Sensitivity of the dynamics of Na + Na₂ collisions on the three-body interaction at ultralow energies

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Abstract. We have studied the quantum dynamics of collisions between spin-stretched Na atoms and Na₂ molecules. Cross-sections and rate coefficients for vibrational relaxation of $Na_2(v, j = 0)$ have been computed in the 1 nK−0.1 mK energy range using an accurate time-independent method based on hyperspherical coordinates. The complex scattering length and the extension of the Wigner region have been determined. A detailed study of the sensitivity of collisional quantities on the three-body interaction at short distance has been performed. They are very sensitive to three-body effects for the vibrational state $v = 1$ of Na₂. Rotational distributions have also been calculated and show a more pronounced sensitivity on the three-body interaction, even for $v = 2$ and 3.

PACS. 34.50.-s Scattering of atoms and molecules

1 Introduction

Whereas all akali atoms have been condensed and extremely low temperatures have been reached (450 pK for sodium atoms [1]), there is currently a substantial research effort in producing ultracold alkali molecules from atomic ultracold gases of bosons or fermions.

Ultracold molecules (below 100 μK) are formed by two different mechanisms: photoassociation of cooled or condensed alkali atoms, or by a mechanism which involves magnetically tuned Feshbach resonances.

A few years ago, Heinzen and co-workers [2] created ultracold molecules ⁸⁷Rb₂ in a rubidium atomic Bose-Einstein condensate (BEC) using a two-photon stimulated Raman transition. More recently, the photoassociation technique has been used in several groups [3–5] to form ultracold ²³Na₂ molecules in their singlet or triplet electronic state from ultracold atomic Na atoms. Caesium molecules have also been created from an ultracold atomic gas in a magneto-optical trap [6].

An alternate route for producing ultracold molecules from ultracold atoms uses the atom-molecule coupling that arises from a Feshbach resonance [7]. Feshbach resonances are a powerful tool to tune the microscopic interactions in ultracold bosonic and fermionic gases. In this technique the scattering length is measured as a function of the magnetic field. The sign and magnitude of the scattering length can be modified by adjusting the value of an external magnetic field near a Feshbach resonance. Formation of molecules using this technique has been reported

for bosons, for example ²³Na₂ [8], ⁸⁵Rb₂ [9], ⁸⁷Rb₂ [10], ¹³³Cs₂ [11]. This technique has also been used to convert an ultracold degenerate Fermi gas of ⁴⁰K and ⁶Li atoms into an ultracold gas of molecules and very recently Bose-Einstein condensates of ⁶Li₂ [12,13] and ⁴⁰K₂ [14] molecules have been produced.

In experiments on ultracold molecules, collisional processes have an important role. The photoassociation or Feshbach resonance techniques lead to molecules in very excited vibrational states. At ultracold temperatures, molecules can deexcite to lower lying levels by inelastic collisions (without atom exchange) or rearrangement collisions (with atom-exchange) with atoms or other molecules present in the trap. These collisional processes which are called quenching processes lead to heating and to trap loss. Quenching collisions often occur at a significant rate. For instance the vibrational quenching rate coefficient for Rb-Rb₂ collisions has been measured with a value of 3×10^{-11} cm³ s⁻¹ [2].

Presently, only a few accurate quantum-mechanical studies of molecular collisions in the ultralow energy range have been reported. Most studies considered vibrational relaxation where rearrangement processes are not involved (He + H₂ [15], He + O₂ [16], He + F₂ [17], He + CO [18], He + CaH [19]) or neglected (H + H₂ [20]). Some theoretical studies involve collisions with atom exchange. However they are restricted to a few light systems (F + H₂ [21], F + D₂ [22]) in which the interactions, equilibrium distances, potential surface topology, masses and rovibrational spacings are very different from those encountered in the Na + Na₂ system. In this paper, we have performed a quantum-dynamical study of elastic, inelastic and rearrangement

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collisions for Na + Na$_2$ $(v, j = 0)$ at energies down to 1 nK.

Hutson and co-workers [23] have investigated the lowest quartet potential energy surfaces of spin-polarized alkali trimers (Li$_3$, Na$_3$, K$_3$, Rb$_3$ and Cs$_3$) at D$_{3h}$ and D$_{\infty h}$ configurations. They found very strong three-body effects. For instance the binding energies of alkali trimers are increased by taking into account the three-body interaction (more than a factor of 4 for Li, 1.3 to 1.5 for heavier alkalis) and the equilibrium distances of trimers are reduced in comparison with those of dimers. For Na$_3$ around the potential minimum, 80% of the total potential comes from the three-body interaction.

