Calculation of scattering parameters for ultracold ^{6}Li–^{7}Li elastic collisions*

Zhang Ji-Cai(张计才)[a)†], Sun Jin-Feng(孙金锋)[a)b)], and Liu Yu-Fang(刘玉芳)[a)]

[a)] *College of Physics and Information Engineering, Henan Normal University, Xinxiang* 453007, *China*
[b)] *Department of Physics, Luoyang Normal College, Luoyang* 471022, *China*

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This paper theoretically studies the elastic scattering properties in a mixture of ^{6}Li and ^{7}Li atoms at cold and ultracold temperatures. Based on the constructed accurate interatomic potential of the triplet state for ^{6}Li^{7}Li mixture by the mass scaling method, it calculates the interspecies s-wave scattering lengths and the p-wave scattering lengths by the variable phase method and the semiclassical method, respectively. The scattering length is in good agreement with the experiment. The partial-wave and total cross sections are also calculated and a rich resonance structure is found.

Keywords: scattering length, elastic cross section, variable phase method

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1. Introduction

Cold and ultracold atomic collisions have special properties[1,2] and play a crucial role in the production of Bose–Fermi ensembles of various homonuclear and heteronuclear alkali-metal dimers and dual species Bose–Einstein condensation.[3−7] The interspecies s-wave scattering length, for example, determines the efficiency of the sympathetic cooling procedure. In addition, knowledge of the scattering length is important in order to predict macroscopic properties of these mixed systems, such as the stability and phase separation of binary degenerate systems, or microscopic properties, such as the occurrence of Feshbach resonances in the interspecies collisions. Therefore the interspecies collisions currently attract many experimental and theoretical researches on several mixtures, such as, NaLi,[3], KLi,[4] CsLi,[5] NaRb,[6] RbCs.[7] Scattering between two heteronuclear atoms at ultracold temperature is characterized by the s-wave scattering length, the effective range, and the p-wave scattering volume, the contributions from higher angular momenta being negligible at very low energy.[8,9]

Among the alkali-metal atoms, lithium has a special status because both bosonic and fermionic isotopes are available and both Bose–Einstein condensation and Fermi degeneracy have been achieved. In recent years cold collisions between ^{7}Li atoms and between ^{6}Li atoms have been studied extensively both experimentally and theoretically. Relatively little attention has been devoted to collisions where an ^{7}Li atom collides with a ^{6}Li atom. In the previous study, we have investigated the cold and ultracold collision properties for ^{7}Li–^{7}Li[10] and ^{6}Li–^{6}Li,[11] respectively. In this paper, we will study the cold ^{6}Li–^{7}Li elastic collision properties in detail. Atomic units are used unless otherwise stated.

2. Cold collision theory

The Schrödinger equation for the two colliding atoms, in the centre-of-mass coordinate systems, can be written as

$$\left[\frac{\mathrm{d}^2}{\mathrm{d}R^2} + k^2 - \frac{l\,(l+1)}{R^2} - \mathrm{V}\,(R)\right] u_l\,(R) = 0, \quad (1)$$

where k is the wave number given in terms of the energy E of relative motion by $k^2 = 2\mu E/\hbar^2$, μ is the reduced mass and $V\,(R)$ is $2\mu/\hbar^2$ times the interaction potential. The solution must be regular and behave asymptotically as

$$u_l\,(R) \sim A_l\left[\mathrm{j}_l\,(kR) + \tan\delta_l \mathrm{n}_l\,(kR)\right], \quad R \to \infty, \quad (2)$$

where A_l is a normalization constant, $\mathrm{j}_l\,(x)$ and $\mathrm{n}_l\,(x)$ are the spherical Bessel and Neumann functions, and

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†Corresponding author. E-mail: jicaiz@gmail.com

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δ_l the scattering phase. The total and partial-wave cross sections may be defined by

$$\sigma = \sum_{l=0}^{\infty} \sigma_l = \sum_{l=0}^{\infty} \frac{4\pi}{k^2}(2l+1)\sin^2\delta_l. \tag{3}$$

In the variable phase approach, the phase δ_l can be expressed in effective range theory by[8]

$$\tan\delta_l(R) = -k^{2l+1}[a_l(R) + k^2 b_l(R) + O\left(k^4\right)], \tag{4}$$

where the coefficients $a_l(R)$ satisfy the differential equation of Riccati type

$$\frac{\mathrm{d}}{\mathrm{d}R}a_l(R) = \left[\frac{1}{(2l+1)!!}R^{l+1} - \frac{1}{(2l-1)!!}R^{-l}a_l(R)\right]^2 V(R). \tag{5}$$

