Brownian motion

We have analyzed many physical systems through the equation of motion of classical dynamical variables; collective variables.

These systems can be quantized by the canonical method, but what about dissipation?

There are terms which represent fluctuations and energy loss that cannot be treated within the canonical quantization procedure. What is the way out?

Review of classical Brownian motion; a paradigm for dissipative systems!

Classical Brownian motion

Particle in a viscous fluid; Langevin equation

$$M\ddot{q} + \eta\dot{q} + V'(q) = f(t)$$

$$\langle f(t)\rangle = 0$$

$$\langle f(t)f(t')\rangle = 2\eta k_B T\delta(t - t')$$

SQUID ring

$$C\ddot{\phi} + \frac{\dot{\phi}}{R} + U'(\phi) = I_f(t)$$

$$\langle I_f(t)\rangle = 0$$

$$\langle I_f(t)I_f(t')\rangle = 2k_B T R^{-1}\delta(t - t')$$

Stochastic processes

Stochastic variable $-\infty < y(t) < \infty$

Infinitesimal probability to find *y* within [*y*, *y*+*dy*]

$$d\mathbf{P}(y) = P(y,t)dy$$

Joint probability density $P_n(y_n, t_n; y_{n-1}, t_{n-1}; ...; y_1, t_1)$

Normalized as

$$\int_{R^n} P_n(y_n, t_n; y_{n-1}, t_{n-1}; ...; y_1, t_1)\, dy_1\, dy_2 ...\, dy_n = 1$$

And integrated over one of its varibles

$$\int P_n(y_n, t_n; y_{n-1}, t_{n-1}; ...; y_1, t_1)\, dy_n = P_{n-1}(y_{n-1}, t_{n-1}; ...; y_1, t_1)$$

N^{th} moment of y at $t_1, t_2, \ldots, t_n$;

$$\mu_n(t_1, t_2, \ldots, t_n) \equiv \langle y(t_1)\ldots y(t_n)\rangle = \int_{R^n} dy_1\, dy_2 \ldots dy_n\, y_1\, y_2 \ldots y_n \times P_n(y_n, t_n; y_{n-1}, t_{n-1}; \ldots; y_1, t_1)$$

First moment of y at $t_1=t$; average or mean $\mu_1(t) = \langle y(t)\rangle$

Second moment of y at $t_1=t_2=t$; $\mu_2(t) = \langle y^2(t)\rangle$

Variance or dispersion; $\sigma^2(t) = \langle (y(t) - \langle y(t)\rangle)^2\rangle = \mu_2 - \mu_1^2$

Stationary process;

$$P_n(y_n, t_n; y_{n-1}, t_{n-1}; \ldots; y_1, t_1) = P_n(y_n, t_n + \tau; y_{n-1}, t_{n-1} + \tau; \ldots; y_1, t_1 + \tau)$$

$$\Downarrow$$

$$P_1(y_1, t_1) = P_1(y_1) \qquad P_2(y_2, t_2; y_1, t_1) = P_2(y_2, t_2 - t_1; y_1, 0)$$

Conditional probability density;

$$P_{11}(y_2, t_2 | y_1, t_1) = \frac{P_2(y_2, t_2; y_1, t_1)}{P_1(y_1, t_1)}$$

⬇

$$P_1(y_2, t_2) = \int dy_1 P_{11}(y_2, t_2 | y_1, t_1) P_1(y_1, t_1)$$

⬇

$$\int dy_2 P_{11}(y_2, t_2 | y_1, t_1) = 1$$

Generalized conditional probability density;

$$P_{lk}(y_{k+l}, t_{k+l}; ...; y_{k+1}, t_{k+1} | y_k, t_k; ...; y_1, t_1) \equiv \frac{P_{k+l}(y_{k+l}, t_{k+l}; ...; y_1, t_1)}{P_k(y_k, t_k; ...; y_1, t_1)}$$

Independent process;

$$P_n(y_n, t_n; y_{n-1}, t_{n-1}; ...; y_1, t_1) = \prod_{i=1}^{n} P_1(y_i, t_i)$$

