^*(x)$  as the microscopic relaxation time over which local equilibrium is established.

$$|1-2x| \equiv e^{-1/\tau^*(x)}$$

$$|1-2x|^n = e^{-n/\tau^*(x)}$$



In the figure, we simulate the Kac ring model dynamics for rings of size  $N = 2,500$  with  $F = 20, 100,$  and  $500$ . The initial conditions are that every spin is in the  $\uparrow$  state. Note how there is an initial exponential relaxation of the magnetization  $m = (N_{\uparrow} - N_{\downarrow})/N = 2p - 1$  to the equilibrium value  $m_{eq} = 0$ , about which  $m$  fluctuates. But at time  $n = N = 2500$ , we have  $m = 1$  once again, and all the spins have returned to their initial  $\uparrow$  state! It is easy to see why: after  $n = N$  time steps, each spin will have gone completely around the ring and

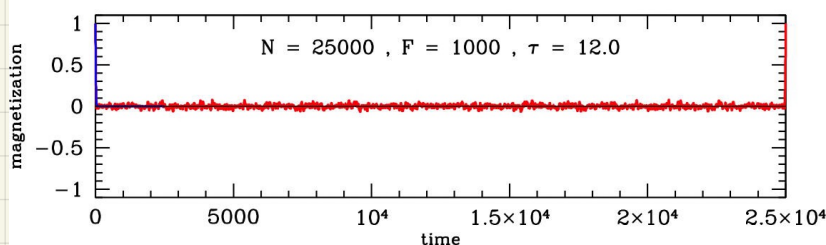
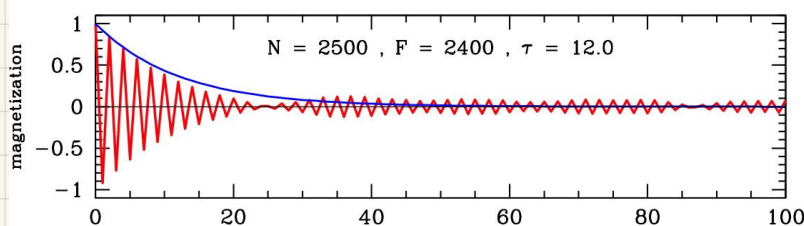
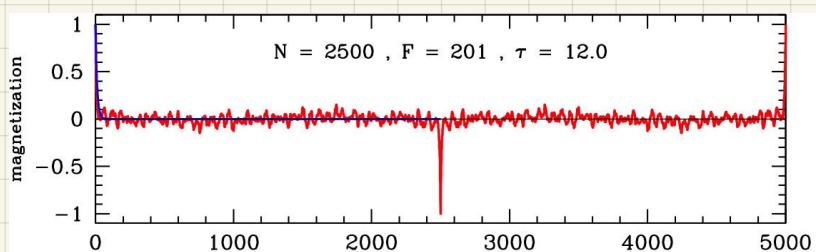
encountered all  $F$  flippers. If  $F$  is even, each spin will have flipped an even number of times, thus returning to its initial state. Thus  $m_N = m_0$ . If  $F$  is odd, each spin flips an odd number of times after  $N$  steps, and  $m_N = -m_0$ . But then  $m_{2N} = m_0$  and the recurrence time is  $2N$ . We emphasize that not only does the magnetization repeat, but the entire initial configuration  $\{\sigma_1, \dots, \sigma_N\}$ , where  $\sigma_j = \pm 1$ , has repeated, and this is true for all  $2^N$  initial conditions. Note that the KRM satisfies the conditions for recurrence:

- map is volume-preserving (one configuration  $\vec{\sigma}$  maps to a unique image  $\vec{\sigma}'$ )
- map is invertible (just run counterclockwise!)
- phase space volume is finite ( $\text{vol}(\Gamma) = 2^N$ )

•  $F$  odd  $\Rightarrow m_N = -m_0$

•  $\chi > \frac{1}{2} \Rightarrow m_n$  oscillates

•  $N = 25,000$ : still recurrent!



