Weak ergodicity and non-equilibrium statistical mechanics

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$\Gamma = \{x_1, \ldots, x_n, y_1, \ldots, y_n\}$ — phase space.

Liouville equation

$$\frac{\partial \rho}{\partial t} + \{H, \rho\} = 0$$

1.
$$\bar{\rho}(x, y) = \lim_{\tau \to \infty} \frac{1}{\tau} \int_0^{\tau} \rho_t(x, y) dt$$

2. ρ_t weakly converges to $\bar{\rho}$ if
$$\int_{\Gamma} \varphi \rho_t d^n x d^n y \to \int_{\Gamma} \varphi \bar{\rho} d^n x d^n y$$
as $t \to \infty$

Weak Ergodicity

$M^n = \{x_1, \ldots, x_n\}$, $\Gamma = T^*M$
$H = \frac{1}{2}(A(x)y, y)$ is a Hamiltonian function

$$\dot{x} = \frac{\partial H}{\partial y}, \quad \dot{y} = -\frac{\partial H}{\partial x}$$

Lemma 1. If $x(t)$, $y(t)$ is a solution, then $t \mapsto x(\lambda t), \lambda y(\lambda t)$ is also a solution for any $\lambda \in \mathbb{R}$.

Gibbs measure γ with density

$$\rho = e^{-\beta H}/Z; \quad \beta = \frac{1}{kT}$$

$$\int_\Gamma \rho d^n x d^n y = 1 \quad \Rightarrow \quad \gamma(\Gamma) = 1$$

Weak Ergodicity

$$\varphi\colon M \to \mathbb{R} \underset{\text{lift}}{\longmapsto} \tilde{\varphi}\colon \Gamma \to \mathbb{R}$$

$$d\nu = |A(x)|^{-1/2} d^n x \quad \text{is a Riemannian volume on } M$$

Lemma 2. If φ is integrable with respect to the measure ν, then $\tilde{\varphi}$ is integrable with respect to the measure γ and

$$\int_\Gamma \tilde{\varphi} d\gamma = \int_M \varphi d\nu \Big/ \int_M d\nu.$$

Here g_H^t is the phase flow.

For almost all $z \in \Gamma$ there exist

$$\lim_{\tau \to \pm\infty} \frac{1}{\tau} \int\limits_0^\tau \tilde{\varphi}(g_H^t(z)) dt = \bar{\varphi}(z) \quad \text{(Birkhoff–Khinchin theorem)}$$

and $\bar{\varphi}$ is integrable with respect to the measure γ; $\bar{\varphi}|_{y=0} = \varphi$.

Weak Ergodicity

Lemma. If $y \neq 0$, then $\bar{\varphi}$ depends only on x and $y/|y|$.

Definition. A system is called *weakly ergodic* if for any integrable function $\varphi\colon M \to \mathbb{R}$ its mean value $\bar{\varphi}\colon \Gamma \to \mathbb{R}$ is constant almost everywhere.

Theorem 1. If the system is weakly ergodic, then

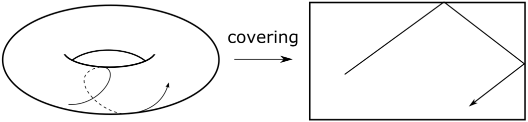
$$\bar{\varphi} = \int_M \varphi d\nu \bigg/ \int_M d\nu \quad \text{(a.e.)}$$

Corollary. Almost all geodesics are everywhere dense on M.

Theorem 2. Every ergodic system is weakly ergodic.

Weak Ergodicity

Example. $M = \mathbb{T}^n$, $H = \frac{1}{2}(y, y) = \frac{1}{2}\sum y_i^2$ is a weakly ergodic system and is not an ergodic system.



Knudsen gas
(1871 - 1949)

$$\rho_t(z) = \rho_0(g_H^{-t}(z)) \quad \text{is a solution of the Liouville equation}$$

If $\rho_0 \in L_p$, then $\rho_t \in L_p$ for all $t \in \mathbb{R}$.
Let $f \in L_q(\Gamma, \mu)$, $d\mu = d^n x d^n y$ is the Liouville measure $\Rightarrow f\rho_t$ is integrable with respect to the measure μ.

