

Interaction potentials and ultracold scattering cross sections for the ${}^7\text{Li}^+ - {}^7\text{Li}$ ion-atom system

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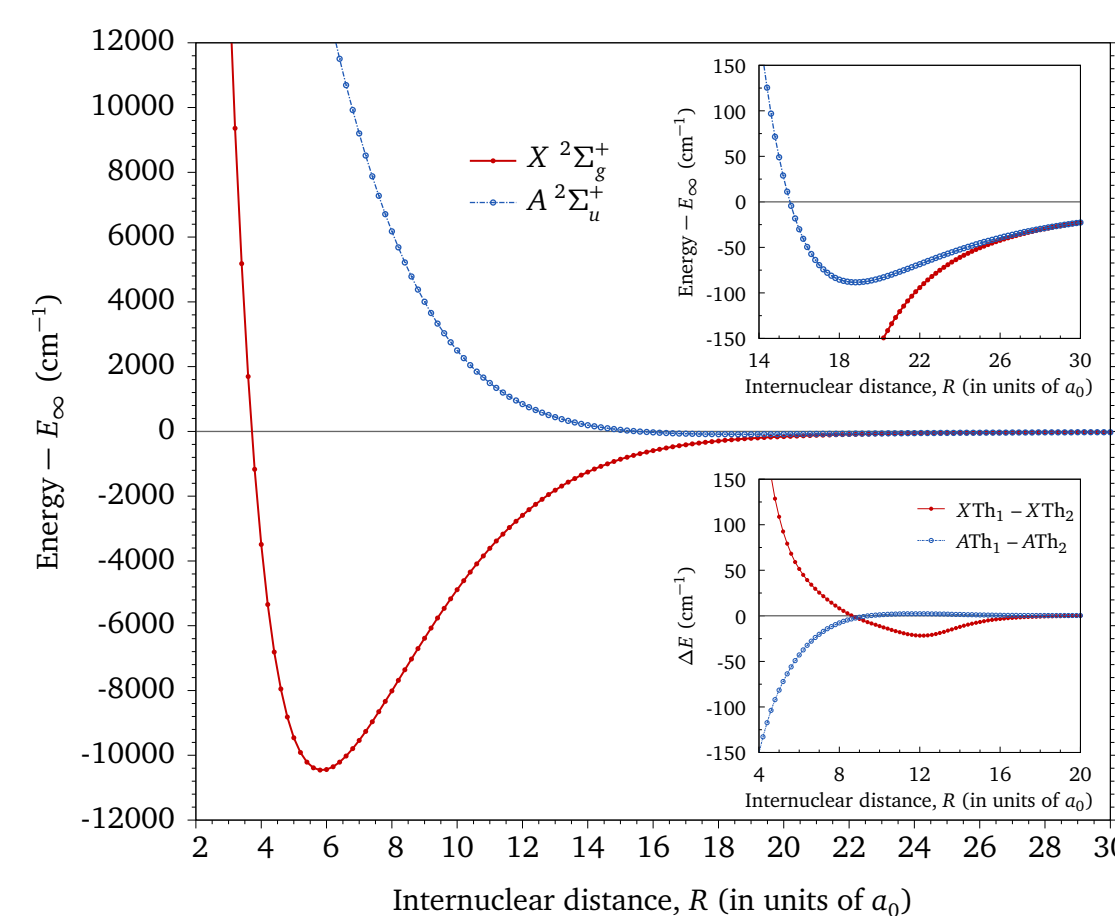
Introduction

Accurate estimation of the scattering parameters at the ultracold temperatures demands precise knowledge of the interactions between the colliding partners. We compute ${}^7\text{Li}^+ - {}^7\text{Li}$ potential energy curves (PECs) for the $X^2\Sigma_g^+$ and $A^2\Sigma_u^+$ states, their low energy scattering phase shifts, and ion-atom total scattering cross section. We examine the effects of minor alterations, within the computational accuracy, in the computed PECs on the scattering parameters. We report a significant change in total cross section in the s -wave limit resulting from the restrained variation in the PECs, and we discuss the primary sources of uncertainties.

