Elastic scattering of sodium and cesium atoms at ultracold temperatures*

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The elastic scattering properties in a mixture of sodium and cesium atoms are investigated at cold and ultracold temperatures. Based on the accurate interatomic potential for the NaCs mixture, the interspecies s-wave scattering lengths, the effective ranges and the p-wave scattering lengths are calculated by the quantal method and the semiclassical method, respectively. The s-wave scattering lengths are $512.7a_0$ for the singlet state and $33.4a_0$ for the triplet state. In addition, the spin-change and elastic cross sections are also calculated, and the g-wave shape resonance is found in the total elastic cross sections.

Keywords: elastic scattering, s-wave scattering length, spin-change cross section

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1. Introduction

The collision between two atoms is a fundamental physical process. With the fast development of laser cooling and trapping techniques, atomic collision properties in the cold and ultracold regime have become directly accessible.[1] Elastic scattering of cold atoms in the ground state has a large variety of applications, for example, evaporative cooling,[2] sympathetic cooling,[3] collisional shift in high precision spectroscopy[4] and in the properties of a weakly interacting Bose gas.[5] In addition to the cold homonuclear collisions extensively studied for most alkali atoms,[6] heteronuclear cold samples also constitute very interesting systems for the investigation of these cold collisional processes.[7−12]

Among the heteonuclear alkali-metal atomic pairs, Na–Cs pairs have attracted the interest of both experimental and theoretical researchers involved in interatomic potentials,[13−16] photoassociative spectroscopy and molecular formation.[17−19] However, relatively little attention has been paid to investigating the elastic scattering between Na and Cs atoms. At ultracold temperatures, scattering between two heteronuclear atoms is characterized by the s-wave scattering length, the effective range and the p-wave scattering length, the contributions from higher angular momenta are negligible at very low energy.[20,21] Those scattering parameters are very sensitive to the interaction potentials between the colliding systems over an extended range of internuclear distances. The elastic scattering and spin-change cross sections are also important for cold atom experiments, which control the thermalisation of the atoms and lead to atom loss, respectively. In this paper, by adopting the accurate potential energy curves constructed in Ref. [16] for the NaCs molecule, the s-wave scattering lengths, the effective ranges and the p-wave scattering lengths are obtained precisely for the singlet $X^1\sum^+$ and triplet $a^3\sum^+$ states. Furthermore, the triplet elastic and spin-change cross sections are also calculated for the collision between sodium and cesium atoms, respectively. Shape resonances occur in the low-temperature atomic collisions. Atomic units are assumed unless otherwise indicated.

2. Cold collision theory

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

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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 given in terms of the energy E by $k^2 = 2\mu E/\hbar^2$, μ is the reduced mass and $U(r) = 2\mu V(r)/\hbar^2$, where $V(r)$ is the interatomic potential. Two ground-state atoms interact via spin-singlet $X^1\sum^+$ and spin-triplet $a^3\sum^+$ molecular potentials, with potential-energy curves V_S and V_T, respectively. Elastic singlet and triplet cross sections may be defined as

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

where δ_l is the partial wave phase shifts, S and T stand for singlet and triplet, respectively. The spin-change cross section is calculated from the singlet and triplet phase shifts by

$$\sigma_{\mathrm{SC}} = \frac{\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)\sin^2(\delta_l^{\mathrm{T}} - \delta_l^{\mathrm{S}}). \quad (3)$$

The low energy s-wave phase shifts δ_s and p-wave phase shifts δ_p satisfy the effective range expansions[22]

$$k\cot\delta_s = -\frac{1}{a} + \frac{1}{2}r_e k^2 + o(k^4), \quad (4)$$

and

$$k^{-3}\cot\delta_p = -V + o(k^2), \quad (5)$$

where the parameters a and r_e are the s-wave scattering length and effective range, respectively, and V is the p-wave scattering volume, which is related to the p-wave scattering length by $V = a_p^3$. The semiclassical results have been derived for the s-wave scattering length,[23] the effective range[24] and the p-wave scattering volume[25] with long-range potentials falling off as fast as $1/R^6$. These parameters can be expressed by the following equations:

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

$$r_e^{\mathrm{sc}} = \frac{\sqrt{2}\beta}{3}\left[\frac{\Gamma\left(\frac{1}{4}\right)}{\Gamma\left(\frac{3}{4}\right)} - 2\frac{\sqrt{2}\beta}{a} + \frac{\Gamma\left(\frac{3}{4}\right)}{\Gamma\left(\frac{1}{4}\right)}\frac{4\beta^2}{a^2}\right], \quad (7)$$

$$V^{\mathrm{SC}} = -\frac{\beta^3\Gamma(1/4)}{12\sqrt{2}\Gamma(7/4)}\frac{\bar{a} - a^{\mathrm{SC}}}{2\bar{a} - a^{\mathrm{SC}}}, \quad (8)$$

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

3. Results and discussion

At ultracold temperatures, atomic scattering properties are very sensitive to the interaction potentials between the colliding atoms. Several experimental and theoretical studies have been performed for the NaCs molecule. An extensive theoretical study of the electronic structure of NaCs has been performed and the potential energy curves were calculated far out to the atomic asymptotes.[13] Diemer *et al.*[14] performed spectroscopic measurements by using a combination of doppler-free polarization, double-resonance and laser-induced fluorescence methods, and they observed 64 vibrational levels of the $X^1\sum^+$ state. Docenko *et al.*[16] used high resolution Fourier transform spectroscopy to greatly improve the experimentally determined ground electronic state potentials. The accuracy of the *ab initio* calculations is still below the state-of-the-art accuracy of the spectroscopic data. In this paper, we use the accurate interatomic potentials given for the $X^1\sum^+$ and $a^3\sum^+$ electric states of the NaCs molecule by Docenko *et al.*. Figure 1 shows the Born–Oppenheimer potential energy curves for the $X^1\sum^+$ and $a^3\sum^+$ states used in our calculations.

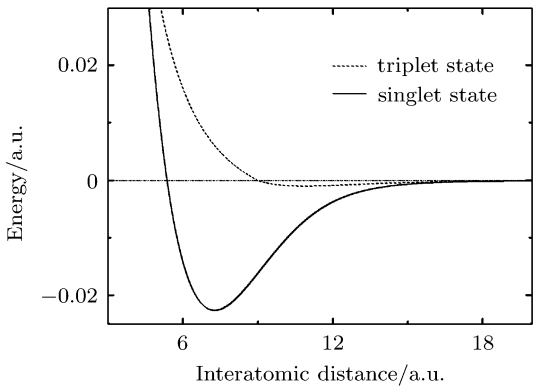


Fig. 1. Adopted potential curves for the singlet $X^1\sum^+$ and triplet $a^3\sum^+$ states.

Equation (1) is solved numerically by the Numerov method with the accurate reduced mass.[26] The s-wave scattering length a and the effective range r_e are determined by fitting the s-wave phase shifts δ_s to the effective range expansion in Eq. (4). The results for the s-wave scattering length, $512.7a_0$ for the singlet state and $33.4a_0$ for the triplet state, are in excellent agreement with the recent accurate values.[16] The p-wave phase shifts in the ultralow collision energies are also calculated and the p-wave scattering length is obtained by Eq. (5). All the calculated results are presented in Table 1. To our knowledge, this

is the first time that the values of r_e and a_p are calculated.

Those scattering parameters are sensitive to numerical error and, as a check, we calculate those data by using the semiclassical method. The results obtained by this method are also listed in Table 1. The majority of the results for a^{SC} and a_p^{SC} shown in Table 1 are within 1.5% of the quantal values. Considering the sensitivity of the semiclassical s-wave 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 s-wave scattering length is certainly encouraging. Overall, these comparisons also suggest that the semiclassical result for the p-wave scattering length can provide a robust estimate of the full result, once the s-wave scattering length and the long-range properties are known.