Here we extend our study to the $v = 2$ and $v = 3$ vibrational states of Na$_2$ and we investigate the three-body effects on the dynamics. Cross-sections and rate coefficients at ultralow temperatures for the elastic collision and for the vibrational relaxation (quenching processes including atom exchange) have been calculated. We have determined the complex scattering length and the extension of the energy region where Wigner threshold laws [24] apply. A detailed study of the sensitivity of these quantities on the three-body interaction has been performed. We show that the cross-sections, rate coefficients and scattering length are very sensitive to three-body effects.

2 Theoretical methods

In this paper, we are interested in collisional processes in an ultracold gas of Na(^{2}S) and Na$_2$($^3\Sigma_u^+$) molecules. In Section 1, we saw that elastic, inelastic and rearrangement processes have different roles in the formation and stability of a molecular BEC. In particular, elastic collisions are favorable collisions because they thermalize the gas and allow for evaporative cooling. We have two kinds of elastic collisions, those without (a) or with (b) atom exchange:

a: Na + Na$_2$($v, j = 0$) → Na + Na$_2$($v_f = v, j_f = j$),
b: Na + Na$_2$($v, j = 0$) → Na$_2$($v_f = v, j_f = j$) + Na.

On the contrary, non-elastic collisions are not favorable and are a source of heating. These collisions convert internal energy into kinetic energy and the molecules can change state and can be ejected from the trap. We have to distinguish two different processes: inelastic collisions, i.e. without atom exchange (c) and rearrangement collisions, i.e. with atom exchange (d):

c: Na + Na$_2$($v, j = 0$) → Na + Na$_2$(v_f, j_f),
d: Na + Na$_2$($v, j = 0$) → Na$_2$(v_f, j_f) + Na.

In both inelastic and rearrangement collisions, final states have rovibrational energies which are smaller than those of initial states. We consider that the electronic spin state of Na atoms is $S = 1/2$ and $m_S = +1/2$ and that the nuclear spin state of Na atoms is $I = 3/2$ and $m_I = +3/2$. We thus have three identical bosons with a total spin $F = F_{max} = I + S = 2$ and $M_F = M_{max} = +2$. All magnetic interactions are neglected, so that the electronic

and nuclear spin orientations are unchanged during the collision.

Because of bosonic symmetry, the spatial part of the Na$_3$ nuclear wavefunction has to be symmetric. As a consequence inelastic and rearrangement contributions cannot be distinguished. Quenching results from interferences between these two processes.

We use a time-independent formalism which is the most appropriate choice for ultralow energy scattering. It is essential to carry out three-dimensional calculations which include all three arrangements. At ultralow energies, only one partial wave with $l = 0$ contributes and since we have initial rotational states $j = 0$, we have to consider only one value of the total Na$_3$ orbital nuclear angular momentum $J = 0$.

The configuration space is divided into an inner and an outer region, depending on the atom-diatom distance.

In the inner region, we use a formalism based on body-frame democratic hyperspherical coordinates [25]. This has previously proved successful in describing atom-diatom insertion reactions such as N(^{2}D) + H$_2$ → NH + H [26,27] and O(^{1}D) + H$_2$ → OH + H [28,29]. These coordinates have also been used recently in studies of three-body recombination of ultracold atoms [30]. At each hyperradius ρ, we determined a set of eigenfunctions of a fixed-hyperradius reference Hamiltonian $H_0 = T + V$, which incorporates the total energy with the kinetic energy T arising from deformation and rotation around the axis of least inertia and the potential energy V. At small hyperradius, the adiabatic states in each sector span a large fraction of configuration space and allow for atom exchange. The scattering wave function is expanded on a set of hyperspherical adiabatic states. This yields a set of close-coupling equations, which are solved using the Johnson-Manolopoulos log-derivative propagator [31].

