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Scattering properties of the ultracold $^{133}Cs_2$ triplet state*

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The elastic scattering properties of ultracold $^{133}Cs_2$ triplet state are investigated in detail. We construct a potential curve of the $^{133}Cs_2$ triplet state, based on the latest *ab initio* molecular potential data and show how the scattering parameters are obtained by using three methods: the Numerov method, the semiclassical method and the variable phase method, where the scattering lengths of the $^{133}Cs_2$ triplet state, i.e. $301.79a_0$, $300.67a_0$ and $310.81a_0$ are obtained respectively, with a_0 being the Bohr radius. We also calculate the effective range and the number of bound states for the $^{133}Cs_2$ triplet state. Our results are in agreement with the recent experimental data and the theoretical calculations. This confirms that the results of the scattering properties of the ultracold $^{133}Cs_2$ triplet state, calculated by using these three methods, are reliable.

Keywords: scattering length, effective range, variable phase method
PACC: 3400, 3420, 3440

1. Introduction

Scattering length is of fundamental importance in the study of ultracold atom–atom collision. The character of the interaction between atoms in low temperatures is determined by signs (±) and magnitude of the scattering length a. The magnitude of a is a measure of the strength of the interaction, and its sign indicates whether the interaction is effectively repulsive ($a > 0$) or attractive ($a < 0$).[1] The stability of Bose–Einstein condensation (BEC) requires repulsive interactions, whereas for attractive interactions it is unstable; only a finite number of atoms can be found in condensate state in a trap.[2] There are several theoretical methods to calculate scattering length. Usually, the scattering length is calculated by solving the single-channel radial Schrödinger equation to find the phase shifts for several small values of the wavenumber of relative motion and by extrapolating from effective range expansions,[3] or by using the semiclassical formula. Ouerdane *et al*[4] developed another method of evaluating the scattering length in which they solved the first-order equation, a Riccati equation, of the variable phase approach to potential scattering. Gao derived the formulas of calculating scattering parameters from the quantum defect theory, based on the exact solutions of the Schrödinger equation for an attractive $1/r^6$ potential, which provides a systematic interpretation for molecular bound states and atom–atom scattering properties and establishes the relationship between them.[5] In the present work, we use the first three methods to revaluate the scattering length of the Cs_2 triplet state.

The coupling of the scattering continuum with molecular states can lead the caesium atom–atom scattering to have many anomalistic properties, such as the large clock shifts,[6] enormous collision cross sections,[7] and the extreme difficulty in reaching the BEC.[8] These have intrigued experimentalists and theorists. The long-range interaction parameters, as well as the molecular structure near threshold can be accurately determined through the detection of multiple Feshbach resonances, or Feshbach spectroscopy. With this information, the cold collision anomalies can be resolved.[9] Caesium molecules have been created by using photoassociation[10−12] or Feshbach resonances,[13,14] and the BEC of dilute ^{133}Cs atomic gases has been investigated and observed by

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Weber *et al.*[15] Despite of the rapid development of the research on the caesium quantum gas, there exists an unusual degree of disagreement between measurements and calculations of scattering length in the $^{133}Cs_2$ triplet state, which can characterize a great many of collision properties of a particle. This disagreement arises from the fact that the ^{133}Cs triplet scattering length exhibits a strong variation with collision energy, due to a nearly bound (above threshold) resonance.[16] The scattering length is very sensitive to the interatomic potential. Hence, constructing the accurate interatomic potential of the $^{133}Cs_2$ triplet state is very important and we will address this point below.

The rest of the present paper is organized as follows. In Section 2, we present the theory of three methods: the Numerov method, the semi-classical method and the variable phase method. In Section 3, we construct a potential curve of the $^{133}Cs_2$ triplet state. In Section 4, we revaluate the scattering parameters of the Cs_2 triplet state by using the three methods. Finally, a brief discussion and some conclusions drawn from the present study are given in Section 5.

