

SIMPLE VERSION:

$$(T_N + H_e) = \sum_i \alpha_i(n; R) \cdot m_i(R) = \epsilon \sum_i \alpha_i(n; R) m_i(R)$$

$$\Rightarrow T_N = \hat{p}_N \cdot \hat{p}_N; \quad \hat{p}_N = \frac{-i \hbar}{\sqrt{M_I}} \nabla_I$$

MULTIPLY
MASS-VARIABLE TRANSFORMATION

$$\Rightarrow \sum_i \hat{p}_N \left[(\hat{p}_N \alpha_i) m_i + \alpha_i (\hat{p}_N m_i) \right] + \sum_i (H_e \alpha_i) m_i$$

$$\Rightarrow \sum_i \left[(T_N \alpha_i) m_i + 2 (\hat{p}_N \alpha_i) \cdot (\hat{p}_N m_i) + \alpha_i (T_N m_i) \right] + \sum_i (\epsilon \alpha_i) m_i$$

$$= \epsilon \sum_i \alpha_i m_i$$

$$+ \sum_i (\epsilon \alpha_i) m_i$$

$$= \epsilon \sum_i \alpha_i m_i \rightarrow \textcircled{1}$$

\Rightarrow ASSUME: $H_e \alpha_i = \epsilon_i \alpha_i$
 IN NOT: ~~REZUM~~ $H_e \alpha_i$
 LEFT MULTI. $\langle m_j |$

$$\Rightarrow \sum_i \left[(T_N \alpha_i) \delta_{ij} + 2 \langle m_j | \hat{p}_N | m_i \rangle (\hat{p}_N \alpha_i) + \alpha_i \langle m_j | T_N | m_i \rangle \right] + \sum_i (H_e \alpha_i) \delta_{ij} = \epsilon \sum_i \alpha_i m_i$$

$$\Rightarrow \underbrace{(H_e + T_N) \alpha_j}_{\text{DBOC}} + \underbrace{\left\{ \sum_i 2 \langle m_j | \hat{p}_N | m_i \rangle (\hat{p}_N \alpha_i) + \alpha_i \langle m_j | T_N | m_i \rangle \right\}}_{\text{NON-BO}} = \epsilon \alpha_j = \epsilon \sum_i \alpha_i m_i \rightarrow \textcircled{2}$$

ALL KEIGHTED BY $\frac{1}{\sqrt{M_I}}$; IF SMALL: $H_e \alpha_j = \epsilon_j \alpha_j$
BO

IF NOT: TERMS IN EG. (2).

NUCLEAR PART :

FROM. Eq. (1) : LEFT MULT. $\langle x_j |$

$$\Rightarrow \sum_i \left[\langle x_j | T_N | x_i \rangle n_i + 2 \langle x_j | \hat{p}_N | x_i \rangle (\hat{p}_N n_i) + S_{ij} T_N n_i \right] \\ + \sum_i \langle x_j | H_e | x_i \rangle n_i = E \sum_i \langle x_j | x_i \rangle n_i$$

$$\Rightarrow (T_N + E_j) n_j + \underbrace{\left\{ \sum_i \left[\langle x_j | T_N | x_i \rangle + 2 \langle x_j | \hat{p}_N | x_i \rangle \cdot \hat{p}_N \right] x_i \right\}}_{\text{NON-BO}} = E n_j \quad \rightarrow (3)$$

ALL HAVE $\frac{1}{\sqrt{M_I}}$ - IF SMALL: $(T_N + E_j) n_j = E n_j$