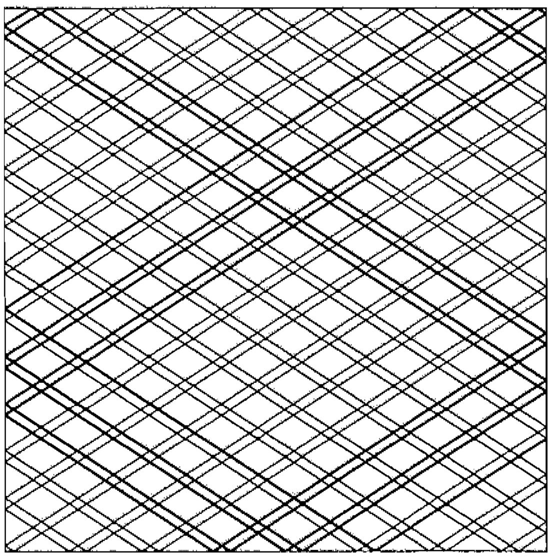
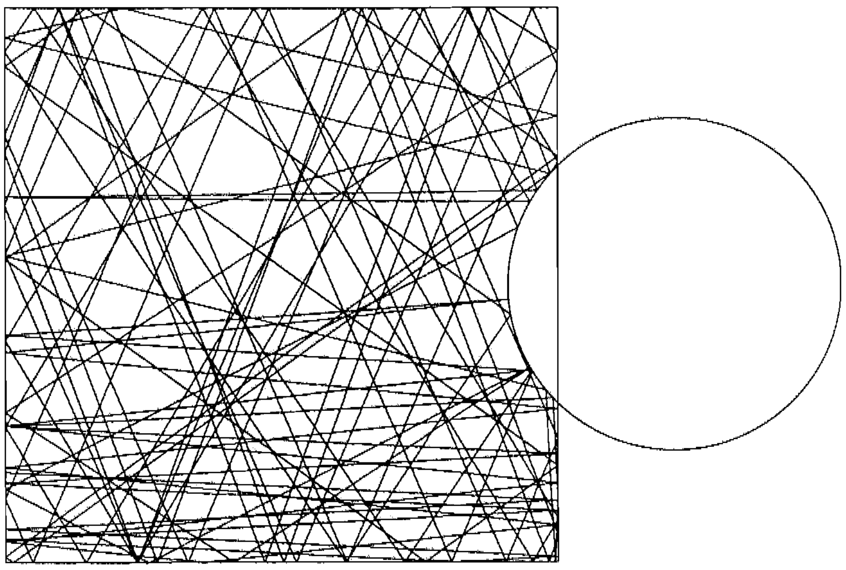
Lecture #5

(1)





