Four-body long-range interactions between ultracold weakly-bound diatomic molecules

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Four-body long-range interactions between ultracold weakly-bound diatomic molecules

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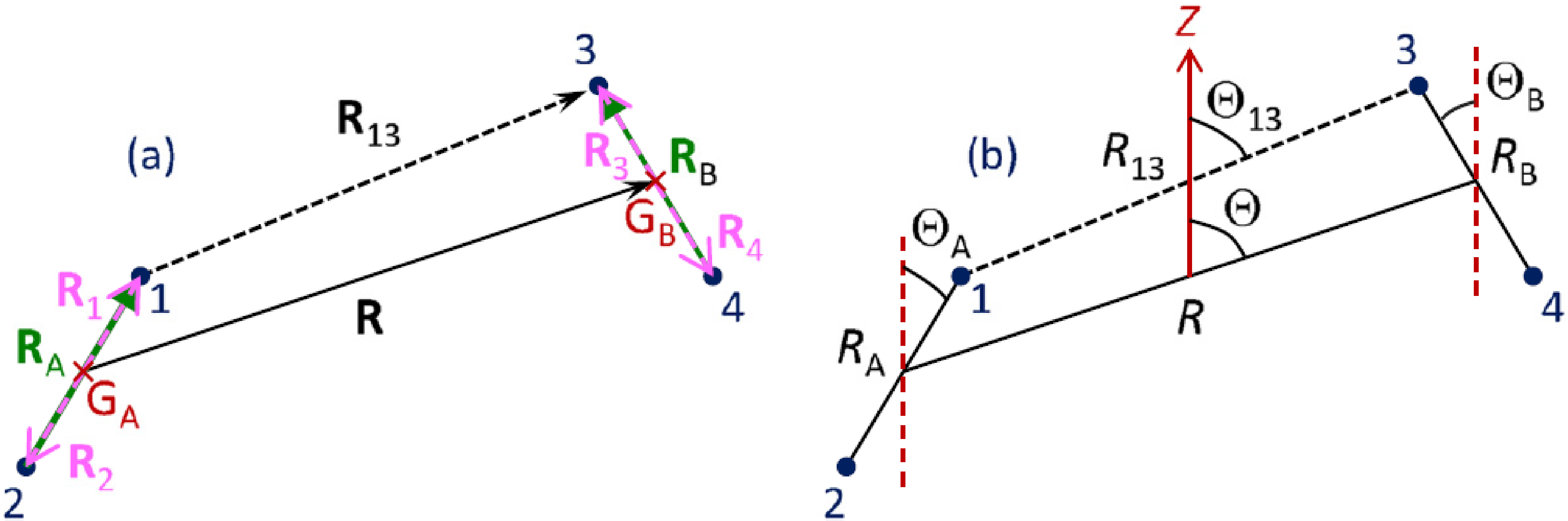
Interacting weakly-bound molecules: Geometry



Atom	$R_i,\ R_j$	$\Theta_i,\ \Theta_j$	$\Phi_i,\ \Phi_j$	$\eta_i,\ \eta_j$
1	$R_1 = \dfrac{\mathcal{M}_2}{\mathcal{M}_1 + \mathcal{M}_2} R_A$	$\Theta_1 = \Theta_A$	$\Phi_1 = \Phi_A$	$\eta_1 = +\dfrac{\mathcal{M}_2}{\mathcal{M}_1 + \mathcal{M}_2}$
2	$R_2 = \dfrac{\mathcal{M}_1}{\mathcal{M}_1 + \mathcal{M}_2} R_A$	$\Theta_2 = \pi - \Theta_A$	$\Phi_2 = \Phi_A + \pi$	$\eta_2 = -\dfrac{\mathcal{M}_1}{\mathcal{M}_1 + \mathcal{M}_2}$
3	$R_3 = \dfrac{\mathcal{M}_4}{\mathcal{M}_3 + \mathcal{M}_4} R_B$	$\Theta_3 = \Theta_B$	$\Phi_3 = \Phi_B$	$\eta_3 = +\dfrac{\mathcal{M}_4}{\mathcal{M}_3 + \mathcal{M}_4}$
4	$R_4 = \dfrac{\mathcal{M}_3}{\mathcal{M}_3 + \mathcal{M}_4} R_B$	$\Theta_4 = \pi - \Theta_B$	$\Phi_4 = \Phi_B + \pi$	$\eta_4 = -\dfrac{\mathcal{M}_3}{\mathcal{M}_3 + \mathcal{M}_4}$

