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Calculation of the elastic collision properties of Na and Li atoms at ultracold temperature*

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This paper firstly reports a theoretical study of elastic scattering properties in a mixture of ^{23}Na and ^{7}Li atoms at cold and ultracold temperatures in detail. Based on the new constructed accurate singlet $X^1\Sigma_g^+$ and the triplet $a^3\Sigma_u^+$ states interatomic potentials for ^{23}Na^{7}Li mixture, it calculates the scattering lengths and the effective ranges by three computational methods, and obtains good agreements. Using the mass scaling method, it also calculates ^{23}Na^{6}Li scattering lengths and s-wave and total elastic cross sections, whose rich resonance structures were found and interpreted in terms of quasibound diatomic levels trapped behind a centrifugal barrier.

Keywords: scattering length, elastic cross section, variable phase method
PACC: 3400, 3420, 3440

1. Introduction

Atomic collisions in the cold and ultracold temperatures have attracted substantial attention in recent years[1] with an interdisciplinary impact on physics, chemistry, and quantum information science.[2] Ultracold atomic collisions have special properties[1] and play a crucial role in the production of Bose–Fermi ensembles of various homonuclear and heteronuclear alkali-metal dimmers and dual species Bose–Einstein condensation (BEC). So they currently attract both experimental and theoretical research in this field, for example NaRb,[3] KRb,[4,5] RbCs,[6] LiCs.[7]

In the very-low-energy region, 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.[8] In particular, for bosonic atoms with $a > 0$ the possible Bose condensate is stable, whereas for $a < 0$ it is unstable,[9] and only a finite number of atoms can be found in the condensate state in a trap. The effective range r_e determines the energy dependence of the scattering length at low collision energies to first order, $-1/a_E \approx -1/a + k^2 r_e/2$, where k is the wave number.

Compared with Li_2 and Na_2 molecules, we know little about the NaLi molecule. Spectroscopic studies of NaLi are hampered by difficulties in generating the mixed molecules at high enough and stable concentration, and also by spectral overlaps with Na_2 and Li_2 dimers presented simultaneously in the vapour. Only in 1971 the first experimental observation of NaLi was reported by Hessel,[10] NaLi molecule is of particular interest for theoretical chemists, as there exist the simplest heteronuclear alkali metal system and numerous calculations on it. Quite recently the Na+Li system has been also considered as a promising candidate for production of ultracold heteronuclear molecules.[11]

In this article, we present the first extensive theoretical study of the elastic scattering properties of Li and ^{23}Na atoms in the temperature range which is typical of degenerate gases (i.e. between 300 mK and 1 μK). Since Li has both fermionic and bosonic isotopes, Na+Li mixtures are of particular interest. The scattering information will be useful for forming a BEC of polar molecules and future experiments on ultracold Na+Li mixtures. Scattering length is very sensitive to the interaction potentials between the colliding systems over an extended range of internuclear distances. Due to the recent theoretical and exper-

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imental investigation of its interatomic potentials, it is possible and needs to perform more precise of calculations collision properties. In this paper, we firstly construct the improved accurate potentials for the singlet and triplet states of Na^7Li molecule, and then precisely calculate the scattering lengths and the effective ranges for the singlet and triplet states. By the mass scaling method, we also calculate the scattering parameters for the scattering between Na and ^{6}Li atom in the ultralow temperature. Shape resonances occur in the ultralow temperature atomic collisions. Atomic units are assumed unless otherwise indicated.

2. Low-energy collision theory

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

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

where $k^2 = 2\mu E/\hbar^2$, μ is the reduced mass of the collision system, and $U(r) = 2\mu V(r)/\hbar^2$, here $V(r)$ is the interatomic 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 normalization constant, $\mathrm{j}_l(x)$ and $\mathrm{n}_l(x)$ are the spherical Bessel and Neumann functions, and δ_l is the partial-wave phase shift. The value of δ_l can be computed by using the formula in Ref.[12]. Elastic singlet and triplet cross sections may be defined by

$$\sigma_{\mathrm{el}}^{\mathrm{S/T}} = \frac{4\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)\sin^2\delta_l^{\mathrm{S/T}}, \quad (3)$$

where S and T stand for singlet and triplet, respectively. The low-energy scattering is described by the $l = 0$ scattering length a and the effective range r_{e}, $\cot\delta_0$ may be expanded in the form

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

The scattering length also satisfies the differential equation in the nuclear separation R of the Riccati type[13,14]

$$\frac{\mathrm{d}a(R)}{\mathrm{d}R} = \left[R - a(R)\right]^2 V(R). \quad (5)$$

The numerical solution of Eq.(5) is non-trivial. The function $a(R)$ contains poles which correspond to the bound states supported by the potential as we illustrate in Fig.1.