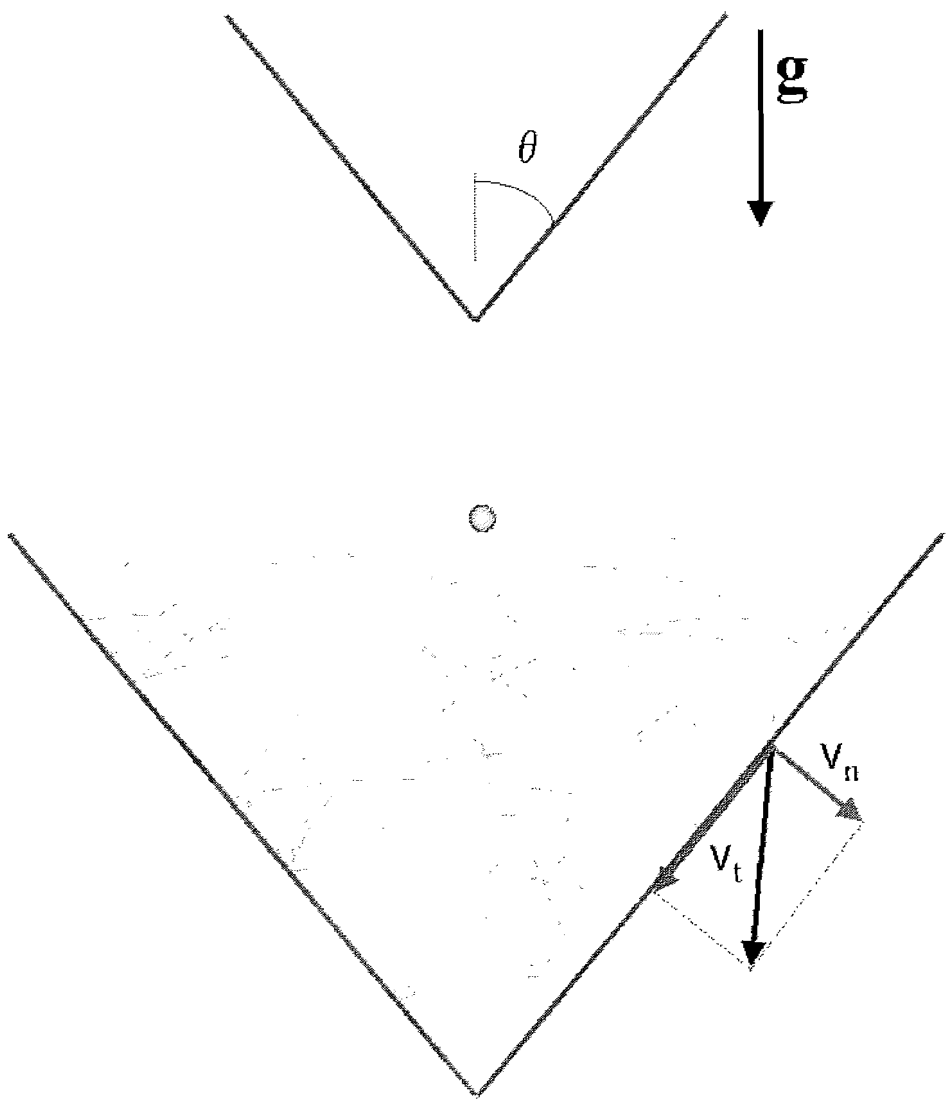
Gravitational Wedge Billiard

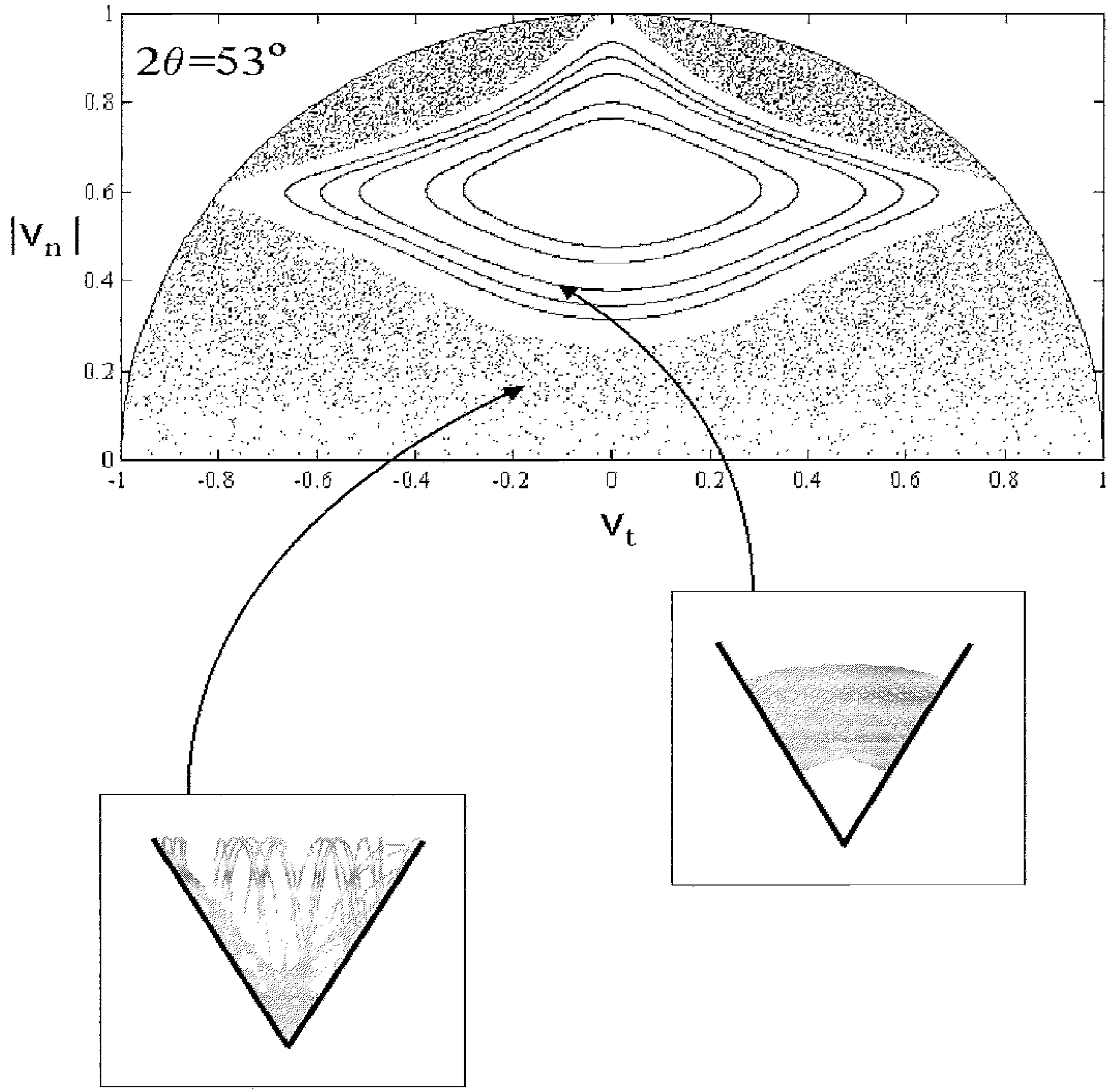
Lehtihet

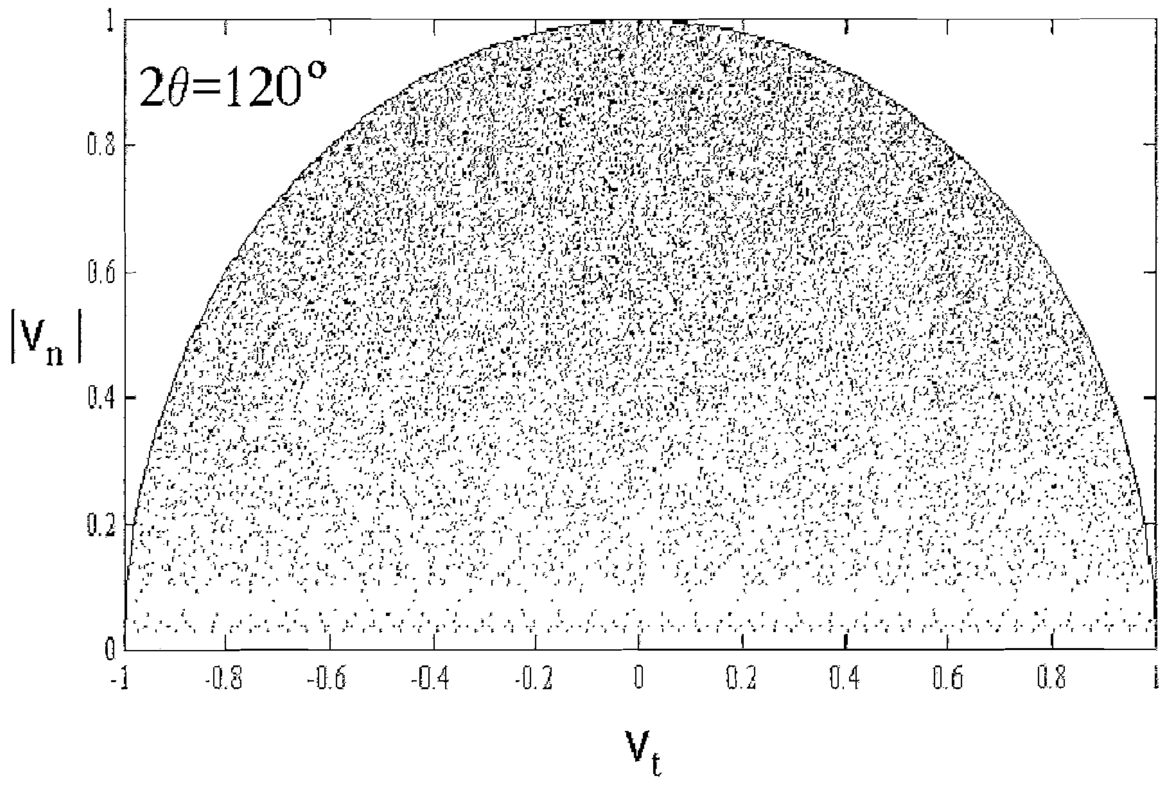
&

Miller

‘86




2θ=53°
|v_n|
v_t