Multipolar expansion, 1st order

$$V\left(\mathbf{R}_A, \mathbf{R}_B, \mathbf{R}\right) = \sum_{i=1}^{2} \sum_{j=3}^{4} V_{ij}\left(\mathbf{R}_{ij}\right),$$

In the space-fixed frame

$$V_{ij}\left(\mathbf{R}_{ij}\right) = \sum_{\ell_{ij}=0}^{+\infty} \sum_{m_{ij}=-\ell_{ij}}^{+\ell_{ij}} F_{\ell_{ij} m_{ij}} G^{*}_{\ell_{ij} m_{ij}}\left(\mathbf{R}_{ij}\right)$$

$$F_{\ell_{ij} m_{ij}} = F_0 \sum_{\ell_i, \ell_j = 0}^{\ell_{ij}} \delta_{\ell_i+\ell_j, \ell_{ij}} (-1)^{\ell_j} \binom{2\ell_{ij}}{2\ell_i}^{1/2} \times \sum_{m_i=-\ell_i}^{+\ell_i} \sum_{m_j=-\ell_j}^{+\ell_j} C^{\ell_{ij} m_{ij}}_{\ell_i m_i \ell_j m_j} Q_{\ell_i m_i} Q_{\ell_j m_j}$$

$$G_{\ell_{ij} m_{ij}}\left(\mathbf{R}_{ij}\right) = \frac{C_{\ell_{ij} m_{ij}}\left(\Theta_{ij}, \Phi_{ij}\right)}{R_{ij}^{1+\ell_{ij}}}$$

$$\mathbf{R}_{ij} = \mathbf{R} - \left(\mathbf{R}_i - \mathbf{R}_j\right) \equiv \mathbf{R} - \mathbf{U}_{ji}$$

$$(U_{ji}, \Xi_{ji}, \Psi_{ji})$$

$$F_0 = 1/4\pi\epsilon_0 \ \ (\mu_0/4\pi)$$

Clebsch-Gordan

Multipole moments in SF

Binomial coefficients

Transformation with R variable

$$G_{\ell_{ij}m_{ij}}(\mathbf{R}_{ij}) = \frac{C_{\ell_{ij}m_{ij}}(\Theta_{ij}, \Phi_{ij})}{R_{ij}^{1+\ell_{ij}}}$$

$$\mathbf{R}_{ij} = \mathbf{R} - (\mathbf{R}_i - \mathbf{R}_j) \equiv \mathbf{R} - \mathbf{U}_{ji}$$

$$G_{\ell_{ij}m_{ij}}(\mathbf{R}_{ij}) = \sum_{\lambda=\ell_{ij}}^{+\infty} (-1)^{\lambda} \times \left(\frac{(2\lambda+1)!}{(2\lambda-2\ell_{ij})!(2\ell_{ij}+1)!} \right)^{1/2} \frac{U_{ji}^{\lambda-\ell_{ij}}}{R^{1+\lambda}} \times \sum_{\mu=-\lambda}^{+\lambda} C^{\ell_{ij}m_{ij}}_{\lambda-\ell_{ij},\mu-m_{ij},\lambda\mu} C_{\lambda-\ell_{ij},\mu-m_{ij}}(\Xi_{ji}, \Psi_{ji}) \times C_{\lambda\mu}(\Theta, \Phi)$$

$U_{ji} < R.$

$R_i + R_j < R$

$$G_{\ell_{ij}m_{ij}}(\mathbf{R}_{ij}) = \sum_{\lambda=\ell_{ij}}^{+\infty} \sum_{\lambda_i,\lambda_j=0}^{\lambda-\ell_{ij}} \delta_{\ell_{ij}+\lambda_i+\lambda_j,\lambda} (-1)^{\lambda+\lambda_j} \times \left[\binom{2\lambda+1}{2\ell_{ij}+1} \binom{2\lambda_i+2\lambda_j}{2\lambda_i} \right]^{1/2} \times \frac{R_i^{\lambda_i} R_j^{\lambda_j}}{R^{1+\lambda}} \sum_{\mu=-\lambda}^{+\lambda} C^{\ell_{ij}m_{ij}}_{\lambda-\ell_{ij},\mu-m_{ij},\lambda\mu} C_{\lambda\mu}(\Theta, \Phi) \times \sum_{\mu_i=-\lambda_i}^{+\lambda_i} \sum_{\mu_j=-\lambda_j}^{+\lambda_j} C^{\lambda-\ell_{ij},\mu-m_{ij}}_{\lambda_i\mu_i\lambda_j\mu_j} C_{\lambda_i\mu_i}(\Theta_i, \Phi_i) C_{\lambda_j\mu_j}(\Theta_j, \Phi_j)$$

$$\sum_{\lambda_i,\lambda_j=0}^{\lambda-\ell_{ij}} \ldots R_i^{\lambda_i} C_{\lambda_i\mu_i}(\Theta_i, \Phi_i)$$ Effective multiple moments