Table 1. Scattering parameters for Na–Cs elastic collision.

	s-wave scattering length/a.u.		Effective range/a.u.		p-wave scattering length/a.u.	
	Quantal	Semiclassical	Quantal	Semiclassical	Quantal	Semiclassical
Singlet	512.7	520.9	138.2	137.4	–78.7	–79.4
Triplet	33.4	33.1	638.9	646.4	–50.3	–51.3

In the ultralow collision energies, only s-wave scattering is expected and the spin-change cross section is about equal to $\pi(a_T - a_S)^2$. The large difference in both scattering lengths leads to significant cross sections for spin-exchange collisions, and the calculated results are shown in Fig. 2. The spin-change total cross sections increase rapidly with decreasing collision energy and display several shape resonances. This trend may inhibit the evaporative cooling of heavy atoms with large magnetic moments.

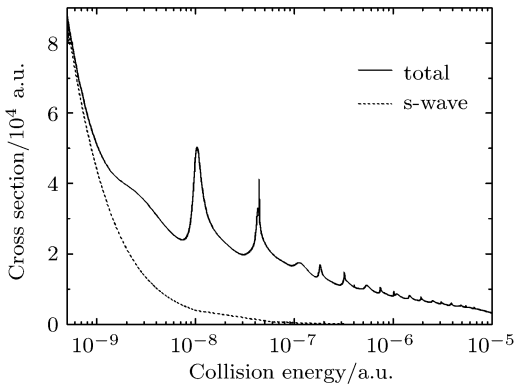


Fig. 2. The s-wave cross sections and total cross section for the spin-change process as functions of collision energy.

The collisional properties of other partial waves are also calculated at non-zero collision energies. Figure 3 shows the energy-dependent cross sections for the collisions of Na and Cs in the triplet state at cold and ultracold temperatures. The total elastic cross sections display typical Wigner-threshold behaviour for s-wave scattering at collision energies less than 1×10^{-10} a.u., where the cross section is a constant given by $\sigma = 4\pi a_T^2$, and then increases slowly before being at higher energies. The s-wave cross section begins to decrease with increasing collision energy, but the total cross section continues to increase owing to the higher partial-wave contributions. Oscillations occur through the addition of a small number of partial waves. Sharper structures are due to shape resonances, which are resonances associated with quasibound diatomic levels trapped behind a centrifugal barrier. A low energy g-wave shape resonance exists for the $a^3\sum^+$ state, giving rise to a peak in the cross section near $E = 1.03 \times 10^{-8}$ a.u.

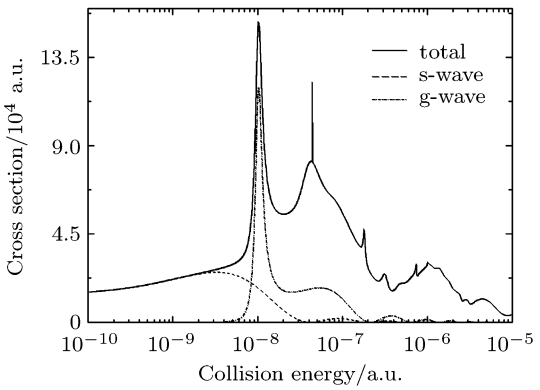


Fig. 3. The s-, g-wave cross sections and total cross section for the scattering in the $a^3\sum^+$ state as functions of collision energy.

4. Conclusion

This paper investigated the elastic scattering between sodium and cesium atoms at cold and ultracold temperatures in detail. It also calculated the interspecies s-wave scattering lengths, the effective ranges and the p-wave scattering lengths for NaCs mixture via the $X^1\sum^+$ and $a^3\sum^+$ states, by the quantal method and the semiclassical method, respectively. The results for the s-wave scattering length are in good agreement with experimental results. This is the first time that the values of r_e and a_p have been obtained. In addition, the triplet elastic and spin-change cross

sections are also calculated. G-wave shape resonance due to angular momentum barriers occurs in the total elastic cross sections and further experimental studies of ultracold collisions will help to test our calculated results.[27−29]

