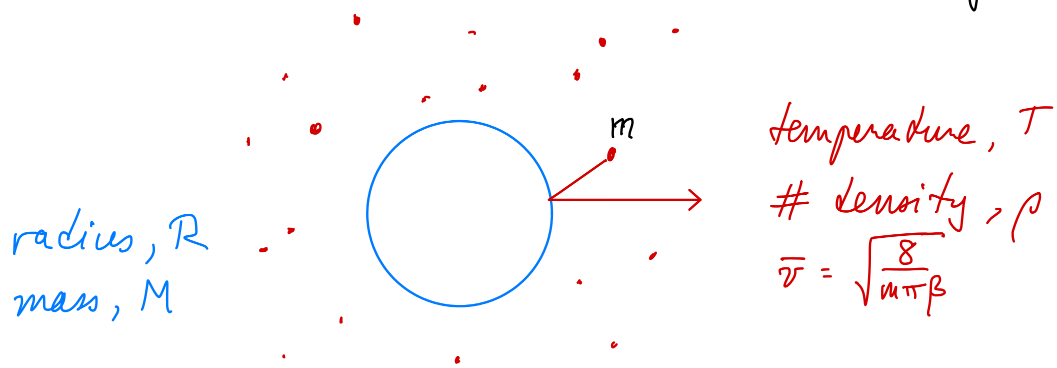
Up the ladder of timescales

Recall the hard sphere immersed in an ideal gas...



Different levels of description:

Hamiltonian $\quad \mathcal{H}(\underbrace{\vec{Q}, \vec{P}}_{\text{hard sphere}}; \underbrace{\vec{q}_1, \cdots \vec{q}_N, \vec{p}_1, \cdots \vec{p}_N}_{\text{ideal gas}})$

$$\boxed{\dot{\vec{Q}} = \frac{\partial \mathcal{H}}{\partial \vec{P}} \quad , \quad \dot{\vec{P}} = -\frac{\partial \mathcal{H}}{\partial \vec{Q}} \quad , \quad \dot{\vec{q}}_n = \frac{\partial \mathcal{H}}{\partial \vec{p}_n} \quad , \quad \dot{\vec{p}}_n = -\frac{\partial \mathcal{H}}{\partial \vec{q}_n}}$$

If $M \gg m$ the we get a separation of timescales: $t_{coll} \ll t_p$

time between collisions

time required for sphere's momentum to change significantly

Taking advantage of the separation, we can model the sphere as a Brownian particle w/ inertia:

$$\boxed{\dot{\vec{Q}} = \frac{\vec{P}}{M} \quad , \quad \dot{\vec{P}} = -\frac{\gamma}{M}\vec{P} - \frac{\partial U}{\partial \vec{Q}}(\vec{Q}) + \vec{\Xi} \qquad \langle \Xi_i(0)\,\Xi_j(t)\rangle = 2D_p\,\delta(t)\,\delta_{ij}}$$

microscopic calculations $\longrightarrow$ $\gamma = \beta D_p = \frac{4\pi}{3} R^2 m \rho \bar{v}$

We've gone from Hamiltonian description in (6N+6)-dimensional phase space to Langevin description in 6-dim'l phase space.

relaxation time in $U(\vec{Q})$

If $t_p \ll t_x$,

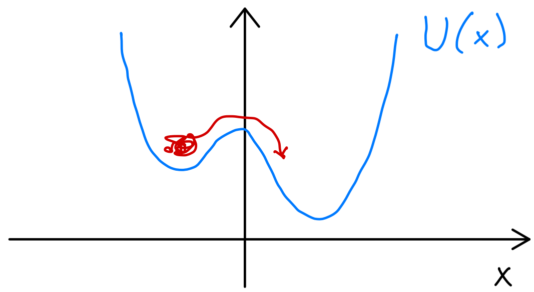
then we can describe the sphere as an overdamped Brownian particle:

$$\boxed{\dot{\vec{Q}} = -\frac{1}{\gamma}\frac{\partial U}{\partial \vec{Q}} + \vec{\zeta} \quad , \quad \langle \zeta_i(0)\,\zeta_j(t)\rangle = 2D\,\delta(t)\,\delta_{ij}}$$

treating $\vec{P}(t)$ as Ornstein-Uhlenbeck process $\longrightarrow$ $D = \frac{1}{\beta\gamma}$

