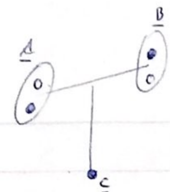

$\hat{=}$ scale-invariant (?) 5-body system

AB - AB - A   dimer - dimer - atom

$$\Psi = \hat{\mathcal{A}}'\Big[\overset{e^{-\frac{\alpha}{2}(\bar r_1^2+\bar r_2^2)}}{\overset{\parallel}{\phi_A}}\,\phi_B\,\overset{1}{\overset{\parallel}{\phi_C}}\;\mathcal{X}(\varsigma_1,\varsigma_2)\,F(R_{cm})\Big]$$

$$= \hat{\mathcal{A}}'\Big[\int d^3(\varsigma_1',\varsigma_2')\; e^{-\alpha_1\bar r_1^2-\alpha_2\bar r_3^2}\,\delta(\varsigma_1-\varsigma_1')\,\delta(\varsigma_2-\varsigma_2')\,\mathcal{X}(\varsigma_1',\varsigma_2')\Big]\,F(R_{cm})$$

$$= \hat{\mathcal{A}}'\Big[\int d^3(\varsigma_{1,2}',s_{1,2})\; e^{-\alpha_1\bar r_1^2-\alpha_2\bar r_3^2-i\underline{s}_1\cdot(\varsigma_1-\varsigma_1')-i\underline{s}_2\cdot(\varsigma_2-\varsigma_2')}\Big]\,\mathcal{X}(\varsigma_{1,2}')\,F_{cm}$$

$\downarrow$ internal averaging

$$\int d^3(\varsigma_{1,2}',s_{1,2},\bar r)\; e^{-\alpha_1\bar r_1^2-\alpha_2\bar r_3^2}\underbrace{\sum_{ij}\hat V_{ij}}_{\sum\delta(r_i-r_j)}\;\Psi$$

$$\overset{\sum_{P\in\hat{\mathcal{A}}'}\sum_{ij}}{=}\int d^3(\varsigma_{1,2}',s_{1,2},\bar r)\; e^{-\alpha_1\bar r_1^2-\alpha_2\bar r_3^2-\lambda(r_i-r_j)^2}\,\hat P\Big[e^{-\alpha_1\bar r_1^2-\alpha_2\bar r_3^2-i\underline{s}_1\cdot\varsigma_1-i\underline{s}_2\cdot\varsigma_2}\Big]e^{i\underline{s}_1\cdot\varsigma_1'+i\underline{s}_2\cdot\varsigma_2'}\,\mathcal{X}F$$

$r_{Jacobi}=T\tilde r$

$$\equiv\int d^3(\varsigma_{1,2}',s_{1,2},\bar r)\; e^{-\frac12\bar r\underline{\underline{A}}\bar r-\frac12\underbrace{\bar r\underline{\underline{V}}\bar r}_{=\sum\lambda(r_i-r_j)^2}-\frac12\underbrace{\bar r\underline{\underline{A}}^P\bar r}_{=P\bar r\underline{\underline{A}}P\bar r}+\underline{S}\cdot\underbrace{\hat P\Big[\Big(\begin{smallmatrix}0\\ \varsigma_1\\ \varsigma_2\\ 0\end{smallmatrix}\Big)\Big]}_{\tilde r_r}}\cdot e^{-\underline{S}\cdot\tilde r_r'}\,\mathcal{X}F$$

$$P_r=\begin{pmatrix}\bar r_1+\varsigma_1-\frac{\varsigma_2}{2}\cdots\\ \cdots\end{pmatrix}\circlearrowleft P$$

$$\bar r_1=\begin{pmatrix}0\\ \bar r_i\\ \bar r_j\\ 0\end{pmatrix}\longrightarrow \bar r_I\begin{pmatrix}2\lambda & -2\lambda\\ -2\lambda & 2\lambda\end{pmatrix}\bar r_I,\quad \begin{pmatrix}2\lambda & -2\lambda\\ -2\lambda & 2\lambda\end{pmatrix}=\underline{\underline{V}}^{ij}$$

$$= \bar r_I\,\underline{\underline{V}}^{ij}\,\bar r_I = \bar r\,\underline{\underline{T}}_{ij}\underline{\underline{V}}^{ij}\underline{\underline{T}}_{ij}\bar r,\quad \bar r_I=\underline{\underline{T}}_{ij}\bar r$$

$$= \tilde r\,\underline{\underline{T}}_{ij}^T\underline{\underline{V}}^{ij}\underline{\underline{T}}_{ij}\,\tilde r$$

$$=P\bar r\underline{\underline{A}}P\bar r = \cancel{\bar r P^T\underline{\underline{A}}P\bar r} = PT^{-1}r\,\underline{\underline{A}}\,PT^{-1}r = T^{-1}P_r\underline{\underline{A}}T^{-1}P_r = r(T^{-1}P)^T\underline{\underline{A}}(T^{-1}P)r = \tilde r\underbrace{(T^{-1}PT)^T\underline{\underline{A}}(T^{-1}PT)}\tilde r$$

$$P\tilde r_r = P\,\cancel{F}\begin{pmatrix}0\\ \varsigma_1(r_{\ldots},r_4)\\ \varsigma_2(r_{\ldots})\\ 0\end{pmatrix} = P\begin{pmatrix}0\\ (T^{-1}r)_{A-F+1}\\ (T^{-1}r)_{A-F+2}\\ 0\end{pmatrix} = P\,T_r^{-1}r = T_r^{-1}P_r = T_r^{-1}PT\,\tilde r$$