So, we make the change of variables

$$a(R) = \tan\theta(R) \quad (6)$$

and

$$R = \tan\phi(R) \quad (7)$$

to obtain the equation

$$\frac{\mathrm{d}\theta(\phi)}{\mathrm{d}\phi} = \sec^4\phi\sin^2\left[\theta(\phi) - \phi\right]V\left[\tan(\phi)\right]. \quad (8)$$

The Runge–Kutta method[15] with a self-adjusting step length was used to solve Eq.(8) over a range $[0,\ \phi_c]$.

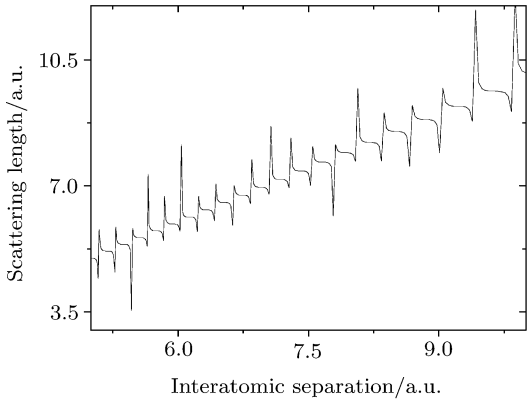


Fig.1. The singlet scattering length in Na-^{7}Li collision as functions of interatomic separation R.

It has been shown[16,17] that for a potential falling off as R^{-6} the semiclassical approximations to the scattering length, a^{sc} and the effective range, $r_{\mathrm{e}}^{\mathrm{sc}}$ are given by

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

where

$$\bar{a} = \sqrt{2\gamma}\,\Gamma\left(\frac{3}{4}\right)\Big/\Gamma\left(\frac{1}{4}\right), \quad \gamma = \sqrt{2\mu C_6}/\hbar,$$
$$\Phi = \int_{R_0}^{\infty}\sqrt{-2\mu U(r)}\mathrm{d}r, \quad V(R_0) = 0, \quad (10)$$

and

$$r_{\mathrm{e}}^{\mathrm{sc}} = \frac{\sqrt{2\gamma}}{3}\left[\frac{\Gamma\left(\frac{1}{4}\right)}{\Gamma\left(\frac{3}{4}\right)} - 2\frac{\sqrt{2\gamma}}{a} + \frac{\Gamma\left(\frac{3}{4}\right)}{\Gamma\left(\frac{1}{4}\right)}\frac{4\gamma}{a^2}\right]. \quad (11)$$

Gribakin and Flambaum have also shown that the number of bound states n_{b} is given by[16,17]

$$n_{\mathrm{b}} = \left[\frac{\Phi}{\pi} - \frac{5}{8}\right] + 1, \quad (12)$$

where [ ] indicates the largest integer.

3. Interatomic potentials

To calculate elastic scattering properties of two alkali metal atoms, we need complete potential energy curves, from the repulsive part up to a few hundred Å interatomic distances (1 Å=0.1 nm). The interaction potentials of lithium and sodium atoms have been discussed in many literatures.[18−22]

For the $X^1\Sigma_g^+$ states, we used the IPA data in Ref.[18], and extended this RKR curve in the short-range region with 2 points from Konowalow[21] at $3.50a_0$ and $3.75a_0$. For $R \leq 3.50a_0$ we used the exponential form

$$V(r) = A\exp(-BR)/R, \tag{13}$$

where A and B are evaluated from a cubic spline fitting of the data points for $V(r)$. We extrapolated the potential to large internuclear separations R by using the dispersion plus exchange form,

$$V_{\rm S}(R) = V_{\rm dis}(R) - V_{\rm ex}(R), \tag{14}$$

where $V_{\rm dis}(R) = -\sum_{n=6,8,10} C_n/R^n$ and $V_{\rm ex}(R) = CR^\alpha \exp(-\beta R)$.

