- GET 2B PES
- FROM 2B PES, EXTRACT EFFECTIVE σ & ε
- FOR ANY TWO PARTICLES i & j, DEFINE

$$\sigma_{ij} = 0.5(\sigma_i + \sigma_j) \qquad r_{c,in} = a\sigma_{ij}, \text{ e.g. } 0.25\sigma_{ij}$$
$$r_{min,ij} = 2^{1/6}\sigma_{ij} \qquad r_{c,out} = b\sigma_{ij}, \text{ e.g } 3.5\sigma_{ij}$$
$$\varepsilon_{ij} = \sqrt{\varepsilon_i \varepsilon_j}$$

NOW SUPPOSE YOUR MODEL HAS 3 DIMENSIONS: E, λ, r SUCH THAT YOUR MODEL HAS THE FORM:

$$E_{2B}(r_{ij}, \sigma_{ij}, \varepsilon_{ij}) \approx \sum_{\alpha}^{\Theta_\lambda} \sum_{\beta}^{\Theta_r} C_{\alpha\beta} T_\alpha(\eta_{ij}) T_\beta(s_{ij})$$

- s_{ij} IS DEFINED VIA MORSE XFORM, BUT $r_{c,in}$ & $r_{c,out}$ VARIES W/ λ
- η_{ij} IS A DIRECT XFORM, e.g. (DEFINED BASED ON YOUR λ)

$$\eta_{ij}(\varepsilon_{ij}) = (\varepsilon_{ij} - \varepsilon_{ij,MIN})/(\varepsilon_{ij,MAX} - \varepsilon_{ij,MIN})$$

HENCE, λ DOESN'T GET DIRECTLY PLUGGED IN, ε_{ij} DOES, WHICH IS A λ PROXY. FOR THIS TO WORK, NEED TO DEFINE A RELATIONSHIP BETWEEN λ & ε, ie $\varepsilon = f(\lambda)$ & $\eta = f(\varepsilon)$.

WE CAN APPLY THIS STRATEGY TO ATOMIC SYSTEMS W/O ISSUE B/C WE CAN DIRECTLY TAKE IONIZATION E FOR ε, & VDW RADIUS FOR σ, & DON'T NEED λ, ie $\lambda = \varepsilon$

FOR NP SYSTEMS, CAN EXTRACT σ + ε FROM 2B PMF, BUT NEED TO DETERMINE THE FUNCTION THAT MAKES $\varepsilon = f(\lambda)$... OR, COULD JUST USE ε AS THE λ DIRECTLY.