Lemma 4.

$$\int_\Gamma \rho_0(g_H^{-t}(z)) f(z) d\mu = \int_\Gamma \rho_0(z) f(g_H^t(z)) d\mu.$$

Let $\rho_0 \in L_1(\Gamma, \mu)$ and $\varphi \in L_\infty(M, \nu)$;

$$K(t) = \int_\Gamma \rho_t \varphi d\mu.$$

Ergodic Theorems

Theorem 3. If the system is weakly ergodic, then

$$\lim_{t \to \pm\infty} K(t) = \bar{\varphi} \quad \left(= \int_M \varphi d\nu \Big/ \int_M d\nu \right).$$

Average Temperature of the Knudsen Gas

$$M = \mathbb{T}^n\{x_1, \ldots, x_n \mod 2\pi\}$$

$$\rho_0(x, y) = \frac{e^{-\frac{y^2}{2\sigma^2(x)}}}{[\sqrt{2\pi}\sigma(x)]^n}\varphi(x), \quad y^2 = \sum y_i^2$$

Let $\int_\Gamma \rho_0 d\mu = 1 \Rightarrow \int_{\mathbb{T}^n} \varphi(x) d^n x = 1$.

$$\sigma^2(x) = kT(x)$$

$$\rho_t(x, y) = \frac{e^{-\frac{y^2}{2\sigma^2(x-yt)}}}{[\sqrt{2\pi}\sigma(x-yt)]^n}\varphi(x - yt)$$

is a solution of the Liouville equation

$$\frac{\partial \rho}{\partial t} + \sum_{i=1}^{n} \frac{\partial \rho}{\partial x_i} y_i = 0.$$

ρ_t weakly converges to $\rho_\infty = \frac{1}{(2\pi)^n} \int_{\mathbb{T}^n} \rho_0(x, y) d^n x$.

Average Temperature of the Knudsen Gas

$$E_0 = \frac{1}{2}\int_{\mathbb{R}^n}\int_{\mathbb{T}^n} y^2\rho_0(x,y)d\mu = \frac{nk}{2}\int_{\mathbb{T}^n} T(x)\varphi(x)d^n x.$$

$$E_\infty = \frac{1}{2}\int_{\mathbb{R}^n}\int_{\mathbb{T}^n} y^2\rho_\infty d\mu = \frac{nk}{2}T_\infty.$$

Theorem 5.

$$T_\infty = \int_{\mathbb{T}^n} T(x)\varphi(x)d^n x \Bigg/ \int_{\mathbb{T}^n}\varphi(x)d^n x$$

Density Homogenization

$$u(x,t) = \int_{\mathrm{R}^n} \rho_t(x,y) d^n y$$

— the density of distribution in the configuration space.

Theorem 6. If $\sigma = \text{const}$, then $u'_t = t\sigma^2 \Delta u$, $u(x,0) = \varphi(x)$, Δ is the Laplace operator.

$$u'_\tau = \sigma^2 \Delta u, \quad \tau = t^2/2$$

— heat equation, which is invariant under the substitution $t \mapsto -t$.

In statistical mechanics, $\sigma^2 = kT$, k is the Boltzmann constant, T is the absolute temperature.

$$\Pi^n = \{x \in \mathbb{R}^n \colon 0 \leqslant x_1 \leqslant l_1, \dots, 0 \leqslant x_n \leqslant l_n\}, \quad l = \max_j l_j.$$

$$\left\| u(x,t) - \frac{1}{\text{mes}\Pi} \int_\Pi \varphi(x) d^n x \right\|_{L_2} \leqslant c e^{-\frac{\pi^2 \sigma^2}{2l^2} t^2}, \quad c = \text{const}.$$

Doklady, 2007, V. 416, №3, pp. 302–305

$$\Gamma = T^*M, \quad \rho_0(x,y) = \frac{e^{-\frac{H}{\sigma^2}}}{(\sqrt{2\pi}\sigma)^n}\varphi \Big/ \int_M \varphi d\nu$$

$$\int_\Gamma \rho_0 d\mu = 1; \quad \int_\Gamma H\rho_t \psi d\mu$$

$\psi(x) \equiv 1 \Rightarrow$ we obtain the mean kinetic energy of the system (which is constant).

Let ψ be the characteristic function of a measurable region $\Psi \subset M$. Then we obtain the mean energy of the systems from the Gibbs ensemble located in Ψ for the moment t.

