

Energy dependence of scattering ground-state polar molecules

Christopher Ticknor*

*ARC Centre of Excellence for Quantum-Atom Optics and Centre for Atom Optics and Ultrafast Spectroscopy,
Swinburne University of Technology, Hawthorn, Victoria 3122, Australia*

(Received 19 July 2007; published 7 November 2007)

We explore the total collisional cross section of ground-state polar molecules in an electric field at various energies, focusing on RbCs and RbK. An external electric field polarizes the molecules and induces strong dipolar interactions, leading to nonzero partial waves contributing to the scattering even as the collision energy goes to zero. This results in the need to compute scattering problems with many different values of total M to converge the total cross section. An accurate and efficient approximate total cross section is introduced and used to study the low-field temperature dependence. To understand the scattering of the polar molecules we compare a semiclassical cross section with the quantum unitarity limit. This comparison leads to the ability to characterize the scattering based on the value of the electric field and the collision energy. General and simple forms of the characteristic electric field and energy are given, enabling characterization of the scattering.

DOI: [10.1103/PhysRevA.76.052703](https://doi.org/10.1103/PhysRevA.76.052703)

PACS number(s): 34.20.Cf, 34.50.-s, 05.30.Fk

I. INTRODUCTION

Recently the ballistic expansion of a Bose-Einstein condensate (BEC) of ^{52}Cr showed the influence of the magnetic dipole-dipole interaction [1]. In these experiments an interplay of trap geometry and magnetic polarization was used to clearly illustrate the interaction of the dipoles. Another example of spin-spin dipolar interactions adding character to ultracold matter is the perturbative effect observed in the p -wave Feshbach resonances in ^{40}K [2] and ^{40}K - ^{87}Rb [3] where different $|m_l\rangle$'s have distinct resonant magnetic field values [4]. These experiments offer a glimpse of the additional character relatively weak dipole-dipole interactions offer in ultracold atomic systems. Attention has begun to turn towards polar molecules which have large electric-dipole moments. Theories predict many novel phase transitions for dipolar gases [5,6]. Further heightening the interest in polar molecules are its applications, which range from quantum computing [7,8] to tests of fundamental symmetries [9,10].

With such remarkable possibilities, it is not surprising that rapid experimental progress should soon produce ultracold ground-state polar molecules. There are many methods of producing cold molecules; for a review, see Ref. [11]. One of the most exciting techniques used to produce cold polar molecules is photoassociation (PA). This method produces cold polar molecules by binding two distinct ultracold alkali-metal atoms through a series of optical transitions which ultimately lead to the formation of a polar molecule such as RbCs [12], KRb [13], or NaCs [14]. Recently RbCs was produced in its absolute vibrational ground state at a temperature of $100\ \mu\text{K}$ [15]. The production of a cold and dense sample of these heteronuclear alkali-metal dimers would constitute the realization of a strongly interacting dipolar system near $T=0$. Considering only the physics of collisions, this system presents a series of exciting experiments, such as the detection of field linked states [16], the study of ultracold rotationally inelastic collisions, the study of fully hydrodynamic systems, and ultracold chemistry [17].

In light of the current experimental progress there is an immediate need to understand the collisions of polar molecules, so that collisional experiments can be understood and control of the molecular interactions can be achieved. Previous theoretical scattering studies looked at how the long-range dipolar interactions are affected by external fields, first those in weak-field-seeking states [16,18,19] and later those in strong-field-seeking states [20]. Other studies looked at the ways magnetic and electric fields can be used to control the molecular state in collisions of atom-molecule systems [21].

For ultracold ground-state polar molecules in an electric field, only long-range interactions at extremely cold temperatures have been studied previously [20]. That work showed potential resonances (PRs) occur with the application of an external field. These resonances emerge from the electric field changing the long-range character of the lowest adiabatic curve, from $1/R^6$ to $1/R^3$, adding many bound states to the system. This mechanism leads to broad semiregular resonances with respect to electric field. These PRs are significantly different from magnetic Feshbach resonances (FRs) in ultracold atomic physics [22]. A FR occurs when an external magnetic field separates the scattering thresholds and alters the molecular structure and changes the number of bound states in the two-body system. This process acts over short range, where spin exchange couples different channels. The long-range character of the interatomic potential remains the same in a magnetic field, in contrast to PRs.

With the experimental reality of ultracold ground-state polar molecules rapidly approaching, it is necessary to understand both the energy and electric field dependence of the scattering. In this paper we obtain total cross sections for the long-range scattering of RbCs and RbK. These molecules are considered to be in their absolute ground state. The rest of the paper is structured as follows: we briefly review the Stark effect and the dipolar interaction. Then results of the scattering are presented with both energy and electric field being varied. We consider the thermally averaged cross section, and finally we explore the character of the scattering as a function of energy and electric field.

*cticknor@swin.edu.au

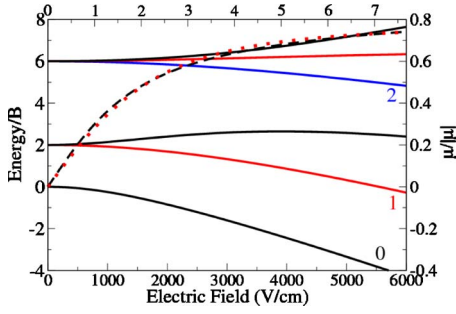


FIG. 1. (Color online) RbCs molecular energies shown as a function of electric field. The energies are normalized by the rotational constant. Different color curves represent values of M : $M=0$ (black), $|M|=1$ (red), and $|M|=2$ (blue). The black dashed line is the projection of the dressed molecular ground state onto the field axis, $\langle 00|\hat{z}|00\rangle$, and its value is given on the right vertical axis. The red dotted curve is a simple and approximate form of $\langle 00|\hat{z}|00\rangle$ given in the text. The top horizontal axis shows the electric field normalized by the critical field value, $\mathcal{E}/\mathcal{E}_0$.

II. STARK EFFECT AND MOLECULAR SCATTERING

We consider the polar molecules to be in their absolute ground state, including vibration, rotation and electronic ground state ($^1\Sigma$). We assume the molecules are rigid rotors best described in the J basis $|JM\rangle$, where J is $J=S+L+N$, S and L are the spin and orbital angular momentum of the electronic system, and N is the rotational state of the molecule. For these systems L and S are zero. M is the projection of J onto the field axis. We ignore the effects nuclear spin.

