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Accurate calculation of the elastic scattering properties of ^{7}Li atoms at ultralow temperatures*

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The elastic scattering properties for collisions between two ^{7}Li atoms are investigated in the cold and ultracold regimes separately. Based on recent theoretical and experimental results, we present the improved hybrid potentials for the singlet $X^1\sum_g^+$ and triplet $a^3\sum_u^+$ ground states of the Li_2. Our calculated values for the scattering lengths a and the effective ranges r_e are compared with previous ones, and found them to be in good agreement. The scattering lengths are $34.6a_0$ for the singlet state and $-27.6a_0$ for the triplet state. Shape resonances occur in the collisions at low energies. We also calculate the total cross sections and the energy positions of shape resonances for both $X^1\sum_g^+$ and $a^3\sum_u^+$ states.

Keywords: scattering length, elastic cross section, shape resonance
PACC: 3400, 3420, 3440

1. Introduction

Atomic collisions are a classical topic of quantum mechanics.[1] With the rapid development of laser cooling and trapping techniques,[2] atomic collision properties in the cold and ultracold regimes have become applicable to some fields. They, for example, play a crucial role in the achieving of Bose–Einstein condensation[3] and Fermi degeneracy[4] in dilute atomic gases. In the very-low-energy regime, elastic collision properties between neutral atoms are determined by the s-wave scattering length and the effective range. The stability of a condensation is indeed controlled by the sign of the scattering length.[5] In particular, for bosonic atoms with $a > 0$ the possible Bose condensate is stable, whereas for $a < 0$ it is unstable,[6] and only a finite number of atoms can be found in the condensate state in a trap. The scattering length is very sensitive to the interaction potentials between the colliding systems over an extended range of internuclear distances. For ^{7}Li atoms, the recent theoretical and experimental investigation of its interatomic potentials have made it feasible to more accurately investigate the collision properties. In this paper, we construct the accurate potentials for the singlet and triplet states of ^{7}Li atoms, and then accurately calculate the scattering lengths and the effective ranges for the singlet $X^1\sum_g^+$ and triplet $a^3\sum_u^+$ states. The potentials can accurately predict the s-wave cross sections and positions of shape resonances. Atomic units are adopted unless otherwise indicated.

2. Low-energy elastic scattering theory

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

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

Here k is the wave number and is related to the energy E of relative motion by $k^2 = 2\mu E/\hbar^2$, μ is the reduced mass of the collision system, and $U(r) = 2\mu V(r)/\hbar^2$, where $V(r)$ is the interatomic potential. The solution must be regular and behave asymptotically as

$$u_l(r) \sim A_l\left[j_l(kr) + \tan\delta_l n_l(kr)\right], \quad r \to \infty, \quad (2)$$

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where A_l is a normalization constant, $j_l(x)$ and $n_l(x)$ are the spherical Bessel and Neumann functions respectively, and δ_l is the partial-wave phase shift. The value of δ_l can be computed using the formula[7]

$$\tan\delta_l = \frac{u_l(r_\mathrm{b})\,s(r_\mathrm{a}) - u_l(r_\mathrm{a})\,s(r_\mathrm{b})}{u_l(r_\mathrm{a})\,c(r_\mathrm{b}) - u_l(r_\mathrm{b})\,c(r_\mathrm{a})}, \tag{3}$$

where r_a and r_b are two distinct points in the asymptotic regime, $s(r) = krj_l(kr)$ and $c(r) = -krn_l(kr)$. Two ^{7}Li atoms in ground-state interact via electronic spin-singlet $\mathrm{X}^1\sum_\mathrm{g}^+$ and spin-triplet $\mathrm{a}^3\sum_\mathrm{u}^+$ molecular potentials, with potential–energy curves $V_\mathrm{g}(r)$ and $V_\mathrm{u}(r)$, respectively. Elastic singlet and triplet cross sections may be defined as

$$\sigma_\mathrm{el}^{\mathrm{S/T}} = \frac{4\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)\sin^2\delta_l^{\mathrm{S/T}}, \tag{4}$$

where S and T stand for singlet and triplet, respectively. At small energies or wave numbers the phase shifts are given by effective range expansions,[8] and the $l = 0$ contribution dominates the cross sections. Hence the low-energy scattering is described by the $l = 0$ scattering length a and the effective range r_e, and $\cot\delta_\mathrm{o}$ may be expanded in the form

$$k\cot\delta_0 = -\frac{1}{a} + \frac{1}{2}r_\mathrm{e}k^2 + O\left(k^4\right). \tag{5}$$