Theorem 7. Under the assumption of weak ergodicity,

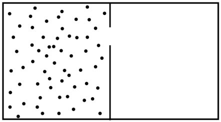
$$\int_\Gamma H\rho_t \psi d\mu \to \frac{n}{2}\int_M \sigma^2 \varphi d\nu \int_M \psi d\nu \Big/ \int_M \varphi d\nu \int_M d\nu$$

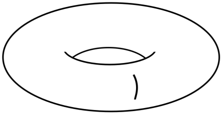
Curved Space

$\psi(x) = 1$; let $E_\infty = \lim_{t\to\infty} E_t = \frac{nkT_\infty}{2}$, $\sigma^2(x) = kT(x) \Rightarrow$

$$T_\infty = \int_M T\varphi d\nu \bigg/ \int_M \varphi d\nu$$

Weak Ergodicity and the Knudsen Gas





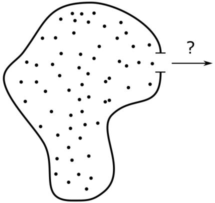
Theorem A. The billiard on a torus with a wall is a weakly ergodic system.

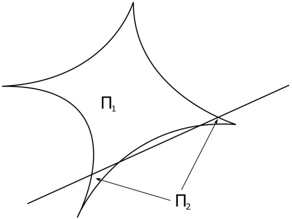
Theorem B. Let $D \subset \mathbb{T}^n$ be a Jordan measurable region, $\varphi\colon \mathbb{T}^n \to \mathbb{R}$ be a Riemannian integrable function. Then for any motion $t \mapsto x(t)$ with non-resonant velocity vector

$$\lim_{\tau\to\infty} \frac{1}{\tau}\int_0^\tau \varphi(x(t))dt = \frac{1}{(2\pi)^n}\int_{\mathbb{T}^n} \varphi(x)d^nx$$

Weak Ergodicity and the Knudsen Gas

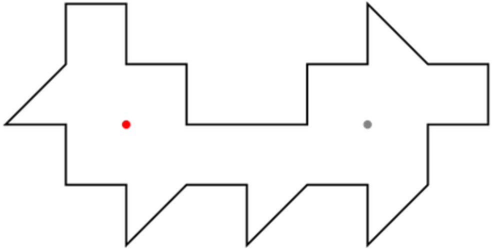
Will the Knudsen gas flow out? $\Pi = \Pi_1 \cup \Pi_2$





Theorem C. If the billiard in Π is weakly ergodic, then almost all Knudsen gas with any integrable density will flow out from Π_1 and Π_2.

Illumination Problem



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Illumination Problem

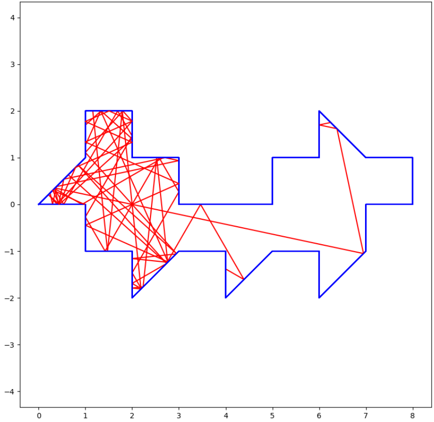

Figure 1: $n = 10$, $T \sim 10$

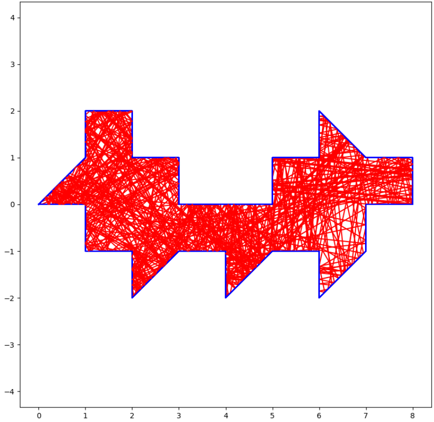

Figure 2: $n = 10$, $T \sim 100$

Illumination Problem

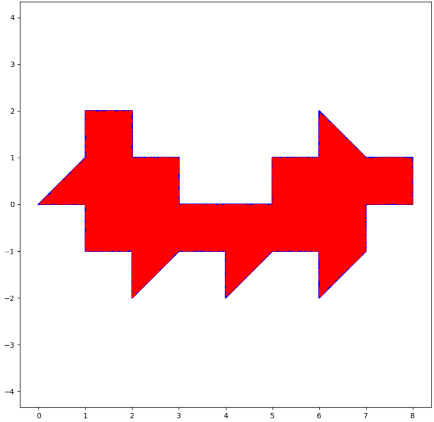

Figure 3: $n = 10$, $T \sim 1000$

Thank you