In this model the only molecular structure is the rotational state; with the electric field accounted for via the Stark effect. In the J basis the matrix elements of the field-molecule Hamiltonian and molecular Hamiltonian are written as [23]

$$\begin{aligned} \langle JM|H_{mol}|J'M'\rangle &= BJ(J+1)\delta_{JJ'}\delta_{MM'} - \mu\mathcal{E}[J,J'] \\ &\times (-1)^M \begin{pmatrix} J & 1 & J' \\ -M & 0 & M' \end{pmatrix} \begin{pmatrix} J & 1 & J' \\ 0 & 0 & 0 \end{pmatrix}, \end{aligned} \quad (1)$$

where $[J]$ is a shorthand notation for $\sqrt{2J+1}$. B is the rotational constant and μ is the electric-dipole moment. In Fig. 1 the Stark energies for RbCs are shown as a function of electric field and the energies are normalized by the rotational constant. At first the energies vary quadratically as the field is varied, then a transition occurs roughly at $\mathcal{E}_0=B/\mu$, when the Stark energy is roughly equal to the energy rotational splitting. Above this field value the energies vary linearly with respect to electric field. The top horizontal axis shows the electric field normalized by the critical field value, $\mathcal{E}/\mathcal{E}_0$. The different color (online) curves represent different values of J projected onto the field axis; the values are $|M|=0$ (black), $|M|=1$ (red), and $|M|=2$ (blue). The black dashed line is the projection of the lowest molecular eigenstate of the molecule/field Hamiltonian from Eq. (1) or the field-dressed ground state onto the field axis, $\langle 00|\hat{z}|00\rangle=\langle\mu\rangle/|\mu|$. An approximate polarization is shown in Fig. 1 as the dotted

red curve. It is used to derive simple analytic results later. This approximate form is

$$\langle\mu\rangle \approx 0.78\mu\sqrt{\frac{x^2}{6.7+x^2}}, \quad (2)$$

where $x=\mathcal{E}/\mathcal{E}_0$. This approximation is within 2% of $\langle\mu\rangle$ for fields less than $6\mathcal{E}_0$.

Throughout this paper we use $^{87}\text{Rb}^{133}\text{Cs}$ and $^{87}\text{Rb}^{41}\text{K}$ as an example of polar molecules. For RbCs we use a dipole of $\mu=1.3$ D, a mass of $m=220$ amu, and a rotational constant of $B=0.0245$ K. For this model the critical field value is $\mathcal{E}_0^{\text{RbCs}} \simeq 780$ V/cm. We also consider RbK with the parameters $\mu=0.76$ D, $m=128$ amu, and $B=0.055$ K [24]. This yields a critical field of $\mathcal{E}_0^{\text{RbK}} \simeq 3000$ V/cm.

The intrigue of polar molecules is their long-range anisotropic dipole-dipole interaction

$$\begin{aligned} V_{\mu\mu} &= -\frac{3(\hat{\mathbf{R}} \cdot \hat{\boldsymbol{\mu}}_1)(\hat{\mathbf{R}} \cdot \hat{\boldsymbol{\mu}}_2) - \hat{\boldsymbol{\mu}}_1 \cdot \hat{\boldsymbol{\mu}}_2}{R^3} \\ &= -\frac{\sqrt{6}}{R^3} \sum_q (-1)^q C_{-q}^2(\boldsymbol{\mu}_1 \otimes \boldsymbol{\mu}_2)_q^2. \end{aligned} \quad (3)$$

Here $C_{-q}^2(\theta, \phi)$ is a reduced spherical harmonic that acts on the relative angular coordinate of the molecules, while $(\boldsymbol{\mu}_1 \otimes \boldsymbol{\mu}_2)_q^2$ is the rank-2 tensor formed from two rank-1 operators which act on the molecular state. The matrix elements of the dipole-dipole interaction are

$$\begin{aligned} &\langle J_1 M_1 J_2 M_2 l M_l | V_{\mu\mu} | J_1' M_1' J_2' M_2' l' M_l' \rangle \\ &= (-1)^{M_1' + M_2' + M_l' + 1} [l, l', J_1, J_1', J_2, J_2'] \\ &\times \begin{pmatrix} \mu^2 \sqrt{6} \\ R^3 \end{pmatrix} \begin{pmatrix} l & 2 & l' \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l & 2 & l' \\ -M_l & M_l - M_l' & M_l' \end{pmatrix} \\ &\times \begin{pmatrix} 1 & 1 & 2 \\ M_1 - M_1' & M_2 - M_2' & M_l - M_l' \end{pmatrix} \begin{pmatrix} J_1 & 1 & J_1' \\ 0 & 0 & 0 \end{pmatrix} \\ &\times \begin{pmatrix} J_1 & 1 & J_1' \\ -M_1 & M_1 - M_1' & M_1' \end{pmatrix} \begin{pmatrix} J_2 & 1 & J_2' \\ 0 & 0 & 0 \end{pmatrix} \\ &\times \begin{pmatrix} J_2 & 1 & J_2' \\ -M_2 & M_2 - M_2' & M_2' \end{pmatrix}. \end{aligned} \quad (4)$$

To perform the scattering calculation we field dress the system which entails using the molecular-field eigenstates from Eq. (1) to compose molecular states in the scattering channels. The basis is also symmetric under interchange because the molecules are identical bosons.

The scattering Hamiltonian can be expressed by the projection of the total angular momentum $M_T=M_1+M_2+M_l$ onto the field axis (\hat{z}), and $V_{\mu\mu}$ is block diagonal due to rotational symmetry about the field axis. To obtain the total cross section σ , the cross sections for each block of total M , $\sigma^{(M)}$, must be calculated. The matrix elements of $V_{\mu\mu}$ differ between blocks of total M and thus are rigorously required to be computed. Thus σ in terms of $\sigma^{(M)}$ is

$$\sigma = \sum_M \sigma^{(M)},$$

$$\sigma^{(M)} = \sum_{ij} \sigma_{ij}^{(M)} = \sum_{ij} \frac{2\pi}{k^2} |T_{ij}^{(M)}|^2, \quad (5)$$

where $\sigma_{ij}^{(M)}$ is the cross section for the system to scatter from the i th to the j th channel for $M_T=M$. $k^2=mE$, where E is the collision energy, and $T_{ij}^{(M)}$ is the scattering T matrix with $M_T=M$ [25]. The factor of 2 in Eq. (6) is present because the molecules are identical particles. We consider collisions in lowest thresholds with two-ground-state molecules and there are no two-body inelastic channels. It is also worth noting that the molecular and scattering Hamiltonian are invariant to the sign of the electric field, thus $\sigma^{(-M)}=\sigma^{(M)}$.