Markovian process;

$$P_{1,n-1}(y_n, t_n | y_{n-1}, t_{n-1}; ...; y_1, t_1) = P_{11}(y_n, t_n | y_{n-1}, t_{n-1})$$

$$P_3(y_3, t_3; y_2, t_2; y_1, t_1) = P_{12}(y_3, t_3 | y_2, t_2; y_1, t_1) P_2(y_2, t_2; y_1, t_1) =$$

$$= P_{11}(y_3, t_3 | y_2, t_2) P_{11}(y_2, t_2 | y_1, t_1) P_1(y_1, t_1)$$

Integrating over y_2

$$P_2(y_3, t_3; y_1, t_1) = \int dy_2 P_3(y_3, t_3; y_2, t_2; y_1, t_1) =$$

$$= P_1(y_1, t_1) \int dy_2 P_{11}(y_3, t_3 | y_2, t_2) P_{11}(y_2, t_2 | y_1, t_1)$$

Chapman-Kolmogorov equation (CK);

$$P_{11}(y_3, t_3|y_1, t_1) = \int dy_2 P_{11}(y_3, t_3|y_2, t_2) P_{11}(y_2, t_2|y_1, t_1)$$

Example 1; Wiener-Lévy (WL) process

$$P_{11}(y_2, t_2|y_1, t_1) = \frac{1}{\sqrt{2\pi(t_2 - t_1)}} \exp - \frac{(y_2 - y_1)^2}{2(t_2 - t_1)}$$

Which obeys CK. If we choose $P_1(y_1, 0) = \delta(y_1)$

$$P_1(y, t) = \frac{1}{\sqrt{2\pi t}} \exp - \frac{y^2}{2t}$$

Einstein-Smoluchovsky (ES) theory of the Brownian motion

Example 2; Ornstein-Uhlenbeck (OU) process $\tau \equiv t_2 - t_1$

$$P_{11}(y_2, t_2 | y_1, t_1) = \frac{1}{\sqrt{2\pi(1 - \exp(-2\tau))}} \exp - \frac{(y_2 - y_1 \exp(-\tau))^2}{2(1 - \exp(-2\tau))}$$

Also obeys CK, and with $P_1(y_1, t_1) = \frac{1}{\sqrt{2\pi}} \exp - \frac{y_1^2}{2}$ maintains the form of $P(y,t)$.

Velocity distribution for Brownian particles proposed by OU.

The only process which is stationary, Gaussian, and Markovian

Master and Fokker-Planck equations

$$P(y,t+\tau) = \int dy_1 P_{11}(y,t+\tau|y_1,t)P(y_1,t)$$

Using that $$\frac{\partial P(y,t)}{\partial t} \equiv \lim_{\tau\to 0} \frac{P(y,t+\tau)-P(y,t)}{\tau}$$

$$\Downarrow$$

$$\frac{\partial P(y,t)}{\partial t} = \lim_{\tau\to 0} \frac{1}{\tau} \int dy' [P_{11}(y,t+\tau|y',t)P(y',t) - P_{11}(y,t|y',t)P(y',t)]$$

Expanding P_{11} $$P_{11}(y,t+\tau;y',t) \approx \frac{\delta(y-y') + \tau W_t(y,y')}{1+\tau\int W_t(y,y')\,dy}$$

$$\approx \delta(y-y')\left[1-\tau\int W_t(y'',y')\,dy''\right] + \tau W_t(y,y')$$

$$P_{11}(y,t|y',t) = \delta(y-y') \qquad W_t(y,y') \equiv \partial P_{11}(y,t|y',t')/\partial t|_{t=t'}$$

Master equation;

$$\frac{\partial P(y,t)}{\partial t} = \int dy' W_t(y,y')P(y',t) - \int dy' W_t(y',y)P(y,t)$$

Defining $\xi \equiv y - y'$ and

$$W_t(y,y') = W_t(y'+\xi, y') \equiv W(\xi, y') = W(\xi, y-\xi)$$

$$W_t(y',y) = W_t(y-\xi, y) \equiv W(-\xi, y)$$

We have

$$\frac{\partial P(y,t)}{\partial t} = \int d\xi W(\xi, y-\xi)P(y-\xi,t) - P(y,t)\int d\xi W(-\xi, y)$$

