$f(g(x))$

$$\frac{df}{dx} = \frac{\partial f}{\partial g}\frac{dg}{dx}$$

Interpretation of overdamped Langevin equation:
In the absence of the stochastic force,

$$\dot{x} = -\frac{1}{m\zeta}\frac{\partial V}{\partial x} \qquad \text{(velocity of particle in downhill direction).}$$

Velocity vanishes at extrema of $V(x)$. The stochastic force then keeps the particle moving — is continually pushed away.
$\Rightarrow$ gives a posibility of making transitions from one minimum to another.

<u>Fokker – Planck Equation</u> from the Langevin Equation. (no external potential)

Given an initial velocity distribution, $P(v, t_0)$, the distribution evolves through time due to Brownian diffusion.

Define $P(v,t) = \langle \delta(v - \upsilon(t)) \rangle$ (Ensemble average).

Stochastic variable
(one function of t for one system in an ensemble) – a single realization.

Derive an equation of motion for $P(v,t)$. (How does P evolve?)

$$\frac{\partial}{\partial t} P(v,t) = \frac{\partial}{\partial t}\langle \delta(v - \upsilon(t))\rangle \qquad \text{use } \frac{\partial}{\partial t} = \frac{\partial \upsilon}{\partial t}\frac{\partial}{\partial \upsilon} = \frac{\partial \upsilon}{\partial t}\frac{-\partial}{\partial v}$$

$$= \frac{-\partial}{\partial v}\left\langle \delta(v - \upsilon(t))\frac{\partial \upsilon}{\partial t}\right\rangle \qquad \text{Langevin: } \frac{\partial \upsilon}{\partial t} = -\zeta \upsilon + \frac{f(t)}{m}$$

$$= -\frac{\partial}{\partial v}\left\langle \delta(v - \upsilon(t))\left(-\zeta \upsilon(t) + \frac{f(t)}{m}\right)\right\rangle$$

delta function
$v = \upsilon(t)$

$$= \frac{-\partial}{\partial v}\left\langle \delta(v - \upsilon(t))\left(-\zeta v + \frac{f(t)}{m}\right)\right\rangle$$

$f(t)$ is stochastic

$$= +\frac{\partial}{\partial v}\underbrace{\langle \delta(v - \upsilon(t))\rangle}_{P(v,t)}\zeta v - \frac{1}{m}\frac{\partial}{\partial v}\langle \delta(v - \upsilon(t)) f(t)\rangle$$

$$= \zeta v \frac{\partial P}{\partial v} - \frac{1}{m}\frac{\partial}{\partial v}\langle \delta(v - \upsilon(t)) f(t)\rangle$$

Characterization of stochastic force:

$$P[f(t)] = e^{-\int_{t_i}^{t_f} dt\, \frac{1}{2} \frac{1}{2m\zeta k_B T} f^2(t)}$$

probability suppressed for large $\int_{t_i}^{t_f} f^2(t)$.

Define a generating functional:

$$Z[j(t)] = \int \mathcal{D}f(t)\, e^{-\int_{t_i}^{t_f} dt \left(\frac{1}{2} f(t) \frac{1}{2m\zeta k_B T} f(t) + j(t) f(t)\right)}$$

$$= e^{-\int_{t_i}^{t_f} dt\, dt' \frac{1}{2} j(t)\, 2m\zeta k_B T\, \delta(t-t')\, j(t')}$$

So, we need

$$-\frac{1}{m}\langle \delta(v - v(t))\, f(t)\rangle = -\frac{1}{m}\int \mathcal{D}f(t')\, \delta(v - v(t))\, f(t)\, e^{-\int_{t_i}^{t_f} dt' \frac{1}{2} f(t') \frac{1}{2m\zeta k_B T} f(t')}$$

Functional integration by parts

$$= \frac{-1}{\cancel{m}}(+2\cancel{m}\zeta k_B T)\int \mathcal{D}f(t')\, \delta(v - v(t))\, \frac{\delta}{\delta f(t)}\, e^{-\int_{t_i}^{t_f} dt' \frac{1}{2} f(t') \frac{1}{2m\zeta k_B T} f(t')}$$

$$= -2\zeta k_B T \int \mathcal{D}f(t')\, \frac{\delta}{\delta f(t)}\, \delta(v - v(t))\, e^{-\int_{t_i}^{t_f} dt' \frac{1}{2} f(t') \frac{1}{2m\zeta k_B T} f(t')}$$

$$= -2\zeta k_B T \left\langle \frac{\delta}{\delta f(t)}\, \delta(v - v(t))\right\rangle$$

$$= +2\zeta k_B T \frac{\partial}{\partial v}\left\langle \frac{\delta v(t)}{\delta f(t)}\, \delta(v - v(t))\right\rangle$$

Use solution

$$v(t) = v_0 e^{-\zeta t} + e^{-\zeta t}\int_t^{\infty} dt'\, e^{\zeta t'} \frac{f(t')}{m}$$

Then

$$\frac{\delta v(t)}{\delta f(t)} = e^{-\zeta t}\int_t^{\infty} dt'\, e^{\zeta t'} \frac{\delta(t-t')}{m}$$

$$= \frac{1}{2m} \quad \text{(half of Delta function)}$$

$$= +\cancel{2}\zeta k_B T \frac{1}{\cancel{2}m} \frac{\partial}{\partial v} \underbrace{\langle \delta(v - v(t))\rangle}_{P}$$

$$\Rightarrow \boxed{\frac{\partial P}{\partial t} = \zeta v \frac{\partial P}{\partial v} + \frac{\zeta k_B T}{m}\frac{\partial^2 P}{\partial v^2}}$$

Fokker–Planck Equation

Can be written in the form of a continuity equation

$$\frac{\partial}{\partial t} P(v,t) = -\zeta \frac{\partial}{\partial v}\Big(\underbrace{-v P(v,t)}_{\text{Drift term}} - \underbrace{\frac{k_B T}{m}\frac{\partial}{\partial v} P(v,t)}_{\text{Diffusion current}}\Big)$$

If $(\dots) = 0$, then $\frac{\partial P}{\partial t} = 0$, and gives an equilibrium distribution. (steady state solution)

$$\frac{\partial P}{\partial v} = \frac{-vm}{k_B T} P(v,t)$$

solution: $P(v,t) = \mathcal{N} e^{-\frac{mv^2}{2k_BT}}$ [Maxwell Distribution] (steady-state solution)

check:

$$\frac{\partial P}{\partial v} = \frac{-mv}{k_B T} \mathcal{N} e^{-\frac{mv^2}{2k_BT}} = \frac{-vm}{k_B T} P(v,t) \checkmark$$