An approximate σ can be obtained by assuming $\sigma^{(M)}$ is equal to $\sigma^{(0)}$ once all the terms with unphysical partial wave terms have been removed—i.e., those with $|M_l|>l$. To clarify this consider $\sigma^{(1)}$ for ground-state molecules, $M_1=M_2=0$, and therefore $M_T=M_l=1$. Since $M_l=1$, it is unphysical to have s -wave channels contribute and these are removed. This approximation results in $\sigma^{(1)}=\sum_{ij}\sigma_{ij}^{(0)}(1-\delta_{l,0})\times(1-\delta_{l,0})$. Using this procedure for all $\sigma^{(M)}$ we find the total approximate cross section is

$$\tilde{\sigma} = \sum_{ij} (2l_{\min} + 1) \sigma_{ij}^{(0)}, \quad (6)$$

where $l_{\min}=\min(l_i, l_j)$. This approximation works well and is a cost-effective method for computing the thermally averaged total cross section. To obtain the thermally averaged cross section we use

$$\langle \sigma \rangle \approx \langle \tilde{\sigma} \rangle = \frac{1}{(kT)^2} \int_0^\infty E \tilde{\sigma}(E) e^{-E/kT} dE, \quad (7)$$

where $\tilde{\sigma}(E)$ is the energy-dependent approximate total cross section, k is Boltzmann's constant, and T is the temperature.

In ultracold atomic collisions there is usually a need to compute only one block of M_T , the one containing s -wave channels. This is due to Wigner threshold laws which state that nonzero partial waves are suppressed as the collision energy goes to zero. However, this is not the case for polar molecules in a nonzero electric field. The electric field mixes the various rotational states and polarizes the scattering molecules. Considering the field-dressed scattering Hamiltonian, we find that there is a direct dipole-dipole coupling between the scattering molecules. The result of this interaction is most clearly seen through the Born approximation, which assumes a long-range potential $C_{ij}R^{-s}$. For small C_{ij} one can approximate the wave functions as spherical Bessel functions and then the Born approximation yields a T matrix [25,26]. From the Born approximation we obtain a partial cross section $\sigma_{ij} \propto E^p$ where $p=\min(2l, s-3)$. For a nonzero electric field, we find $s=3$ and C_{ij} denotes the field-dressed couplings derived from Eq. (4). In the Born approximation when $C_{ij} \neq 0$ the partial cross section for degenerate channels is

$$\sigma_{ij} = \text{const.} \quad (8)$$

This result is independent of energy for all l and implies that the dipole-dipole interaction leads to a scattering cross section where many partial waves might contribute even at low

energy. For a complete discussion of this result see Ref. [26].

A worthwhile estimate of the total cross section is with a semiclassical approach. This approach offers scaling of σ on the physical parameters of the system, such as μ , m , and E [27]. This yields a total cross section of

$$\sigma_{SC} = \langle \mu \rangle^2 \sqrt{\frac{m}{E}} c_{SC}, \quad (9)$$

where c_{SC} is a constant chosen so the units of μ , m , E , and σ_{SC} are in De, amu, K, and cm^2 , respectively. Using Eq. (2) for $\langle \mu \rangle$ and comparing the approximation to the full scattering calculation with many different initial boundary conditions at R_{in} with large \mathcal{E} we obtain $c_{SC}=1.5 \times 10^{-13}$. This is roughly an order of magnitude less than what is obtained from the semiclassical calculation [27], but as we shall see this value of c_{SC} offers a good representation of the scattering in an electric field for both RbCs and RbK.

In quantum mechanical scattering the unitarity limit provides an upper limit for any single partial-wave contribution. This limit is obtained when the T matrix takes on its maximum value of 4, yielding

$$\sigma_Q = \frac{8\pi}{mE} c_Q. \quad (10)$$

$c_Q=4.85 \times 10^{-15}$ and has been chosen so the units of m , E , and σ_Q are in amu, K, and cm^2 , respectively. The comparison of σ_{SC} and σ_Q offers insight into the scattering process and is explored at length below. The primary difference between these two cross sections is the energy dependence, and this indicates there will be a transition from semiclassical to quantum mechanical scattering as the collision energy is lowered.

To numerically solve the scattering problem we use Johnson's log derivative [28]. We start the scattering calculation at $R_{in}=20a_0$, which is inside of where the molecular interaction deviates from $V_{\mu\mu}$ due to van der Waals interactions. At R_{in} we impose the boundary condition that the wave function must be zero. This is not a physical boundary condition; rather, it is a starting point to systematically study the long-range scattering. We also include a diagonal $-C_6/r^6$ potential, where a value of $C_6=10^3$ a.u. is used. We propagate the log derivative to $R_\infty=10^5a_0$. To converge $\sigma^{(M)}$ we need a large number of partial waves. For RbCs (RbK) we use $l_{max}=18$ ($l_{max}=14$). Furthermore, many values of the total M are required; RbCs (RbK) needs up to $M_T=10$ ($M_T=6$) to converge for field values up to $4\mathcal{E}_0$ and collision energies ranging from 10^{-7} to 10^{-4} K. We use up to $J=2$; additional rotational states make the calculations very computationally cumbersome to converge with respect to the number of partial waves. On physical grounds collisions in the ground state are coupled at third order to $J=3$ rotational states and for these reasons are omitted.

Using the above parameters we find all $\sigma^{(M)}$'s are converged to better than 1% and the total cross section is converged to better than 10% for electric field values up to $4\mathcal{E}_0$ with collision energies ranging from 10^{-7} to 10^{-4} K. For low field and low energy σ is converged to a much better percentage. For energies below 10^{-7} K we need a larger R_∞ to

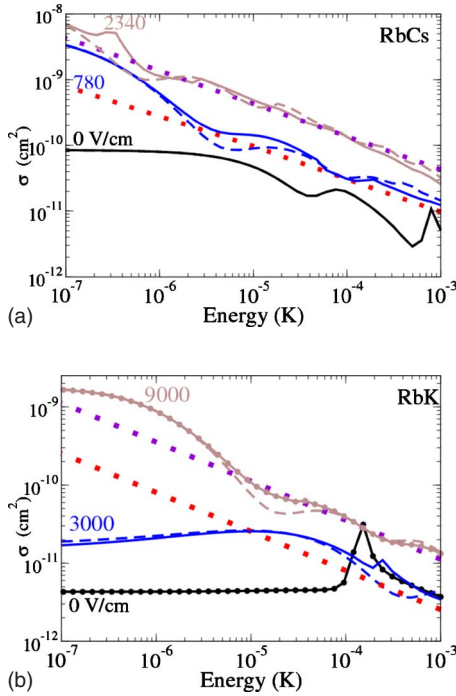


FIG. 2. (Color online) The energy dependence of σ (solid lines) and $\tilde{\sigma}$ (dashed lines) for various electric fields. In ascending order the fields are 0 (black), \mathcal{E}_0 (blue), and $3\mathcal{E}_0$ (brown) for (a) RbCs and (b) RbK where $\mathcal{E}_0^{\text{RbCs}} \approx 780$ V/cm and $\mathcal{E}_0^{\text{RbK}} \approx 3000$ V/cm. The dotted lines are σ_{SC} from Eq. (9) for different electric fields. In ascending order they are \mathcal{E}_0 (red) and $3\mathcal{E}_0$ (purple).

converge the calculations, and at higher collision energies $E > 10^{-4}$ K, more partial waves and $\sigma^{(M)}$ are required. With this model, we explore the field dependence and energy dependence of the molecular scattering.

