Statistical physics

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Statistical physics of many-body systems

- **equilibrium**
- **non-equilibrium**

Statistical properties may be tackled from three levels

- **Fundamental level**

Solve microscopic equations of motion, such as Newton, Hamiltonian, Heisenberg Eqs..

Difficulties

* **too many degrees of freedom**
* **microscopic initial conditions and boundary conditions**
* **irregular disturbance from environments**

Here the time t is microscopic.

- **Quasi-fundamental level**

Do not trace the motion of each molecule, and consider only the time-dependent probability distribution in phase space, $\rho(p_i, q_i, t)$

Equations of motion

* **Liouville's eq.**
* **Boltzmann eq.**

These eqs. can be solved only in simple cases, such as dilute gases.

The time t is mesoscopic.

- **Statistical mechanics**

*** Equilibrium: Do not solve any eqs. of motion, but assume a form of** $\rho(p_i, q_i, \infty) = \rho(p_i, q_i)$

* **it can be tested by experiments**
* **it can be derived from eqs. of motion in some special cases.**

More strictly, this is the so-called ensemble theory.

The time t is macroscopic.

*** Non-equilibrium: one usually assumes certain effective equations of motion, e.g., Monte Carlo dynamics, Langevin eq., KPZ eq. etc**

The time scale depends on the equations.

Non-equilibrium phenomena

- **Dynamic relaxation**

For example, t＝0, the system is at high temperature; t > 0, suddenly quenched to low temperature. Obviously, properties and observables are time-dependent.

- **Dynamic transportation**

The system is a stationary state, but with ‘current’, such as particle current, electric current, energy current. It needs also dynamic equations.

- **Other dynamic systems.**

For example, a system driven by macroscopic external forces, or the external forces can not be described by a Hamiltonian etc.

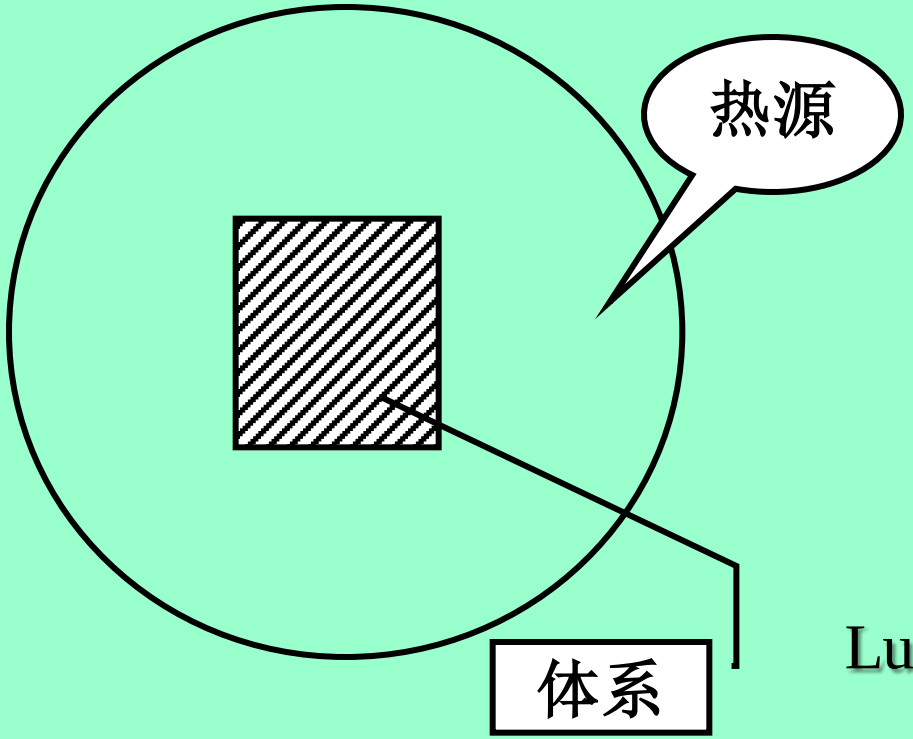
Dynamic fluctuations around equilibrium or stationary states belong also to non-equilibrium phenomena.

In our lectures, Monte Carlo simulations, and molecular dynamics simulations based on fundamental equations of motion are mainly used to tackle the non-equilibrium dynamics.

