Quantum Correlation Functions

$$C_{AB}(t) = \mathrm{tr}\left(\hat{A}\, e^{i\hat{H}t/\hbar}\hat{B}\, e^{-i\hat{H}t/\hbar}\right)$$

Quantum correlation functions describe many experiments:

- electrical current
- transport properties
- position distributions
- populations of states
- reaction rates
- spectra

… and much, much more!

Semiclassical Initial Value Representation

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

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

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