III. ENERGY DEPENDENCE

In Fig. 2 we show the energy dependence of the total cross section σ (solid lines) and the approximate cross section $\tilde{\sigma}$ (dashed lines) for both RbCs (a) and RbK (b) at three electric field values: 0 (black), \mathcal{E}_0 (blue), and $3\mathcal{E}_0$ (brown) where $\mathcal{E}_0^{\text{RbCs}} \approx 780$ V/cm and $\mathcal{E}_0^{\text{RbK}} \approx 3000$ V/cm. The dotted lines are σ_{SC} from Eq. (9) for the electric field values of \mathcal{E}_0 (red) and $3\mathcal{E}_0$ (purple). There are general comments which can be made about both (a) and (b), but the effects of dipolar scattering are more prominent in the heavier, more polar RbCs.

The solid black curve shows the energy-dependent scattering for zero electric field. In zero field there is no dipolar coupling between degenerate channels containing ground-state molecules. This fact implies that the zero-field scattering will behave like the familiar ultracold atomic systems, where the low-energy scattering is s -wave dominated. This means as the energy goes to zero, $\sigma \rightarrow 8\pi a^2$ where a is the s -wave scattering length. Furthermore, channels with non-zero partial waves are suppressed as the collision energy goes to zero. The zero-field collisions will contain information about the short-range interactions. However, the dipolar

interaction does influence the scattering at short range when $V_{\mu\mu}$ becomes larger than the threshold separation between channels containing two ground-state molecules, $J_1=J_2=0$, and two rotationally excited molecules, $J'_1=J'_2=1$.

Once there is an electric field, the nonzero partial-wave terms contribute to the total cross section even at low energy. This can be seen in all of the curves in (a) with $\mathcal{E} \neq 0$. The blue and brown curves have significantly different profiles than the black curve in both (a) and (b). The change in profile is only slightly due to the change in the s -wave scattering length. Predominantly the change is due to the additional contribution of nonzero partial waves to the total cross section. Generally in a strong field the scattering is made up of many partial-wave contributions at low energies. The total cross section for large electric field is fairly well represented by $\sigma_{SC} \propto E^{-1/2}$. This is seen in (a) and (b) when the field is $3\mathcal{E}_0$, in the similar energy dependence of the purple dotted lines and the brown curves.

At low energy quantum mechanical scattering must dominate, $\sigma_Q > \sigma_{SC}$ as $E \rightarrow 0$. This fact does not imply that σ must be larger than σ_{SC} or $\sigma = \sigma_Q$. Rather it implies that the scattering will depend on the phase it acquires at short range and only when resonant will a single partial wave obtain the value of σ_Q .

$\tilde{\sigma}$ from Eq. (6) works well as a cost-effective method to determine the total scattering cross section. This approximation fails when there are resonances in any of the $\sigma^{(M)}$'s. If a resonance is in $\sigma^{(0)}$, then $\tilde{\sigma}$ overestimates σ , or if there is a resonance in $\sigma^{(M \neq 0)}$, then $\tilde{\sigma}$ will underestimate σ . Aside from these drawbacks $\tilde{\sigma}$ offers a cost-effective method to estimate $\tilde{\sigma}$ over a wide range of energies and electric fields.

In Fig. 3 we explore the behavior of particular $\sigma^{(M)}$'s as a function of energy at various electric fields. (a) and (b) show σ and several $\sigma^{(M)}$'s for RbK at two different field values: (a) $\mathcal{E}=0$ and (b) $\mathcal{E}=3\mathcal{E}_0$. The circles are the total cross section and are the same points in Fig. 2(b). The other curves are the different $\sigma^{(M)}$'s, where M_T is 0 (solid lines), 2 (dashed lines), and 4 (dash-dotted lines).

The total cross section at zero field (black circles) and a few of its components are shown in Fig. 3(a). The most important feature of this figure is that only $M=0$ is significant at low collision energy. $\sigma^{(0)}$ is the only calculation containing s -wave scattering. In zero field colliding ground-state molecules are unpolarized and therefore the dipolar interaction is confined to short range. This fact results in all nonzero partial waves being suppressed as the collision energy goes to zero. This can clearly be seen in the $\sigma^{(2)}$ (dashed line) and $\sigma^{(4)}$ (dash-dotted line) where these cross sections go to zero as the collision energy is decreased. Note the vertical axes of (a) and (b) have significantly different scales.

The result of the scattering is significantly different when there is a nonzero field. In Fig. 3(b) $\mathcal{E}=3\mathcal{E}_0$, and we have plotted σ (brown circles) from Fig. 2(b) and $\sigma^{(0)}$ (solid line), $\sigma^{(2)}$ (dashed line), and $\sigma^{(4)}$ (dash-dotted line). In this situation there is direct dipolar coupling between two scattering ground-state molecules, which means these are couplings between degenerate channels in the field-dressed basis. This coupling dramatically alters the low-energy behavior of all nonzero partial waves and $\sigma^{(M)}$'s; they are constant at low energy as predicted by the Born approximation in Eq. (8).

