§36

Eigenvalue spectrum

$$\dot P = L P \qquad P = P(x,t)$$

$$\lambda_n \psi_n(x) = L \psi_n(x)$$

general solution

$$P(x,0) = \sum a_n \psi_n(x)$$

$$P(x,t) = \sum a_n \psi_n(x) \exp(\lambda_n t)$$

- $\lambda_0 = 0 \Leftrightarrow \psi_0$ steady-state solution
- Fact: $0 \ge \lambda_1 \ge \lambda_2 \ge \dots$

Proof:

- $1 \overset{!}{=} \int dx\, P(x,t)$

$$= \sum a_n \exp(-\lambda_n t) \int dx\, \psi_n(x)$$

$$\lambda_n \neq 0 \Rightarrow \int dx\, \psi_n(x) = 0$$

$$\Rightarrow \exists x \quad \psi_n(x) < 0$$

- $0 \overset{!}{\le} P(x,t) \Rightarrow \mathrm{Re}\,\lambda_n \le 0$
- Why λ_n real?

Adjoint operator L^*.

$$\int dx\, Lg\, h = \int dx\, g\, L^* h \quad \forall g(x), h(x)$$

$$Lg = -\frac{\partial}{\partial x}(fg) + D \frac{\partial^2}{\partial x^2} g$$

$$L^* h = +f \frac{\partial}{\partial x} h + D \frac{\partial^2}{\partial x^2} h$$

(partial integration)

$$f(x) = -\frac{\partial U(x)}{\partial x}$$

Define.

$$A = \exp\left(-\frac{\beta u}{2}\right) L \exp\left(+\frac{\beta u}{2}\right).$$

Then

$A = A^*$ self-adjoint (Hermitean)

$\Rightarrow$ all eigenvalues real.

But A and L have same eigenvalues.

q.e.d.

<u>Backward Fokker Planck equation</u>

$$P = P(x_1, t \mid x_0, 0) = P(x_1, 0 \mid x_0, -t).$$

$$\dot{P} = L_{x_1} P \qquad \text{forward}$$

$$= L^*_{x_0} P \qquad \text{backward.}$$

(without proof)

$$\left[L^*_{x_0} g = +f \frac{\partial}{\partial x_0} g + D \frac{\partial^2}{\partial x_0^2} g . \right]$$

$\Phi = \beta u(x)$,

$P^* \sim \exp(-\beta u)$,

$$L = \frac{\partial}{\partial x} D \exp(-\Phi) \frac{\partial}{\partial x} \exp(+\Phi)$$

$$(\exp \Phi\, L)^+ = L^* \exp \Phi = \exp \Phi\, L.$$

$\Rightarrow$

$A = \exp(+\Phi/2)\, L \exp(-\Phi/2)$ Hermitean

$$A = T^{-1} L T \qquad , \; Lg = -\nabla(fg) + D\nabla^2 g.$$

$$\nabla T = +\frac{f}{2D} T.$$

$$\langle Ag, h\rangle - \langle g, Ah\rangle \stackrel{?}{=} 0 \iff A = A^*.$$

$$\cdot\, L(Tg) = -(\nabla T) fg + T Lg.$$
$$+ (\nabla^2 T) Dg + 2D(\nabla T)(\nabla g)$$

$$\circ\, \langle Ag, h\rangle - \langle g, Ah\rangle =$$

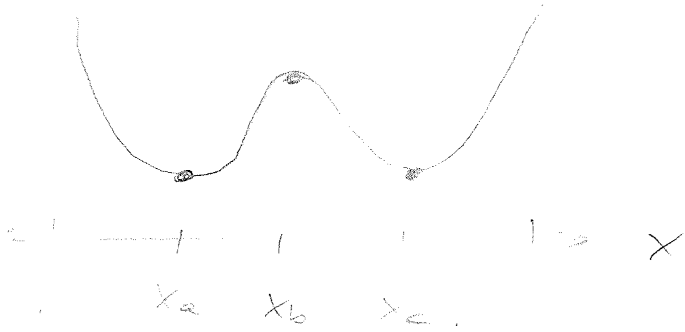
$$- \langle T^{-1}\cancel{(\nabla T)} fg, h\rangle + \langle Lg, h\rangle$$
$$+ \langle T^{-1}(\cancel{\nabla^2 T}) Dg, h\rangle + 2D\langle T^{-1}(\nabla T)(\nabla g), h\rangle$$
$$+ \langle g, T^{-1}\cancel{(\nabla T)} fh\rangle - \langle g, Lh\rangle$$
$$- \langle g, T^{-1}(\cancel{\nabla^2 T}) Dh\rangle - 2D\langle g\, T^{-1}(\nabla T)(\nabla h)\rangle$$
$$= \langle g, (L^* - L) h\rangle.$$

