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Calculation of the elastic scattering properties for cold and ultracold ^{39}K atoms in a triplet state*

Hu Qiu-Bo(胡秋波)[a)], Wang Xiao-Fei(王晓飞)[a)],
Sun Jin-Feng(孙金锋)[a)b)†], and Zhu Zun-Lue(朱遵略)[a)c)]

[a)] *College of Physics and Information Engineering, Henan Normal University, Xinxiang* 453007, *China*
[b)] *Department of Physics, Luoyang Normal College, Luoyang* 471022, *China*
[c)] *Institute of Atomic and Molecular Physics, Sichuan University, Chengdu* 610064, *China*

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The elastic scattering properties for collisions between cold and ultracold ^{39}K atoms in a triplet state are investigated. Based on the recent theoretical and experimental results, the improved hybrid potential is presented for a triplet $a^3\Sigma_u^+$ ground state of K_2. Our calculated value of the s-wave scattering length a by using the Numerov method for the triplet state is $79.578a_0$ and found to be in good agreement with the previous ones. The numbers of bound states are supported by the molecular potential. Pronounced shape resonances appear for the $l = 3$ partial waves for the $a^3\Sigma_u^+$ state. Furthermore, the s-wave scattering cross section, the total cross section and energy positions of shape resonances for the $a^3\Sigma_u^+$ state are calculated.

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

1. Introduction

Owing to the rapid development of laser cooling and trapping techniques,[1] collisions of the alkali atoms in dilute gases have been investigated at cold and ultracold temperatures. For instance, they play a crucial role in achieving the Bose–Einstein condensate[2−4] and Fermi degeneracy[5] in dilute atomic gases. In a low-energy regime, the elastic collision properties between neutral atoms are determined by the s-wave scattering length a and the effective range r_e.[6,7] The stability of a condensation is controlled by the sign of the scattering length.[8] For bosonic atoms, when $a > 0$, the possible Bose condensation is stable, but for $a < 0$, it is unstable. There is only a finite number of atoms found to be in the condensate state in a trap. The s-wave scattering length is very sensitive to the interaction potentials of atom-atom collisions at ultralow temperatures, so the accurate interaction potentials must be constructed. For ^{39}K atoms, the recent theoretical and experimental investigations of their interatomic potentials have made it feasible to more accurately investigate the collision properties.[8] In this paper, we construct the improved hybrid potential for the triplet state of ^{39}K atoms, and then calculate the scattering length a and effective range r_e for the triplet $a^3\Sigma_u^+$ state accurately. The potentials can be used to accurately predict the s-wave scattering cross section and position of the shape resonance. We adopt atomic units unless otherwise specified.

The outline of this paper is as follows. A brief review of the theoretical knowledge and the computational method, and then the description of the interaction potential are given in Section 2. The computational results for the $a^3\Sigma_u^+$ state are presented and discussed in Section 3, in which included are all of the main results for scattering properties together with a detailed comparison with other calculations and experimental data wherever available. Conclusions drawn from the present study are given in Section 4.

2. Low-energy elastic scattering theory

The scattering length is determined from the asymptotic behaviour of the solution of the radial

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†Corresponding author. E-mail: xfw628@yahoo.com.cn

Schrödinger equation at zero energy

$$\Big[\frac{\mathrm{d}^2}{\mathrm{d}r^2}+k^2-\frac{l(l+1)}{r^2}-2\mu V(r)/\hbar^2\Big]u_l(r)=0. \quad (1)$$

Here, k is the wave number which is related to the collisional energy E by $k^2=2\mu\mathrm{E}/\hbar^2$, μ is the reduced mass of the collision system and $V(r)$ is the interatomic potential. The solutions must be regular and behave asymptotically as

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

where A_l is a normalization constant, $j_l(x)$ and $n_l(x)$ are the spherical Bessel and Neumann functions, and δ_l is the partial-wave phase shift which can be computed using the formula[6,8,9]

$$\tan\delta_l=\frac{u_l(r_2)s(r_1)-u_l(r_1)s(r_2)}{u_l(r_1)c(r_2)-u_l(r_2)c(r_1)}, \quad (3)$$

where r_1 and r_2 are two distinct points in an asymptotic region, $s(r)=krj_l(kr)$ and $c(r)=-krn_l(kr)$. Two ^{39}K atoms in a ground state interact with each other via electronic spin-triplet $a^3\Sigma_u^+$ molecular potential with a potential curve $V_T(R)$. Elastic triplet cross sections may be defined as[6]