Calculation of PECs

■ We compute *ab initio* $X^2\Sigma_g^+$ and $A^2\Sigma_u^+$ curves under the BO approximation using the MOLPRO program package.

■ The complete active space self-consistent field (CASSCF) and multi-reference configuration interaction (MRCI) methods are employed for a set of augmented correlation-consistent basis sets.



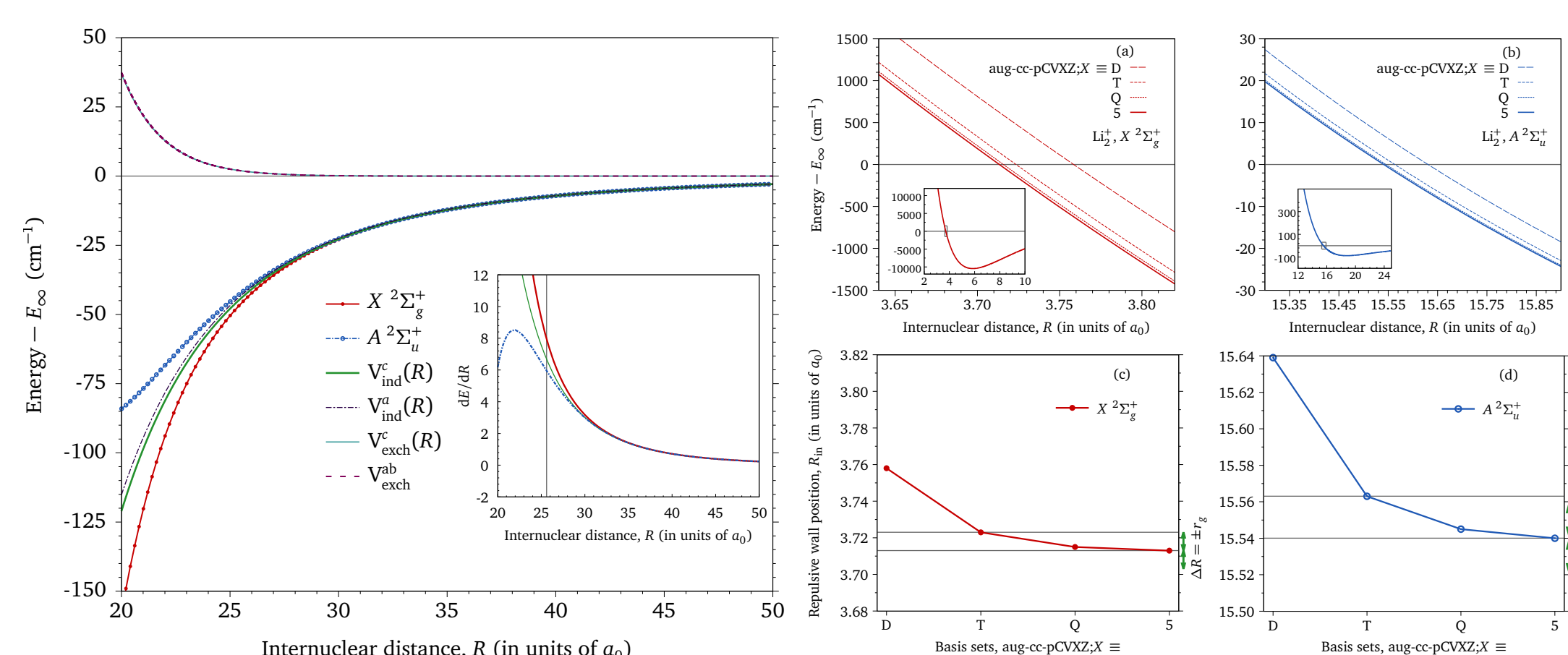
■ Full-valence type CASSCF wave functions are calculated and used as the reference function for the MRCI calculations.

