

Initial distribution

$$\rho^{(I)}(\vec{q}, \vec{p}) = \frac{1}{(\pi\hbar)^N} \exp\left(-\frac{2}{\hbar}W(\vec{q}, \vec{p})\right),$$

$$W(\vec{q}, \vec{p}) = \frac{1}{2} \sum_{i=1}^N \left(\frac{1}{\omega_i} p_i^2 + \omega_i q_i^2 \right)$$

Final distribution

$$\rho_E^{(F)}(\vec{q}, \vec{p}) = \delta(E - H^{(F)}(\vec{q}, \vec{p}))$$

Transition rate

$$I(E) = \frac{1}{(\pi\hbar)^N} \int_{H^{(F)}(\vec{q}, \vec{p})=E} d\vec{q} d\vec{p} \exp\left(-\frac{2}{\hbar}W(\vec{q}, \vec{p})\right)$$

Jumping point (q^*, p^*)

$W(\vec{q}, \vec{p})$ minimal under constraint $H^{(F)}(\vec{q}, \vec{p}) = E$.

$$\vec{\nabla}W(\vec{q}^*, \vec{p}^*) = \lambda \vec{\nabla}H^{(F)}(\vec{q}^*, \vec{p}^*)$$

Result of integration around (q^*, p^*)

$$I(E) = \frac{f_0^*}{H_1} (\pi\hbar \text{Det } \mathbf{F})^{-1/2} \exp\left(-\frac{2}{\hbar}W^*\right)$$

$$f_0^* = f_0(\vec{q}^*, \vec{p}^*), \quad W^* = W_0(\vec{q}^*, \vec{p}^*),$$

$$H_1 = |\vec{\nabla}H(\vec{q}^*, \vec{p}^*)|, \quad F_{ij} = \frac{\partial^2}{\partial \xi_{i+1} \partial \xi_{j+1}} (W - \lambda H)$$

Logarithm of the rate

$$I = \exp\left(-\frac{2}{\hbar}w\right)$$

$$w = W^* - \frac{\hbar}{2} \ln \left((\pi\hbar H_1^2 \text{Det } \mathbf{F})^{-1/2} f_0^* \right)$$