Spin depolarization of N_2^+ ($^2\Sigma^+$) in collisions with ^{3}He and ^{4}He in a magnetic field

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We study the effect of a magnetic field on the spin-depolarization cross sections of $N_2^+(^2\Sigma)$ in collisions with ^{3}He and ^{4}He at very low collision energy. The fundamental states of the two nuclear spin isomers of N_2^+ are shown to respond quite differently to the application of the field. When the applied magnetic filed increases, the spin-depolarization cross sections are found to monotonously decrease for the fundamental paralevel $N=0$ of N_2^+ whereas they monotonously increase for the fundamental ortholevel $N=1$ of N_2^+. This effect is found to be amplified around the resonances and an explanation based on the different mechanism of spin flipping acting for these two levels is proposed. We discuss the sensitivity of the results on the change of relative mass when ^{3}He is replaced by ^{4}He. We also explore the tuning of the inelastic cross sections by examining the variation of the scattering length as a function of the magnetic field and locate several narrow Feshbach resonances.

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I. INTRODUCTION

The possibility of tuning the interactions between atoms using a magnetic field or atoms and molecules using applied electromagnetic fields has opened new perspectives of controlling collisional energy transfer at very low temperature. Several groups had first shown that the probabilities of elastic collisions and inelastic energy transfer for atom diatom collisions undergo dramatic changes near Feshbach resonances [1,2]. The tuning of the Feshbach resonances using a magnetic field was first considered by Volpi and Bohn in their study dedicated to the He-$O_2(^3\Sigma)$ [3] collision. They obtained a very strong enhancement of the spin-flipping transitions even for very small magnitude of the magnetic field. The formal theory of collisions between atom and molecule in the presence of a magnetic field was developed by Krems and Dalgarno [4] and applied by them to the He+CaH($^2\Sigma^+$) and Ar+NH($^3\Sigma^-$) collisions. These two systems appeared to be quite less sensitive to the applied magnetic field. The He-NH($^3\Sigma^-$) collision was then the subject of three detailed studies [5–7]. Two zero energy resonances were located by the team of Hutson for this system as a function of the magnetic field. The effect of the hyperfine structure of the diatomic molecule was even considered in several recent studies dedicated to Rb+OH($^2\Pi$) [8] and He-YbF($^2\Sigma$) [9]. In two previous papers we recently investigated the effect of the spin-rotation interaction [10] as well as the collision induced Zeeman relaxation [11] for a collision involving an ionic molecule: The He+N_2^+ collision. The very strong isotope effect exhibited by this collision at very low energy which results from the strongly attractive long-range charge-induced dipole potential gives a peculiar interest to this system. The deep well ($\cong -84.5$ cm^{-1}) produces also a large number of resonances which can be studied in the presence of a field. This system is furthermore comparable to the He+CaH($^2\Sigma^+$) collision as the electronic states $^2\Sigma$ of the two diatomic molecules are the same and the ratio B/γ of $N_2^+(^2\Sigma)$ is 2 times as large as for CaH. But the central reason to study this system in the presence of a field is that the two nuclear spin isomers of N_2^+ can be studied separately. As a matter of fact, in the absence of an applied magnetic field, the spin-flipping transitions in the fundamental rotational state ($N=0$) was shown by Krems to be induced through the coupling to the excited rotational levels whereas the Zeeman relaxation of excited rotational levels follows a direct mechanism. This is indeed what we found in the case of N_2^+. This system then offers a unique opportunity to compare the action of an applied magnetic field on the two lowest-lying ortho-($N=1$) and para-($N=0$) states of N_2^+ which are expected to behave in a very different way. Although the theory of collisions of charges in the presence of a magnetic field is known for a long time, there are to our knowledge no studies available of collisions involving an atom and a diatomic ion in the presence of magnetic field. This is due to the complication of the exact treatment when all of the terms of interaction with the field are taken into account [12]. In the present study we ignore the cyclotron motion of the center of mass of the ion. We will discuss the validity of this approximation which is acceptable at very low collision energy as the cyclotron radius is quite small. We will then solve the close-coupling equations describing an atom colliding with a neutral $^2\Sigma$ molecule in the presence of a magnetic field but using the He N_2^+ potential. The paper is organized as follows. In Sec. II we shortly review the main features and the parameters of the method suggested by Krems and Dalgarno which we use to solve the scattering calculations. Our results are then presented and analyzed in Sec. III.