2. Theoretical methods

2.1. Numerov method

The radial part of the Schrödinger equation (in atomic units) for collision between two atoms with $V(R)$ as an interatomic potential is written as

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

Here, k is the wave number and is related to the energy E of the relative motion by $k = \sqrt{2\mu E}$, with μ being the reduced mass of the collision system. The wavefunction of each partial wave has the asymptotic form,[17]

$$u_l(k,R) \sim \sin(kR + \delta_l(k)), \quad (2)$$

where δ_l is the phase shift introduced by the potential. Total cross section is given by

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

At the value of k close to zero, the s-wave phase shift can be written as a power-series expansion in k

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

where a and r_e are the scattering length and the effective range, respectively.

2.2. Semiclassical method

Owing to the large reduced mass of the collision pair, the interaction between atoms behaves as $-C_6/R^6$ at large distances and allows a semiclassical treatment within the potential well. As a result, the low-energy scattering is governed by two large parameters: the asymptotic parameter $\gamma = \sqrt{2\mu C_6} \gg a_0^2$ and the semiclassical zero-energy phase $\Phi = \int_{R_0}^{\infty}\sqrt{2\mu\left(-V(R)\right)}\mathrm{d}R \gg 1$ (R_0 is the classical turning point, where the interaction potential $V(R_0) = 0$). The parameters a and r_e are obtained by using the semiclassical method (Wentzel–Kramers–Brillouin (WKB) method)[18] as

$$a = \cos\left(\frac{\pi}{4}\right)\left(\frac{\gamma}{4}\right)^{\frac{1}{2}}\frac{\Gamma(3/4)}{\Gamma(5/4)} \times\left[1 - \tan\frac{\pi}{4}\tan\left(\Phi - \frac{\pi}{8}\right)\right], \quad (5)$$

$$r_\mathrm{e} = \frac{\sqrt{2\gamma}}{3}\left[\frac{\Gamma(1/4)}{\Gamma(3/4)} - 2\frac{\sqrt{2\gamma}}{a} + \frac{\Gamma(3/4)}{\Gamma(1/4)}\frac{4\gamma}{a^2}\right]. \quad (6)$$

The total number of bound states with zero orbital angular momentum is given by

$$N_\mathrm{b} = [\Phi/\pi - 5/8] + 1, \quad (7)$$

where $[\Phi/\pi - 5/8]$ is the integer part.

2.3. Variable phase method

In the variable phase approach, the accumulated s-wave phase shift $\delta_{k,0}(R)$ satisfies the equation at the nuclear separation R[19]

$$\frac{\mathrm{d}\delta_{k,0}(R)}{\mathrm{d}R} = -\frac{\nu(R)}{k}\sin^2\left[kR + \delta_{k,0}(R)\right], \quad (8)$$

where $\nu(R) = 2\mu V(R)$. The accumulated phase shift is the limit of $\delta_{k,0}(R)$ as $R_\mathrm{C} \to \infty$; it suffers no mod $[\pi]$ ambiguity.

The scattering length $a(R_\mathrm{C})$ is a corresponding limit of $-\tan\delta_k(R_\mathrm{C})/k$[3] and $a(R_\mathrm{C}) \to a$ as $R_\mathrm{C} \to \infty$. $a(R_\mathrm{C})$ satisfies the Riccati equation in R_C.[20] Dropping the subscript C, the Riccati equation is

$$\frac{\mathrm{d}a(R)}{\mathrm{d}R} = \left[R - a(R)\right]^2\nu(R). \quad (9)$$

The function $a(R)$ contains poles that correspond to the bound states, shown in Fig.1, so finite difference

methods such as the Runge–Kutta method are unsuitable. Ouerdane *et al*[4] gave two possible ways, i.e. the change of variables and the log-derivative method,[21] to solve Eq.(9). In Eq.(9), we make the change of variables

$$a(R) = \tan\theta(R) \quad \text{and} \quad R = \tan\phi(R) \tag{10}$$

to obtain the equation

$$\frac{\mathrm{d}\theta(\phi)}{\mathrm{d}\phi} = \sec^4\phi \sin^2\left(\theta(\phi) - \phi\right) \nu\left(\tan(\phi)\right). \tag{11}$$