In the outer region, we use the standard Arthurs-Dalgarno formalism [32] based on Jacobi coordinates and assume that the atom-molecule interaction can be described by an isotropic potential $U(R)$ and therefore induces only elastic scattering. Radial channel wavefunctions are a solution of the following equation:

$$\left(-\frac{1}{2\mu} \frac{d^2}{dR^2} + \frac{l(l+1)}{2\mu R^2} + U(R) \right) F(R) = \frac{k^2}{2\mu} F(R) \quad (1)$$

where μ is the Na-Na$_2$ reduced mass and k and l are the channel wavenumber and orbital angular momentum quantum number. The potential $U(R)$ behaves asymptotically as C/R^6 with a coefficient $C = 3174$ au which is close to a recent ab initio value of 3216 au [33].

The equation (1) is solved by a finite difference method in the range $50-10000a_0$. The matching of the inner and outer wavefunctions is performed on a boundary which is an hypersphere of radius $50a_0$. This yields the reactance K, scattering S and transition T matrices. The inner region starts at a hyperradius of $8a_0$ and is split into 297 intervals. In the middle of each interval we compute eigenstates of the fixed-ρ Hamiltonian H_0 by a variational expansion on a basis of hyperspherical harmonics with A_1 symmetry of the nuclear P$_3$ permutation group. They are

fully symmetric with respect to spatial coordinate permutations to account for the indistinguishability of atoms. In each interval we expand the Na$_3$ nuclear wavefunction on a set of 135 eigenstates of H_0.

At large hyperradius, the eigenstates concentrate into the arrangement channels and describe Na$_2$ molecules in even j states. The hyperspherical harmonic basis is truncated at Λ_{max}, the maximum value of the grand angular momentum. Λ_{max} varies from 198 (867 harmonics) at small hyperradius to 398 (3400 harmonics) at large hyperradius. At the boundary between the inner and outer regions, the nuclear wavefunction is projected onto a set of Na$_2$ rovibrational states with vibrational quantum numbers $v = 0, 1, ..., 7$ and maximum rotational quantum numbers $j_{max} = 48, 44, ..., 10$ for each vibrational manifold.

Elastic and quenching cross-sections are given as a function of the diagonal elements of the transition T-matrix:

$$\sigma_E = \frac{\pi}{k^2}|T_{ii}|^2 \quad \sigma_Q = \frac{\pi}{k^2}(1 - |1 - T_{ii}|^2). \tag{2}$$

Here, at ultralow energies, we consider only T_{ii} elements with a relative atom-diatom orbital angular momentum $l = 0$. The complex scattering length can be written as

$$a = \frac{1}{2i} \lim_{k \to 0} \left(\frac{T_{ii}}{k} \right). \tag{3}$$

Then, the elastic and quenching cross-sections at threshold can be written respectively as the modulus squared of the scattering length and as the imaginary part of the scattering length:

$$\sigma_E = 4\pi|a|^2, \quad \sigma_Q = -\frac{4\pi}{k}\text{Im}(a). \tag{4}$$

From the cross-sections we deduce the elastic and quenching rate coefficients $K = \sigma v$ where v is the atom-diatom relative velocity and the Wigner laws for these quantities are

$$K_E = \frac{4\pi\hbar|a|^2}{\mu}k \sim E_{coll}^{1/2}, \quad K_Q = -\frac{4\pi\hbar}{\mu}\text{Im}(a) \sim \; const. \tag{5}$$

We note that the imaginary part of the scattering length is directly linked to quenching processes.

State-to-state cross-sections for the partial wave $J = 0$ are generated from the T-matrix using the standard formula:

$$\sigma_{vj \to v_f j_f} = \frac{\pi}{k_{vj}^2}|T_{v_f j_f, vj}^{J=0}|^2. \tag{6}$$

3 Results and discussion

In this work we use a potential energy surface (PES) which depends parametrically on a dimensionless parameter λ. It can be written as a many-body expansion [34]:

$$V_\lambda(r_1, r_2, r_3) = V(r_1) + V(r_2) + V(r_3) + \lambda W(r_1, r_2, r_3) \tag{7}$$