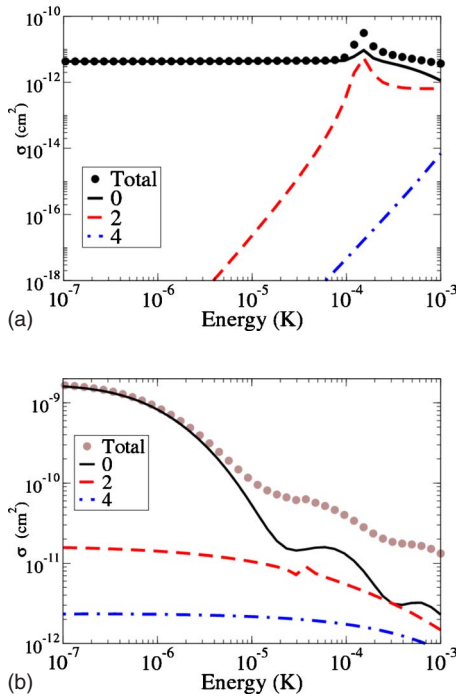


FIG. 3. (Color online) The total cross section (solid circles) for RbK decomposed into three $\sigma^{(M)}$'s for different field values. The fields are (a) $\mathcal{E}=0$ and (b) $\mathcal{E}=3\mathcal{E}_0$, and their comparison clearly shows the change in threshold behavior induced by the electric field. The different $\sigma^{(M)}$'s are for M equal to 0 (solid lines), 2 (dashed lines), and 4 (dash-dotted lines). The total cross section is also shown as circles in Fig. 2(a).

These two figures, (a) and (b), show the essential difference between polar molecules with and without an electric field and allude to why partial waves and many total M 's are required to converge σ , especially at high collision energies.

We have shown the dramatic effect an electric field has on the energy-dependent scattering. We now study the scattering of polar molecules as a function of electric field at various energies and temperatures.

IV. ELECTRIC FIELD DEPENDENCE

In ultracold atomic physics it is more experimentally feasible to change an external field rather than the temperature of the gas. To this end we study the total cross section and approximate total cross section as a function of electric field at several different energies and temperatures. In Figs. 4(a) and 4(b) the electric field dependence of σ (solid lines) and $\bar{\sigma}$ (dashed lines) are shown for different energy values. In descending order they are 0.1 (brown), 1 (red), 10 (blue), and 100 μK (black). Primarily, the influence of the electric field is to make the cross section large and induce potential resonances, which are clearly seen in the brown curves in (a) and (b). The heavier, more polar RbCs has many more than RbK for a field range of 0 to $4\mathcal{E}_0$.

At the collision energy of 100 μK (black curves) the dominant effect of the electric field is to increase the cross section without pronounced PRs. The result of decreasing the

energy an order of magnitude (blue) is to make the PRs emerge at low field, but not at high field. Then at 1 μK (red) many more PRs become distinguishable and the variation in the cross section becomes significant at low field. Finally at 0.1 μK (brown) the PRs are very distinct and there is significant variation in σ between the PRs at low field. At high field, especially in RbCs, the minima between PRs are less deep. The decrease in variation of σ is clearly seen in the brown curve in both (a) and (b). This result is simply due to the larger number of partial waves contributing to the scattering cross section. Ultimately, the electric field does not offer control of the scattering length as has been seen with the magnetic Feshbach resonance. Rather it induces a large number of partial waves to significantly contribute to σ , thus resulting in large total cross sections, but they are not necessarily resonant.

In a magnetic Feshbach resonance the field alters the molecular structure so the colliding pair of atoms can access an alternate pathway (closed-channel quasibound state). The pathways can interfere constructively or destructively depending on the value of the magnetic field, and this leads to the ability to tune the scattering.

The possibility of resonantly “turning off” the two-body interactions in a system of polar molecules with an electric field does not truly exist. The electric field might effectively turn off the two-body interaction if the zero-field scattering length is greater than zero. This can be seen in Fig. 4(a). This system and its particular parameters result in a large positive scattering length ($\sim 350a_0$). This results in a minimum in the cross section as the electric field evolves the system toward the addition of another bound state. This fact offers a simple means to determine the sign of the zero-field scattering length by varying the electric field. Overall, the effect of an electric field is to activate the dipoles and make many partial waves significant in the scattering. This fact prevents the cross section from rigorously being zero due to the contribution of nonzero partial waves.

In both Figs. 4(a) and 4(b) we see that $\bar{\sigma}$ (dashed lines) offers a good approximation to σ (solid lines). It works especially well at low field and low energy. Even at high field and high energy it offers a reasonable estimate of the total scattering cross section. Also seen in Fig. 2, $\bar{\sigma}$ does not get the resonant values of σ , but still offers a cost-effective means to achieve a total cross section. We have used $\bar{\sigma}$ to estimate a thermally averaged total cross section at low field, and this is shown in Fig. 4(c) for RbCs and (d) for RbK. The temperatures of the curves are 1 (circle), 5 (open circle), 10 (square), 25 (open square), 50 (open triangle), and 100 (triangle) μK .

The thermally averaged cross sections for both RbCs (c) and RbK (d) show that as the temperature is lowered from 100 μK resonant features emerge in the cross section. When the temperature is decreased, the RbCs cross section develops PRs at low field first. One can clearly see the emergence of the PRs as the temperature is decreased at low field along with the minimum. This shows that if the zero-field scattering length is greater than zero, there will be an observable minimum before the first PR below $T \sim 25$ μK . Then as the temperature is further decreased the other PRs at high field become distinguishable. In the thermally averaged system