## • Canonical transformations

In Lagrangian mechanics, we are free to redefine our generalized coordinates, viz.

$$Q_\sigma = Q_\sigma(q_1, \dots, q_n, t)$$

This is called a "point transformation". It is locally invertible provided  $\det(\partial Q_\alpha / \partial q_\beta) \neq 0$ . Assuming the transformation is everywhere invertible, so we can write  $q_\sigma = q_\sigma(Q, t)$ , the Lagrangian is

$$\tilde{L}(Q, \dot{Q}, t) = L(q(Q, t), \dot{q}(Q, \dot{Q}, t), t) + \frac{d}{dt} F(q(Q, t), t)$$

Note that  $q = q(Q, t) \Rightarrow \dot{q} = \dot{q}(q, \dot{Q}, t)$ . For example,

$$\phi(x, y) = \tan^{-1}(y/x)$$

$$\dot{\phi}(x, y, \dot{x}, \dot{y}) = (x\dot{y} - y\dot{x}) / (x^2 + y^2)$$

We can always add to  $L$  a total derivative of any function of coordinates and time. If  $\delta q_\sigma(t_a) = \delta q_\sigma(t_b) = 0 \forall \sigma$ , then  $\delta Q_\sigma(t_a) = \delta Q_\sigma(t_b) = 0 \forall \sigma$ , and Hamilton's principle,

$$\delta \int_{t_a}^{t_b} dt \tilde{L}(Q, \dot{Q}, t) = 0$$

yields the EL eqns

$$\frac{\partial \tilde{L}}{\partial \Phi_\sigma} - \frac{d}{dt} \left( \frac{\partial \tilde{L}}{\partial \dot{\Phi}_\sigma} \right) = 0$$

This may also be derived starting with the EL eqns for the original generalized coordinates (see Eqs 15.36-37) in the notes.

In Hamiltonian mechanics, we deal with a much broader class of transformations. These are called **canonical transformations** (CTs). The word "canonical" means "conforming to a general rule or accepted procedure" (Webster). What is canonical about CTs is that they preserve a particular structure, namely that of the Poisson bracket. The general form of a CT is

$$q_\sigma = q_\sigma(Q_1, \dots, Q_n, P_1, \dots, P_n, t)$$

$$p_\sigma = p_\sigma(Q_1, \dots, Q_n, P_1, \dots, P_n, t)$$

We may write this as

$$\xi_i = \xi_i(\bar{\xi}_1, \dots, \bar{\xi}_{2n}, t) \quad ; \quad \begin{matrix} \swarrow x_i \\ \xi = \begin{pmatrix} \vec{q} \\ \vec{p} \end{pmatrix} \end{matrix} \quad , \quad \begin{matrix} \swarrow x_i \\ \bar{\xi} = \begin{pmatrix} \vec{Q} \\ \vec{P} \end{pmatrix} \end{matrix}$$

where  $i \in \{1, \dots, 2n\}$ . We shall see that the transformed Hamiltonian is

$$\tilde{H}(Q, P, t) = H(q, p, t) + \frac{\partial}{\partial t} F(q, Q, t)$$



where  $F(q, \dot{q}, t)$  is a function of the old and new coordinates, and of time.

We know that  $\dot{\xi}_j = J_{jk} \frac{\partial H}{\partial \xi_k}$ . Now consider a canonical transformation to new phase space

coordinates  $\Xi_a = \Xi_a(\vec{\xi}, t)$ . We have

$$J = \begin{pmatrix} 0_{n \times n} & 1_{n \times n} \\ -1_{n \times n} & 0_{n \times n} \end{pmatrix}$$

$$\frac{d\Xi_a}{dt} = \frac{\partial \Xi_a}{\partial \xi_j} J_{jk} \frac{\partial H}{\partial \xi_k} + \frac{\partial \Xi_a}{\partial t}$$

But if the transformation is canonical, we must have

$$\begin{aligned} \frac{d\Xi_a}{dt} &= J_{ab} \frac{\partial \tilde{H}}{\partial \Xi_b} = J_{ab} \frac{\partial \xi_k}{\partial \Xi_b} \frac{\partial}{\partial \xi_k} \left( H(\vec{\xi}, t) + \frac{\partial}{\partial t} F(\vec{q}, \vec{Q}, t) \right) \\ &= J_{ab} \frac{\partial \xi_k}{\partial \Xi_b} \frac{\partial H}{\partial \xi_k} + J_{ab} \frac{\partial^2}{\partial t \partial \Xi_b} F(\vec{q}, \vec{Q}, t) \end{aligned}$$