If $R_i, R_j \ll R$,

$\lambda_i = \lambda_j = 0 \quad \lambda = \ell_{ij}$

Usual multipolar expansion

Final expression of potential energy (1st order)

$$
\begin{aligned}
&V(\mathbf{R}_A, \mathbf{R}_B, \mathbf{R}) \\
&= F_0 \sum_{\ell=0}^{+\infty} \sum_{\lambda=\ell}^{+\infty} \sum_{\lambda_A,\lambda_B=0}^{\lambda-\ell} \delta_{\lambda_A+\lambda_B+\ell,\lambda} (-1)^{\lambda_B} \frac{R_A^{\lambda_A} R_B^{\lambda_B}}{R^{1+\lambda}} \\
&\times \sum_{\mu=-\lambda}^{+\lambda} \sqrt{(\lambda+\mu)!(\lambda-\mu)!} \times C^*_{\lambda\mu}(\Theta, \Phi) \\
&\times \sum_{\mu_A=-\lambda_A}^{+\lambda_A} \sum_{\mu_B=-\lambda_B}^{+\lambda_B} \\
&\frac{C_{\lambda_A\mu_A}(\Theta_A, \Phi_A) C_{\lambda_B\mu_B}(\Theta_B, \Phi_B)}{\sqrt{(\lambda_A+\mu_A)!(\lambda_A-\mu_A)!(\lambda_B+\mu_B)!(\lambda_B-\mu_B)!}} \\
&\times \sum_{i=1}^{2} \sum_{j=3}^{4} \eta_i^{\lambda_A} \eta_j^{\lambda_B} \sum_{\ell_i,\ell_j=0}^{\ell} \delta_{\ell_i+\ell_j,\ell} (-1)^{\ell_i} \\
&\times \sum_{m_i=-\ell_i}^{+\ell_i} \sum_{m_j=-\ell_j}^{+\ell_j} \\
&\times \frac{\delta_{\mu_A+\mu_B+m_i+m_j,\mu} Q_{\ell_i m_i} Q_{\ell_j m_j}}{\sqrt{(\ell_i+m_i)!(\ell_i-m_i)!(\ell_j+m_j)!(\ell_j-m_j)!}}
\end{aligned}
$$

Final expression of potential energy (2nd order)