0
0.2
0.4
0.6
0.8
1
-1
-0.8
-0.6
-0.4
-0.2
0
0.2
0.4
0.6
0.8
1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v_t
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0.6
0.4
0.2
0
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-0.8
-0.6
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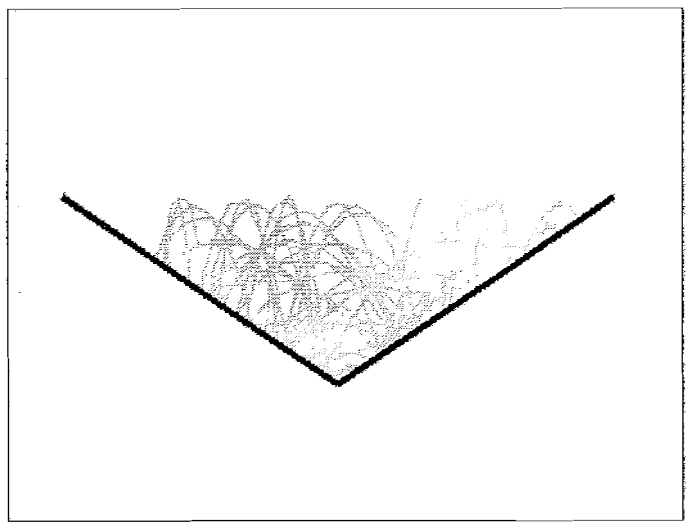
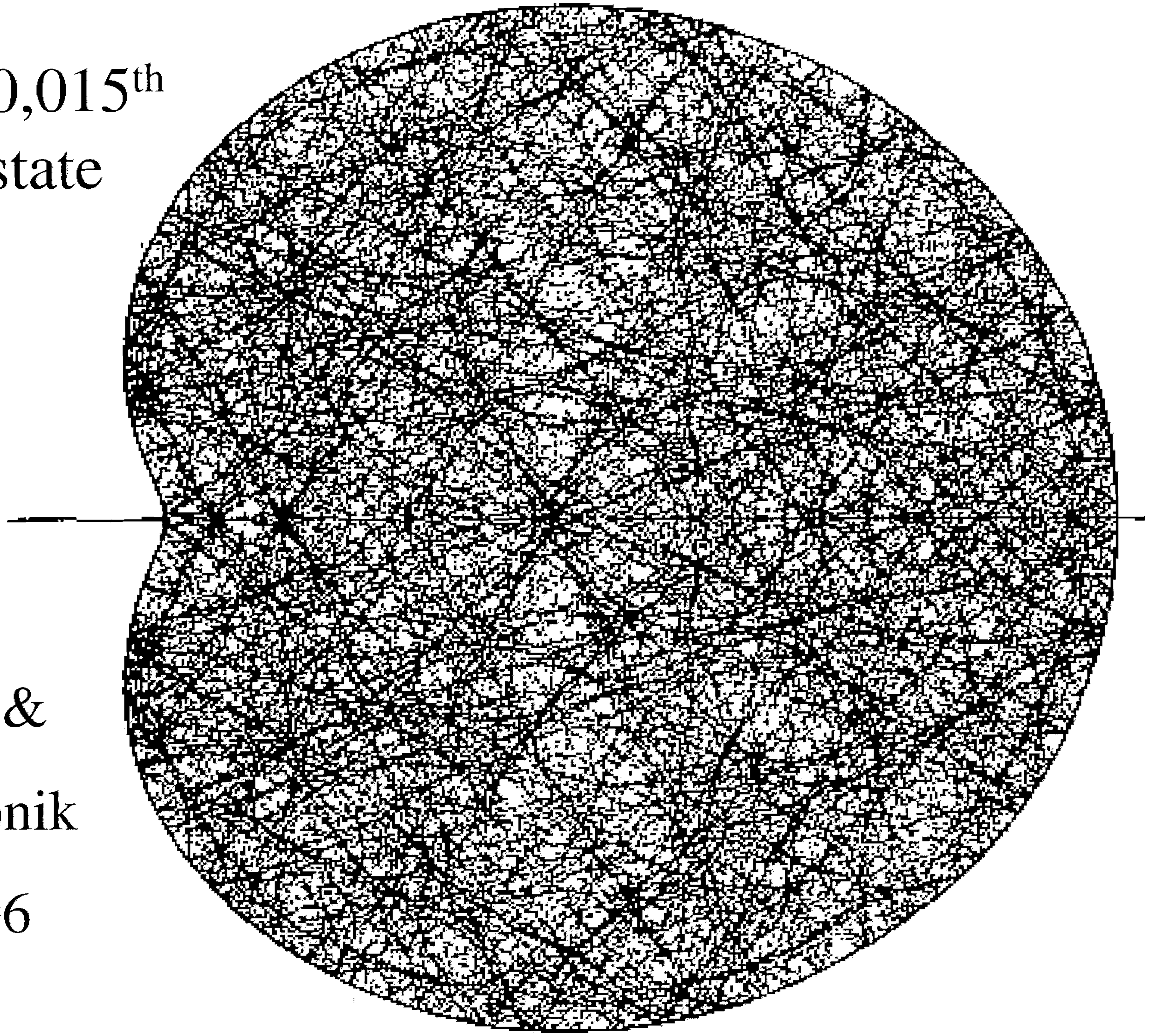
0.4
0.6
0.8
1