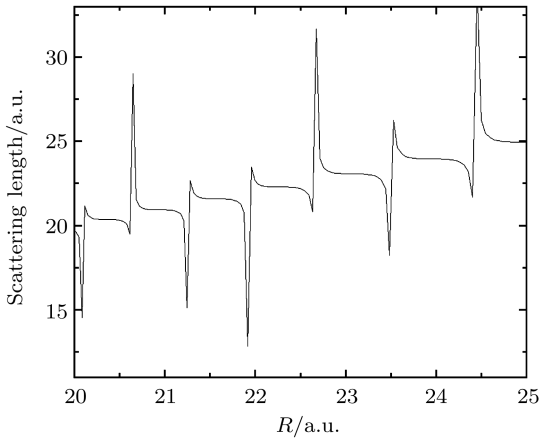


Fig.1. Scattering length for $^{133}Cs_2$ in triplet state $[a^3\Sigma_u^+]$ as a function of interatomic separation R.

3. Interatomic potential

Since scattering length is determined by the condition of vanishing asymptotic kinetic energy, it is exclusively determined by the potential. Although accurate molecular constants of the $^{133}Cs_2$ singlet state are available, much less has been known about the $a^3\Sigma_u^+$ state. Hence, it is difficult to determine the energy curve of the $^{133}Cs_2$ triplet state. The *ab initio* potential energy curve of the $a^3\Sigma_u^+$ state of Cs_2 has been determined in the framework of the pseudopotential method in Ref.[22]. Their theoretical molecular constants are in good agreement with the measurements and the ones given by Weickenmeier *et al*.[23] New *ab initio* molecular potential for the $^{133}Cs_2$ triplet state will be extremely useful for allowing a comparison between the experimental results and hence for confirming the physical implications of the signs of the scattering parameter, and the number of bound states. This is important for $^{133}Cs_2$. So we use their potential data to construct the potential of the Cs_2 triplet state.

In the calculation of the interaction energy between two caesium atoms we consider several ranges of internuclear separations. For $0.2117\,\mathrm{nm} \leq R \leq 0.889\,\mathrm{nm}$, we use the latest *ab initio* interatomic potential curve given by Li *et al*.[22] For $R \leq 0.2117\,\mathrm{nm}$, we extend the *ab initio* potential curve in the exponential form

$$V(R) = AR^{-1}\exp(-BR), \tag{12}$$

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

$$V(R) = V_{\mathrm{dis}}(R) + V_{\mathrm{ex}}(R), \tag{13}$$

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

The major uncertainties in the calculation of scattering parameters arise from the poorly constrained C_6 and C_8 coefficients. Accurate knowledge of the van der Waals coefficients C_6 and C_8, which control the interaction between ground state atoms, is also crucial for scattering length determination. In the present paper, we use the optimizing C_8 dispersion coefficient in addition to the C_6 coefficient in Ref.[24]. The C_{10} coefficient is taken from Ref.[25]. The exchange potential is from Ref.[26] where the exchange parameters are $C = 0.0008$, $\alpha = 5.53$ and $\beta = 1.072$,[27] respectively.

4. Numerical results

The Numerov method is used to solve Eq.(1) with the constructed potential, and the wavefunctions at different energies are obtained. Figure 2 shows the s-wave wavefunctions as the energy changes from $E = 1.0 \times 10^{-10}$ a.u. to $E = 1.0 \times 10^{-15}$ a.u.. The wavelengths and amplitudes of wavefunctions increase with energy decreasing. For energy $E = 1.0 \times 10^{-15}$ a.u. and $E = 1.0 \times 10^{-12}$ a.u., the wavefunctions overlap and almost become a straight line for large values of R. The intercept of the line, projected back to the R-axis, is the scattering length. Hence, we can roughly evaluate the scattering length from wavefunction. It is about $300a_0$. Outside the interaction range, the s-wave wavefunction is a simple spherical wave. Clearly, the concept of scattering length is useful only at a sufficiently low temperature and we can describe the system by using the identical wavefunctions at the ultralow energies.

