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

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Experimental research on the ion-atom interactions in dilute, trapped gas systems at ultracold temperatures is rapidly evolving towards detailed probes of the quantum dynamics of the resulting products [1-5]. One of the main experimental goals is to thermalize an atomic ion within the ultracold atomic gas. Despite continuous progress regarding the precise control of the trapped ion motion, reaching the ultra-low relative energy regime ($E/k_B \approx 1\mu K$ or lower) for ion-atom collisions is still challenging. At these energies, quantum effects emerge as only few partial waves contribute to the collision [6]. Due to ion heating as a result of interactions and trap imperfections in dynamical trapping, it is experimentally advantageous to investigate the full quantum regime at the highest possible temperatures. We therefore focus this study on the scattering properties of $^7Li^+$-^7Li as this is a light system, with isotopic abundance, for going toward the quantum regime. We calculate Li^+-Li potential energy curves for the electronic ground and first excited states – $X^2\Sigma^+_g$ and $A^2\Sigma^+_u$ respectively. Scattering phase shifts and total scattering cross section for the $^7Li^+$-^7Li collision are calculated with emphasis on the ultra-low energy domain down to the *s*-wave regime. The effect of physically motivated alterations on the calculated potential energy curves is used to determine the bound of accuracy of the low-energy scattering parameters for the ion-atom system. Accurate large scattering lengths with their bounds are determined. The computed scattering length for the $A^2\Sigma^+_u$ state, $a_u = 1325\ a_0$, is positive and has well-constrained bounds. For the $X^2\Sigma^+_g$ state, the scattering length, $a_g = 20465\ a_0$ has a large magnitude, and it is sensitive to the restrained change of the potential, due to the presence of a vibrational state in the vicinity of the dissociation limit. Study of $^7Li^+$-^7Li is published recently in Pandey *et al.* [7].

References

[1] Z. Meir, T. Sikorsky, R. Ben-Shlomi, N. Akerman, Y. Dallal, and R. Ozeri, Phys. Rev. Lett. 117, 243401 (2016).
[2] S. Haze, S. Hata, M. Fujinaga, and T. Mukaiyama, Phys. Rev. A 87, 052715 (2013).
[3] K. Ravi, S. Lee, A. Sharma, G. Werth, and S. Rangwala, Nat. Commun. 3, 1126 (2012).
[4] R. Côté and A. Dalgarno, Phys. Rev. A 62, 012709 (2000).
[5] P. Zhang, E. Bodo, and A. Dalgarno, J. Phys. Chem. A 113, 15085 (2009).
[6] R. Côté, in Advances in Atomic, Molecular, and Optical Physics, edited by E. Arimondo, C. C. Lin, and S. F. Yelin (Academic Press, San Diego, CA, 2016), Vol. 65, pp. 67–126.
[7] A. Pandey, M. Niranjan, N. Joshi, S. A. Rangwala, R. Vexiau, O. Dulieu, Phys. Rev. A 101, 052702 (2020)