

Semiclassical Initial Value Representation

$$C_{AB}(t) \approx (2\pi)^{-F} \int d\mathbf{q}_0 \int d\mathbf{p}_0 \int d\mathbf{q}'_0 \int d\mathbf{p}'_0$$

$$\times \underbrace{\langle \mathbf{q}_0 \mathbf{p}_0 | \hat{A} | \mathbf{q}'_0 \mathbf{p}'_0 \rangle}_{A(x)} \underbrace{\langle \mathbf{q}'_t \mathbf{p}'_t | \hat{B} | \mathbf{q}_t \mathbf{p}_t \rangle}_{B(x)} \underbrace{c_t^{\text{HK}} c_{t'}^{\text{HK}*} e^{i(S_t - S'_t)}}_{C(x)}$$

- $A(x)$ requires no trajectory, just matrix element
- $B(x)$ requires “classical trajectory” (forces)
- $C(x)$ requires “semiclassical trajectory” (Hessian)

Monte Carlo Integration

$$\int dx f(x)g(x) = \left\langle \frac{1}{\rho(x)} f(x)g(x) \right\rangle_{\rho(x)}$$

This average will give us the integral,
but how to do it efficiently?