where r_i are the interatomic distances, V is the $^3\Sigma_u^+$ potential of Na$_2$ and λW is a three-body term. When $\lambda = 0$, we obtain an additive potential V_0 and when $\lambda = 1$, V_1 reproduces the PES of Higgins et al. [35] for the lowest $1^4A_2'$ quartet electronic state of Na$_3$ [36]. The full potential V_1 has a global minimum of -1222 K for an equilateral triangle configuration with interatomic distances of $8.3a_0$. This value is much larger than for V_0 (-760 K at $9.8a_0$). For collinear geometries, the minimum is reached when two interatomic distances are equal. The respective values are -554 K at $9.6a_0$ for V_1 and -516 K at $9.8a_0$ for V_0. The Na$_3$ PES is attractive at large distances and all approaches of a Na atom towards a Na$_2$ molecule are possible at ultralow energies. Atom exchange can therefore proceed through two mechanisms: abstraction and insertion [37]. In order to study the effect of the three-body interaction on the dynamics of Na + Na$_2$ collisions, we change the strength of the three-body term λW by varying the parameter λ.
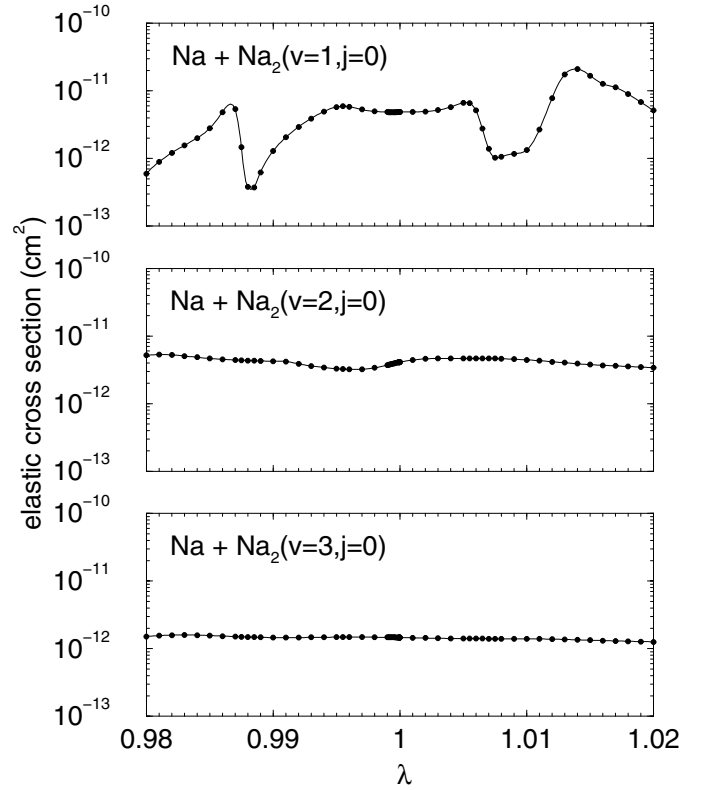
For $\lambda = 1$, we computed elastic and quenching probabilities at collision energies lying between 1 nK and 1 K for the $J^\Pi = 0^+$ partial wave. At energies higher than 0.1 mK, partial waves with $J \geq 1$ are needed to obtain converged cross-sections. This will be reported in a future paper. Rate coefficients for three initial rovibrational states ($v = 1, 2, 3, j = 0$) of the Na$_2$ molecules are shown in Figure 1 as a function of the collision energy. Figure 1 corresponds to calculations using the full nonadditive potential V_1. Both elastic and quenching rate coefficients decrease when the initial vibrational quantum number v increases from 1 to 3. In contrast, if we only use the additive potential V_0, rate coefficients (not shown here) do not present a clear dependence on the initial vibrational quantum number v. Moreover the magnitude of the rate coefficients is not the same. For instance at 1 nK the elastic rate coefficient for $v = 1$ obtained with the additive potential is 20 times smaller than that obtained on the full potential. So these results show that the inclusion of the three-body term has a large influence on the magnitude of elastic and quenching rate coefficients and on their dependence on the initial vibrational state of Na$_2$. This conclusion is consistent with our previous calculations [38] which were restricted to the initial ($v = 1, j = 0$) rovibrational state of Na$_2$. Figure 1 exhibits another striking feature. For the three first excited initial vibrational states the quenching rate coefficients are more important than the elastic ones below 100 μK so that evaporative cooling (where elastic collisions should predominate) would not be efficient. The oscillations which occur in the elastic rate coefficient for collision energies larger than 1 mK arise from small values of the complex scattering phase-shift. Finally we determined the upper limit of the Wigner region. Wigner threshold laws are valid for collision energy below 10^{-6} K, 10^{-5} K, 10^{-4} K respectively for $v = 1, 2, 3$. The Wigner region spreads more and more as the initial v increases because quenching probabilities reach their upper limit 1 at larger energies as v increases. By using the equation (3) with the T_{ii} matrix elements calculated with the full potential, we extract the complex scattering
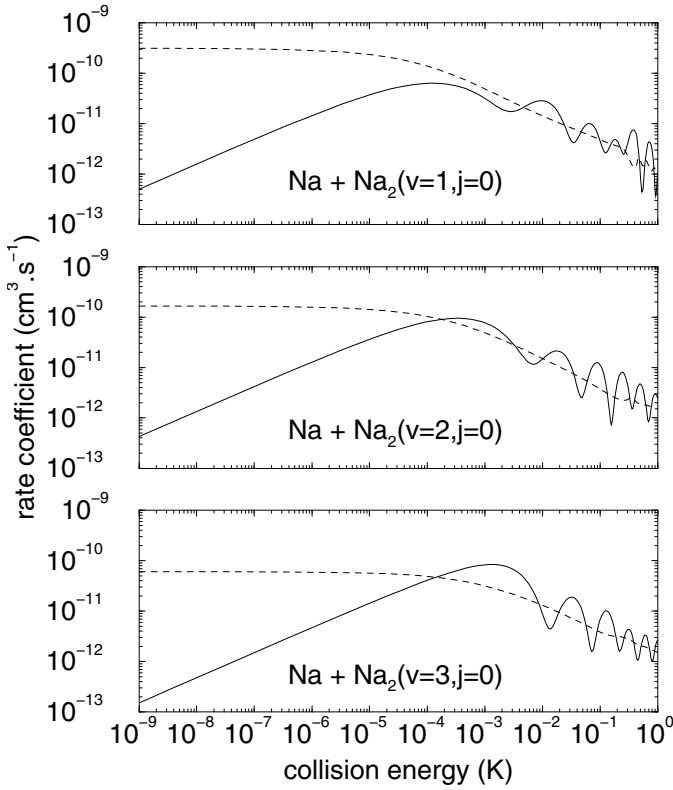
Fig. 1. Elastic (solid line) and quenching (dashed line) $J = 0$ rate coefficients for Na + Na$_2$ collisions for three initial rovibrational states $(v = 1, j = 0)$, $(v = 2, j = 0)$, $(v = 3, j = 0)$ of Na$_2$ as a function of the collision energy. The full non-additive potential (two-body terms + three-body term, $\lambda = 1$) is used here.

