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随机过程.

$\bar{x} = \frac{1}{n}\sum x_i$.

~~Rew~~ Review. 中心极限定理. $\lim\limits_{n\to\infty} P\{|\bar{x} - \mu| < \epsilon\} = 1$.

大数定理. $\bar{x} \sim N(\mu, \frac{\sigma^2}{n})$

大偏差.

Brown motion.

① 历史

② 1905 Einstein 工作.

③ 朗之万方程.

意义: 微观变化 <—> 宏观.

牛顿运动 $\frac{\partial \phi}{\partial t} = D\frac{\partial^2 \phi}{\partial x^2}$

定律. 扩散方程.

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

阻力. 势场力. 随机力.

$\langle \xi(t) \rangle = 0$, $\langle \xi(t)\xi(t') \rangle = D\delta(t-t')$. 白噪声.

<1> $f=0$ 的情况.

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

$\dot{x} = v$.

$m\dot{v} = -\alpha v + \xi$.

1) green ~~δ~~-function. $\mathcal{L}u = f$. $\mathcal{L}g(x-x') = \delta(x-x')$

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

$\mathcal{L} = (m\frac{d}{dt} + \alpha)$ $\mathcal{L}u_0 = 0$

$m\dot{v} = -\alpha v + \xi$

$v \sim e^{-(\alpha/m)t}$.

$v = e^{-(\alpha/m)t} u$.

$v(0) = u(0)$.

$\Rightarrow m e^{-\frac{\alpha}{m}t}\dot{u} - m\frac{\alpha}{m} e^{-\frac{\alpha}{m}t} u = -\alpha e^{-\frac{\alpha}{m}t} u + \xi$.

$\dot{u} = \frac{1}{m} e^{\frac{\alpha}{m}t}\xi$.

$u = u_0 + \int_0^t \frac{1}{m} e^{\frac{\alpha}{m}t'} \xi(t') dt'$

完整解：$v = v_0 e^{-\frac{\alpha}{m}t} + \frac{1}{m}\int_0^t e^{-\frac{\alpha}{m}(t-t')} \xi(t') dt'$.

1）有解，但解是随机的（非确定的）.

2）观测量只在平均上有意义

平均值 [P(ξ(t))]

① $\bar{v}(t) = \langle v_0 e^{-\frac{\alpha}{m}t} \rangle + \int_0^t \frac{1}{m} e^{-\frac{\alpha}{m}(t-t')} \overset{0}{\overset{\shortparallel}{\langle \xi(t') \rangle}} dt'$.

$= v_0 e^{-\frac{\alpha}{m}t}$.

② $\overline{v^2}$ $\left(v = A + B \qquad \overline{v^2} = \overline{A^2} + \overline{B^2} + 2\overline{AB} \right)$

$= v_0^2 e^{-\frac{2\alpha}{m}t} + \left\langle \left(\int_0^t e^{-\frac{\alpha}{m}(t-t')} \xi(t') dt' \right)^2 \right\rangle \frac{1}{m^2}$

$= v_0^2 e^{-\frac{2\alpha}{m}t} + \int_0^t dt_1' dt_2' e^{-\frac{\alpha}{m}(t-t_1') - \frac{\alpha}{m}(t-t_2')} \frac{1}{m^2} \underset{D\delta(t_1'-t_2')}{\underset{\shortparallel}{\langle \xi(t_1') \xi(t_2') \rangle}}$

$= v_0^2 e^{-\frac{2\alpha}{m}t} + \frac{D}{m^2} \int_0^t dt_1 e^{-\frac{2\alpha}{m}(t-t_1)}$

$\int_0^t e^{-\alpha t'} dt' = -\frac{1}{\alpha} e^{-\alpha t'} \Big|_0^t = \frac{1}{\alpha}(1 - e^{-\alpha t})$

若 $\alpha = 0$ $\quad \bar{v}(t) = v_0 \quad \overline{v^2} = v_0^2 + (t - t_0)\frac{D}{m^2} = v_0^2 + \frac{D}{m^2} t$.

平均速度不变，方差正比于 t

定义上的区别：

~~$\bar{X} = \frac{1}{n}(x_1 + \cdots + x_n) \sim N(\mu, \frac{\sigma^2}{n})$~~

~~$X = x_1 + \cdots + x_n \sim N(n\mu, \frac{n^2\sigma^2}{n})$~~

$\bar{X} = \frac{1}{n}(\xi_1 + \cdots + \xi_n) \sim N(\mu, \frac{\sigma^2}{n})$

$X = \xi_1 + \cdots + \xi_n \sim N(n\mu, \frac{n^2\sigma^2}{n}) = N(n\mu, n\sigma^2)$

σ_X^2 即X的方差 $= n\sigma^2 \propto n$.

$Y = (\xi_1 + \cdots + \xi_n)\,dt = \int_0^t d\xi(t')\,dt' \sim N(n\mu\,dt, n\sigma^2 dt)$

$\Downarrow$

$n\,dt = t$.

~~$\Rightarrow \overline{(\int_0^t \xi(t')dt')^2}$~~

$\Rightarrow \overline{(\int_0^t \xi(t')dt')^2} \propto t.$

回答：实验上测量的物理量 C_v, χ 到底是什么？
平均值？方差？

$$C_v = \left(\frac{\partial \bar{E}}{\partial T}\right)_v = -\frac{\partial \beta}{\partial T}\left(\frac{\partial \bar{E}}{\partial \beta}\right)_v$$
$$= -\frac{1}{T^2}\left(\frac{\partial \bar{E}}{\partial \beta}\right)_v$$

$$\bar{E} = \frac{Tr(e^{-\beta H} H)}{Tr(e^{-\beta H})}$$

$$\left(\frac{\partial \bar{E}}{\partial \beta}\right)_v = -\frac{Tr(H^2 e^{-\beta H})}{Tr(e^{-\beta H})} + \frac{[Tr(H e^{-\beta H})]^2}{[Tr(e^{-\beta H})]^2}$$

$$\Rightarrow \left(\frac{\partial \bar{E}}{\partial \beta}\right)_v = -(\langle E^2\rangle - \langle E\rangle^2)$$

$$C_v = \frac{1}{T^2}(\langle E^2\rangle - \langle E\rangle^2) \propto V$$ 系统体积

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离散化

令: $m=1 \quad \alpha=0$.

