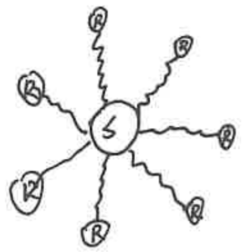
随机微分方程

I. 布朗运动 : $M\ddot{q} + 2m\gamma\dot{q} + \frac{\partial V}{\partial q} = \xi(t)$

II. 开放系统 $H_{tot} = H_S + H_R + H_I$



$$H_S = \frac{p^2}{2m} + V(q) \qquad H_R = \sum_{\alpha=1}^{N}\left(\frac{p_\alpha^2}{2m_\alpha} + \frac{1}{2}m_\alpha\omega_\alpha^2 x_\alpha^2\right)$$

$$H_I = -\sum_{\alpha=1}^{N} c_\alpha q\cdot x_\alpha + \Delta V(q) \longrightarrow \Delta V(q) = \sum_{\alpha=1}^{N}\frac{c_\alpha^2 q^2}{2m_\alpha\omega_\alpha^2}$$

$$H = \frac{p^2}{2m} + V(q) + \frac{1}{2}\sum_{\alpha=1}^{N}\left[\frac{p_\alpha^2}{m_\alpha} + m\omega_\alpha^2\left(x_\alpha - \frac{c_\alpha q}{m_\alpha\omega_\alpha^2}\right)^2\right]$$

$$\begin{cases} M\ddot{q} + \frac{\partial V(q)}{\partial q} + \sum_\alpha \frac{c_\alpha^2}{m_\alpha\omega_\alpha^2}q(t) = \sum_\alpha c_\alpha x_\alpha \\ m_\alpha\ddot{x}_\alpha + m_\alpha\omega_\alpha^2 x_\alpha = c_\alpha q(t) \end{cases}$$

$$x_\alpha(t) = x_\alpha^{(0)}\cos\omega_\alpha t + \frac{p_\alpha^{(0)}}{m_\alpha\omega_\alpha}\sin\omega_\alpha t + \frac{c_\alpha}{m_\alpha\omega_\alpha}\int_0^t dt'\sin\omega_\alpha(t-t')\,q(t')$$

$$= x_\alpha^{(0)}\cos\omega_\alpha t + \frac{p_\alpha^{(0)}}{m_\alpha\omega_\alpha}\sin\omega_\alpha t + \frac{c_\alpha}{m_\alpha\omega_\alpha^2}\left[q(t) - \cos\omega_\alpha t\cdot q(0)\right] - \frac{c_\alpha}{m_\alpha\omega_\alpha^2}\int_0^t dt'\cos\omega_\alpha(t-t')\,\dot{q}(t')$$

$$M\ddot{q}(t) + M\int_0^t dt'\,\gamma(t-t')\,\dot{q}(t') + V'(q) = -M\gamma(t)\,q(0) + \xi(t)$$

memory-friction kernel:

$$\gamma(t-t') = \Theta(t-t')\frac{1}{M}\sum_\alpha\frac{c_\alpha^2}{m_\alpha\omega_\alpha^2}\cos\omega_\alpha(t-t')$$

and the force:

$$\xi(t) = \sum_\alpha c_\alpha\left(x_\alpha^{(0)}\cos\omega_\alpha t + \frac{p_\alpha^{(0)}}{m_\alpha\omega_\alpha}\sin\omega_\alpha t\right).$$

Assuming initially, the bath oscillators are in thermodynamic equilibrium.

thus: $\rho_R = \frac{1}{Z} e^{-\beta \sum_\alpha \left[\frac{P_\alpha^{(0)2}}{2m_\alpha} + \frac{m_\alpha \omega_\alpha^2}{2} (x_\alpha^{(0)})^2 \right]}$

$\langle \xi(t) \rangle_{\rho_R} = 0 \qquad \langle \xi(t)\xi(t') \rangle_{\rho_R} = M k_B T \, \gamma(t-t')$

$$\gamma(t) = \Theta(t) \frac{1}{M} \frac{2}{\pi} \int_0^\infty d\omega \frac{J(\omega)}{\omega} \cos\omega t$$

$$J(\omega) = \cancel{M\omega \int_0^\infty dt} \; \frac{\pi}{2} \sum_\alpha \frac{C_\alpha^2}{m_\alpha \omega_\alpha} \delta(\omega - \omega_\alpha)$$

$$J(\omega) = M\gamma\omega \rightarrow \text{Ohmic dissipation.}$$

$$M\ddot{q}(t) + \gamma M \dot{q}(t) + \frac{\partial V(q)}{\partial q} = \xi(t)$$

(经典朗之万方程

量子 ? → legget).