$\cdots \rightarrow$ 3-dim'l config. space

Going further, let's imagine the sphere is trapped in a double-well potential. (For simplicity, work in 1d now.)



$$\dot{x} = -\frac{1}{\gamma}\frac{\partial U}{\partial x} + \tilde{\zeta} \quad , \quad \frac{\partial f}{\partial t} = \frac{1}{\gamma}\frac{\partial}{\partial x}\left(\frac{\partial U}{\partial x} f\right) + D\frac{\partial^2 f}{\partial x^2}$$

$$= D\frac{\partial}{\partial x}\left[e^{-\beta U}\frac{\partial}{\partial x}\left(e^{\beta U} f\right)\right]$$

$$= \hat{\mathcal{L}} f$$

eigenvalues of $\hat{\mathcal{L}}$: $0 = \lambda_0 > \lambda_1 \geq \lambda_2 \geq \cdots$ (all real)

timescales: $t_n = \frac{1}{|\lambda_n|} \quad , n \geq 0$

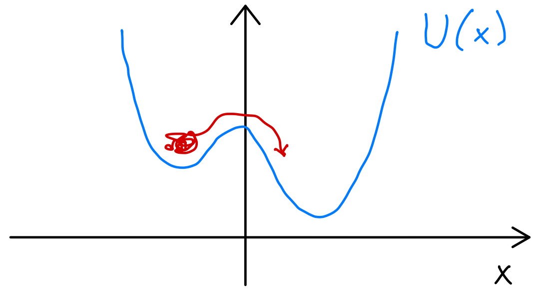
$$t_0 = \text{"}\infty\text{"} \gg t_1 \geq t_2 \geq \cdots$$

<u>Suppose</u> $t_1 \gg t_2, t_3, \cdots$

$$f(x,0) = \pi(x) + \sum_{n=1}^{\infty} c_n u_n(x)$$

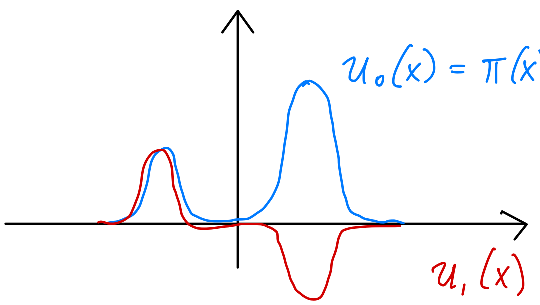
$$f(x,t) = \pi(x) + \sum_{n=1}^{\infty} c_n u_n(x) e^{-|\lambda_n| t}$$

$$\approx \pi(x) + c_1 u_1(x) e^{-|\lambda_1| t} \quad , \; t \gtrsim t_2$$



$$\frac{\partial f}{\partial t} = \hat{\mathcal{L}} f$$

$$\hat{\mathcal{L}}\, u_n(x) = \lambda_n u_n(x)$$



$$u_0(x) = \pi(x) \quad = \alpha_L \pi_L(x) + \alpha_R \pi_R(x)$$

$$\alpha_L + \alpha_R = 1$$

$$u_1(x) \quad = \pi_L(x) - \pi_R(x)$$

$$f(x,t) \cong \pi(x) + c_1 u_1(x) e^{-|\lambda_1| t}$$

$$= p_L \pi_L(x) + p_R \pi_R(x) \qquad \begin{cases} p_L = \alpha_L + c_1 e^{-|\lambda_1| t} \\ p_R = \alpha_R - c_1 e^{-|\lambda_1| t} \end{cases}$$

$$\dot{p}_L = -|\lambda_1| (p_L - \alpha_L)$$

$$\dot{p}_R = +|\lambda_1| (p_R - \alpha_R)$$

... which is equivalent to :

$$\boxed{\frac{d\vec{p}}{dt} = \mathcal{R}\vec{p}, \quad \mathcal{R} = |\lambda_1| \begin{pmatrix} -\alpha_R & \alpha_L \\ \alpha_R & -\alpha_L \end{pmatrix}}$$

$$\vec{p} = \begin{pmatrix} p_L \\ p_R \end{pmatrix}$$

... two-state system !