Q1. Prove $L_{SSM} = E_{x\sim p(x)} E_{v\sim p(v)} [\| v^T S(x;\theta)\|^2 + 2v^T \nabla_x (v^T S(x;\theta))]$

step1. From Original def.

$L_{SSM} = E_{v\sim p(v)} E_{x\sim p(x)} [\| v^T S(x;\theta) - v^T \nabla_x \log p(x) \|^2]$

step2. $\|A-B\|^2 = \|A\|^2 - 2A^T B + \|B\|^2$

$L_{SSM}(\theta) = E_{v,x} [\| v^T S(x;\theta)\|^2 - 2(v^T S(x;\theta))(v^T \nabla_x \log p(x)) + \| v^T \nabla_x \log p(x)\|^2]$

step3. $E_{v,x}[\| v^T \nabla_x \log p(x)\|^2] = \text{const}$

step4. $E_{p(x)}[g(x)^T \nabla \log p(x)] = -E_{p(x)}[\nabla_x p(x)]$

5. $E_x[(v^T S(x;\theta))(v^T \nabla_x \log p(x))]$

令 $g(x) = v(v^T S(x;\theta))$ v for x is a const vector

$v^T S$ for x is a ~~cons~~ scalar func. $\Rightarrow g(x)$ is a vec func

$g(x)^T \nabla_x \log p(x) = [v(v^T S)]^T \nabla_x \log p(x) = \cancel{(v^T S) v^T \nabla_x \log}$

$= (v^T S) v^T \nabla_x \log p(x)$

代入 step4, $E_x[(v^T S)(v^T \nabla_x \log p(x))] = -E_x[\nabla_x (v(v^T S(x;\theta)))]$

6.

$\nabla_x \cdot (v\, c(x))$, where $v \leftarrow$ const vec

$c(x) = v^T s(x;\theta) \leftarrow$ scalar func.

$$\nabla_x (v\, c(x)) = \sum_i \frac{\partial}{\partial x_i}(v_i\, c(x)) = \sum_i v_i \frac{\partial c(x)}{\partial x_i} = v^T (\nabla_x c(x))$$

$$\Rightarrow \nabla_x (v (v^T s(x;\theta))) = v^T \nabla_x (v^T s(x;\theta))$$

7.

$$E_x[(v^T s)(v^T \nabla_x \log p(x))] = -E_x[v^T \nabla_x (v^T s(x;\theta))]$$

$$\Rightarrow L_{SSM} = E_{v,x}[\|v^T s(x;\theta)\|^2 - 2\cdot(-E_x[v^T \nabla_x (v^T s(x;\theta))])]$$

$$L_{SSM} = E_{v,x}[\|v^T s(x;\theta)\|^2 + 2 v^T \nabla_x (v^T s(x;\theta))]$$

Q2.

SDE: $dx_t = \underbrace{f(x_t,t)\,dt}_{\substack{\text{Drift} \\ \text{(deterministic)}}} + \underbrace{G(x_t,t)\,dW_t}_{\substack{\text{diffusion} \\ \text{(stochastic)}}}$

W_t: $W_0 = 0$

$W_{t+u} - W_t \sim N(0, uI)$

dW_t is indep for each other

W_t is continuous (but ~~all~~ no where differenciable)

4 solve: $\int G\, dW_s$ is a Ito Integral

5 find solution: SDE 很難找解析解

Q3.

1 SDE 與材料中的原子擴散关係

$\frac{\partial p}{\partial t}=\frac{\sigma^2}{2}\frac{\partial^2 p}{\partial x^2}$ vs $\left(\frac{\partial C}{\partial t}=D\frac{\partial^2 C}{\partial x^2}\right)$ Fick's 2nd law

2. SDE與材料的相变能核化
           总

$f(x,t)dt$ with ~~自由能~~
表面能

$G(x,t)dW_t$ with 熱波動隨机力.

SDE is the 成核過程的 math tool?

3. 我們可以將一個材料的結構 (x_t 原子座標)
視為SDE的解 x_t, train NN to learn 反向SDE
, 循而從 $N(0,1)$ 生成出一個全新物理上穩定的
structure.