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

The low-energy scattering is determined by the $l=0$ partial wave contribution, which is so called s-wave scattering. As values of k are close to zero, the $l=0$ phase shift δ_0 can be represented by the effective range expansion[10]

$$k\cot\delta_0=-\frac{1}{a}+\frac{1}{2}r_{\mathrm{e}}k^2+o(k^4). \quad (5)$$

This is the Numerov method of solving the parameters a and r_{e}, which are the scattering length and the effective range, respectively. In addition, we use another computational method, the semiclassical method (WKB), to calculate the two parameters, which are given by

$$a^{\mathrm{sc}}=\bar{a}\Big[1-\tan\Big(\Phi-\frac{\pi}{8}\Big)\Big], \quad (6)$$

where

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

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

and

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

And the number of bound states n_{b} is given by

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

where [ ] presents the largest integer. When [ ] in the expression (10) is an integer, the scattering length is infinite, which corresponds to the appearance of a new bound state.

3. Interaction potentials

The computed scattering parameters crucially depend on the interaction potential. It is important to compare the results obtained with a variety of interaction potentials.[11] The interaction potentials of two ^{39}K atoms have been discussed in Refs.[12,13]. In this paper, for the $a^3\Sigma_u^+$ state, we adopt the more accurate experimental Rydberg–Klein–Rees (RKR) data from Zhao *et al*,[14] the recent *ab initio* data from Ahmed *et al*,[15] and the more accurate dispersion coefficient for K_2.

We construct a more accurate interaction potential, which is a hybrid potential and consists of four parts. We use the new RKR data ($10.80a_0<R<15a_0$) from Ref.[14], and extend this RKR curve in a short-range region with 18 *ab initio* points from Ref.[15] (between $5.40a_0$ and $10.80a_0$). For $R\le 5.40a_0$, we adopt the exponential form

$$V(R)=A\exp(-BR), \quad (11)$$

where A and B are evaluated from a cubic spline fitting of the values for $V(R)$. In a long-range region ($R>15a_0$), the triplet potential $V_{\mathrm{T}}(R)$ may be expressed as a sum of dispersion term r^{-n} and an exchange potential $V_{\mathrm{EX}}(R)$ which decreases exponentially. Thus at large distances we have

$$V_{\mathrm{T}}(R)=-\frac{C_6}{R^6}-\frac{C_8}{R^8}-\frac{C_{10}}{R^{10}}+V_{\mathrm{EX}}(R), \quad (12)$$

where the dispersion coefficients C_6, C_8 and C_{10} are cited from Refs.[16,17]. The exchange term $V_{\mathrm{EX}}(R)$ is fitted to the form in Ref.[18]

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

where the values of α, β and C are the same as ones in Ref.[18]. Our adopted hybrid potential curve for the

triplet state is illustrated in Fig.1 and the potential parameters are listed in Table 1.

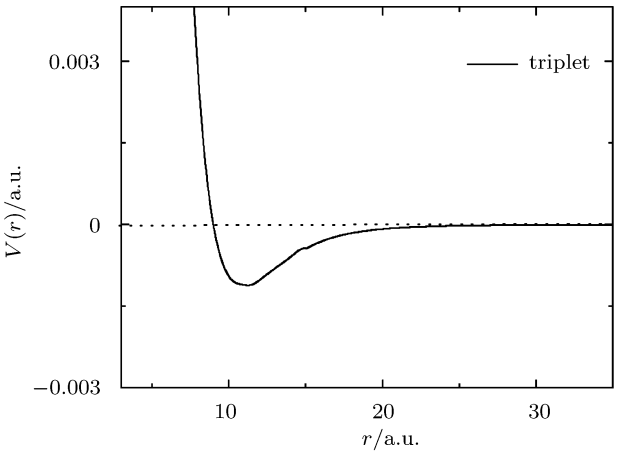


Fig.1. The adopted hybrid potential curve of the triplet $a^3\Sigma_u^+$ state of K_2.

Table 1. Long-range dispersion coefficients and exchange interaction parameters in atomic unit used for $a^3\Sigma_u^+$ potential.