References

[1] Burnett K, Julienne P S, Lett P D, Tiesinga E and Williams C J 2002 *Nature* **416** 225

[2] Ketterle W and van Druten N J 1996 *Adv. At. Mol. Opt. Phy.* **37** 181

[3] Modugno G, Ferrari G, Roati G, Brecha R J, Simoni A and Inguscio M 2001 *Science* **294** 1320

[4] Fertig C and Gibble K 2000 *Phys. Rev. Lett.* **85** 1622

[5] Dalfovo F, Giorgini S, Pitaevkii L and Stringari S 1999 *Rev. Mod. Phy.* **71** 463

[6] Weiner J, Bagnato V S, Zilio S and Julienne P S 1999 *Rev. Mod. Phys.* **71** 1

[7] Zhang J C, Sun J F and Liu Y F 2011 *Chin. Phys.* B **20** 023401

[8] Zhang J C, Zhang Y, Du B G and Sun J F 2009 *Chin. Phys.* B **18** 1486

[9] Voigt A C, Taglieber M, Costa L, Aoki T, Wieser W, T Hänsch W and Dieckmann K 2009 *Phys. Rev. Lett.* **102** 020405

[10] Staanum P, Pashov A, Knöckel H and Tiemann E 2007 *Phys. Rev.* A **75** 042513

[11] Pashov A, Docenko O, Tamanis M, Ferber R, Knöckel H and Tiemann E 2005 *Phys. Rev.* A **72** 062505

[12] Anderlini M, Courtade E, Cristiani M, Cossart D, Ciampini D, Sias C, Morsch O and Arimondo E 2005 *Phys. Rev.* A **71** 061401

[13] Diemer U, Weickenmeier H, Wahl M and Demtroder W 1984 *Chem. Phys. Lett.* **104** 489

[14] Korek M, Allouche A R, Fakhreddine K and Chaalan A 2000 *Can. J. Phys.* **78** 977

[15] Docenko O, Tamanis M, Ferber R, Pashov A, Knockel H and Tiemann E 2004 *Eur. Phys. J.* D **31** 205

[16] Docenko O, Tamanis M, Zaharova J, Ferber R, Pashov A, Knockel H and Tiemann E 2006 *J. Phys.* B **39** S929

[17] Haimberger C, Kleinert J, Bhattacharya M and Bigelow N P 2004 *Phys. Rev.* A **70** 021402

[18] Haimberger C, Kleinert J, Zabawa P, Wakim A and Bigelow N P 2009 *New J. Phys.* **11** 055042

[19] Zabawa P, Wakim A, Neukirch A, Haimberger C, Bigelow N P, Stolyarov A V, Pazyuk E A, Tamanis M and Ferber R 2010 *Phys. Rev.* A **82** 040501

[20] Ouerdane H and Jamieson M J 2004 *Phys. Rev.* A **70** 022712

[21] Ouerdane H and Jamieson M J 2009 *Eur. Phys. J.* D **53** 27

[22] Mott N F and Massey H S W 1965 *The Theory of Atomic Collisons* (Oxford: Clarendon)

[23] Gribakin G F and Flambaum V V 1993 *Phys. Rev.* A **48** 546

[24] Flambaum V V, Gribakin G F and Harabati C 1999 *Phys. Rev.* A **59** 1998

[25] Dickinson A S 2008 *J. Phys.* B **41** 175302

[26] Londono B E, Mahecha J E, Luc-Koenig E and Crubellier A 2010 *Phys. Rev.* A **82** 012510

[27] Monroe C R, Cornell E A, Sackett C A, Myatt C J and Wieman C E 1993 *Phys. Rev. Lett.* **70** 414

[28] Baumgarten C, Braun B, Capiluppi M, Ciullo G, Dalpiaz P F, Kolster H, Lenisa P, Marukyan H, Nass A, Reggiani D, Stancari M and Steffens E 2008 *Eur. Phys. J.* D **48** 343

[29] Boesten H M J M, Tsai C C, Verhaar B J and Heinzen D J 1996 *Phys. Rev. Lett.* **77** 5194