Which expanded about $\xi = 0$ gives

$$\frac{\partial P(y,t)}{\partial t} = \sum_{n=1}^{\infty} \frac{(-1)^n}{n!} \frac{\partial^n}{\partial y^n}[\alpha_n(y)P(y,t)]$$

Kramers-Moyal (KM) expansion

$$\frac{\partial P(y,t)}{\partial t} = \sum_{n=1}^{\infty} \frac{(-1)^n}{n!} \frac{\partial^n}{\partial y^n} [\alpha_n(y) P(y,t)]$$

$$\alpha_n(y) \equiv \int d\xi \, \xi^n \, W(\xi, y) = \lim_{\tau \to 0} \frac{1}{\tau} \int dy' (y - y')^n \, P_{11}(y, t + \tau | y', t)$$

In the multidimensional case the KM, up to 2^{nd} order, reads

$$\frac{\partial P(\mathbf{y},t)}{\partial t} = -\sum_{i=1}^{N} \frac{\partial}{\partial y_i} [\alpha_i(\mathbf{y}) P(\mathbf{y},t)] + \frac{1}{2} \sum_{i,j=1}^{N} \frac{\partial^2}{\partial y_i \partial y_j} [\alpha_{ij}(\mathbf{y}) P(\mathbf{y},t)] + \ldots$$

$$\alpha_i(\mathbf{y}) \equiv \int d\xi_i \, \xi_i \, W(\xi, \mathbf{y}) \qquad \text{and} \qquad \alpha_{ij}(\mathbf{y}) \equiv \int d\xi_i \, d\xi_j \, \xi_i \, \xi_j \, W(\xi)$$

Example 1; Free Brownian particle

$$M\frac{dv}{dt} + \eta v = f(t) \qquad \langle f(t) \rangle = 0$$

$$\langle f(t) f(t') \rangle = 2D_{pp}\, \delta(t - t') \qquad D_{pp} = \eta k_B T$$

Integrating over Δt: $$\Delta v = -\frac{\eta v}{M}\Delta t + \frac{1}{M}\int_t^{t+\Delta t} d\xi\, f(\xi)$$

Allows us to compute $$\alpha_1 \equiv \lim_{\Delta t \to 0} \frac{\langle \Delta v \rangle}{\Delta t} = -\frac{\eta v}{M}$$

$$\alpha_2 \equiv \lim_{\Delta t \to 0} \frac{\langle (\Delta v)^2 \rangle}{\Delta t} = \lim_{\Delta t \to 0} \left[\frac{1}{M^2} \int_t^{t+\Delta t} d\xi \int_t^{t+\Delta t} d\lambda\, 2D_{pp}\, \delta(\xi - \lambda) \right] =$$

$$= \frac{2D_{pp}}{M^2}$$

$$\alpha_n = 0 \text{ if } n \geq 3$$

$$\frac{\partial P(v,t)}{\partial t} = \frac{\eta}{M}\frac{\partial}{\partial v}[vP(v,t)] + \frac{D_{pp}}{M^2}\frac{\partial^2 P(v,t)}{\partial v^2}$$

Which is also obeyed by $P_{11}(v,t|v_0,t_0)$

Solution

$$P_{11}(v,t|v_0,0) = \frac{1}{\sqrt{2\pi\,\langle(\Delta\,v(t))^2\rangle}}\exp - \frac{(v - v_0\exp - (\eta\,t/M))^2}{2\,\langle(\Delta\,v(t))^2\rangle}$$

with $\langle(\Delta\,v(t))^2\rangle = \frac{k_B T}{M}\left[1 - \exp - \left(\frac{2\eta\,t}{M}\right)\right]$

OU with $\tau = \eta\,t/M$ and $y = v$. MB velocity distribution for the Brownian particle when $t \to \infty$

For long times $\eta \frac{dx}{dt} = f(t)$

Diffusion equation

$$\frac{\partial P(x,t)}{\partial t} = D_{xx} \frac{\partial^2 P(x,t)}{\partial x^2} \qquad \text{with} \qquad D_{xx} = k_B T/\eta$$