Fig. 2. Elastic cross-sections for Na + Na$_2$ collisions for three initial rovibrational states $(v = 1, j = 0)$, $(v = 2, j = 0)$, $(v = 3, j = 0)$ of Na$_2$ as a function of λ at a collision energy of 1 nK.

length a. The complex scattering length in nanometer is then $a = 1.51 - i\,6.04$, $4.74 - i\,3.18$ and $3.20 - i\,1.17$ for respectively $v = 1, 2, 3$. If we use the additive potential only, we find $a = 0.48 - i\,1.29$, $5.77 - i\,2.84$ and $0.19 - i\,0.63$.

Then we studied the sensitivity of the elastic and quenching cross-section for Na + Na$_2(v = 1, 2, 3)$ collisions at ultracold energies on the parameter λ. We generated bases of hyperspherical states for 65 values of λ between 0.98 and 1.02 and computed cross-sections at a collision energy $E_{coll} = 1$ nK. For the elastic processes (Fig. 2), cross-sections are less sensitive on λ as the initial vibrational quantum number v increases. For $v = 1$, the elastic cross-section presents a strong dependence on λ. For instance, a change of 1% in λ yields a change of about 75% in the cross-section. This change of 1% corresponds to a variation of around 10 K (7 cm^{-1}) in the minimum of the full potential. Presently, ab initio calculations are not accurate enough to give the magnitude of cross-sections for this vibrational state. In contrast for $v = 2$ the elastic cross-section is less sensitive to λ and for $v = 3$ it is almost constant. The quenching processes (Fig. 3) exhibit similar features. Sensitivity with λ decreases as the initial vibrational quantum number v increases. Quenching processes involve all open final rovibrational channels except the initial one. The final vibrational distributions for the