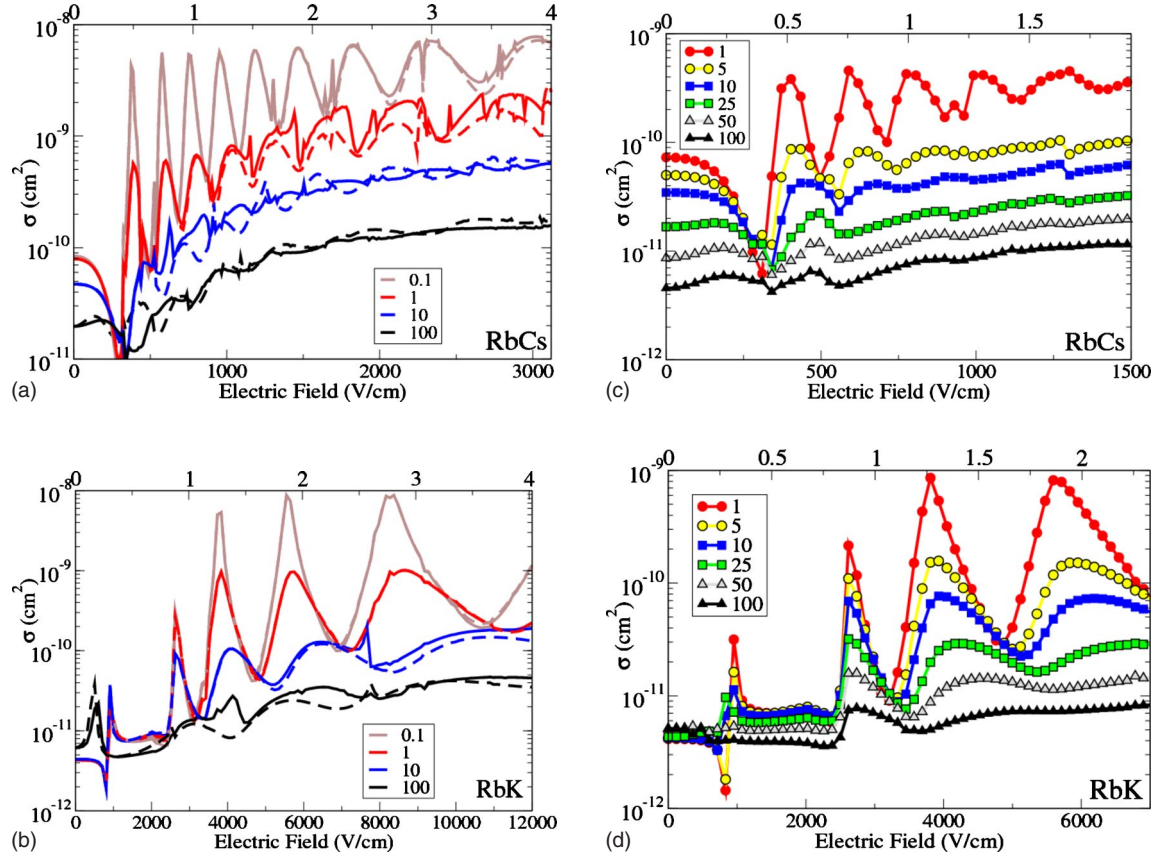


FIG. 4. (Color online) Electric field dependence of the total cross section (solid lines) and approximate total cross section (dashed lines) at various energies for RbCs in (a) and RbK in (b). In (a) and (b) the energies of the curves in descending order are 0.1 (brown), 1 (red), 10 (blue), and 100 (black) μK . Electric field dependence of the approximate thermally averaged cross at various temperatures for RbCs (c) and RbK (d). The temperatures of the curves in descending order are 1 (circle), 5 (open circle), 10 (square), 25 (open square), 50 (open triangle), and 100 (triangle) μK .

the dominant effect of increasing the electric field is to raise the total values of the cross section.

V. TRANSITION IN CHARACTER OF SCATTERING

To understand the scattering of polar molecules, we compare the total cross section, semiclassical cross section, and quantum unitarity limit. We make this comparison for both RbCs in Fig. 5(a) and for RbK in Fig. 5(b). In each plot we show all three cross sections, σ (solid lines), σ_{SC} (dashed lines), and σ_Q (dotted lines), at three energies: 1 (red), 10 (blue), and 100 μK (black). To make σ_{SC} simple, use Eq. (2).

There is an intriguing interplay between the energy and electric field in this system. Equations (9) and (10) show us $\sigma_{SC} \propto \frac{(\mu)^2}{\sqrt{E}}$ and $\sigma_Q \propto \frac{1}{E}$. When σ_{SC} is larger than σ_Q , the σ will be made up of a large number of partial waves and have roughly the same simple energy and electric field dependence of σ_{SC} . In contrast to when σ_Q is larger than σ_{SC} , the scattering will sensitively depend on the scattering process which occurs, making the energy and electric field dependence nontrivial.

To begin the analysis we look at RbCs in Fig. 5(a). First we look at the 100- μK system: σ is the solid black curve and

its behavior closely follows σ_{SC} , the dashed black line. Note how large the cross section becomes for large electric field values. It is much larger than σ_Q , the dotted black line. This shows a large number of partial waves are contributing to the scattering. The electric field where $\sigma_{SC} = \sigma_Q$ is marked by a square and is called the critical field \mathcal{E}_X . Above this field σ closely follows σ_{SC} .

When the energy is lowered by an order of magnitude to 10 μK , σ_Q (blue dotted line) is larger by an order of magnitude, but σ_{SC} (blue dashed line) only increases by a factor of $\sqrt{10}$. For this system, the σ_{SC} quickly becomes larger than σ_Q as the electric field is increased and \mathcal{E}_X is marked by a circle for this energy. Above \mathcal{E}_X we again see σ closely follows σ_{SC} .

At 1 μK we see there are many potential resonances before \mathcal{E}_X , marked by a triangle. Below the critical field σ (red solid line) has a series of potential resonances which reach up to σ_Q (red dotted line). Then as the electric field is increased near and above \mathcal{E}_X , σ becomes larger than σ_Q and roughly follows the trend of σ_{SC} (red dashed line). It is worth noting that σ has many fluctuations due to potential resonances in many partial waves and $\sigma^{(M)}$'s.

Now turning our attention to RbK, we have plotted σ (solid lines), σ_{SC} (dashed lines), and σ_Q (dotted lines) for the