100,015th
state



Li &
Robnik
‘96

⑥

If the system is ergodic, the ~~enty~~ 6N-1 ~~system~~ phase space will be explored uniformly.

If one wants to compute a time-average -

$$\langle f \rangle_t = \frac{1}{\tau}\int_{t_0}^{t_0+\tau} dt\, f(q_i(t), p_i(t)),$$

we invoke the ergodic hypothesis and argue that the system is equally likely to be anywhere on the constant energy surface.

$$\langle f \rangle_t = \langle f \rangle_\rho = \int dp_i\, dq_i\, f(q_i, p_i)\, \rho(q_i, p_i) \Big/ \int dp\, dq\, \rho$$

* $\dfrac{\rho}{\int dp\, dq\, \rho}$ is probability distribution in phase-space

$$\rho \propto \delta(E - H(p_i, q_i)), \quad \delta(x) \text{ is Dirac-}\delta \text{ function}$$

$$\cancel{\int dp_i\, dq_i\, \rho = 1 = c \int dp_i\, dq_i\, \delta(E - H(p_i, q_i))}$$

$$\therefore \rho = c\, \delta[E - H(p_i, q_i)]$$

$\Rightarrow$ uniform-distribution on the constant E surface.

It is important to stress that the ensemble-average will coincide with the time average only if the system is ergodic, and the time-average is over a time longer than any microscopic time.

If the ergodic hypothesis is false, there would be parts of phase space that are effectively disconnected from one another.
→ they might have thermodynamically distinguishable states ⇒ more variables besides Energy U are important

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If we generalize ρ to describe the probability of a configuration of $\{q,p\}$ it will evolve in time as

$$\frac{d\rho}{dt} = \frac{\partial\rho}{\partial t} + \{\rho, H\} \; ; \quad \{A,B\} = \sum_i \left(\frac{\partial A}{\partial q_i}\frac{\partial B}{\partial p_i} - \frac{\partial A}{\partial p_i}\frac{\partial B}{\partial q_i}\right)$$

(Poisson bracket)

In Equilibrium, ρ reaches a steady-state, $\frac{d\rho}{dt} = \frac{\partial\rho}{\partial t} = 0$

$\Rightarrow \{\rho, H\} = 0$; one way is for $\rho = \rho(H(p;q))$

Micro-Canonical Ensemble

$$\rho \sim \delta(E-H)$$

Canonical Ensemble,

$$\rho \sim e^{-H/k_BT}$$

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From a microscopic point of view, $\rho(q_i,p_i)/\int dp\,dq\,\rho(p,q)$ is the probability density that the system will be found in phase-space at (q_i, p_i)

Write $g(E) = \int \frac{dp_i\,dq_i}{h^{3N}}\,\delta[E-H(p_i q_i)]$; $= \int dp_i\,dq_i\,\rho$

$[h] \sim [p][q]$, so $[g] = \frac{1}{E}$

$g(E)$ is the normalization of the distribution $\rho(q,p)$

$= \frac{\text{total \# of "micro-states"}}{\text{Energy interval}}$. Classically, h is arbitrary,

Quantum-Mechanically, $g(E)$ is the density of states, and h is Planck's constant.