Basics of Monte Carlo simulations

与温度T的大热源接触的体系，在平衡态时，正则分布由体系的Hamiltonian决定。

$$\rho(\{S_i\}) \propto \mathrm{e}^{-H(\{S_i\})/kT}$$



Ludwig Boltzmann, 1844-1906

宏观物理量是对所有微观状态平均的结果。

例如， 对Ising模型，磁化强度

$$M = \frac{1}{Z}\sum_{\{S_i\}} \frac{1}{N}\sum_i S_i \; e^{-H/kT}$$

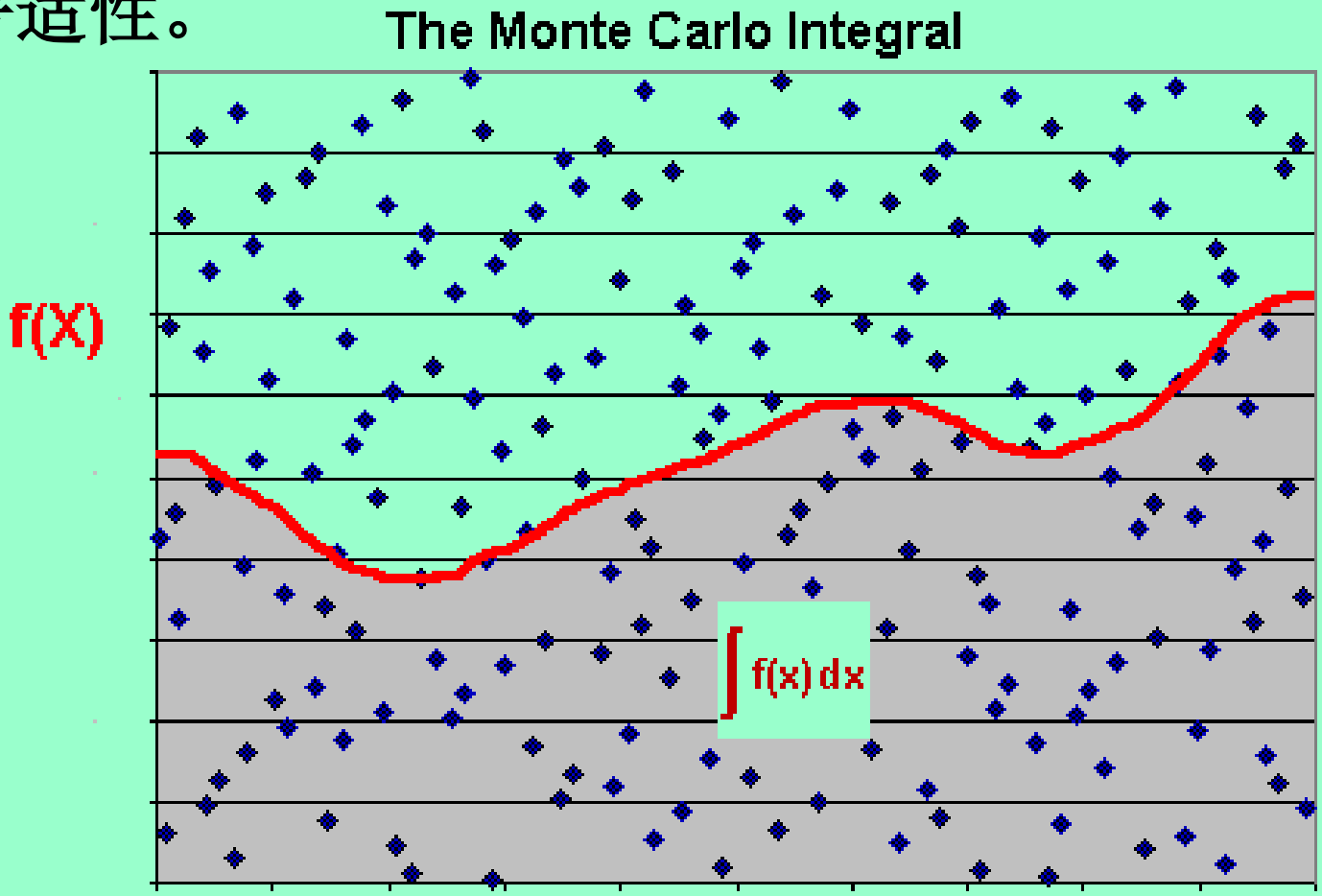
$$-\frac{1}{kT}H = K\sum_{\langle i\, j\rangle} S_i\, S_j + h\sum S_i$$

$$Z = \sum_{\{S_i\}} e^{-H/kT} \qquad S_i = \pm 1$$

对多体系统，计算统计平均十分困难

如何用随机的Monte Carlo 方法求积分？

例如，可用‘抛石子’方法。对单自由度，这方法不比简单的数值积分或近似方法有效。但具有普适性。



对多自由度 ***d*** ，

随机的“Monte Carlo”方法

$$\Delta S \propto 1/\sqrt{M}$$

数值积分Trapezoid方法

$$\Delta S \propto 1/M^{2/d} \qquad (h^d = 1/M)$$

当***d***非常大，数值积分方法根本没法和 **Monte Carlo方法比较！**

但是，两种方法都存在“平均主义”的弱点。只是数值积分“太仔细”了。

重要抽样的Monte Carlo 方法

如果被积函数 ***f(x)*** 是均匀的函数，则简单抽样方法已经可以得到相当准确的积分值。

如果被积函数 ***f(x)*** 不是均匀的函数----这在高维积分十分常见，则必须引入重要抽样。我们希望在对积分贡献大的区域多取样品，在贡献小的区域少取样品。

