

随机过程

Brownian motion

宏观扩散 / Fokker-Planck eq.

微观朗之万方程  $dx = v dt$

$$dv = -\alpha v + f + \sigma dw$$

数学基础 Ito lemma

中心极限定理. 大数定律.

$$\langle x^2 \rangle = 2Dt$$

↓  
误差  $\propto \sqrt{t}$

$$df(x,t) = \frac{\partial f}{\partial t} dt + \frac{\partial f}{\partial x} dx + \frac{1}{2} \frac{\partial^2 f}{\partial x^2} dx^2$$

↳ break chain rule

Ito: 1915 - 2008

1935 - 1938 本科

39 - 43 统计局

43 - 54 副教授

45 博士

42 - 43 Ito lemma

Runge

MC solution 随机数做计算

量子扩散 (量子 Monte Carlo)

蒙特计算: 1)  $dx = f dt + \sigma dw$

2)  $dx = v dt$

3)  $dv = (-\alpha v + f) dt + \sigma dw$

4)  $\int f(x_1, \dots, x_n) dx_1 \dots dx_n, \quad 3 \leq n \leq 10$

5)  $Z = \text{Tr}(e^{-\beta H}) = \int dx_1 \dots dx_n e^{-\beta H(x_1, \dots, x_n)}$

简单的问题.

Iring Model 用 MC 模拟.

### Fokker-Planck

宏观 - 微观.

$PV = NRT$

$\rho(x, p, t) \Rightarrow dp = 0 \Rightarrow$  动态平衡.

$\frac{\partial \rho}{\partial t} + \nabla \cdot \vec{J} = 0 \Rightarrow \vec{J} = (\vec{v} \rho, \vec{a} \rho)$

只有一阶导数.

$\frac{\partial \phi}{\partial t} = D \frac{\partial^2 \phi}{\partial x^2} =$  二阶导数 (Ito lemma).

Coupled Langevin eq.

$\frac{dx}{dt} = F(x, y) + \xi_1$

$\frac{dy}{dt} = G(x, y) + \xi_2$

drift term      diffusion term

$\frac{\partial}{\partial t} P(x, y, t) =$  线性 + 扩散项.

$\left( -\frac{\partial}{\partial x} (FP) - \frac{\partial}{\partial y} (GP) \right) + \left( D_1 \frac{\partial^2 P}{\partial x^2} + D_2 \frac{\partial^2 P}{\partial y^2} \right)$

两个 Langevin eq.

1)  $F=0, G=0$  此 Langevin eq = 0.

2)  $D_1=0, D_2=0$  Liouville eq = 0.

$$\frac{d}{dt} P(x, y, t) = 0 \Rightarrow \frac{\partial P}{\partial t} + \frac{\partial}{\partial x} (FP) + \frac{\partial}{\partial y} (GP) = 0.$$

量子 Langevin eq.

Caldeira - Leggett model (CL model)

一个振子与环耦合 (4.14)  
 1 可解.

ref: 1) Caldeira - Leggett model. wiki

2) Caldeira Leggett PRL 1981.

3) Benguria, Kac, PRL, 1981. "Quantum Langevin eq"

(4) Ford, Kac, 1987, "On the Quantum Langevin eq"

振子: Feynman - Kac Integral.

$$m\ddot{x} = -\alpha \dot{x} + f + \xi$$

$\alpha$ : 阻力  
 $\xi$ : 随机力.

① 有阻尼次微分方程.

② 量子化.  $H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 = \hbar\omega (a + a^\dagger + \frac{1}{2})$

$a$  表示  $x$  与  $p$  函数.

$$x \propto (a + a^\dagger)$$

$x \sim a + a^\dagger$ ,  $f, \xi$  怎么表示?

$$a+a+\frac{1}{2} = \frac{p^2}{2m\hbar\omega} + \frac{m\omega}{2\hbar} x^2$$

$$c^2 - d^2 = (c+d)(c-d)$$

$$c^2 + d^2 = (c+id)(c-id)$$

$$+icd - idc$$

$$= (c+id)(c-id) + i[c,d]$$

$$= a+a+\frac{1}{2}$$

$$c = \sqrt{\frac{m\omega}{2\hbar}} x$$

$$d = \frac{i p}{\sqrt{2m\hbar\omega}}$$

$$\left. \begin{aligned} a &= \sqrt{\frac{m\omega}{2\hbar}} x - \frac{i p}{\sqrt{2m\hbar\omega}} \\ a^+ &= \sqrt{\frac{m\omega}{2\hbar}} x + \frac{i p}{\sqrt{2m\hbar\omega}} \end{aligned} \right\}$$

$$x = \sqrt{\frac{\hbar}{2m\omega}} (a+a^+)$$

$$m\ddot{x} = -\alpha x - m\omega^2 x + \mathcal{F} \quad U = \frac{1}{2} kx^2 \quad f = -\nabla U = kx$$

$$x = \sqrt{\frac{\hbar}{2m\omega}} (a+a^+)$$

$$\mathcal{F} = \eta (b+b^+) \quad \leftarrow \text{Bath 自由度}$$

b 的这动力学方程在哪里?