The major uncertainties in the calculation of scattering parameters arise from the poorly constrained C_6 and C_8 coefficients. Precise knowledge of the Van der Waals coefficients C_6, C_8, which control the interaction between ground state atoms, is also crucial for scattering length determination. In this paper, the optimizing C_6 dispersion coefficient used by us is taken from Ref.[23], whereas the C_8 dispersion coefficient and the C_{10} coefficient are taken from Ref.[24]. The exchange potential is taken from Ref.[25] where the exchange parameters are $C = 0.0124$, $\alpha = 4.626$ and $\beta = 1.2445$,[28] respectively.

Although accurate molecular constants of the NaLi singlet state are available, much less has been known about the $a^3\Sigma_u^+$ state, since there was no experimental work for the triplet potential. Theoretically, potential energy curves of the triplet ground states of NaLi have been investigated by Davies and Jones[26] through many-body perturbation theory calculations, and by Schmidt–Mink *et al* who have combined all-electron (SCF) calculations, valence CI calculations and have included an effective core polarization potential. The results of Schmidt–Mink *et al* [21] are believed to be of the highest quality, and we adopted at intermediate distances, the short and long-range form is the same as V_S, except the exchange term is repulsive. Due to the $X^1\Sigma_g^+$ potential well is much deeper than the $a^3\Sigma_u^+$ well, and we find 32 bound levels for the state and 8 bound levels for the state by calculating bound levels for each potential using Eq.(12) of Gribakin and Flambaum.

4. Results and discussion

We solve Eq.(1) numerically by the Numerov method and determine the scattering length a and the effective range $r_{\rm e}$ by fitting the scattering phase shifts δ_0 to the effective range expansion formula (4). The value of the atomic mass is taken from Ref. [27]. Our results for a, $-10.87a_0$ for the triplet state and $19.25a_0$ for the singlet state, are very consistent with the semiclassical results from which we calculate the scattering lengths a and the effective ranges $r_{\rm e}$ by using Eqs.(9) and (11), respectively. Considering the sensitivity of a to Φ for the values arising here, we find that the success of the semiclassical estimate is certainly encouraging. The scattering lengths and the effective ranges for the singlet $X^1\Sigma_g^+$ and triplet $a^3\Sigma_u^+$ states are presented in Table 1. The results in Table 1, where we calculate a from Eqs.(4) and (9) and $r_{\rm e}$ from Eqs.(4) and (11), demonstrate generally good agreement between the quantal and the semi-classical calculations.

Table 1. Scattering lengths a and effective ranges $r_{\rm e}$ in units of a.u. for (a) triplet and (b) singlet of ^{23}Na^{7}Li.

Ref.	scattering length	effective range
	(a) triplet	
present	–10.87	1808.92
Present: semiclassical	–10.30	1977.79
Present: variable	–11.05	
	(b) singlet	
Present	19.25	224.87
Present: semiclassical	19.05	230.57
Present: variable	19.2	

For variable phase method, equation (8) was solved over a range [0, ϕ_c]. The value of ϕ_c corresponds to R_C and is close to $\pi/2$. The scattering length varies with interatomic distance R. Corresponding to every bound state supported by the potential, we find hat scattering length contains a pole. The variable phase function is illustrated by the curve for a in Fig.2. The last pole is located at around $28a_0$, and for $R > 28a_0$ the function is smooth and approaches its limit ultimately. The results are presented in Table 1. We did not apply any corrections

to the scattering length,[14] however, we also have obtained good results. It illustrated that the corrections to the scattering length only have a little effect on numerical results.

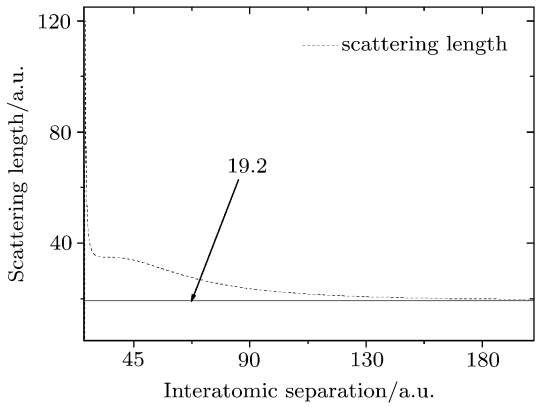


Fig.2. The scattering length as functions of interatomic separation R.