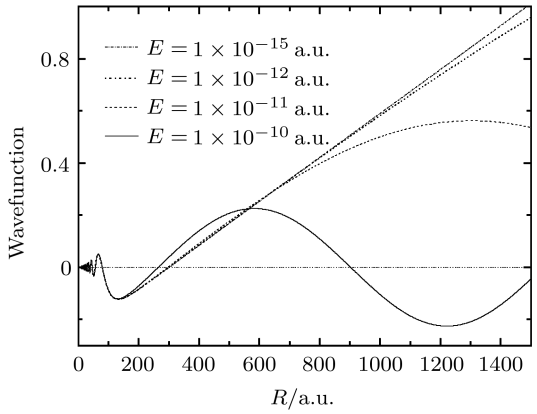


Fig.2. Wavefunctions of $^{133}Cs_2$ triplet states at different energies.

From expression (2), the phase shift can be obtained at low energies by using the numerical calculation. The s-wave scattering length is related to the phase shift and the effective range by effective range expansion formula (4). The effective range, r_e, is important because it implies that there is a relative contribution to the elastic scattering cross section at energy E.[28] We calculate the scattering length and the effective range by fitting the scattering phase shift to expression (4). The results are displayed in Table 1. Using the obtained phase shift, the elastic partial-wave cross sections and total cross section for the $^{133}Cs_2$ triplet state are calculated from Eq.(3). The total elastic cross section is constant at very low speeds, where only s-wave scattering is significant.

For very low energies, the s-wave cross section is constant and decreases with energy increasing, but the decrease is overcome by higher partial-wave contributions which initially increase with energy from zero before passing through maxima and decreasing as shown in Fig.3. The s-wave cross-section at zero energy is the same as that of a hard sphere with radius a. So we can also carry out the rough calculation of scattering length via $\sigma = 4\pi a^2$. It is about $300a_0$.

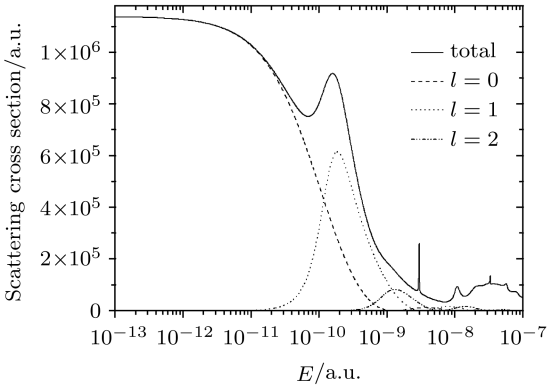


Fig.3. Total cross section and individual partial wave cross sections for the scattering in the $a^3\Sigma_u^+$ state as functions of collision energy.

The semiclassical phase $\Phi = \int_{R_0}^{\infty} \sqrt{2\mu\,(-V(R))}\mathrm{d}R$ is calculated from R_0 to a large value of R, where the reduced mass $\mu = 121135.828 m_e$.[29] Then, the scattering length and the effective range can be obtained from expressions (5) and (6). We list the results in Table 1. We use expression (7) to obtain the number of bound states. It is 59.

Table 1. Scattering length and effective range calculated by using the Numerov method, the WKB method and the variable phase method and their comparison with the results cited from Refs.[30, 31].

	Numerov method	WKB	variable phase method	Ref.[30]	Ref.[31]
a/a.u.	301.79	300.67	310.81	$\|a_T\| > 260$	$\|a_T\| > 140$Å
r_e/a.u.	159.10	158.85			

For the variable phase method, Eqs.(8) and (11) are solved by using the Runge–Kutta method with a self-adjusting step length.[32] Phase shift increases with R increasing. After passing through the potential well, phase shift approaches its limit ultimately, 185.35, from below. To calculate the number of bound states supported by the potential, the simplest formulation of Levinson's theorem can be used,[20] which links the scattering phase shift to the number of bound states, N_b, via $N_b\pi = \delta_{k,0}|_{k=0}$. Hence, we obtain 59 bound states. In Ref.[33], triplet potential curves[34] led to a number of bound vibrational levels, 58 ± 2. As shown in Ref.[23], there were about 60 bound levels in a shallow well of the $a^3\Sigma_u^+$ state. The number of bound states, which is obtained in the present paper, is in good agreement with other calculated results.