$$
\begin{aligned}
W(\mathbf{R}_A, \mathbf{R}_B, \mathbf{R})
&= -F_0^2 \sum_{\ell\lambda\lambda_A\lambda_B} \sum_{\ell'\lambda'\lambda_A'\lambda_B'} \\
&\times \delta_{\lambda_A'+\lambda_B'+\ell',\lambda'}\delta_{\lambda_A+\lambda_B+\ell,\lambda} \frac{R_A^{\lambda_A+\lambda_A'} R_B^{\lambda_B+\lambda_B'}}{R^{2+\lambda+\lambda'}} \\
&\times \sqrt{\binom{2\lambda+1}{2\ell+1}\binom{2\lambda_A+2\lambda_B}{2\lambda_A}} \\
&\times \sqrt{\binom{2\lambda'+1}{2\ell'+1}\binom{2\lambda_A'+2\lambda_B'}{2\lambda_A'}} \\
&\times \sum_{k\kappa\pi\kappa_A\kappa_B} (-1)^{\kappa+\kappa_B} \\
&\times \left[(\lambda_A+\lambda_B)(\lambda_A'+\lambda_B')\kappa_A\kappa_B\kappa\pi\right]^{1/2} \\
&\times \begin{Bmatrix} \lambda_A & \lambda_B & \lambda_A+\lambda_B \\ \lambda_A' & \lambda_B' & \lambda_A'+\lambda_B' \\ \kappa_A & \kappa_B & \pi \end{Bmatrix} \\
&\times \begin{Bmatrix} \lambda_A+\lambda_B & \lambda & \ell \\ \lambda_A'+\lambda_B' & \lambda' & \ell' \\ \pi & \kappa & k \end{Bmatrix} C^{\kappa_A 0}_{\lambda_A 0 \lambda_A' 0} C^{\kappa_B 0}_{\lambda_B 0 \lambda_B' 0} C^{\kappa 0}_{\lambda 0 \lambda'} \\
&\times \sum_{q\varrho\sigma\varrho_A\varrho_B} C^{\pi\sigma}_{\kappa_A\varrho_A\kappa_B\varrho_B} C^{kq}_{\pi\sigma\kappa\varrho} C^{*}_{\kappa\varrho}(\Theta, \Phi) \\
&\times C^{*}_{\kappa_A\varrho_A}(\Theta_A, \Phi_A) C^{*}_{\kappa_B\varrho_B}(\Theta_B, \Phi_B) \\
&\times \sum_{ii'jj'} \eta_i^{\lambda_A}\eta_{i'}^{\lambda_A'}\eta_j^{\lambda_B}\eta_{j'}^{\lambda_B'} \\
&\times \sum_{\ell_i\ell_{i'}\ell_j\ell_{j'}} \delta_{\ell_i+\ell_j,\ell}\delta_{\ell_{i'}+\ell_{j'},\ell'}(-1)^{\ell_j+\ell_{j'}} \\
&\times \sqrt{\binom{2\ell}{2\ell_i}\binom{2\ell'}{2\ell_{i'}}}\left[\ell\ell'\right] \\
&\times \sum_{k_A k_B} \left[k_A k_B\right]^{1/2} \begin{Bmatrix} \ell_i & \ell_j & \ell \\ \ell_{i'} & \ell_{j'} & \ell' \\ k_A & k_B & k \end{Bmatrix} \\
&\times \sum_{q_A q_B} C^{kq}_{k_A q_A k_B q_B} \\
&\times \sum_{1'',2'',3'',4''}{}' \frac{Q''_{(\ell_i,\ell_{i'})k_A q_A} Q''_{(\ell_j,\ell_{j'})k_B q_B}}{\Delta_{1''}+\Delta_{2''}+\Delta_{3''}+\Delta_{4''}},
\end{aligned}
$$

Application to Er_2

$$\left|v_A\right\rangle = \sum_{M_{J_1}M_{J_2}} \sum_{N_A M_{N_A}} \chi^{v_A}_{M_{J_1}M_{J_2}N_A M_{N_A}}(R_A) \times \left|M_{J_1}M_{J_2}N_A M_{N_A}\right\rangle$$