$$+ 2D\langle \left(\frac{\nabla T}{T}\right)(\nabla g), h\rangle - 2D\langle g, \left(\frac{\nabla T}{T}\right)(\nabla h)\rangle$$
$$= \langle g, 2f(\nabla h) + (\nabla f) h\rangle$$
$$+ \cancel{2D}\langle +\frac{f}{\cancel{2D}}(\nabla g), h\rangle - \cancel{2D}\langle g, \frac{+f}{\cancel{2D}}(\nabla h)\rangle$$

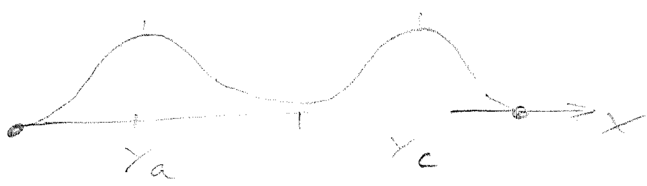
$$= \langle g, 2f(\nabla h) + (\nabla f) h\rangle$$

$$\cancel{=} \langle g, (\nabla f) h + f(\nabla h)\rangle \cancel{=} \langle g, f, (\nabla h)\rangle.$$

Example: Double-well potential

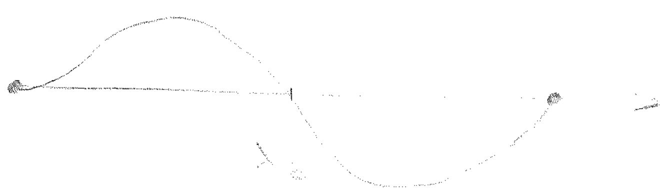


ψ_0



$\lambda_0 = 0$

ψ_1



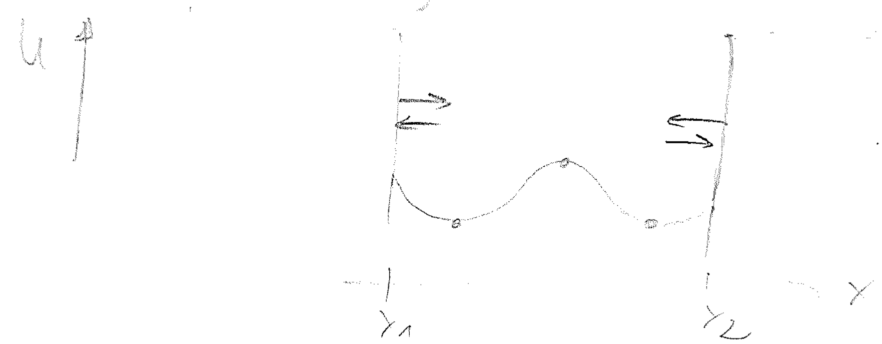
$r = -\lambda_1$

transition rate

Boundary conditions matter.

$$\dot{P} = -\nabla J, \quad J \equiv \text{current}$$

- reflecting b.c.

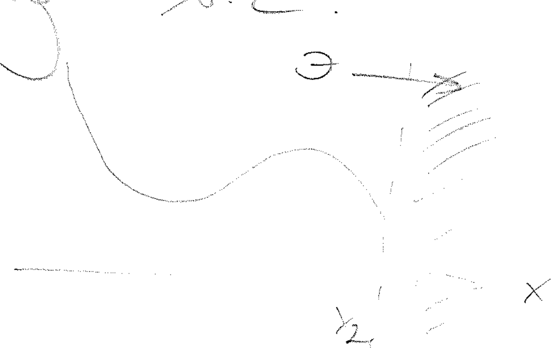


no-flux boundary condition
$J(x_1) = J(x_2) = 0.$
Robin b.c.

$\Rightarrow \int dx \; P(x,t) = 1.$

Steady state distribution
$P^*(x)$ exists.
Similar for confinement potential $\lim_{x \to \pm\infty} U(x) \to \infty$
[not for free diffusion].

- absorbing b.c.



$P(x_2, t) = 0.$
Dirichlet b.c.

$$0 > \frac{d}{dt} \int dx \; P(x,t) = \int dx \; \frac{d}{dt} P(x,t) = -J(x_2)$$

$$\dot{P} = -\nabla J$$