For $l=0$ and $l=1$, and $R\to\infty$, these coefficients are the s-wave scattering length a_{s} and p-wave scattering volume a_{p} (or V). The numerical solution of Eq. (5) is non-trivial. The function $a_l(R)$ contains poles which correspond to the bound states supported by the potential illustrated in Fig. 1. The finite difference methods such as the Runge–Kutta method are unsuitable, and equation (5) can be solved by changing the variable. Substituting

$$a_l(R) = \tan\theta(R) \quad \text{and} \quad R = \tan\phi(R), \tag{6}$$

into Eq. (5), we obtain[8,12,13]

$$\frac{\mathrm{d}\theta(\phi)}{\mathrm{d}\phi} = \sec^4\phi\sin^2\left[\theta(\phi)-\phi\right]V\left[\tan(\phi)\right], \quad l=0, \tag{7}$$

$$\frac{\mathrm{d}\theta(\phi)}{\mathrm{d}\phi} = \frac{\cos^2(\theta)}{\sin^2(\phi)}\left[\frac{\tan^3(\phi)}{3} - \tan(\theta)\right]V\left[\tan(\phi)\right], \quad l=1, \tag{8}$$

which can be solved over a range $[0,\phi_{\mathrm{c}}]$ by the Runge–Kutta method where the value of ϕ_{c}, corresponding to $\arctan R_{\mathrm{C}}$ is close to $\pi/2$.

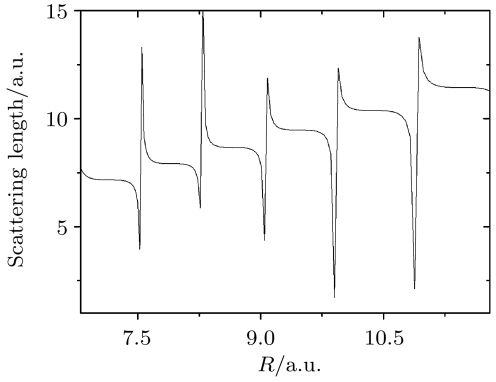


Fig. 1. The scattering length for ^{6}Li–^{7}Li in ground state, as a function of the interatomic separation R.

The semiclassical results have been derived for the s-wave scattering length[14] and the p-wave scattering volume[15] with long-range potentials falling off as fast as $1/R^6$. These parameters can be expressed by the following equations:

$$a^{\mathrm{SC}} = \bar{a}\left[1 - \tan\left(\Phi - \pi/8\right)\right], \tag{9}$$

$$V^{\mathrm{SC}} = -\frac{\beta_6^3\Gamma(1/4)}{12\sqrt{2}\Gamma(7/4)}\frac{\bar{a}-a^{\mathrm{SC}}}{2\bar{a}-a^{\mathrm{SC}}}, \tag{10}$$

where $\bar{a} = \sqrt{2}\beta_6\Gamma(3/4)/\Gamma(1/4)$ is the mean scattering length with $\beta_6 = (2\mu C_6)^{1/4}$, and $\Phi = \int_{R_0}^{\infty}\sqrt{2\mu V(R)}\mathrm{d}R$ is the semiclassical phase with $V(R_0) = 0$.

3. Results and discussion

To calculate elastic scattering properties of two atoms, the complete potential energy curve is needed. The interaction potential curve of two neutral atoms is due to the electronic interactions of electrons and the two nuclei. Changing the number of neutrons in the nuclei should therefore not alter the interaction potential curve if the nuclei are regarded as infinitely heavy in comparison with the electrons. So it is possible to predict the scattering length from one isotope combination to another, this method is often referred to as mass-scaling. The Li_2 interatomic potentials have been extensively studied experimentally and theoretically for the lowest electronic triplet state. Using the accurate interatomic potential energy curve constructed in Ref. [10], we calculate the scattering parameters for the triplet states of ^{6}Li–^{7}Li mixture by mass scaling method. In order to calculate the scattering length and the scattering volume by using the Riccati equations (7) and (8), we must obtain solutions at infinite values of the interatomic

separation. In practice, the calculation stops at some value R_C, but R_C must be chosen very large, and such choices increase computation time and accumulated error. Ouerdane *et al.*[8,13] showed how the Riccati equation can be used to predict corrections, and calculate scattering length, thus compensate for stopping the calculation at finite distance R_C. Such corrections enable us to make calculations with smaller values of R_C while maintaining the desired accuracy. For $R > R_C$, the lower $a_0^{(L)}$ and upper $a_0^{(U)}$ corrections of the scattering length are given by Eqs. (28) and (29) in Ref. [13], respectively, and a better approximation value of the scattering length $a_0^{(I)}$ is obtained in Eq. (33) of the same paper. The results are shown in Fig. 2. The curve $a_0^{(L)}$ (or $a_0^{(U)}$) illustrates how the lower (upper) bound correction leads to the scattering length that approaches $a_0 = 40.8$ a.u. from below (above), $a_0^{(I)}$ is faster than $a_0^{(U,L)}$ to approach its limit. Our obtained s-wave scattering length is in good agreement with the recent accurate measurement in Ref. [15], which clearly demonstrates the accuracy of our potential curve newly constructed by mass scaling method. Table 1 shows the results for the s-wave scattering lengths and the p-wave scattering volumes for the ^{6}Li–^{7}Li triplet state.