Solution for $P_{11}(v,t|v_0,t_0)$

$$P_{11}(x,t|x_0,0) = \frac{1}{\sqrt{2\pi\,\sigma^2(t)}} \exp - \frac{(x-x_0)^2}{2\,\sigma^2(t)}$$

with $\sigma^2(t) = \langle(\Delta x(t))^2\rangle = 2\,D_{xx}\,t$

Which is a WL process with $x = y$ and $D_{xx} = \frac{1}{4}$

OU x ES

$$s(t) = x(t) - x_0 = \frac{M v_0}{\eta}\left[1 - \exp - \left(\frac{\eta\, t}{M}\right)\right] -$$

$$- \int_0^t dt' \int_0^{t'} dt''\, \frac{f(t'')}{M}\, \exp - \frac{\eta(t' - t'')}{M}$$

$$\langle s(t)\rangle = \frac{M v_0}{\eta}\left[1 - \exp - \left(\frac{\eta\, t}{M}\right)\right]$$

$$\langle s^2(t)\rangle = \frac{2 k_B T}{\eta} t + \frac{M^2 v_0}{\eta^2}\left[1 - \exp - \left(\frac{\eta\, t}{M}\right)\right]^2 - \frac{M k_B T}{\eta^2} \times$$

$$\times \left[3 - 4 \exp - \left(\frac{\eta\, t}{M}\right) - \exp - \left(\frac{2\eta\, t}{M}\right)\right]$$

$t \to \infty \quad \langle s^2(t)\rangle = 2\, D_{xx}\, t$ — diffusive ES

$t \to 0 \quad \langle s^2(t)\rangle = v_0^2\, t^2$ — ballistic OU

Example 2; Brownian particle in a potential $V(q)$

$$\frac{dq}{dt} = \frac{p}{M}$$

$$\frac{dp}{dt} = -\frac{\eta p}{M} - V'(q) + f(t)$$

Integrating over Δt allows us to compute

$$\alpha_1 = \lim_{\Delta t \to 0} \frac{\langle \Delta q \rangle}{\Delta t} = \frac{p}{M}$$

$$\alpha_2 = \lim_{\Delta t \to 0} \frac{\langle \Delta p \rangle}{\Delta t} = -\frac{\eta p}{M} - V'(q)$$

$$\alpha_{11} = \lim_{\Delta t \to 0} \frac{\langle (\Delta q)^2 \rangle}{\Delta t} = 0$$

$$\alpha_{12} = \alpha_{21} = \lim_{\Delta t \to 0} \frac{\langle \Delta q \Delta p \rangle}{\Delta t} = 0$$

$$\alpha_{22} = \lim_{\Delta t \to 0} \frac{\langle (\Delta p)^2 \rangle}{\Delta t} = 2D_{pp}$$

Fokker-Planck (FP) equation

$$\frac{\partial P}{\partial t} = -\frac{\partial}{\partial q}(pP) + \frac{\partial}{\partial p}\left[\left(\frac{\eta}{M}p + V'(q)\right)P\right] + D_{pp}\,\frac{\partial^2 P}{\partial p^2}$$

How to generalize it to quantum mechanics?

Classically all we need is the equation of motion and the concept of stochastic Processes, but in quantum mechanics...

Quantum Brownian motion

i) There is no time independent Hamiltonian or Lagrangian from which we can get the Langevin equation. Time dependent functions?

ii) New schemes of quantization or system-plus-reservoir (S-R) approach. The latter is more realistic!

iii) If S-R, first principle or model Hamiltonians?

iv) If simple model, what method should be applied? Schrödinger or Heisenberg picture?