C_6	C_8	C_{10}	C	α	β
3.905×10^3	4.907×10^5	5.374×10^7	2.725×10^{-3}	5.195	1.130

4. Results and discussion

Equation (1) is numerically solved by the Numerov method with the automatic selection of step size, and the partial-wave phase shift δ_l is obtained at low energies by using the formula (3). The scattering length a and effective range r_e are determined by fitting the s-wave scattering phase shift δ_0 to the effective range expansion formula (5). Our value of a is $79.578a_0$ for the triplet state, and it is in good agreement with the values reported recently in Ref.[18], showing that our constructed hybrid potential curve is accurate. We also calculate the scattering length a and effective range r_e using the semiclassical method (Eq.(6) and Eq.(10)), respectively. We take the value for the reduced mass of two ^{39}K atoms as 71026.4739 atomic mass units, corresponding to the collision of two potassium atoms. The values of the two parameters are listed in Table 2.

In Table 2, the values of scattering length a calculated from Eqs.(5) and (6), and the values of effective range r_e obtained from Eq.(5) and Eq.(9) are nearly the same, which demonstrate the results obtained by using the Numerov and semiclassical methods are in good agreement. Our scattering lengths are in a range the same as that in Ref.[18], so we believe that our values are reliable. And we find 27 bound levels for the $a^3\Sigma_u^+$ state by computing Eq.(10), which is consistent with Levinson's theorem, indicating that as the binding energy of the highest level approaches a zero value, the scattering length tends to $\pm\infty$. Nevertheless, we have not found any effective ranges and bound levels in the literature at present.

Table 2. The scattering length a and effective range r_e in atomic unit for triplet state.

Reference	Scattering length	Effective range
Present study (using Numerov method)	79.578	117.255
Present study (using WKB method)	80.312	115.870
Ref.[18]	81.1 ± 2.4	

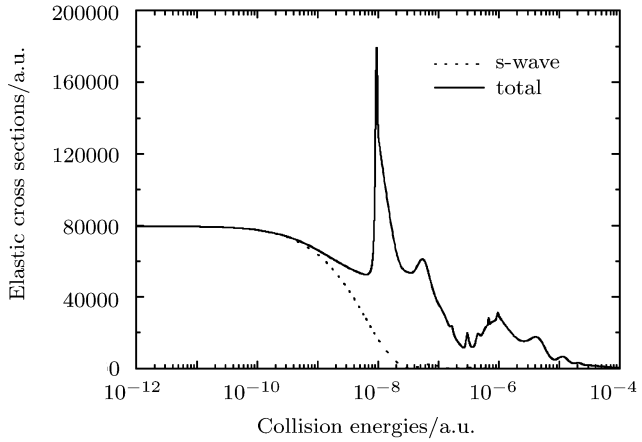


Fig.2. The s-wave scattering cross section and total cross section versus collision energy in the $a^3\Sigma_u^+$ state.

Figure 2 presents the relation between the elastic cross sections, including the s-wave scattering cross section and total cross section, and collision energy. At temperatures less than 1mk, the total elastic cross section is dominated only by the s-wave scattering cross section, which 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 using the values of a and r_e. For $l = 0$, Eq.(4) becomes

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

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

$$\sigma_{\rm el}^{\rm T} \approx \frac{4\pi}{(ka)^2 + [1 - r_e a k^2/2]^2} \approx 4\pi a^2[1 + ak^2(r_e - a)]. \qquad (15)$$

As energy increases, high angular momentum waves contribute to the scattering. And the s-wave cross section tends to decrease with energy increasing but the reduction is overcome by the high partial-wave contribution which initially increases with energy from zero before passing through maximum and decreasing. Oscillations occur through the addition of a small number of partial waves. The appearance of sharper structures is due to shape resonances.[19] The most prominent is the f-wave resonance corresponding to a quasi-bound-state trapped by the $l = 3$ centrifugal barrier. The f-wave resonance for the $a^3\Sigma_u^+$ state occurs at an energy of 9.49×10^{-9} a.u. and has a width of 1.1×10^{-9}a.u.[20]

5. Conclusions

In our calculations we have employed a more accurate interaction potential curve for a triplet ground state of potassium molecule, available from the literature, and investigated the elastic properties by using the potential curve of two ^{39}K atoms at the cold and ultracold temperatures, which are sensitive to the details of the interaction potential. Because of the high accuracy of the potential, we have obtained the most probable values for the s-wave scattering lengths and effective ranges. We have figured out the scattering lengths by using the Numerov and WKB methods, and found them to be in good agreement with the experimental results. In addition, we have presented the calculated total elastic cross sections which are very large and dominated by the s-wave scattering at ultracold temperatures.[19] It is found that the shape resonance, trapped within the centrifugal barrier, imposes a structure on the cross section. And we have computed the position of the shape resonance theoretically and it may be possible to be confirmed experimentally in the future.

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