Now define the matrix

$$M_{aj} M_{jb}^{-1} = \frac{\partial \Xi_a}{\partial \xi_j} \frac{\partial \xi_j}{\partial \Xi_b} = \frac{\partial \Xi_a}{\partial \Xi_b} = \delta_{ab}$$

$$M_{aj} \equiv \frac{\partial \Xi_a}{\partial \xi_j} \Rightarrow M_{kb}^{-1} = \frac{\partial \xi_k}{\partial \Xi_b} = (M^t)^{-1}_{bk}$$

Equating the two expressions for  $d\Xi_a/dt$ , we have

$$M_{aj} J_{jk} \frac{\partial H}{\partial \xi_k} + \frac{\partial \Xi_a}{\partial t} = J_{ab} (M^t)^{-1}_{bk} \frac{\partial H}{\partial \xi_k} + J_{ab} \frac{\partial^2 F}{\partial t \partial \Xi_b}$$

Since  $\vec{\xi}$  is arbitrary, the coefficients of  $\frac{\partial H}{\partial \xi_k}$  on each side must match, which says

$$MJ = J(M^t)^{-1} \Rightarrow MJM^t = J$$

What about the terms in blue? We must also have

$$\frac{\partial \Xi_a}{\partial t} = J_{ab} \frac{\partial}{\partial \Xi_b} \frac{\partial}{\partial t} F(\vec{q}(\vec{\Xi}), \vec{p}, t)$$

This is true, but the proof requires results from the next section on generating functions. For now, let's focus on the result  $\mathbf{M}\mathbf{J}\mathbf{M}^t = \mathbf{J}$ . (Note this entails  $\mathbf{M}^t\mathbf{J}\mathbf{M} = \mathbf{J}$  (exercise!). An  $N \times N$  real-valued matrix  $R$  which satisfies  $R^t R = \mathbf{1}$  is called orthogonal, and  $N \times N$  orthogonal matrices form a Lie group,  $O(N)$ . Thus  $R^t R = \mathbf{1} \Leftrightarrow R \in O(N)$ . A  $2n \times 2n$  real-valued matrix  $M$  satisfying  $\mathbf{M}^t \mathbf{J} \mathbf{M} = \mathbf{J}$  with  $\mathbf{J} = \begin{pmatrix} 0_{n \times n} & \mathbf{1}_{n \times n} \\ -\mathbf{1}_{n \times n} & 0_{n \times n} \end{pmatrix}$  is called **symplectic**, and we write  $M \in Sp(2n)$ , the Lie group of real symplectic matrices of rank  $2n$ . With  $M_{aj} = \partial \Xi_a / \partial \xi_j$ , the Poisson bracket is preserved:

$$\begin{aligned} \{A, B\}_{\xi} &= J_{ij} \frac{\partial A}{\partial \xi_i} \frac{\partial B}{\partial \xi_j} = J_{ij} \frac{\partial A}{\partial \Xi_a} \overbrace{\frac{\partial \Xi_a}{\partial \xi_i}}^{M_{ai}} \frac{\partial B}{\partial \Xi_b} \overbrace{\frac{\partial \Xi_b}{\partial \xi_j}}^{M_{bj} = M_{jb}^t} \\ &= M_{ai} J_{ij} M_{jb}^t \frac{\partial A}{\partial \Xi_a} \frac{\partial B}{\partial \Xi_b} = J_{ab} \frac{\partial A}{\partial \Xi_a} \frac{\partial B}{\partial \Xi_b} = \{A, B\}_{\Xi} \end{aligned}$$

We next consider how to manufacture a canonical transformation. But before doing so, let us first show that Hamiltonian evolution itself generates a CT.