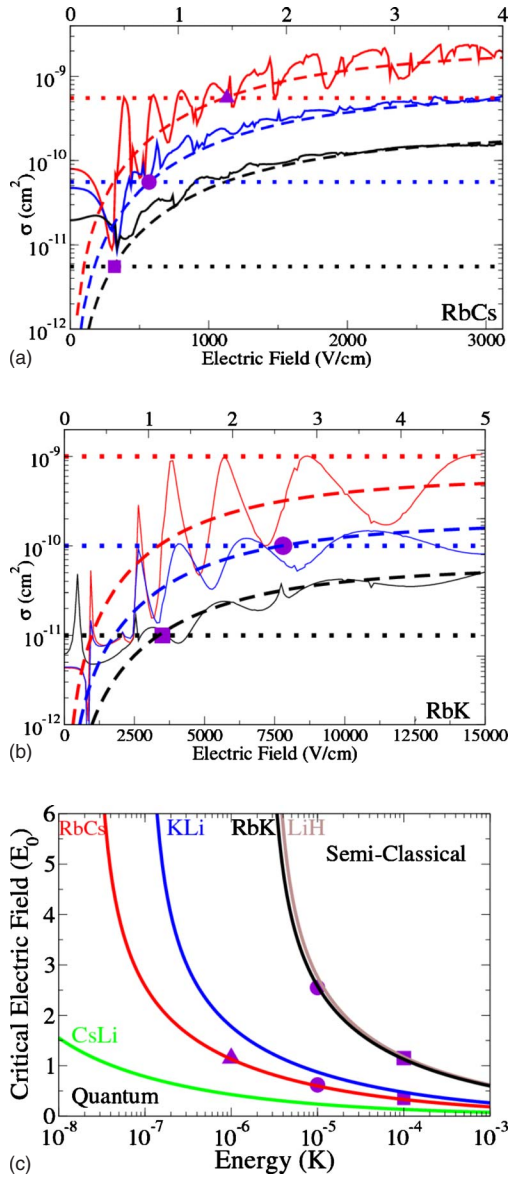


FIG. 5. (Color online) Comparisons of σ (solid lines), σ_{SC} (dashed lines), and σ_Q (dotted lines) show the change of character in scattering for both RbCs (a) and RbK (b). Sets of curves (σ , σ_{SC} , and σ_Q) are given for different energies, and in descending order the sets are for 1 (red), 10 (blue), and 100 (black) μK . The critical electric field, when $\sigma_{SC} = \sigma_Q$, is indicated by a symbol for each energy, and these symbols are also shown in (c). (c) The critical electric field in units of E_0 is plotted as a function of energy for various molecules. For a particular molecule, the scattering is semiclassical in character when the electric field is greater than \mathcal{E}_X and the collision energy is greater than E_Q . The scattering is quantum mechanical when either the electric field is less than \mathcal{E}_X or the collision energy is less than E_Q . The parameters of the molecules are given in the text.

same collision energies, 1 (red), 10 (blue), and 100 μK (black). There are some similarities to RbCs, but there is a very important difference in the behavior of the scattering cross section at 1 μK : for all electric fields $\sigma_Q > \sigma_{SC}$. This fact brings up an important quantity E_Q , the energy at which

$\sigma_Q = \sigma_{SC}(\mathcal{E} \rightarrow \infty)$ or, for a maximally polarized molecule σ_{SC} , E_Q is the energy at which σ_Q equals σ_{SC} . For collision energies below E_Q the scattering will always be dependent on the details of the interaction, $\sigma_Q > \sigma_{SC}$.

To explore Fig. 5(b) more thoroughly we look at the cross sections for 100 μK . We see that σ (solid black line) roughly follows σ_{SC} (dashed black line) when the field is greater than \mathcal{E}_X . Here many partial waves are contributing to the scattering. Again the critical field is marked by a circle and square for both 10 and 100 μK , respectively. As the collision energy is decreased the variation in the cross section as a function of electric field is greater. This can be seen in both 1- and 10- μK cross sections. At 1 μK for all electric fields σ_Q (dotted red line) is greater than σ_{SC} (dashed red line), because $E < E_Q$. Satisfying the inequality $\sigma_Q > \sigma_{SC}$ does not imply that $\sigma > \sigma_{SC}$ or $\sigma = \sigma_Q$. Rather it signifies the scattering will be sensitive to the scattering processes which occur. Thus when the scattering is in the quantum mechanical regime it depends on the short range details of the system and will exhibit resonance behavior. This is in contrast to when $\sigma_{SC} > \sigma_Q$. When this inequality is true, we expect $\sigma \sim \sigma_{SC}$ as is shown in Figs. 5(a) and 5(b).

To explore the interplay of σ_{SC} and σ_Q we analytically determine \mathcal{E}_X as a function of energy. The critical field is of fundamental importance because it denotes the field near which the character of the scattering changes from interaction sensitive to semiclassical. Equating $\sigma_{SC}(\mathcal{E})$ and σ_Q and solving for the critical field we find

$$\frac{\mathcal{E}_X}{E_0} = \sqrt{\frac{6.7b}{\sqrt{m^3 \mu^4 E - b}}}, \quad (11)$$

where $b = (8\pi c_Q / 0.608 c_{SC}) = 1.29$ and m , μ , and E are in units of amu, D, and K, respectively. We have plotted this critical field in Fig. 5(c) for many different molecules including LiH (brown), RbK (black), KLi (blue), RbCs (red), and CsLi (green). The parameters used for this figure are listed below:

Molecule	μ (D)	E_0 (V/cm)	m (amu)	E_Q (μK)
LiH	5.88	77500	8	2.7
RbK	0.76	3000	128	2.4
KLi	3.53	4320	48	0.1
RbCs	1.30	780	220	0.06
CsLi	5.51	1850	140	0.0007

Fig. 5(c) has interesting features, the most important of which is that it divides the electric-field–energy parameter space into two regions which have qualitatively different scattering character. Above the curve with a large electric field or high energy, the scattering is semiclassical and the scattering is essentially determined by physical parameters of the system: m , E , and $\langle \mu \rangle$ as shown in Eq. (9). Below the curve, for low energy or low electric field, the molecular scattering is sensitive to the details of the interaction and will be characterized by resonances and large variations in σ .

The two regions are labeled such that above the curves the scattering is semiclassical and below the scattering is quantum mechanical. Relating these curves back to the total cross section shown in Figs. 5(a) and 5(b), we have included the symbols in (c). This offers a feel for how the character changes above and below \mathcal{E}_X for a few energies.

The energy below which all scattering is quantum mechanical, E_Q , is determined when $\sigma_Q = \sigma_{SC}(\mathcal{E}_X \rightarrow \infty)$. This energy is most easily determined as the denominator on the right-hand side of Eq. (11) goes to zero and is

$$E_Q = \frac{b^2}{m^3 \mu^4}. \quad (12)$$

This reveals for heavier and more polar molecules that the semiclassical scattering will occur at a lower energy, suppressing quantum mechanical scattering. This is most evident in Fig. 5(c) for CsLi, a heavy and very polar molecule, whose E_Q is 0.7 nK compared with the polar but light LiH for which E_Q is 2.7 μ K or the not very polar RbK for which E_Q is 2.4 μ K. It is important to notice that the scaling of E_Q is m^{-3} and μ^{-4} . This shows that the mass of the molecule plays a significant role, almost as significant as the dipole, in determining the character of the scattering as the collision energy it lowered.

To show polar molecules present a unique opportunity to study semiclassical scattering consider ^{52}Cr [1]. This system has a magnetic-dipole moment of 6 bohr magneton. If we make the appropriate conversions for this magnetic-dipole moment and put it into the current theory, we find $E_Q \sim 1$ K. This shows the scattering will always be quantum mechanical ($E \ll E_Q$) and there will never be scattering of a semiclassical character in this atomic system.

VI. CONCLUSION

We have studied the collisions of RbCs and RbK in an electric field at various energies and temperatures. This work found the full scattering cross section is a computationally intense calculation where a large number of partial waves and many blocks of total M are required to converge the total cross section. An approximate cross section is introduced and

works well to provide a cost effective method to obtain a thermally averaged cross section. At large electric fields and at relatively high energies the semiclassical scattering cross section approximates the total cross section well.