$$M_{J_1} = M_{J_2} = -J = -6,\ N_A = M_{N_A} = 0$$

Matrix elements of the magnetic dipole interaction

Leading term: R^{-3} $\quad \lambda_A = \lambda_B = 0$ and $\lambda = 2$

$\lambda_{max}=10$ R^{-3}, R^{-5}, R^{-7}, R^{-9}, R^{-11}

$$\begin{aligned}
\langle v'_A v'_B L' M'_L | \hat{V}_{md} | v_A v_B L M_L \rangle &= -\frac{\mu_0}{4\pi R^3}(\mu_B g_J)^2 J(J+1) \\
&\times \sum_{\lambda=2}^{+\infty} \sum_{\lambda_A,\lambda_B=0,2,\ldots}^{\lambda-2} \delta_{\lambda_A+\lambda_B+2,\lambda} \frac{(-1)^{\lambda_B}}{(2R)^{\lambda_A+\lambda_B}} \\
&\times \sum_{M_{J_1}M_{J_2}} \sum_{M'_{J_1}M'_{J_2}} \left(\frac{\delta_{M_{J_2}M'_{J_2}} C^{JM'_{J_1}}_{JM_{J_1}1,M'_{J_1}-M_{J_1}}}{\sqrt{(1+M'_{J_1}-M_{J_1})!(1-M'_{J_1}+M_{J_1})!}} \right. \\
&+ \left. \frac{\delta_{M_{J_1}M'_{J_1}} C^{JM'_{J_2}}_{JM_{J_2}1,M'_{J_2}-M_{J_2}}}{\sqrt{(1+M'_{J_2}-M_{J_2})!(1-M'_{J_2}+M_{J_2})!}} \right) \\
&\times \sum_{M_{J_3}M_{J_4}} \sum_{M'_{J_3}M'_{J_4}} \left(\frac{\delta_{M_{J_4}M'_{J_4}} C^{JM'_{J_3}}_{JM_{J_3}1,M'_{J_3}-M_{J_3}}}{\sqrt{(1+M'_{J_3}-M_{J_3})!(1-M'_{J_3}+M_{J_3})!}} \right. \\
&+ \left. \frac{\delta_{M_{J_3}M'_{J_3}} C^{JM'_{J_4}}_{JM_{J_4}1,M'_{J_4}-M_{J_4}}}{\sqrt{(1+M'_{J_4}-M_{J_4})!(1-M'_{J_4}+M_{J_4})!}} \right) \\
&\times \sum_{N_A M_{N_A}} \sum_{N'_A M'_{N_A}} \\
&\times \int_0^{+\infty} dR_A\, R_A^{\lambda_A} \chi^{v'_A}_{M'_{J_1}M'_{J_2}N'_A M'_{N_A}}(R_A)\, \chi^{v_A}_{M_{J_1}M_{J_2}N_A M_{N_A}}(R_A) \\
&\times \sum_{N_B M_{N_B}} \sum_{N'_B M'_{N_B}} \\
&\times \int_0^{+\infty} dR_B\, R_B^{\lambda_B} \chi^{v'_B}_{M'_{J_3}M'_{J_4}N'_B M'_{N_B}}(R_B)\, \chi^{v_B}_{M_{J_3}M_{J_4}N_B M_{N_B}}(R_B) \\
&\times \sqrt{(\lambda+M_L-M'_L)!(\lambda-M_L+M'_L)!} \\
&\times \sqrt{\frac{2L'+1}{2L+1}} C^{L0}_{L'0\lambda0} C^{LM_L}_{L'M'_L\lambda,M_L-M'_L} \\
&\times \sqrt{\frac{2N_A+1}{2N'_A+1}} \\
&\times \frac{C^{N'_A0}_{N_A0\lambda_A0} C^{N'_AM'_{N_A}}_{N_AM_{N_A}\lambda_A,M'_{N_A}-M_{N_A}}}{\sqrt{(\lambda_A+M'_{N_A}-M_{N_A})!(\lambda_A-M'_{N_A}+M_{N_A})!}} \\
&\times \sqrt{\frac{2N_B+1}{2N'_B+1}} \\
&\times \frac{C^{N'_B0}_{N_B0\lambda_B0} C^{N'_BM'_{N_B}}_{N_BM_{N_B}\lambda_B,M'_{N_B}-M_{N_B}}}{\sqrt{(\lambda_B+M'_{N_B}-M_{N_B})!(\lambda_B-M'_{N_B}+M_{N_B})!}}.
\end{aligned} \tag{18}$$