Asymptotic extension and small-R nature of the PECs.

$$V_{g,u}^a(R) = V_{\text{disp}}^a(R) \mp V_{\text{exch}}^a(R)$$

$$V_{\text{disp}}^a(R) = -\frac{1}{2} \left[\frac{C_4}{R^4} + \frac{C_6}{R^6} + \frac{C_8}{R^8} + \dots \right] \quad \&$$

$$V_{\text{exch}}^a(R) = \frac{1}{2} AR^\alpha e^{-\beta R} \left[1 + \frac{B}{R} + \frac{C}{R^2} + \dots \right]$$



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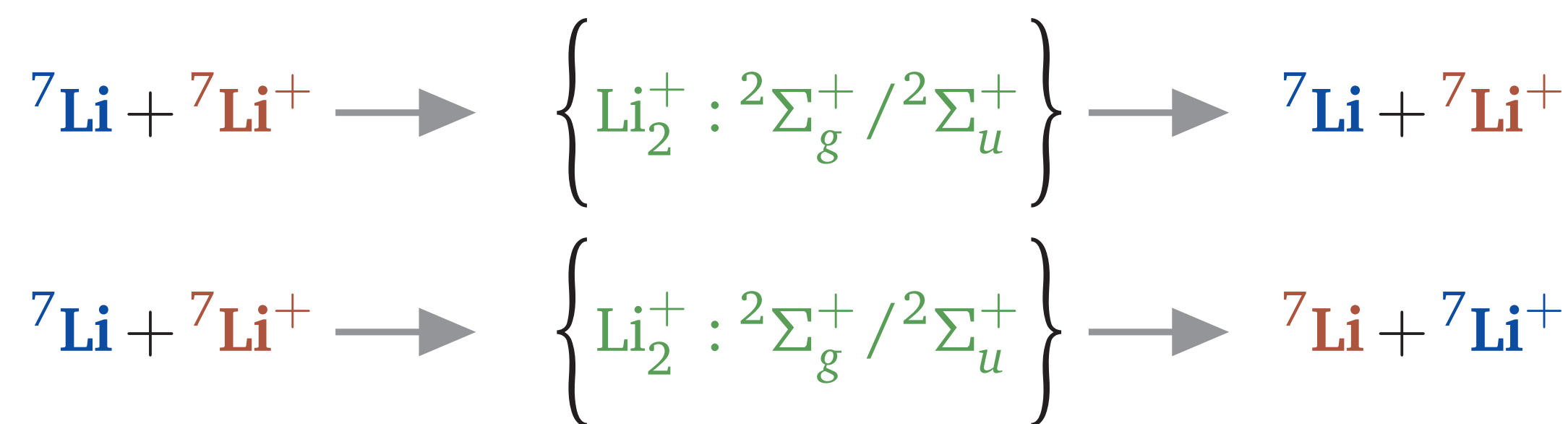
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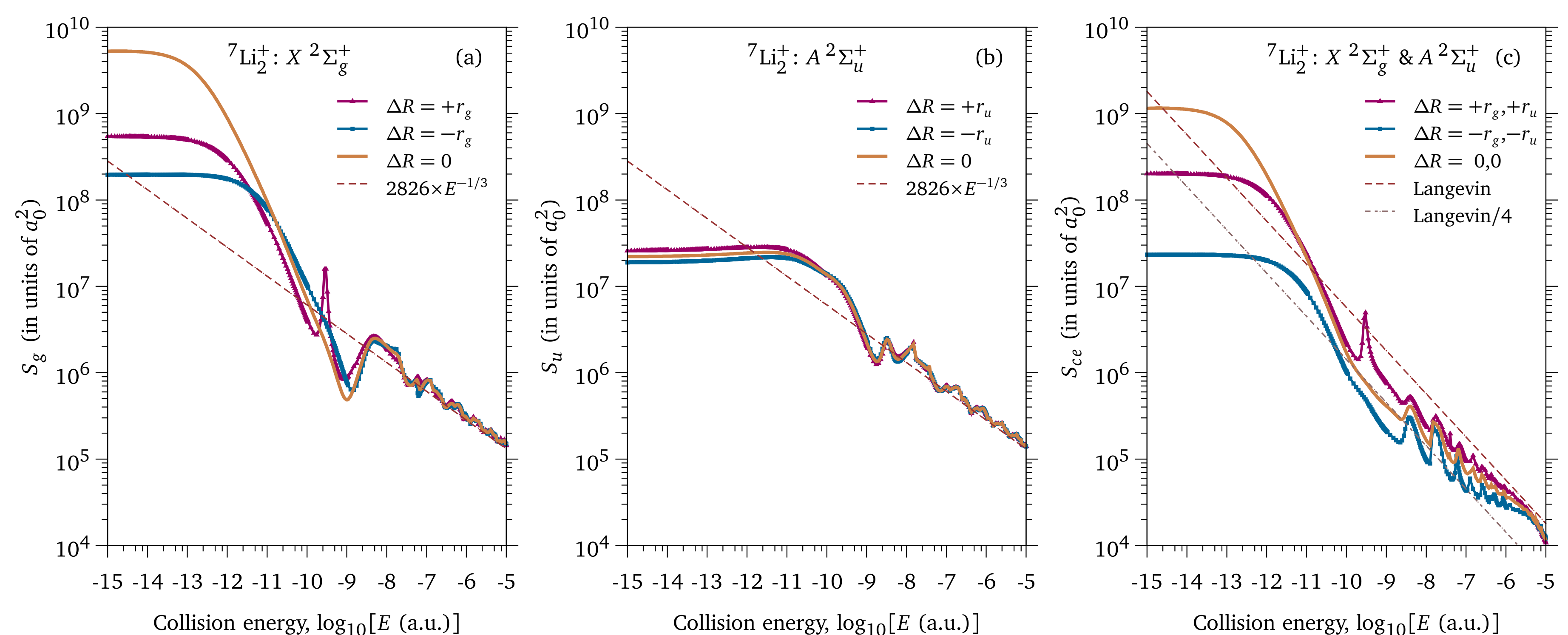
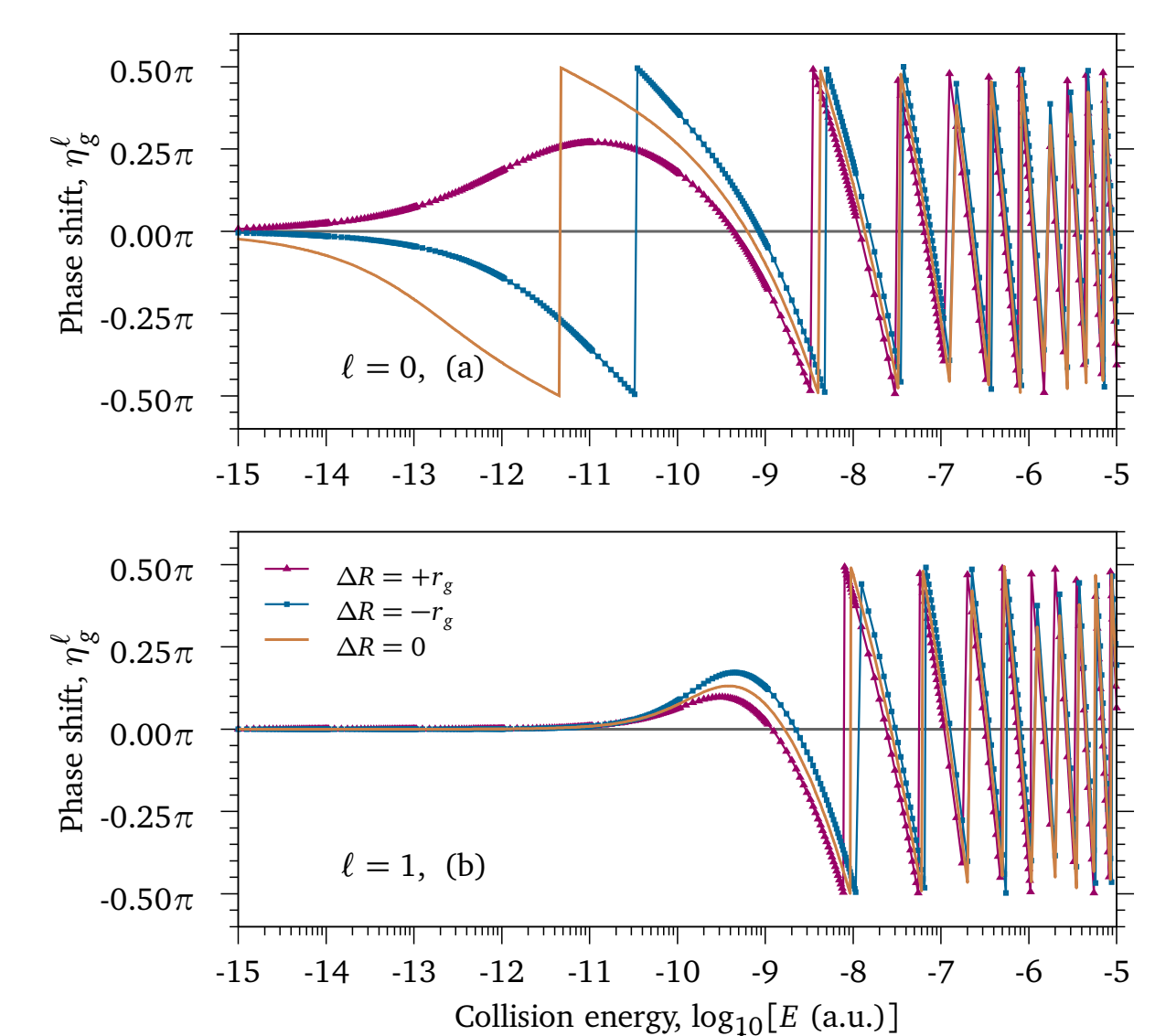
Scattering phase shifts and cross sections