$\dot{v}=\xi \Rightarrow v=v_0+\int_0^t \xi(t')dt'$

对比: $\bar{v}=v_0 \qquad \xi(t)=0$

$\overline{v^2}=v_0^2+Dt. \qquad \langle \xi(t)\xi(t')\rangle = D\delta(t-t')$

$v_{n+1}=v_n+\xi_n\Delta t. \qquad \langle \xi_n \xi_m\rangle = D\,\delta_{nm}$

$v_n=v_{n-1}+\xi_{n-1}\Delta t. \qquad \langle \xi_n\rangle=0.$

$\vdots$

$v_1=v_0+\xi_0\Delta t.$

$v_n=\left(\sum_{i=0}^{n-1}\xi_i\right)\Delta t+v_0.$

$\Rightarrow \bar{v}_n=v_0$

$\overline{v_n^2}=v_0^2+\sum_{i=0}^{n-1}\sum_{j=0}^{n-1}\langle \xi_i\xi_j\rangle(\Delta t)^2.$

$=v_0^2+(\Delta t)^2 n\langle\xi^2\rangle$

$=v_0^2+Dt \quad (n\Delta t=t)$

另一种写法:

$v_n=v_{n-1}+\sqrt{\frac{D}{dt}}\,dt\,\xi_{n-1} \qquad \langle\xi^2\rangle=\frac{D}{dt}$

$\xi_n\sim N(0,1)$ 的随机数.

讨论 $m\ddot{x}=-\alpha\dot{x}+f(x)+\xi(t)$

$\Rightarrow$ ~~$\dot{x}=v$~~

$\Rightarrow$ ~~$m\dot{v}=-\alpha v+f(x)$~~

$$\Rightarrow \begin{cases}\dot{x}=v\\ \dot{v}=-\frac{\alpha}{m}v+f(x)+\xi(t)\end{cases}$$

$$\Rightarrow \begin{cases}x_{n+1}=x_n+v_n dt.\\ v_{n+1}=v_n-\frac{\alpha}{m}v_n dt+f(x_n)dt+\sqrt{\frac{D}{dt}}\,dt\,\xi_n.\end{cases}$$

$\xi_n\sim N(0,1)$

扩散方程的演化过程.

$$\frac{\partial}{\partial t}\phi = D\frac{\partial^2\phi}{\partial x^2}$$

解: $\phi = A(t)\, e^{-ax^2/t} = \sqrt{\frac{\pi t}{a}}\, e^{-ax^2/t}$ $\quad a = \frac{1}{4D}$

$\int \phi(x)\, dx = 1.$ $\quad = \frac{1}{\sqrt{4D\pi t}}\, e^{-\left(\frac{x^2}{4Dt}\right)}$

$\int \phi(x)\, x^2\, dx = 2Dt = \langle x^2 \rangle$

推导: Fick's law + 流守恒.

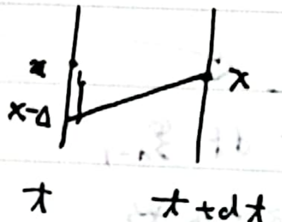
$\downarrow \qquad \downarrow$

$j = -D\frac{\partial \rho}{\partial x} \qquad \frac{\partial \rho}{\partial t} + \frac{\partial j}{\partial x} = 0$

Einstein 1905.

$\phi(x, t)$

$\phi(x, t+dt)$



t+dt时刻 x位置的粒子来自于 t时刻 x-Δ和x+Δ 位置.

则 $\phi(x, t+dt) = \int p(\Delta)\, \phi(x+\Delta, t)\, d\Delta$

$= \int p(\Delta)\left[\phi(x,t) + \frac{\partial \phi}{\partial x}\Delta + \frac{1}{2}\frac{\partial^2\phi}{\partial x^2}\Delta^2\right] d\Delta$

$= \phi(x,t) + \frac{1}{2}\frac{\partial^2\phi}{\partial x^2}\underbrace{\int p(\Delta)\,\Delta^2\, d\Delta}_{\text{方差}}$ 记为 $2Ddt$.

$= \phi(x,t) + \frac{1}{2}\frac{\partial^2\phi}{\partial x^2}\, 2Ddt.$

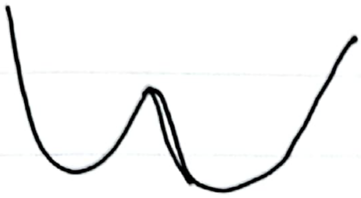
$\Rightarrow \frac{\phi(x, t+dt) - \phi(x,t)}{dt} = D\frac{\partial^2\phi}{\partial x^2}$

$\Rightarrow \frac{\partial \phi}{\partial t} = D\frac{\partial^2\phi}{\partial x^2}$ $\Leftarrow$ 扩散方程.

Fokker-Plank eq.

作业：$U = ax^2 + bx^4$.

$a<0$, $m=1$.



$\ddot{x} = -\alpha x - \nabla U + \xi(t)$

讨论 double-well 中的动力学过程.

a, b 自己设置. ξ：自己调节.