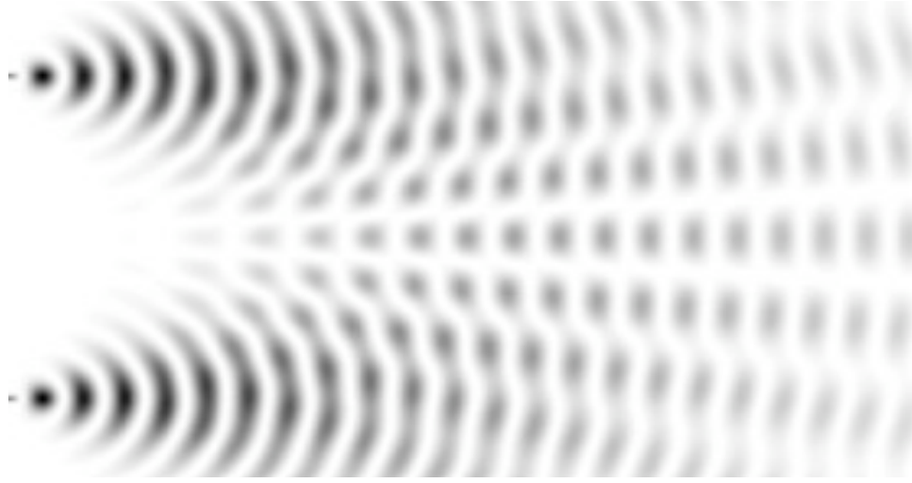
SC w/ interference

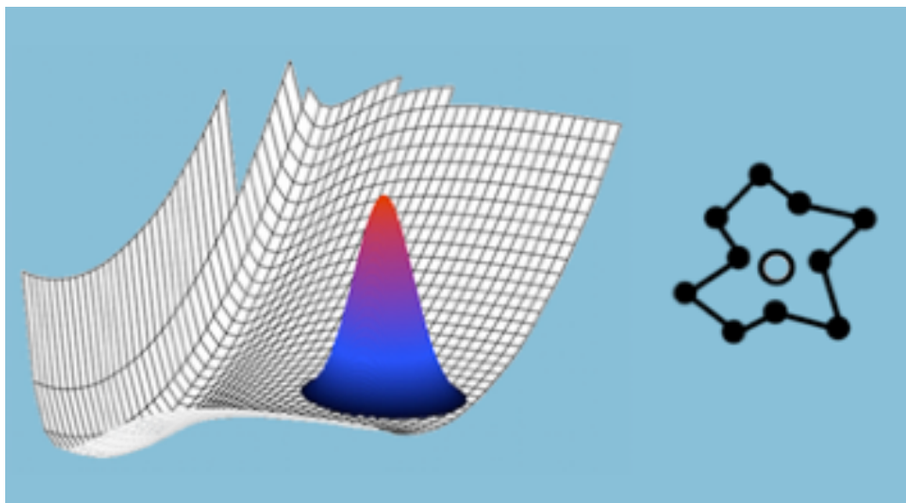
DHK-IVR, FB-IVR



Can we learn anything about this for the computational cost of this?

SC w/out interference

LSC-IVR, RPMD, centroid MD



Correlation Functions

Quantum:

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

Double Herman-Kluk:

$$C_{AB}^{\mathrm{DHK}}(t) = \int \mathrm{d}\Omega_0 \int \mathrm{d}\Omega_0' \left\langle \Omega_0 \middle| \hat{A} \middle| \Omega_0' \right\rangle \left\langle \Omega_t' \middle| \hat{B} \middle| \Omega_t \right\rangle \mathcal{C}_t^{\mathrm{HK}} \mathcal{C}_{t'}^{\mathrm{HK}\,*} e^{i\Delta S}$$

Linearized SC-IVR (Classical Wigner):

$$C_{AB}^{\mathrm{LSC}}(t) = \int \mathrm{d}\Omega_0\, A_{\mathrm{W}}(\Omega_0) B_{\mathrm{W}}(\Omega_t)$$