It has been shown[9,10] that for a potential falling off as R^{-6} the scattering length, a^sc and the effective range, r_e^sc in the semiclassical approximations are given by

$$a^\mathrm{sc} = \bar{a}\left[1 - \tan(\Phi - \pi/8)\right], \tag{6}$$

where

$$\bar{a} = \sqrt{2\gamma}\Gamma\left(\frac{3}{4}\right)\Big/\Gamma\left(\frac{1}{4}\right), \quad \gamma = \sqrt{2\mu C_6}/\hbar, \tag{7}$$

$$\Phi = \int_{R_0}^{\infty}\sqrt{-2\mu U(r)}\mathrm{d}r, \quad V(R_0) = 0, \tag{8}$$

and

$$r_\mathrm{e}^\mathrm{sc} = \frac{\sqrt{2\gamma}}{3}\left[\frac{\Gamma\left(\frac{1}{4}\right)}{\Gamma\left(\frac{3}{4}\right)} - 2\frac{\sqrt{2\gamma}}{a} + \frac{\Gamma\left(\frac{3}{4}\right)}{\Gamma\left(\frac{1}{4}\right)}\frac{4\gamma}{a^2}\right]. \tag{9}$$

Gribakin and Flambaum have also shown that the number of bound state n_b is given by

$$n_\mathrm{b} = \left[\frac{\Phi}{\pi} - \frac{n-1}{2(n-2)}\right] + 1, \tag{10}$$

where [ ] denotes the largest integer.

3. Interatomic potentials

To investigate elastic scattering properties of lithium atoms, complete potential energy curves from the repulsive part up to a few hundred Å of interatomic distance are needed. The interaction potentials of two lithium atoms have been discussed in a vast literature.[11–14] What is more, more accurate experimental RKR (Rydberg–Klein–Rees) potential values and *ab initio* values for the triplet state, and a more accurate estimate of the C_n coefficients for Li_2 are available. Thus it is feasible to improve the hybrid potentials for both the $\mathrm{X}^1\sum_\mathrm{g}^+$ and $\mathrm{a}^3\sum_\mathrm{u}^+$ states.

For the $\mathrm{a}^3\sum_\mathrm{u}^+$ state, we use the new RKR data in Ref.[15], and we extend this RKR curve in a short-range region with 6 points from Konowalow, Regan, and Rosen Krantz[16] (at $3.00a_0$), Schmidt–Mink, Müller, and Meyer[17] (at $3.25a_0$ and $3.50a_0$) and Halls *et al*[18] (between $3.78a_0$ and $5.67a_0$). For ($R \le 5.67a_0$) we use the exponential form

$$V(r) = A\exp(-BR), \tag{11}$$

where A and B are evaluated from a cubic spline fitting of the data points for $V(r)$.

At large internuclear distance, the long-range singlet and triplet potentials V_S and V_T are written in the form

$$V_\mathrm{S,T} = -\frac{C_6}{R^6} - \frac{C_8}{R^8} - \frac{C_{10}}{R^{10}} \mp V_\mathrm{EX}, \tag{12}$$

where the Smirnov and Chibisov[19] exchange part is

$$V_\mathrm{EX} = CR^\alpha\exp(-\beta R) \tag{13}$$

in which the values of α and β are the same as those in Ref.[20]. C_6, C_8 and C_{10} are taken as the recent accurate values calculated by Mitroy and Bromley.[21] Our potential for the $\mathrm{X}^1\sum_\mathrm{g}^+$ state is very identical to the singlet potential in Ref.[22] in short and intermediate ranges, and is the same as V_T in long ranges, except the exchange term is attractive. The adopted hybrid potential curves for the singlet and triplet states are illustrated in Fig.1 and the potential parameters are listed in Table 1.