Na + Na$_2(v = 2, j = 0) \rightarrow$ Na + Na$_2(v_f = 0, 1)$ and Na + Na$_2(v = 3, j = 0) \rightarrow$ Na + Na$_2(v_f = 0, 1, 2)$ are plotted in Figure 3. The sensitivity of quenching cross-sections for $v = 2$ and $v = 3$ on λ depends on the final vibrational states v_f. For instance, for $v = 2$ cross-section for the final vibrational state $v_f = 1$ dominates when $\lambda = 0.98$ or 1.02 whereas cross-section for the final vibrational state $v_f = 0$ dominates when $\lambda = 1$. For $v = 3$, the $v_f = 2$ cross-section dominates at $\lambda = 1.02$ whereas the $v_f = 0$ cross-section dominates at $\lambda = 0.98$, but both of them equally contribute when $\lambda = 1$. Furthermore, for $v = 2$ and $v = 3$, variations with λ are more pronounced for vibrationally state-resolved cross-sections than for total cross-section (summed over v_f). However, this effect is minor for $v = 3$ where each final vibrational distribution is almost constant with λ. This behaviour could be either due to a flat behaviour with λ of each rotationally state-resolved cross-section or due to a compensation effect (the vibrationally state-resolved cross-section is a constant although each rotationally state-resolved cross-section depends on λ).
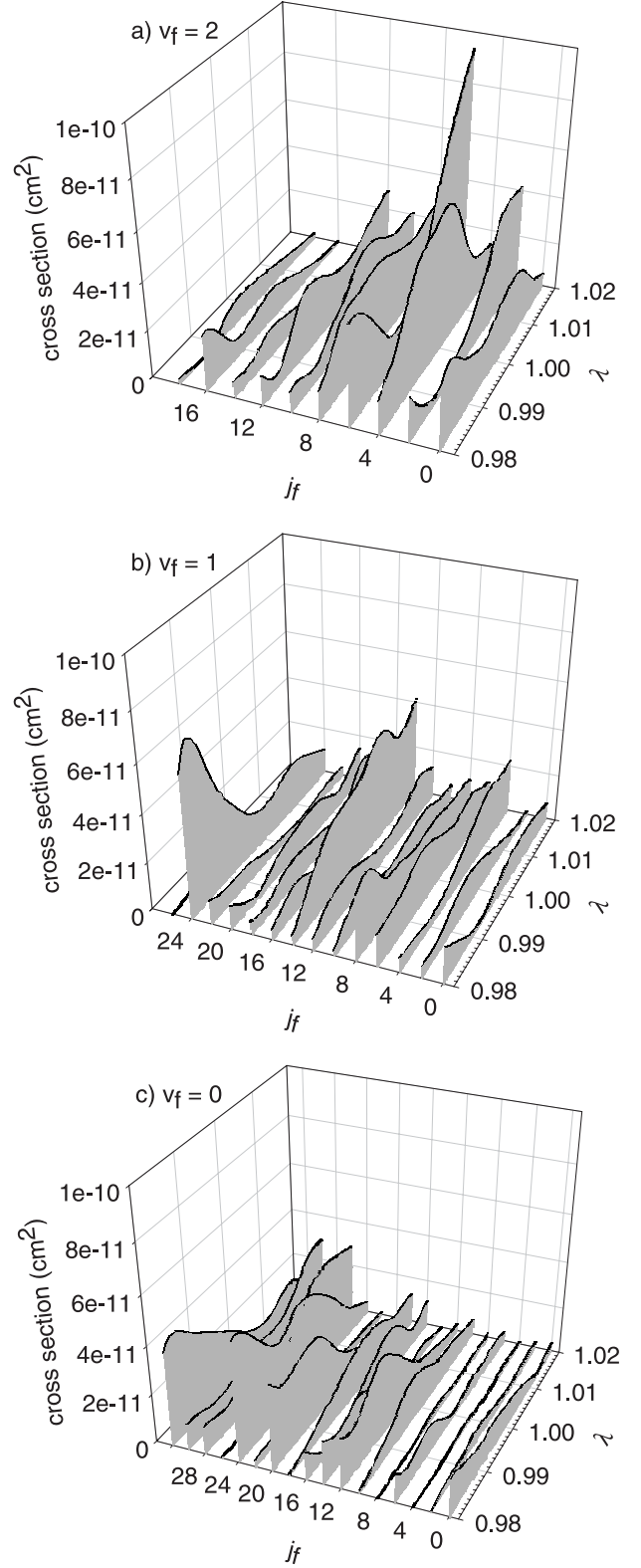
Rotational distributions for Na + Na$_2(v = 3, j = 0) \rightarrow$ Na + Na$_2(v_f = 0, 1, 2)$ collisions have therefore been calculated as a function of λ. Figure 4 shows many structures. For each v_f, the final rotational distribution is very sensitive to λ although the final vibrational distribution is not. For $v_f = 2$ (Fig. 4a), the cross-section is peaked at $j_f = 6$
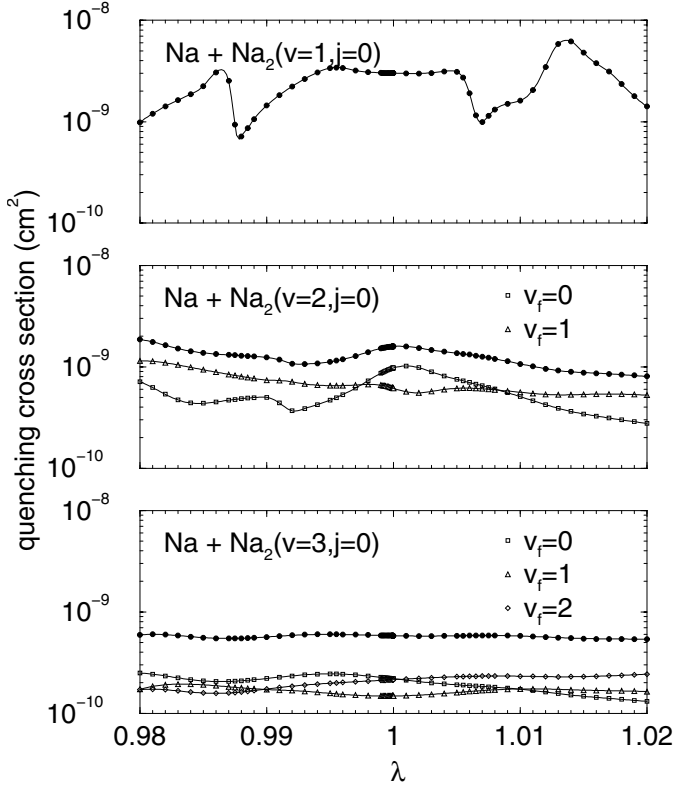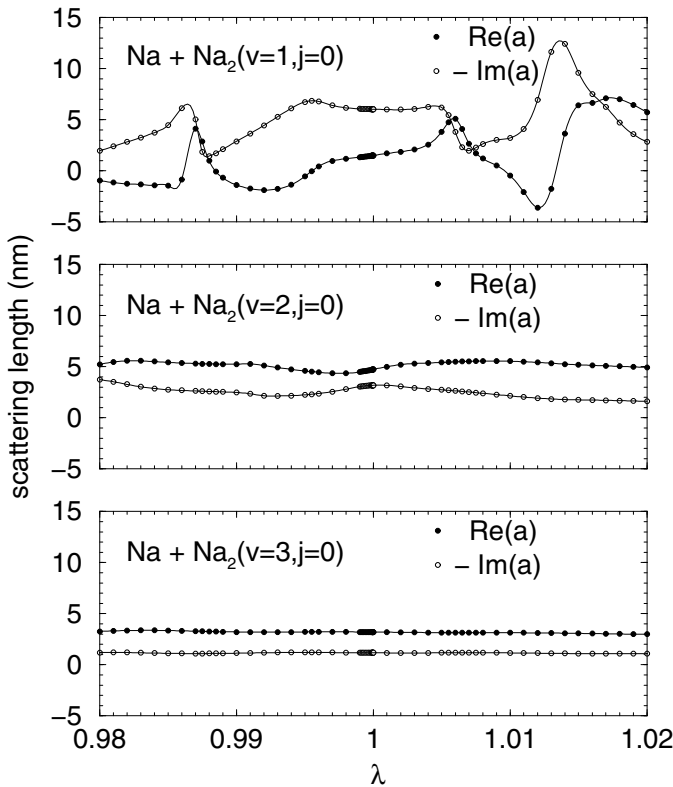
Fig. 3. Quenching cross-sections (full circle) for Na + Na₂ collisions for three initial rovibrational states $(v = 1, j = 0)$, $(v = 2, j = 0)$, $(v = 3, j = 0)$ of Na₂ as a function of λ at a collision energy of 1 nK. For initial vibrational states $v = 2$ and $v = 3$, quenching cross-sections for a final vibrational state $v_f = 0$ (square), $v_f = 1$ (triangle), $v_f = 2$ (cross) are also shown.