III. 朗之万方程. $(M \to 0)$. 例子: $[u = \dot{q}(t)$ 速度$]$

$M \to 0 \qquad \frac{du}{dt} = -\gamma u + \sqrt{f}\,\xi(t) \qquad \langle \xi(t) \rangle = 0; \quad \langle \xi(t)\xi(t') \rangle = \delta(t-t')$

$$u(t) = u(0) e^{-\gamma t} + \sqrt{f} \int_0^t dt' e^{-\gamma(t-t')} \xi(t)$$

(a) Mean velocity $\langle u(t) \rangle = u(0) e^{-\gamma t}$.

(b) Mean Square Velocity.

$$\langle [u(t) - u(0) e^{-\gamma t}]^2 \rangle = f \int_0^t dt \int_0^t dt'' e^{-\gamma(t-t')} e^{-\gamma(t-t'')} \underbrace{\langle \xi(t')\xi(t'') \rangle}_{\delta(t'-t'')}$$

$$= f \int_0^t dt' e^{-\gamma(t-t')} = \frac{f}{2\gamma} \{1 - e^{-2\gamma t}\}$$

$$\langle u(t)^2 \rangle = u^2(0)\, e^{-2\gamma t} + \frac{f}{2\gamma}\left(1 - e^{-2\gamma t}\right)$$

small t $\quad \langle u(t)^2 \rangle = u^2(0)$ $\qquad t \to \infty \quad \langle u(t)^2 \rangle = \frac{f}{2\gamma}$

(c) Fluctuation- Dissipation theorem:

$$t \to \infty \qquad \lim_{t\to\infty}\left(\tfrac{1}{2} M u^2(t)\right) = \frac{fM}{4\gamma} = \frac{1}{2} k_B T$$

(d). Diffusion as a result of Brownian Motion

$$x(t) = \int_0^t ds\, u(s)$$

$$\langle x(t) \rangle = u(0)\, \frac{1 - e^{-\gamma t}}{\gamma} \rightarrow \frac{u(0)}{\gamma} \ (t \to \infty)$$

$$\langle x^2(t) \rangle = u(0)^2 \left(\frac{1 - e^{-\gamma t}}{\gamma}\right)^2 + \frac{ft}{\gamma^2} - \frac{2f}{\gamma^3}\left(1 - e^{-\gamma t}\right) + \frac{f}{2\gamma^3}\left(1 - e^{-2\gamma t}\right)$$

$$D = \lim_{t\to\infty} \frac{\langle x(t)^2 \rangle}{2t} = \frac{f}{2\gamma^2}$$

$$\langle x(t)^2 \rangle \xrightarrow[t\to\infty]{} 2Dt + \left(\frac{u(0)}{\gamma}\right)^2 - \frac{3f}{2\gamma^3} + \cdots$$

扩散方程: $\quad \frac{\partial p(x,t)}{\partial t} = D\, \frac{\partial^2 p(x,t)}{\partial x^2}$

IV 随机微分方程：(数值解法)

$$\dot{x}(t) = a(x(t), t) + b(x(t), t)) \xi(t)$$

$$\Delta t = \frac{t - t_0}{N} \qquad t_i = t_0 + i \Delta t$$

$$\Delta W_i = \int_{t_i}^{t_i + \Delta t} \xi(t) \, dt'$$

$$\langle \Delta W_i \rangle = 0 \qquad \langle (\Delta W_i)^2 \rangle = \Delta t$$

$$\int_{t_i}^{t_i+\Delta t} dt \int_{t_j}^{t_j+\Delta t} dt' \langle \xi(t_i) \xi(t_j') \rangle dt dt'$$

$$= \int_{t_i}^{t_i+\Delta t} dt = \Delta t.$$

Ito: $x_{i+1} = x_i + a_i \Delta t + b_i \Delta W_i$

Stratonovich: $x_{i+1} = x_i + a_i \Delta t + \frac{b_i + b_{i+1}}{2} \Delta W_i$

Heun algorithm: $\dot{x} = a(x(t), t) + b(x(t), t) \xi(t) \qquad \langle \xi(t) \xi(t') \rangle = f \delta(t - t')$

$$\tilde{x}_{n+1} = x_n + a(x_n, t_n) \Delta t + b(x_n, t_n) \sqrt{f} \sqrt{\Delta t} \, \xi_n$$

ξ_n is a random number satisfying the Gaussian distribution with $N(0,1)$

$$\langle \xi_n \rangle = 0 \qquad \langle \xi_n^2 \rangle = 1$$

$$x_{n+1} = x_n + \frac{\Delta t}{2} [a(x_n, t_n) + a(\tilde{x}_{n+1}, t_{n+1})]$$

$$+ \frac{\sqrt{\Delta t f}}{2} [b(x_n, t_n) + b(\tilde{x}_{n+1}, t_{n+1})] \xi_n.$$