$$S_{g,u}(E) = \frac{4\pi}{k^2} \sum_{l=0}^{\infty} (2l+1) \sin^2(\eta_{g,u}^l); \quad S_{ce}(E) = \frac{\pi}{k^2} \sum_{l=0}^{\infty} (2l+1) \sin^2(\eta_g^l - \eta_u^l)$$

$$\sigma_{\text{tot}}(E) = \frac{4\pi}{k^2} \left[x \left[\sum_{\text{even}} (2l+1) \sin^2(\eta_g^l) + \sum_{\text{odd}} (2l+1) \sin^2(\eta_u^l) \right] + (1-x) \left[\sum_{\text{odd}} (2l+1) \sin^2(\eta_g^l) + \sum_{\text{even}} (2l+1) \sin^2(\eta_u^l) \right] \right]$$

- A careful analysis has been performed to obtain the asymptotic form of the scattering potentials.
- The phase shifts, cross section components, and total scattering cross section at different collision energies for PECs, $X^2\Sigma_g^+$: $\Delta R = \pm r_g$, and **unaltered** $X^2\Sigma_g^+$: $\Delta R = 0$ and for $A^2\Sigma_u^+$: $\Delta R = \pm r_u$, and **unaltered** $A^2\Sigma_u^+$: $\Delta R = 0$ are computed.
- We provide the scattering cross sections for **Direct Elastic Collision**, $\sigma_{\text{tot}}(E)$, and **Resonant Charge Exchange**, $S_{ce}(E)$.



■ Extension of the asymptotic region of PECs and modification to the small-R region are observed to be crucial factors in determining the ultra-cold scattering properties.

■ Contribution of the core electrons of the two nuclei to the small-R region of the PECs, $X^2\Sigma_g^+$ and $A^2\Sigma_u^+$, is large. It plays a significant role in the scattering calculation.

■ Determination of the uncertainty around the computed values is essential in providing the reliable cross section estimates for the future experiments.

■ The scattering lengths, a_g , for the bound PECs $X^2\Sigma_g^+$: $\Delta R = \pm r_g$ are $-6582/3948 a_0$ respectively. a_u for $A^2\Sigma_u^+$: $\Delta R = \pm r_u$ are $1432/1227 a_0$ respectively.

■ Scattering lengths for *ab initio* curves $X^2\Sigma_g^+$: $\Delta R = 0$ and $A^2\Sigma_u^+$: $\Delta R = 0$ are $20465 a_0$ and $1325 a_0$ respectively.

■ Total cross section for ${}^7\text{Li}^+ - {}^7\text{Li}$ system, evaluated for *ab initio* $X^2\Sigma_g^+$: $\Delta R = 0$, $A^2\Sigma_u^+$: $\Delta R = 0$, in the low energy limit is $1.9 \times 10^9 a_0^2$.

■ The study is recently published in Phys. Rev. A **101**, 052702 (2020).