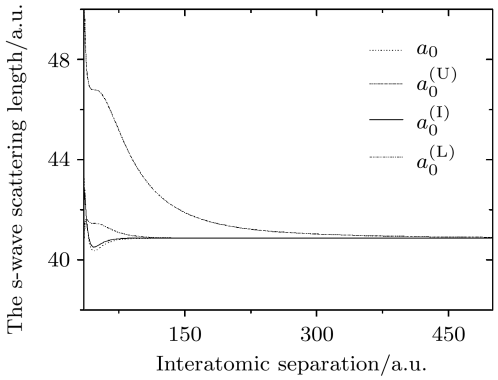


Fig. 2. The accumulated and corrected scattering lengths for ^{6}Li–^{7}Li in the ground state, as functions of the interatomic distance R.

Table 1. The s-wave scattering length and the p-wave scattering length for the triplet state of ^{6}Li–^{7}Li mixture.

	variable phase method	semicalssical method	Ref. [16]
s-wave scattering length	40.8	41.2	40.9 ± 0.2
p-wave scattering length*	30.5	30.1	

* The p-wave scattering length $a_p = \sqrt[3]{V}$.

Those data are also calculated by using the semiclassical method, and the majority of the results for a^{SC} and V^{SC} shown in Table 1 is within 2%, of the variable phase values. Considering the sensitivity of the semiclassical scattering length a^{SC}, to the semiclassical phase Φ for the values arising here, we find that the success of the semiclassical estimate for the scattering length is certainly encouraging. Overall, these comparisons also suggest that the semiclassical result for the scattering volume can provide a robust estimate of the full result, once the scattering length and the long-range properties are known.

Using our constructed potential, we can also calculate the collisional properties of other partial waves at non-zero energies. Figure 3 shows the energy-dependent cross sections for the collisions of ^{7}Li and ^{6}Li. In atom–atom collisions, the fundamental difference between bosons and fermions is seen in the behaviour of cross sections. For two identical spin-polarized bosons, the elastic cross section becomes constant as the collision energy goes to zero because only the s-wave contributes. In contrast, for two fermions, the elastic cross section decreases as the collision energy decreases because there is no s-wave and only p-wave contributes at ultracold temperature. This means that the dominant interaction is via p-wave collisions. However, p-wave scattering cross sections are very small in ultracold temperature and evapourative cooling fails to work. The large cross section between ^{7}Li and ^{6}Li atoms at the ultralow energies is consistent with the large s-wave scattering length and the efficient sympathetic cooling.[17] The

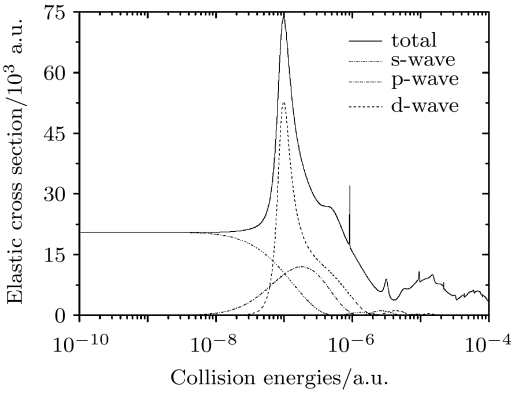


Fig. 3. Total cross section and s-, p- and d-wave cross sections versus collision energies for ^{6}Li–^{7}Li atoms scattering in the $a^3\Sigma^+$ state.

elastic cross sections display typical Wigner-threshold behaviour for s-wave scattering at temperature less than 1 mK, where the elastic cross section is a content given by $\sigma = 4\pi a^2$, and then increases slowly before at higher energies. The s-wave cross section tends to decrease with increasing energy, but the decrease is overcome by higher partial-wave contributions which initially increase with energy from zero before passing through maxima and decrease. The $l = 1$ partial wave starts to contribute at an energy of 1.0×10^{-9} a.u., corresponding to a temperature of 0.3 mK, and higher l becomes important at larger energies. The cross section can be resonantly enhanced by shape resonance, caused by the existence of quasibound rovibrational levels by the centrifugal barrier. We predict that a strong resonance appears in the $l = 2$ partial wave at an energy of 9.8×10^{-8} a.u.

4. Summary

By mass scaling method the accurate potential curves for the triplet ground states of the ^{6}Li–^{7}Li mixture have been constructed, and the elastic scattering parameters between ^{6}Li and ^{7}Li atoms are calculated by means of the variable phase method and the semiclassical method, respectively, a good agreement is obtained. Our results are in good agreements with experimental work for the triplet state. The partial wave (l = s, p, d) and total elastic cross sections are also calculated. Total elastic cross sections are very large and dominated by s-wave scattering at ultracold temperature. Shape resonance due to angular momentum barriers occurs and further experimental studies of ultracold collisions will help us to test those resonances. In the cold atom experiment the scattering length in the hyperfine state and its dependence on the magnetic field[18] are important quantities, So we shall investigate those problems in the future work.

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