正确的结果:

环境中无穷多小振子:  $\frac{1}{m} + \frac{1}{m} = 1/\mu$

↳ Environment. / Bath.

$$H = \frac{1}{2m} \dot{x}^2 + V(x) + \sum_{j=1}^n \left[ \frac{p_j^2}{2m_j} + \frac{1}{2} k_j (q_j - x)^2 \right]$$

1 可解的

1 可数值计算

作业：模拟以上述方程：  $N=100$ ...  $m_i, k_i$ ; 随机取

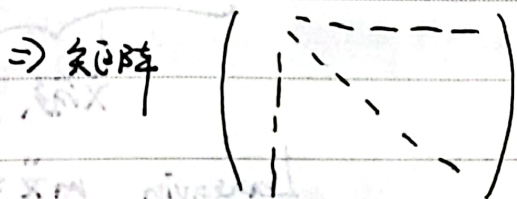
$$\dot{p}_i = -\frac{\partial H}{\partial q_i} \Rightarrow \dot{p}_i = -\frac{\partial H}{\partial q_i} = -k_i (q_i - x)$$

$$\dot{q}_i = \frac{\partial H}{\partial p_i}$$

$$\dot{q}_i = \frac{\partial H}{\partial p_i} = \frac{p_i}{m_i}$$

$$\dot{x} = \frac{\partial H}{\partial p} = \frac{p}{m}$$

$$\dot{p} = -\frac{\partial H}{\partial x} = -V'(x) - \sum_j k_j (x - q_j)$$



$$\dot{p}_i = -k_i (q_i - x)$$

$$\dot{q}_i = \frac{p_i}{m_i}$$

$$m_i \ddot{q}_i = -k_i (q_i - x)$$

$m_i \ddot{q}_i + k_i q_i = k_i x$  Langevin eq:  $m \ddot{x} = -\alpha \dot{x} + \xi$

线性,  $= \beta \ddot{q}_i$

$q_i / \sigma$

$\uparrow$   
 $2/\sigma$

$$\Delta u = f$$

$$u = u_0 + \int g(x-x') f(x') dx'$$

~~$\Delta u_0 = 0$  齐次解~~

$$m_i \ddot{q}_i + k_i q_i = 0$$

特解:  $q_i = A \cos(\omega_i t) + B \sin(\omega_i t)$

$$q_i \propto e^{i\omega_i t}$$

$$m_i \omega_i^2 = k_i$$

$$q_i(0) = A$$

$$m_i \dot{q}_i(0) = p_i 0$$

$$q_j(t) = q_j(0) \cos(\omega_j t) + p_j(0) \sin(\omega_j t) / m_j \omega_j$$

无耗散, 非耗散力

$$+ X(t) - X(0) \cos(\omega_j t) - \int_0^t \cos(\omega_j(t-t')) \dot{X}(t') dt'$$

X(0)

X(0)

Langevin  $m\ddot{x} = -\alpha\dot{x} + \xi$

$$\dot{X} = \frac{p}{m}$$

$$\dot{p} = -V'(x) - \sum_j k_j [-q_j^0 + X(0) \cos(\omega_j t) + \int_0^t \cos(\omega_j(t-t')) \dot{X}(t') dt']$$

$$\dot{p} = -V'(x) + \sum_j k_j q_j^0 - \left[ \sum_j k_j \cos(\omega_j t) \right] X(0)$$

$$- \int_0^t \sum_j k_j \cos(\omega_j(t-t')) \dot{X}(t') dt'$$

$$\dot{p} = -V'(x) + \xi - B(t) X(0)$$

$$- \int_0^t B(t-t') \dot{X}(t') dt'$$

$$\dot{X} = \frac{p}{m}$$

$\delta(t-t') \Rightarrow \alpha \dot{x}$

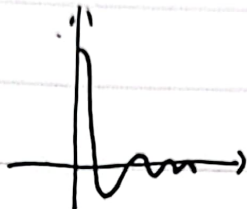
$$B(x) = \sum_j |p_j| \cos(\omega_j t)$$

$$= \sum_j m_j \omega_j^2 \cos(\omega_j t)$$

$$m\ddot{x} + \int_0^x B(x-t') \dot{x}(t') dt' + V'(x) + B(x)x(0) = F$$

$$F = \sum_i k_i q_i^{(0)} \text{ 驱动项.}$$

如果 ~~驱动~~



$$m\ddot{x} + \alpha\dot{x} + V'(x) = F$$

(阻尼  $\frac{\alpha}{2}$  项)

$$F = \sum_j k_j q_j^0$$

$$= \sum_j k_j \left[ q_j(0) \cos(\omega_j t) + \frac{p_j(0)}{m_j \omega_j} \sin(\omega_j t) \right]$$

$$\frac{1}{2} \langle [q_j, p_j] \rangle = i\hbar \delta_{jj}$$

$$\begin{cases} q_j = \sqrt{\frac{\hbar}{2m_j \omega_j}} (b_j + b_j^\dagger) \\ p_j = i \sqrt{\frac{\hbar m_j \omega_j}{2}} (b_j - b_j^\dagger) \end{cases}$$

$$F = \sum_j \hbar \omega_j (b_j e^{-i\omega_j t} + b_j^\dagger e^{i\omega_j t})$$

$$\langle F^2(t) \rangle \sim \eta^2 \langle (b + b^\dagger)^2 \rangle$$

$$\propto \eta^2 \langle b b^\dagger + b^\dagger b + b^2 + b^{\dagger 2} \rangle$$

$$\langle F(t) F(t') \rangle = D \delta(t-t')$$

$$\propto \sqrt{D}$$

$$\langle \int_0^t F(t') dt' \int_0^t F(t'') dt'' \rangle = \frac{D}{2} t^2$$

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Graph of  $\sqrt{t}$

$$\langle \int_0^t F(t') dt' \int_0^t F(t'') dt'' \rangle = \frac{D}{2} t^2$$

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