This work has illustrated how dipolar interactions alter the scattering. The most notable is that an electric-field nonzero partial-wave cross section does not go to zero as the scattering energy goes to zero. Furthermore, resonant control of the interaction will only exist to a limited extent for polar molecules. The electric field in general induces large total cross sections. It cannot be used to “turn off” the two-body interactions unless the zero-field scattering length is greater than zero.

The primary finding of this work is that scattering can be classified as semiclassical and quantum mechanical. Semiclassical scattering is relatively simple where the scattering is determined by the scattering energy (E), the molecular mass (m), and induced dipole moment of the molecule ($\langle\mu\rangle$) as shown in Eq. (9). Quantum mechanical scattering is behavior defined by resonantly large cross sections and is sensitive to the phase shift acquired by the scattering process. We have found a simple form of the critical electric field (\mathcal{E}_X) at which the character of the scattering changes as a function of energy. Additionally we have found the collision energy (E_Q) below which all scattering will be quantum mechanical.

An exciting feature of Fig. 5 is one can study the transition of a gas from quantum mechanical to semiclassical scattering, simply by turning on an electric field. This transition in scattering character might signify a phase transition as was recently suggested for a two-dimensional gas of polar molecules when their interactions have been modified with microwave fields [6].

ACKNOWLEDGMENTS

The author is grateful for support from the ARC through ACQAO and computing resources from Victorian Partnership for Advanced Computing (VPAC) and the Centre for Astrophysics and Supercomputing at Swinburne University. The author thanks Peter Hannaford and Andy Martin for critically reading the manuscript.

-
- [1] J. Stuhler, A. Griesmaier, T. Koch, M. Fattori, T. Pfau, S. Giovanazzi, P. Pedri, and L. Santos, Phys. Rev. Lett. **95**, 150406 (2005); T. Lahaye *et al.*, arXiv:quant-ph/706.1670.
- [2] C. A. Regal, C. Ticknor, J. L. Bohn, and D. S. Jin, Phys. Rev. Lett. **90**, 053201 (2003).
- [3] S. Ospelkaus, C. Ospelkaus, L. Humbert, K. Sengstock, and K. Bongs, Phys. Rev. Lett. **97**, 120403 (2006).
- [4] C. Ticknor, C. A. Regal, D. S. Jin, and J. L. Bohn, Phys. Rev. A **69**, 042712 (2004).
- [5] L. Santos, G. V. Shlyapnikov, P. Zoller, and M. Lewenstein, Phys. Rev. Lett. **85**, 1791 (2000); L. Santos, G. V. Shlyapnikov, and M. Lewenstein, *ibid.* **90**, 250403 (2003).
- [6] H. P. Buchler, E. Demler, M. Lukin, A. Micheli, N. Prokofev, G. Pupillo, and P. Zoller, Phys. Rev. Lett. **98**, 060404 (2007).
- [7] D. DeMille, Phys. Rev. Lett. **88**, 067901 (2002).
- [8] A. Micheli, G. K. Brennen, and P. Zoller, Nat. Phys. **2**, 341 (2006).
- [9] M. Kozlov and L. Labzowsky, J. Phys. B **28**, 133001 (1995); E. A. Hinds, Phys. Scr. **T70**, 34 (1997); M. G. Kozlov and D. DeMille, Phys. Rev. Lett. **89**, 133001 (2002).
- [10] E. R. Hudson, H. J. Lewandowski, B. C. Sayer, and J. Ye, Phys. Rev. Lett. **96**, 143004 (2006).
- [11] J. Doyle, B. Friedrich, R. V. Krems, and F. Masnou-Seeuws, Eur. Phys. J. D **31**, 149 (2004).
- [12] A. J. Kerman, J. M. Sage, S. Sainis, T. Bergeman, and D. DeMille, Phys. Rev. Lett. **92**, 153001 (2004).

- [13] D. Wang *et al.* Eur. Phys. J. D **31**, 165 (2004); D. Wang, J. T. Kim, C. Ashbaugh, E. E. Eyler, P. L. Gould, and W. C. Stwalley, Phys. Rev. A **75**, 032511 (2007).
- [14] C. Haimberger, J. Kleinert, M. Bhattacharya, and N. P. Bigelow, Phys. Rev. A **70**, 021402(R) (2004).
- [15] J. M. Sage, S. Sainis, T. Bergeman, and D. DeMille, Phys. Rev. Lett. **94**, 203001 (2005).
- [16] A. V. Avdeenkov and J. L. Bohn, Phys. Rev. Lett. **90**, 043006 (2003); A. V. Avdeenkov, D. C. E. Bortolotti, and J. L. Bohn, Phys. Rev. A **69**, 012710 (2004).
- [17] N. Balakrishnan and A. Dalgarno, Chem. Phys. Lett. **341**, 652 (2001).
- [18] C. Ticknor and J. L. Bohn, Phys. Rev. A **71**, 022709 (2005).
- [19] A. V. Avdeenkov, M. Kajita, and J. L. Bohn, Phys. Rev. A **73**, 022707 (2006).
- [20] C. Ticknor and J. L. Bohn, Phys. Rev. A **72**, 032717 (2005).
- [21] R. V. Krems, Phys. Rev. Lett. **96**, 123202 (2006); T. V. Tscherebul and R. V. Krems, *ibid.* **97**, 083201 (2006); J. Chem. Phys. **125**, 194311 (2006).
- [22] S. Inouye *et al.*, Nature (London) **392**, 151 (1998); T. Loftus, C. A. Regal, C. Ticknor, J. L. Bohn, and D. S. Jin, Phys. Rev. Lett. **88**, 173201 (2002).
- [23] J. Brown and A. Carrington, *Rotational Spectroscopy of Diatomic Molecules* Cambridge University Press, Cambridge, England, (2003).
- [24] G. Igel-Mann, U. Wedig, P. Fuentealba, and H. Stoll, J. Chem. Phys. **84**, 5007 (1986); S. Kotochigova, P. S. Julienne, and E. Tiesinga, Phys. Rev. A **68**, 022501 (2003).
- [25] John Taylor, *Scattering Theory, The Quantum Theory of Nonrelativistic Collisions* (Dover, Mineola, NY, 2006).
- [26] H. R. Sadeghpour *et al.*, J. Phys. B **33**, R93 (2000).
- [27] D. DeMille, D. R. Glenn, and J. Petricka, Eur. Phys. J. D **31**, 275 (2004); M. Kajita, *ibid.* **20**, 55 (2002).
- [28] B. R. Johnson, J. Comput. Phys. **13**, 445 (1973).