Equation (11) was solved over a range $[0, \phi_c]$.The value of ϕ_c corresponds to R_C and is close to $\pi/2$. The scattering length varies with interatomic separation$R$. Corresponding to every bound state supported by the potential, scattering length contains a pole. So we can also acquire the number of bound states through counting the number of poles. The result is the same as the result calculated from $N_b\pi = \delta_{k,l=0}|_{k=0}$. The

last pole is located at about $210a_0$. For $R > 210a_0$, the scattering length $a(R)$ is illustrated by a short dot curve in Fig.4. and becomes smooth and constant as the value of R increases.

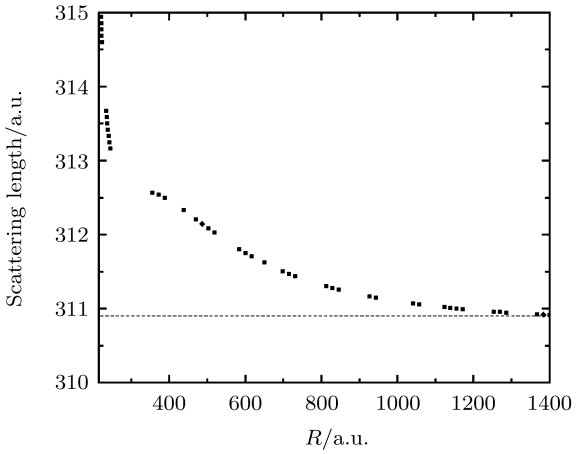


Fig.4. Scattering length for $^{133}Cs_2$ in triplet state $[a^3\Sigma_u^+]$ as a function of interatomic distance R.

The triplet scattering length of ^{133}Cs has been predicted to have many different values ranging from $-1100a_0$ to $2400a_0$.[16] The scattering lengths calculated by using the above three methods are consistent with the recent experimental data.[30,31] We tabulate the calculated scattering parameters from different methods in Table 1.

For the Numerov method, we can obtain the scattering parameters and wavefunctions through solving the Schrödinger equation. When the energy approaches to zero, we calculate the scattering length. In practice, we solve Eq.(1) at some value E. If we choose the value of E to be too small, computation time increases greatly. We usually stop the calculation as the scattering cross section almost becomes constant. The semiclassical formulas are convenient to calculate scattering parameters and give much more accurate results than the extrapolation of the phase shift.

In the variable phase method, one needs to solve a differential equation only once, but in the Numerov method a differential equation must be solved several times at different small wave-numbers and the phase shifts are extracted from the asymptotic solutions. Because of the rapid variation of the local wave number over the potential well, a variable step of integration is used to economize on computation and minimize accumulated truncation error. In the variable phase method, we do not make any correction to scattering length and phase shift, however, this method has already produced results which are in agreement with those given by experiments and other two kinds of methods. This method has a good stability. Its results vary only with potential and mass. The internal parameters of program for investigating the scattering properties almost do not change the results.

5. Conclusion

The Numerov method, the WKB method and the variable phase method are used to investigate the elastic scattering properties for the collision of the caesium atoms in a triplet state with by using a constructed potential. The results obtained by using these three methods are consistent with each other, thereby showing that these methods are reliable for the study of very slow atomic collisions. For $^{133}Cs_2$ in the triplet state, the calculated results show that there is a big collision cross section and the cross section is extremely sensitive to the details of the interaction potentials. Its scattering length a is positive, so caesium Bose gas is stable. We obtain 59 bound states through the semiclassical method and the variable phase method. These results consist with the experimental data and the theoretical calculations. The *ab initio* molecular potential data for $^{133}Cs_2$ triplet state have some uncertainty. A further study is needed to provide a potential for the $a^3\Sigma_u^+$ molecular state of the $^{133}Cs_2$ dimmer, thereby yielding a description of scattering of caesium atoms in ultracold environments with a reduced uncertainty.

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