for $\lambda = 0.98$ and 1.02, whereas it is peaked at $j_f = 4$ for $\lambda = 1$. For $v_f = 1$ (Fig. 4b), the cross-section is peaked at $j_f = 24$ for $\lambda = 0.98$, whereas it is peaked at $j_f = 14$ for $\lambda = 1.02$. The situation is similar for $v_f = 0$ (Fig. 4c) with a peak at $j_f = 24$ and 32 for $\lambda = 0.98$, and a peak at $j_f = 26$ and 30 for $\lambda = 1.02$. Finally we see that the rotational distributions do not show a regular behaviour with λ, and for fixed λ depend strongly on the final vibrational state.

An important feature is the variation of the scattering length with the potential. The real and the imaginary part of the scattering length calculated using equation (3) are shown in Figure 5 as a function of λ. The variations are strong for $v = 1$ as it has already seen in the $v = 1$ cross-sections (Figs. 2 and 3), while they become much weaker for $v = 2$ and nearly disappear for $v = 3$. Here, the complexity of the collisional processes does not allow us to directly explain the origin of these dependences on λ. However a simple model with an absorbing complex square-well potential [39] gives a similar behaviour for the real and imaginary parts of the scattering length. These variations are due to a lowering of the energy of resonant states which fall down to threshold and cross it as λ increases.

Fig. 4. Three-dimensional plots for rotational distributions for the vibrational relaxation Na + Na₂$(v = 3, j = 0) \rightarrow$ Na + Na₂(v_f, j_f) or Na₂(v_f, j_f) + Na with $v_f = 2$ (panel a), $v_f = 1$ (panel b) and $v_f = 0$ (panel c) as a function of λ at a collision energy of 1 nK.

Fig. 5. Real part (black circle) and imaginary part (white circle) of the scattering length a for Na + Na$_2$ collisions for three initial rovibrational states $(v = 1, j = 0)$, $(v = 2, j = 0)$, $(v = 3, j = 0)$ of Na$_2$ as a function of λ.

4 Conclusion

We have performed accurate $J = 0$ quantum-mechanical calculations of elastic scattering and vibrational relaxation of Na$_2(v, j = 0)$ molecules in collisions with Na atoms using a formalism based on hyperspherical coordinates which incorporates rearrangement. In the Wigner regime, below 10^{-6} K, 10^{-5} K, and 10^{-4} K for respectively $v = 1, 2, 3$, the elastic cross-sections and the quenching rate coefficients are constant. Quenching rate coefficients for initial excited vibrational states $v = 1, 2, 3$ of Na$_2$ are larger than the elastic rate coefficients in the Wigner region.

Cross-sections, rate coefficients and scattering lengths depend strongly on the three-body interaction. They are very sensitive to small changes in the three-body term of the many-body expansion of the potential energy surface. This effect is more pronounced for the vibrational distribution involving initial Na$_2$ molecules in their $v = 1$ vibrational state. However rotational distributions are modified by a slight change of the three-body term even for the initial excited vibrational states $v = 2$ and $v = 3$ of Na$_2$. These results exhibit two main points. First the three-body interaction term is required in the many-body expansion of potential energy surface to describe accurately dynamics of ultracold atom-diatom collisions and maybe also the related three-body processes such as the three-body recombination. Second an accurate three-body term

is needed to obtain rigorous cross-sections at the rotational level whereas a fairly good description of the three-body interaction is sufficient to obtain reliable vibrational distributions, especially for the highest initial vibrational states considered in this study.

In a near future we plan the study of vibrational relaxation with initial high vibrational states of Na$_2$ in order to see if the ratio elastic/quenching rate coefficients will be inverted as in recent experiments on molecular BEC. Rotational relaxation will be also investigated. For that we have to include higher partial waves ($J \geq 1$) in the quantum-mechanical treatment. Others systems which are of experimental interest will be considered. For instance, the study of ultracold collisions involving fermionic and bosonic potassium atoms and molecules is currently under way in our group.

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