S-R approach

Full Hamiltonian $\mathcal{H} = \mathcal{H}_0(q,p) + \mathcal{H}_I(q,q_k) + \mathcal{H}_R(q_k,p_k)$

Time evolution of an observable (Heisenberg picture) $\hat{O}(t) = e^{i\,\mathcal{H}\,t/\hbar}\,\hat{O}(0)\,e^{-i\,\mathcal{H}\,t/\hbar}$

Equation of motion $$i\hbar\frac{d\hat{O}(t)}{dt} = i\hbar\frac{\partial\hat{O}(t)}{\partial t} + [\hat{O}(t),\mathcal{H}]$$

Mean value $\langle\hat{O}(t)\rangle = \langle\Psi(0)|\hat{O}(t)|\Psi(0)\rangle$

Or if $\hat{\rho}(0) \equiv \sum_{\Psi} p_{\Psi}|\Psi(0)\rangle\langle\Psi(0)|$

$$\langle\hat{O}(t)\rangle = \mathrm{tr}\left\{\hat{\rho}(0)\hat{O}(t)\right\}$$

S-R approach

Full Schrödinger equation

$$i\hbar\frac{\partial\Psi(q,q_k)}{\partial t} = \mathcal{H}\left(q, q_k, -i\hbar\frac{\partial}{\partial q}, -i\hbar\frac{\partial}{\partial q_k}\right)$$

Schrödinger picture

$$|\Psi(t)\rangle = e^{-i\mathcal{H}t/\hbar}|\Psi(0)\rangle$$

Or

$$\hat{\rho}(t) \equiv \sum_{\Psi} p_{\Psi}|\Psi(t)\rangle\langle\Psi(t)| = e^{-i\mathcal{H}t/\hbar}\hat{\rho}(0)e^{i\mathcal{H}t/\hbar}$$

Then

$$\frac{d\hat{\rho}(t)}{dt} = \frac{1}{i\hbar}\left[\mathcal{H}, \hat{\rho}(t)\right]$$

and

$$\langle\hat{O}(t)\rangle = \mathrm{tr}\left\{\hat{\rho}(0)\hat{O}(t)\right\} = \mathrm{tr}\left\{\hat{\rho}(t)\hat{O}(0)\right\}$$

Propagator method

Reduced dynamics of a sub-system

$$\langle \hat{O}(q,p) \rangle = \mathrm{tr}_{RS}\{\hat{\rho}(t)\hat{O}\} = \mathrm{tr}_S\{[\mathrm{tr}_R \hat{\rho}(t)]\hat{O}\} = \mathrm{tr}_S\{\tilde{\rho}(t)\hat{O}\}$$

where $\tilde{\rho}(t) \equiv \mathrm{tr}_R \hat{\rho}(t)$

Coordinate representation

$$\hat{\rho}(x,\mathbf{R},y,\mathbf{Q},t) = \int\int\int\int dx' dy' d\mathbf{R}' d\mathbf{Q}' \, K(x,\mathbf{R},t;x',\mathbf{R}',0)$$
$$\times K^*(y,\mathbf{Q},t;y',\mathbf{Q}',0) \times \hat{\rho}(x',\mathbf{R}',y',\mathbf{Q}',0)$$

Propagator $\quad K(x,\mathbf{R},t;x',\mathbf{R}',0) = \left\langle x,\mathbf{R} \left| e^{-i\,\mathcal{H}\,t/\hbar} \right| x',\mathbf{R}' \right\rangle$

Initial condition $\quad \hat{\rho}(x',\mathbf{R}',y',\mathbf{Q}',0) = \langle x',\mathbf{R}'|\hat{\rho}(0)|y',\mathbf{Q}'\rangle$

separability $\quad \hat{\rho}(x',\mathbf{R}',y',\mathbf{Q}',0) = \hat{\rho}_S(x',y',0)\,\hat{\rho}_R(\mathbf{R}',\mathbf{Q}',0)$

Propagator method

Reduced density operator evolution

$$\tilde{\rho}(x,y,t) = \int\int dx'dy'\, \mathcal{J}(x,y,t;x',y',0)\, \tilde{\rho}(x',y',0)$$

Super-propagator

$$\mathcal{J}(x,y,t;x',y',0) = \int\int\int d\mathbf{R}'d\mathbf{Q}'d\mathbf{R}\,\Big\{K(x,\mathbf{R},t;x',\mathbf{R}',0)$$

$$\times K^*(y,\mathbf{R},t;y',\mathbf{Q}',0)\,\tilde{\rho}_R(\mathbf{R}',\mathbf{Q}',0)\Big\}.$$

For an isolated system

$$\mathcal{J}(x,y,t;x',y',0) = K_0(x,t;x',0)\,K_0^*(y,t;y',0)$$