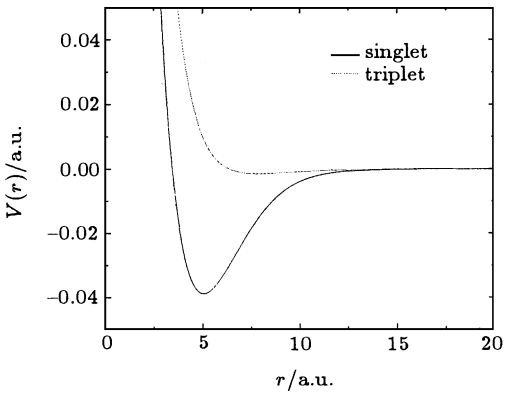


Fig.1. Adopted potential curves for the singlet $X^1\sum_g^+$ and triplet $a^3\sum_u^+$ states.

Table 1. Long-range dispersion coefficients and exchange interaction parameters used for both $X^1\sum_g^+$ and $a^3\sum_u^+$ potentials.

C_6	C_8	C_{10}	C	α	β
1394.60	83515	7381100	0.01141	4.55988	1.25902

4. Results and discussion

Equation (1) is numerically solved by the Numerov method, and the phase shift δ_l is calculated by using the formula (3). We determine the scattering lengths a and the effective range r_e by fitting the scattering phase shifts δ_0 to the effective range expansion formula (5). Our values of a are $34.558a_0$ for the singlet state and $-27.623a_0$ for the triplet state; they are very consistent with the recent accurate measurements in Ref.[13], which clearly demonstrates the accuracy of our potential curves newly constructed. We also calculate the scattering lengths a and the effective ranges r_e using Eq.(6) and Eq.(10), respectively. The scattering lengths and the effective ranges for the singlet $X^1\sum_g^+$ and triplet $a^3\sum_u^+$ states are presented in Table 2.

Table 2. Scattering lengths a and effective ranges r_e in units of atomic units for (a) singlets and (b) triplets.

Ref	scattering length	effective range
	(a) singlet	
present	34.558	71.5
present: semiclassical	34.856	73.1
Ref.[12]	36.9	66±1
Ref.[13]	33±2	
	(b) triplet	
present	−27.623	524.2
present: Semiclassical	−27.619	523.8
Ref.[12]	−17.2	1024±4
Ref.[13]	−27.6±0.5	

The results in Table 2, in which a is calculated from Eqs.(5) and (6) and r_e from Eqs.(5) and (10), demonstrate generally good agreement between the quantal and the semiclassical calculations, but the scattering lengths we obtained are different, especially for the triplet state, from those presented by Côté *et al*[12] using different potentials. Nevertheless we believe our scattering lengths and effective ranges are more reliable. Due to the $X^1\sum_g^+$ potential well being much deeper than the $a^3\sum_u^+$ well, we find 42 bound levels for the $X^1\sum_g^+$ state and 11 bound levels for the $a^3\sum_u^+$ state by calculating bound levels for each potential using the formula (10) of Gribakin and Flambaum.[9]

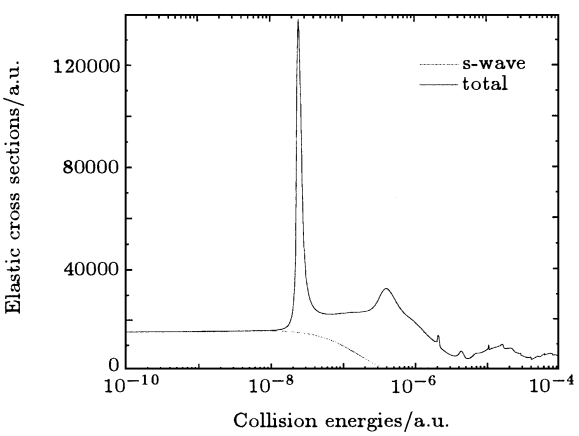


Fig.2. Total cross section and s-wave cross section *versus* collision energy for scattering in the $X^1\sum_g^+$ state.