设积分为

$$S =< f(x) >= \int_a^b f(x)W(x)\,dx$$

其中 ***f(x)*** 是均匀函数，***W(x)*** 是非负不均匀函数，而且可以归一化，给予概率分布的含义。

假设我们可以按照分布**W(x)**得到 ***M*** 个点 $\{x_k\}$

$$S=\frac{1}{M}\sum_{l=1}^{M}f(x_l)+O(1/\sqrt{M})$$

关键：如何按分布 $W(x)$，产生 ***M*** 个 $\{x_k\}$

Markov 过程产生 $\{x_k\}$ 的方法：

构造一个**Markov过程**，即给出一个动力学规则，由 x_t 随机地产生 x_{t+1}。那么，给一个 x_0 可产生

$$x_0, x_1, \cdots x_{M_0}, \cdots x_{M_0+M}$$

如果随机过程满足一定条件，则当 M_0 足够大时，即达到平衡态时，$x_{M_0+1}, \cdots x_{M_0+M}$ 按 **W(x)** 分布

两个条件：

- 各态历经

  从概率上说，在有限时间内 x_t 可走遍 **[a, b]**

- 细致平衡

$$\frac{T\left(x \to x'\right)}{T\left(x' \to x\right)} = \frac{W\left(x'\right)}{W\left(x\right)}$$

$T\left(x \to x'\right)$ 为过程从 x 跃迁到 x' 的概率

Metropolis算法

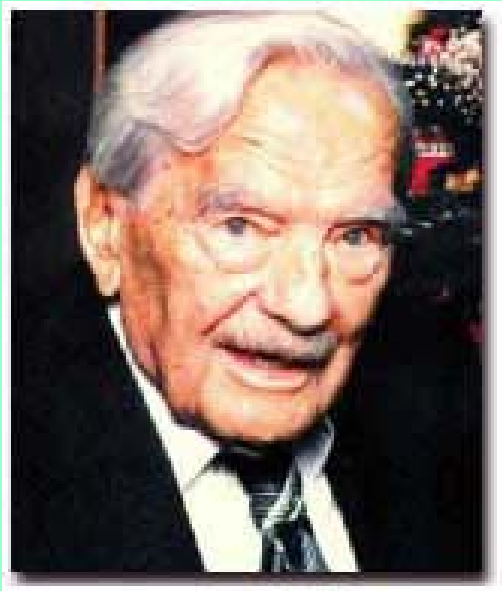
Metropolis (1915-1999)
the Paper was cited 7500 times from 1988 to 2003

$$T_m\left(x \to x'\right)$$

$$= \begin{cases} W(x')/W(x) & W\left(x'\right) < W\left(x\right) \\ 1 & W\left(x'\right) \geq W\left(x\right) \end{cases}$$

$$= Min\ (1,\ W(x')/W(x))$$

$$T\left(x \to x'\right) = S(x \to x')\ T_m\left(x \to x'\right)$$



其中 $S(x \to x')$ 是从 x 选取 x' 的概率

例如，

1、 $S(x \to x') = 常数$

2、 $$S\left(x \to x'\right) = \begin{cases} 常数 & x' \in [x-\varepsilon, x+\varepsilon] \\ 0 & x' \notin [x-\varepsilon, x+\varepsilon] \end{cases}$$

Metropolis算法非常普遍

对正则分布 $W(x) \propto e^{-H(x)/kT}$

$$T_m\left(x \to x'\right) = \begin{cases} e^{-\left(H\left(x'\right)-H\left(x\right)\right)/kT} & H\left(x'\right) > H\left(x\right) \\ 1 & H\left(x'\right) \le H\left(x\right) \end{cases}$$

$$= Min\ (1,\ e^{-\left(H\left(x'\right)-H\left(x\right)\right)/kT})$$

Monte Carlo模拟不但可以计算平衡态的统计平均，事实上还给出变量随时间演化的动力学。在一定条件下，这一动力学可以描述或近似描述实际的物理动力学过程。但是，

- 不是所有的Monte Carlo算法的动力学都有物理意义。例如， cluster 算法没有物理意义。
- 初始状态必须设定为有物理意义的宏观状态。例如， 给定温度和磁化强度等
- Monte Carlo动力学的适用范围需要仔细研究