We also have applied a mass scaling method to calculate the elastic scattering properties of ^{6}Li and ^{23}Na atoms. The mass used in our calculations is $M(^6\text{Li})$=6.015123.[28] The values of a and r_e, which were obtained by the Numerov method, the semiclassical method and the variable phase method, respectively, are tabulated in Table 2.

Table 2. Scattering lengths a and effective ranges r_e in units of a.u. for (a) triplet and (b) singlet of ^{23}Na^{6}Li.

Ref.	scattering length	effective range
	(a) triplet	
present	48.82	44.76
present: semiclassical	48.45	43.01
present: variable	48.76	
Ref.[25]	39.2	
	(b) singlet	
present	18.41	225.7
present: semiclassical	18.83	214.03
present: variable	18.6	
Ref.[25]	31.1	

Our results were in good agreements with each other but those values were different from the previous theoretical result. Although the triplet scattering length $a = 48.82a_0$, which we obtained from the Numerov method, differs by 19.6% from the previous theoretical result,[25] but we believe that we obtain the more reliable values for scattering length because we used the more accurate C_n values. For the singlet state, owning to the experimental potential energy curves are more reliable than the theoretical curves, our values are more reliable. This result showed that the scattering length is very sensitive to small changes of the interatomic potential.

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 ^{23}Na and ^{6}Li. For identical fermionic ^{6}Li the Pauli exclusion principle forbids s-wave collisions. This means that the dominant interaction is via p-wave collisions. However, p-wave scattering cross section is very small at ultracold temperature and evaporative cooling fails to work. The large cross section between ^{23}Na and ^{6}Li atoms at the ultralow energies is consistent with the large s-wave scattering length and the efficient sympathetic cooling.[25] 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 reaching 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 then decreases. The $l = 2$ partial wave starts to contribute at $\log_{10} E \simeq -7.5$, corresponding to a temperature of 9 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 a broad peak in the collisions cross section near $E/k_\text{B} = 5\,\text{mK}$.

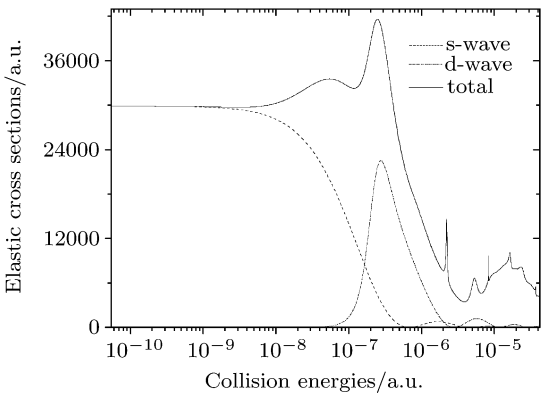


Fig.3. Total cross section and s- and d-wave cross section versus collision energies for ^{6}Li and ^{23}Na atoms scattering in the $a^3\Sigma_u^+$ state.

5. Summary

In conclusion, we have constructed the more accurate potential curves for the singlet and triplet ground states of the Na^7Li molecule, and used them to calculate the elastic scattering properties between Na and ^7Li atoms by the Numerov method, the semiclassical method and the variable phase method, respectively, good agreements were obtained. Because of the high accuracy of the potentials, we obtain the most probable values for the s-wave scattering lengths and the effective ranges at first. Using the same methods, we also calculated Na^6Li elastic scattering length and s-wave and total elastic cross sections by the mass scaling method. Our results were in good agreements with experimental work for the triplet state. Since the *ab initio* molecular potential data for the singlet Na^6Li state have some uncertainty, our results were in good agreements with each other but were different from the previous theoretical results. So further experimental study is very needed to provide more accurate interatomic potentials and to yield a description of scattering of Na and ^6Li atoms in ultracold environments with reduced uncertainty. Total elastic cross sections are very large and dominated by s-wave scattering at ultralow temperature. Shape resonance due to angular momentum barriers occurs and further experimental studies of ultracold collisions will help test those resonances.

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