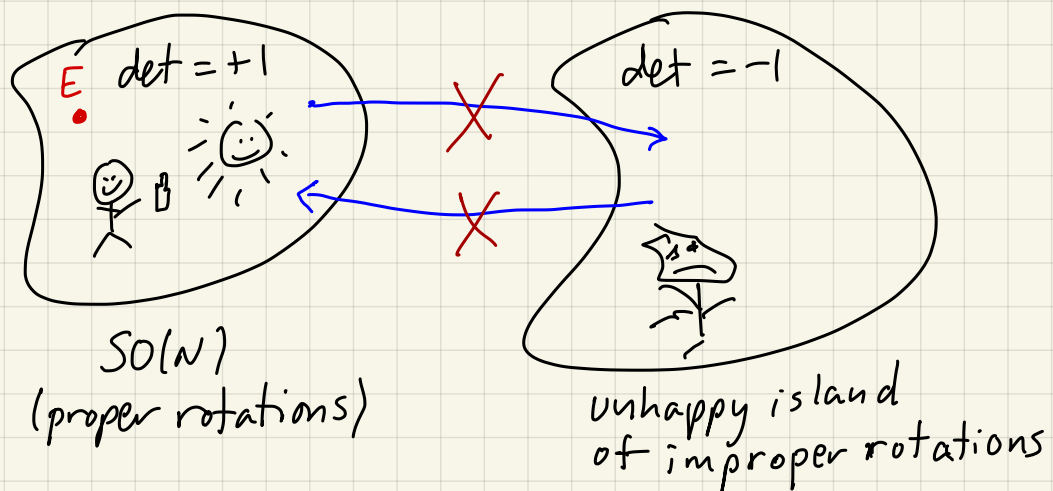


# Scratch

$$O(N) : R^t R = \mathbb{1} \Rightarrow \det R = \pm 1$$

$$SO(N) : R^t R = \mathbb{1} \text{ and } \det R = +1$$

$$O(N) \subset GL(N, \mathbb{R})$$



$$M^t J M = J \Rightarrow \det M = \pm 1$$

$\det M = -1$  excluded (no unhappy island)

$$\text{Pf } A = \frac{1}{2^n n!} \sum_{\sigma \in S_{2n}} \text{sgn}(\sigma) A_{\sigma(1)\sigma(2)} \cdots A_{\sigma(2n-1)\sigma(2n)}$$

$\uparrow$   
 $2n \times 2n$

$$\det A = (\text{Pf } A)^2$$

$$\text{Pf}(A^t J A) = \det A \text{ Pf } J$$

$$M \in Sp(2N) \Rightarrow \text{Pf}(M^t J M) = \cancel{\text{Pf } J} = \det M \cancel{\det J}$$

- Proof Hamiltonian evolution generates a CT

We consider an infinitesimal evolution:

$$\begin{array}{ccc} \xi_i(t) & \rightarrow & \xi_i(t+dt) = \xi_i(t) + J_{ik} \left. \frac{\partial H}{\partial \xi_k} \right|_{\xi(t)} dt + O(dt^2) \\ \parallel & & \parallel \\ \xi_i & & \xi'_i \end{array}$$

We have that  $M_{ij} = \frac{\partial \xi'_i}{\partial \xi_j} = \delta_{ij} + J_{ir} \frac{\partial^2 H}{\partial \xi_j \partial \xi_r} dt + O(dt^2)$

Thus  $M_{kl}^t = \delta_{kl} + J_{ls} \frac{\partial^2 H}{\partial \xi_k \partial \xi_s} dt$  and

$$\begin{aligned} M_{ij} J_{jk} M_{kl}^t &= \left( \delta_{ij} + J_{ir} \frac{\partial^2 H}{\partial \xi_j \partial \xi_r} dt \right) J_{jk} \left( \delta_{kl} + J_{ls} \frac{\partial^2 H}{\partial \xi_k \partial \xi_s} dt \right) \\ &= J_{il} + \underbrace{\left( J_{ir} J_{jl} \frac{\partial^2 H}{\partial \xi_j \partial \xi_r} + J_{ik} J_{ls} \frac{\partial^2 H}{\partial \xi_k \partial \xi_s} dt \right)}_{\text{take } k \rightarrow r, s \rightarrow j} + O(dt^2) \\ &= J_{il} + O(dt^2) \end{aligned}$$

### Lecture 15 (November 23)

#### • Generating functions for canonical transformations

For a transformation to be canonical, we require

$$\delta \int_{t_a}^{t_b} dt \left[ p_\sigma \dot{q}_\sigma - H(\vec{q}, \vec{p}, t) \right] = 0 = \delta \int_{t_a}^{t_b} dt \left[ P_\sigma \dot{Q}_\sigma - \tilde{H}(\vec{Q}, \vec{P}, t) \right]$$

This is satisfied for all motions provided

$$p_\sigma \dot{q}_\sigma - H(\vec{q}, \vec{p}, t) = \lambda \left[ P_\sigma \dot{Q}_\sigma - \tilde{H}(\vec{Q}, \vec{P}, t) + \frac{d}{dt} F(\vec{q}, \vec{Q}, t) \right]$$

where  $\lambda$  is a constant. We can always rescale coordinates