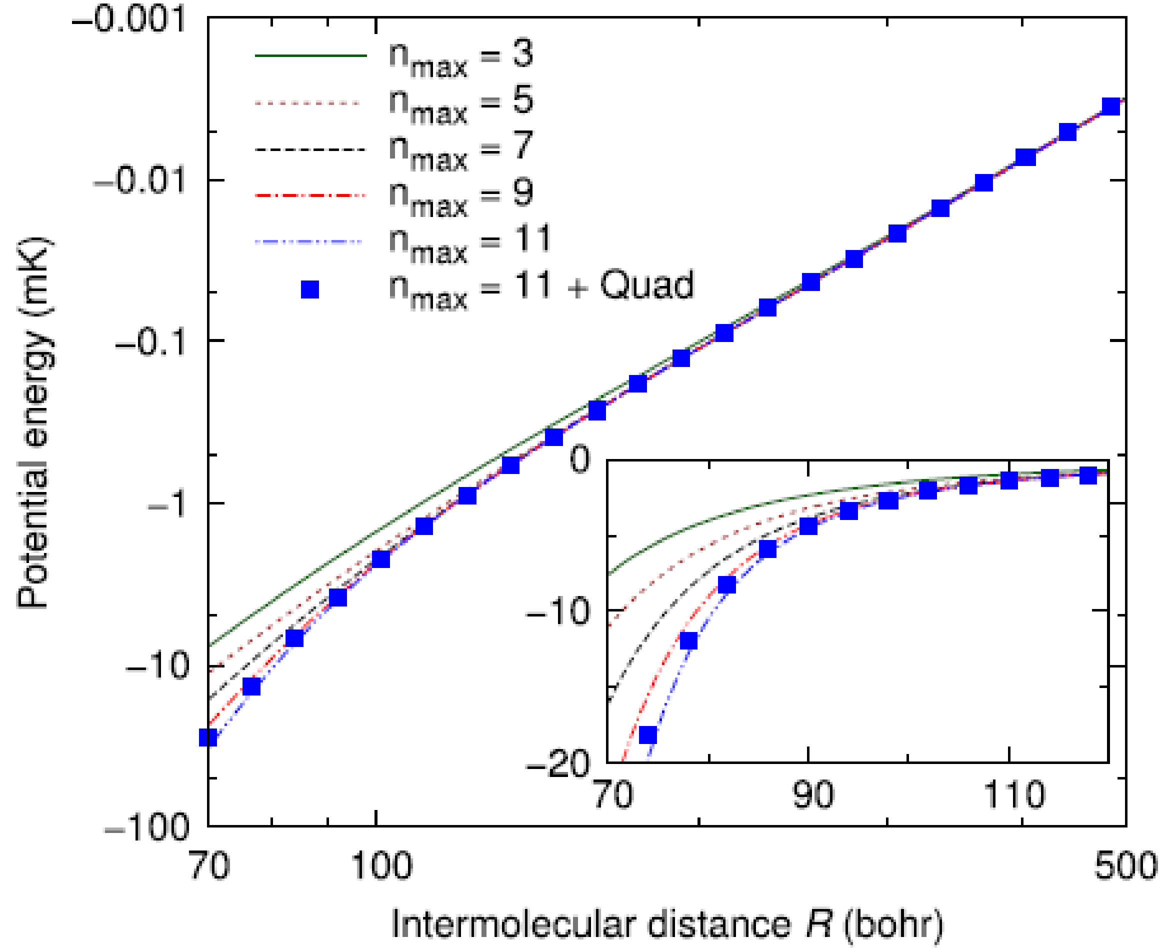
Application to $^{166}Er_2$

Lowest adiabatic curve for

$$M_{J_1} = M_{J_2} = -J = -6,\ N_A = M_{N_A} = 0$$

$$\langle v_A |\ R_A\ | v_A \rangle = \langle v_B |\ R_B\ | v_B \rangle = R_0 \quad 80a_0$$

1st order correction



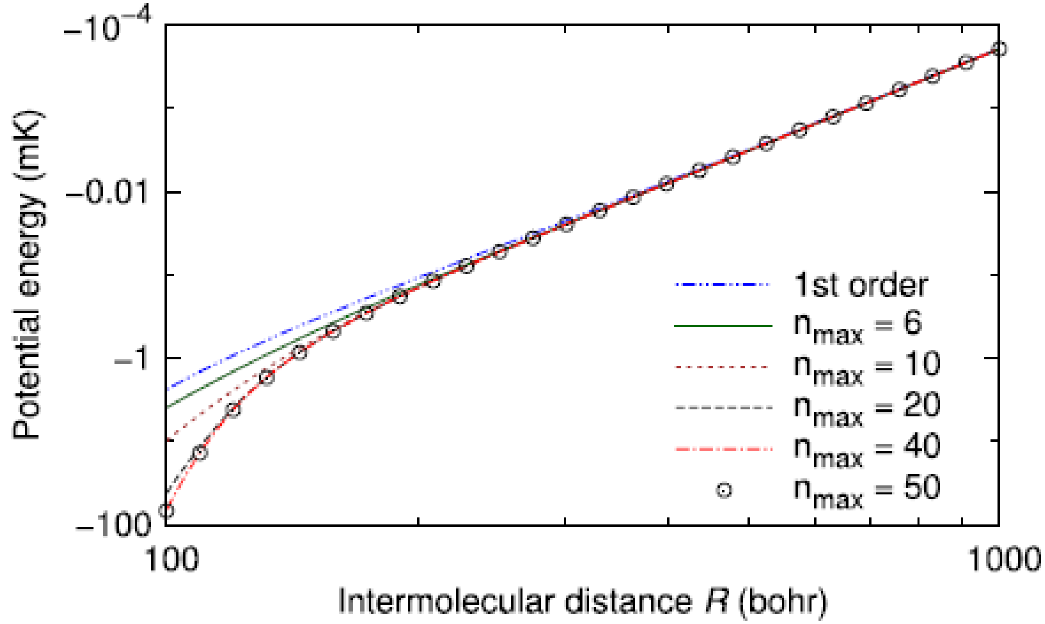
Application to $^{166}Er_2$

Lowest adiabatic curve for

$$M_{J_1} = M_{J_2} = -J = -6,\ N_A = M_{N_A} = 0$$

$$\langle v_A | R_A | v_A \rangle = \langle v_B | R_B | v_B \rangle = R_0 \quad 80a_0$$

Similar curves for the 2nd order correction



Théomol

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