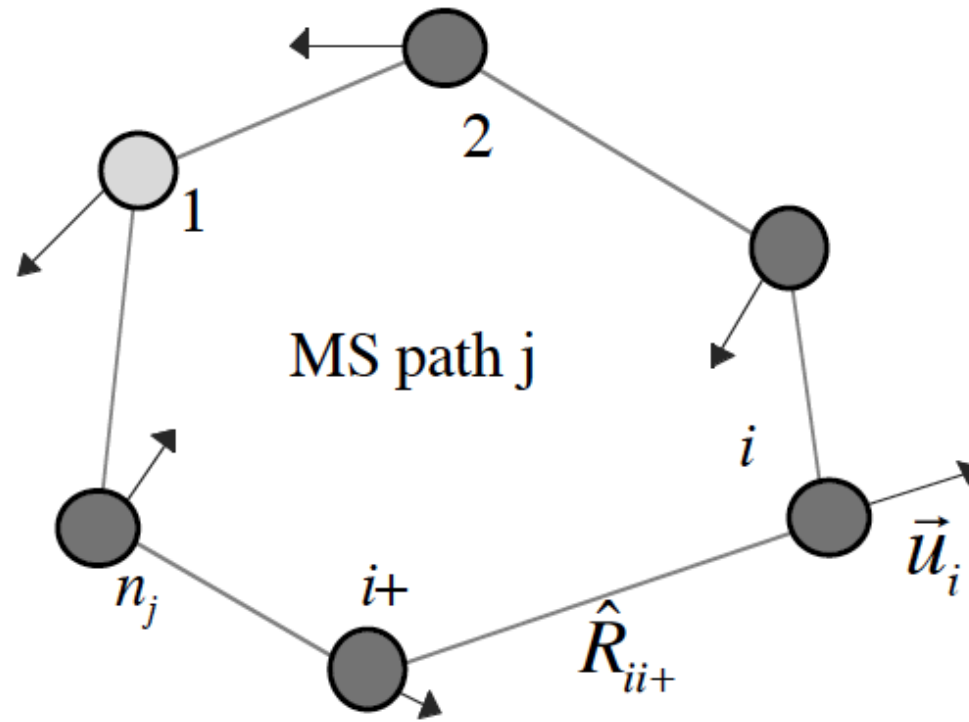# XAFS

$$\chi(k) = \sum_j \frac{N_j S_0^2}{k R_j^2} \left| f_j^{eff}(k, R_j) \right| \sin(2kR_j + \varphi_j(k)) e^{-2R_j/\lambda} e^{-2\sigma_j^2 k^2}$$

$$\sigma_j^2 = \frac{1}{4} \left\langle \left[\sum_{i=1}^{n_j} (\vec{u}_i - \vec{u}_{i+}) \cdot \hat{R}_{ii+} \right]^2 \right\rangle$$

Debye-Waller factors

MS path j

$$\sigma_j^2(T) = \frac{\hbar}{2\mu_j} \int \frac{d\omega}{\omega} \rho_j(\omega) \coth \frac{\hbar\omega}{2k_B T}$$

projected reduced mass:

projected vibrational density of states

$$\frac{1}{\mu_j} \equiv \sum_{i=1}^{n_j} \frac{1}{M_i} \left(\frac{\hat{R}_{ii-} + \hat{R}_{ii+}}{2} \right)^2$$

local
geometric + vibrational
structures

N_R, R $\qquad$ σ^2

dynamical model
local force constants, k_i