We now turn to a quantum mechanical treatment of the problem.

Start with simple observation that quantum mechanics gives quantization: There are many micro states that correspond to given Macro state.

Example: N spins on a 1D lattice:

$$\uparrow \quad \uparrow \quad \downarrow \quad \downarrow \quad \uparrow \quad \uparrow \quad \uparrow \quad \cdots$$

$i=1$, $i=2$, $i=3$ ---- $i=N$

The Magnetization $M \equiv N_\uparrow - N_\downarrow$ is just the number "up" − the number "down"

$$\hat{S}_z |\chi_s\rangle = \pm\frac{\hbar}{2} |\chi_s\rangle$$

$\uparrow\downarrow\downarrow$, $\downarrow\downarrow\uparrow$, $\downarrow\uparrow\downarrow$ are 3 different configurations that have the same "Magnetization"

Underlying Assumption of statistical mechanics is that every microstate corresponding to the same macrostate is equally probable.

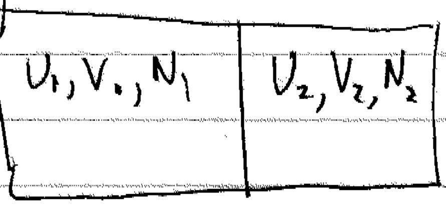
A.K.A. Ergodic Hypothesis.

Denote the total number of microstates corresponding to the thermodynamic variables $\Rightarrow$ U, V, N as

$$\Omega(U,V,N).$$

Now, imagine two physical systems that are seperatly in equilibrium:

now, let heat flow between the systems:



$U = U_1 + U_2$

the total # of microstates of the total combined system is simply

$$\Omega(U,V,N) = \Omega_1(U_1,V_1,N_1)\,\Omega_2(U_2,V_2,N_2)$$

$$= \Omega_1(U_1,V_1,N_1)\,\Omega_2(U-U_1,V_2,N_2)$$

However, U_1 is undetermined, $0 \le U_1 \le U$.

What state do we actually see?

The system should occupy the macrostate that has the largest number of microstates

$\Rightarrow$ Maximize Ω over values of U_1.

$$d\Omega = \left.\frac{\partial\Omega_1}{\partial U_1}\right|_{V,N} \Omega_2\, dU_1 + \frac{\partial\Omega_2}{\partial U_2}\Omega_1\, dU_2 = 0$$

$$U = U_1 + U_2 \Rightarrow dU_1 = -dU_2$$

$$d\Omega = \left(\frac{\partial\Omega_1}{\partial U_1}\Omega_2 - \frac{\partial\Omega_2}{\partial U_2}\Omega_1\right) dU_1 = 0 \quad \forall\, dU_1$$

$$\Rightarrow \left.\frac{\partial \ln\Omega_1}{\partial U_1}\right|_{V,N} = \left.\frac{\partial \ln\Omega_2}{\partial U_2}\right|_{V,N} \;;\text{ or } \beta_1 = \beta_2 \qquad \beta = \frac{\partial \ln\Omega}{\partial U}$$

So the condition for Equilibrium should be the common temperature.

$\Rightarrow$ we associate β with $1/T$.

$$\Leftrightarrow \left.\frac{\partial \ln\Omega}{\partial U}\right|_{V,N} = \left.\frac{\partial S}{\partial U}\right|_{V,N} = \frac{1}{T} \Rightarrow \frac{\Delta S}{\Delta \ln\Omega} \sim \text{const} \;\text{(Boltzmann)}$$

$$\text{or} \quad S = k_B \ln\Omega \quad \text{(Planck)}$$

$\uparrow$ (Boltzmann constant) (no additive constant)

$\Rightarrow$ if the system is perfectly ordered, there is no entropy, $S = 0$

e.g. $\uparrow\uparrow\uparrow\uparrow\uparrow \Rightarrow$ only 1 microstate.