$$=\int d^3(\varsigma_{1,2}',s_{1,2},\bar r)\; e^{-\frac12\tilde r\left(\underline{\underline{A}}+T_{ij}^TV^{ij}T_{ij}+\cancel{P^T\underline{\underline{A}}P}\right)\tilde r+\underline{S}P\tilde r_r}\cdot e^{-\underline{S}\cdot\tilde r_r'}\,\mathcal{X}F$$

$$=\int d^3(\varsigma_{1,2}',s_{1,2})\,\mathcal{X}F\,e^{-\underline{S}\cdot\tilde r_r'}\int d\{\bar r\}\; e^{-\frac12\tilde r\underbrace{\left(\underline{\underline{A}}+T_{ij}^TV^{ij}T_{ij}+(T^{-1}PT)^T\underline{\underline{A}}(T^{-1}PT)\right)}\tilde r+\underbrace{\underline{S}\cdot(T_r^{-1}PT)}\tilde r}$$

$$= \boxed{\underline{S}_A}\cdot\begin{pmatrix}\bar r\\ \bar r_{A-F}\\ \varsigma\\ \varsigma\end{pmatrix}$$

$$\begin{array}{c|c}
 & \begin{array}{cccc}\bar r_1 & \bar r_{A-F}\ \varsigma_1 & \varsigma_{F-1} & R_{cm}\end{array}\\
\begin{array}{c}\bar r_1\\ \vdots\\ \bar r_{A-F}\\ \varsigma_1\\ \varsigma_{F-1}\\ R_{cm}\end{array} & \begin{pmatrix}\underline{\underline{A}} & \underline{\underline{B}} & \underline{\underline{D}}\\ & \underline{\underline{C}} & \underline{\underline{E}}\\ & & \underline{\underline{I}}\end{pmatrix}
\end{array}$$

$\sqcup\!\sqcup$ $\hat{=}$ relevant terms for the $\bar r$ integration

$$=\underbrace{-\frac12\bar r\underline{\underline{A}}\bar r-\frac12\left(\bar r\underline{\underline{B}}\varsigma+\varsigma\underline{\underline{B}}\bar r\right)}-\frac12\varsigma\underline{\underline{C}}\varsigma\underbrace{-\frac12\left(\bar r\underline{\underline{D}}R_{cm}+R_{cm}\underline{\underline{D}}\bar r\right)}-\frac12(\varsigma DR_{cm}+R_{cm}D\varsigma)-\frac12 I R_{cm}^2$$

The average over the internal coordinates yields a structure as follows for the interaction kernel:

$$\langle \phi_A \phi_B \phi_c | \hat{V} \hat{A}[\phi_A \phi_B \phi_c \chi(\underline{\rho}_1, \underline{\rho}_2)] \rangle$$

$$= \int d^3(\rho_1', \rho_2') \sum_{k=1}^{N_0} C_k(\lambda)\, e^{-\alpha_k^{(1)} \rho_1^2 - \beta_k^{(1)} \rho_2^2 - \gamma_k^{(1)} \underline{\rho}_1 \cdot \underline{\rho}_2 - \gamma_k^{(2)} \underline{\rho}_1 \cdot \underline{\rho}_1' - \gamma_k^{(3)} \underline{\rho}_1 \cdot \underline{\rho}_2' - \gamma_k^{(4)} \underline{\rho}_2 \cdot \underline{\rho}_1'}$$

$$\cdot e^{-\gamma_k^{(5)} \underline{\rho}_2 \cdot \underline{\rho}_2' - \gamma_k^{(6)} \underline{\rho}_1' \cdot \underline{\rho}_2' - \alpha_k^{(2)} \rho_1'^2 - \beta_k^{(2)} \rho_2'^2} \quad \chi(\rho_1', \rho_2')$$

$$= \int d^3(\rho_{1,2}') \sum_k C_k\, e^{-\frac{1}{2} \bar{\rho}^T \underline{\underline{A}}\, \bar{\rho}} \quad \chi(\rho_{1,2}')$$

with $\bar{\rho} = \begin{pmatrix} \rho_1 \\ \rho_2 \\ \rho_1' \\ \rho_2' \end{pmatrix}$ and $\underline{\underline{A}} = \begin{pmatrix} 2\alpha_k^{(1)} & \gamma_k^{(1)} & \gamma_k^{(2)} & \gamma_k^{(3)} \\ \gamma_k^{(1)} & 2\beta_k^{(1)} & \gamma_k^{(4)} & \gamma_k^{(5)} \\ \gamma_k^{(2)} & \gamma_k^{(4)} & 2\alpha_k^{(2)} & \gamma_k^{(6)} \\ \gamma_k^{(3)} & \gamma_k^{(5)} & \gamma_k^{(6)} & 2\beta_k^{(2)} \end{pmatrix}$

Notes: ν) $V_{local} \Rightarrow$ ~~γ_k and $\beta_k^{(1)} \neq 0$~~
only $\alpha_k^{(1)}$ and $\beta_k^{(1)}$ <u>may</u> be $\neq 0$

ʒ) all α, β are $f(\lambda, a_{1,2})$ with a well define
$\phi_{A,B}$ wave-function parameter!

$$\lim_{\lambda \to a} \alpha_k^{(1)} = \#_1 a + \#_2 \lambda$$

i.e. in the zero-range limit the interaction becomes δ-like or approaches a fixed well which is controlled by the dimer / fragment size;

λ) $$\lim_{\lambda \to \infty} (\pm) C_k^\lambda = \begin{cases} 0 \\ \infty \end{cases}$$

the sign is the inverse of the original interaction LEC, e.g. $C_0 \to -C_k^\lambda$
$D_1 \to -C_k^\lambda$