Langevin equation:

$$\lambda \frac{dX_t}{dt} = -\frac{\partial V(x)}{\partial x} + \eta(t) \qquad (1)$$

where X_t is the position of a particle in a potential $V(x)$ and $\eta(t)$ is a noise term.

(1) is also written as:

$$dX_t = -\nabla V(x)\,dt + \sqrt{2}\,dW_t \qquad (2)$$

W_t: Brownian motion.

It can shown that the SDE in (2) has a unique invariant measure (steady-state distribution) that does not change along the trajectory (X_t) of the particle. This means that if X_0 is distributed according to some pdf p_∞, then X_t is also distributed according to p_∞ for all $t \geq 0$. If we set the potential V s.t. $p_\infty = \pi$, then we can simulate the SDE (2) to generate samples from π.

Choosing the potential:

By Fokker-Plank eqn, the prob density of X_t in (2) satisfies

$$\frac{\partial p(x,t)}{\partial t} = \frac{\partial}{\partial x}\left[\frac{\partial V(x)}{\partial x} p(x,t)\right] + \frac{\partial^2 p(x,t)}{\partial x^2} \qquad (3)$$

The steady-state solution for (3) is given by $\frac{\partial p(x,t)}{\partial t} = 0$

If p_∞ is the steady-state distribution, we have

$$0 = \frac{\partial p(x,t)}{\partial t} = \frac{\partial}{\partial x}\left[\frac{\partial V(x)}{\partial x} p_\infty(x) + \frac{\partial p_\infty(x)}{\partial x}\right] = \frac{\partial}{\partial x} J(x)$$

$\Rightarrow$ $J(x)$ is a constant. Since $p_\infty(x)$ and $\frac{\partial p_\infty(x)}{\partial x}$ must satisfy certain boundary conditions

$\Rightarrow$ Boundary condition: $J(x) = 0$ at infinity.

$$\Rightarrow J(x) \equiv 0 \Rightarrow \frac{\partial V(x)}{\partial x} p_\infty(x) + \frac{\partial p_\infty(x)}{\partial x} = 0 \Rightarrow p_\infty(x) \propto \exp(-V(x)) \qquad (4)$$

(4) represents a Gibbs distribution. This means we can sample from energy-based models of the form $\pi(x) = \exp\{-E(x)\}/Z$ by setting $V(x) = E(x)$. We can also write $\pi(x)$ as $\exp[\log \pi(x)]$, which means that we can set $V(x) = -\log \pi(x)$

$$\Rightarrow \quad dX_t = \nabla \log \pi(x)\, dt + \sqrt{2}\, dW_t.$$