Figure 2 presents the energy dependences of cross section for the elastic s-wave scattering between two ^{7}Li atoms at cold and ultracold collision energies for the $X^1\sum_g^+$ state. The total cross section is also presented in Fig.2. The elastic cross section displays typical Wigner-threshold behaviour for s-wave scattering at temperature less than 1 mK, where the elastic cross section is a constant given by $\sigma = 4\pi a^2$, and then increases slowly before decreasing at higher energies. This behaviour can be explained by the values of a and r_e. For $l = 0$ Eq.(4) becomes

$$\sigma_{el}^S = \frac{4\pi}{k^2}\sin^2\delta_o = \frac{4\pi}{k^2 + k^2\cot^2\delta_0}. \qquad (14)$$

Using the effective range expansion and retaining terms up to the order of k^2, we find

$$\sigma_{el}^S \approx 4\pi a^2\left[1 + ak^2(r_e - a)\right]. \qquad (15)$$

Since $(r_e - a)$ and a are positive, Eq.(15) shows the feature consistent with the calculated behaviour. The s-wave cross section tends to decrease with energy increasing, but the decrease is supplemented by higher partial-wave contributions which initially increase with energy form zero before passing through maxima and the decrease. We also calculate the elastic s-wave cross section and total cross section for the $a^3\sum_u^+$ state, and the results are illustrated in Fig.3. With the increase of collision energy, higher angular momentum waves makes a contribution to the scattering. Oscillations occur through the addition of small number of partial waves. Sharper structures result from shape resonances, the resonances that are associated with quasibound diatomic levels trapped behind a centrifugal barrier and are important because the collision energies of ultracold atoms are typically lower than the centrifugal barrier even for the lowest partial waves. Using our new potential curves for the $X^1\sum_g^+$ and $a^3\sum_u^+$ states of lithium molecules, we compute the energy positions the shape resonances, and the results are listed in Table 3. The present predictions for the resonance energy positions are in good agreement with those given by Côté *et al.*[23] Strong resonances appear in the $l = 2$ partial wave at an energy of 2.45×10^{-8}a.u. for the $X^1\sum_g^+$ state and in the $l = 4$ and $l = 5$ partial waves for the $a^3\sum_u^+$ state, respectively, at an energy of 5.1×10^{-7}a.u. and 1.4×10^{-6}a.u.

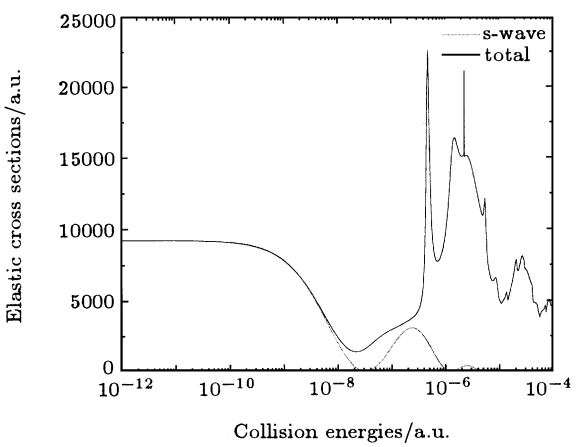


Fig.3. Total cross section and s-wave cross section *versus* collision energy for scattering in the $a^3\sum_u^+$ state.

Table 3. Shape resonance energies for the singlet $X^1\sum_g^+$ and triplet $a^3\sum_u^+$ potentials.

State	l	$\log_{10} E_\Gamma$	$\log_{10} E_\Gamma$ (Ref.[23])
$X^1\sum_g^+$	2	–7.61	–7.64
	3	–6.43	–6.47
	7	–5.68	–5.70
$a^3\sum_u^+$	4	–6.29	–6.23
	5	–5.83	–5.87

5. Conclusions

We have constructed the more accurate potential curves for the singlet and triplet ground states of the lithium molecule, and used these curves to investigate the elastic scattering properties, which are very sensitive to the details of the interatomic potentials, of two ^{7}Li atoms at the cold and ultracold temperatures. Because of the high accuracy of the potentials, we obtain the most probable values for the s-wave scattering lengths and effective ranges. The scattering lengths obtained by using numerical and semiclassical methods are in good agreement with the experimental values. Total elastic cross sections are very large and dominated by s-wave scattering at ultralow temperatures. Shape resonance due to angular momentum barrier is important in low-energy atomic collisions. We compute the positions of several shape resonances theoretically and it may be possible to detect them experimentally.

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