II. THEORY AND PARAMETER CALCULATIONS

As mentioned in the introduction, a complication arises for an ion moving in a magnetic field as a result of the velocity dependence of the Lorentzian force. This point was discussed by several authors [13–15] and we will only remind the reader of some of the problems which still must be solved. In this case, the motion of the center of mass (c.m.) of the whole collision system cannot in principle be separated from the relative translational motion between He and N_2^+. Consequently, the center-of-mass reference frame which is used for field free collisions should be, strictly speaking,

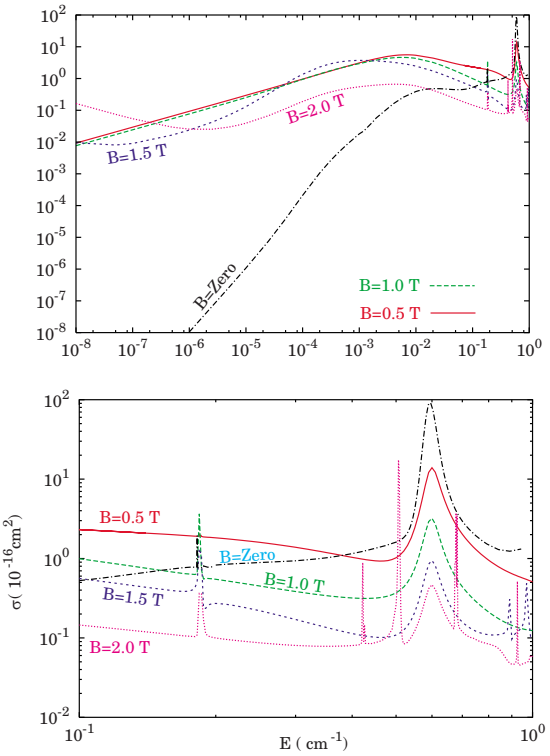

FIG. 1. (Color online) Comparison of the spin-depolarization cross sections of $N_2^+[N=0,\alpha=2,M_J=1/2\rightarrow\alpha=1,\ M_J(\alpha=1)=-1/2]$ in collisions with ^{3}He as a function of collision energy with and without an applied magnetic field. The values of the magnetic field represented are 0; 0.5; 1; 1.5, and 2 T.

abandoned. The dynamics of the collision does depend on the motion of the center of mass of the system, the center-of-mass reference frame being no longer an inertial frame as it rotates with a gyration radius of Mv/eB and a cyclotron frequency eB/M. Nevertheless, in the case of a homonuclear diatomic ion the center of charge coincides with the center of mass and the treatment of the collision can be simplified. Asymptotically (when the helium atom is far from the diatomic ion), in the global c.m. reference frame, the c.m. motion of N_2^+ is completely decoupled from the pure internal motion of N_2^+ [13]. The c.m. motion of the system is in this case simply the Landau motion of a free pseudoparticle with charge $+e$ and mass $2m_N$ in the constant magnetic field. In the present study, we will simply solve the close-coupling equations describing an atom colliding with a neutral $^2\Sigma$ molecule in the presence of a magnetic field but using the He N_2^+ potential and we expect that this approximation should be valid at very low collision energy and for moderate values of the applied magnetic field.

We choose to use the formalism developed by Krems and Dalgarno [4] for an atom colliding with a $^2\Sigma$ diatom in the presence of a magnetic field, taking into account the fine structure of the diatomic molecule but disregarding the molecular hyperfine interaction. We assume that the total nuclear spin of the diatomic molecule is conserved in the collision implying that the even molecular rotational states N are separated from the odd ones. We also ignore the small interaction between the field and the rotational angular momentum. In what follows we will only remind the reader of the main steps of our calculations in order to define the notations used in this paper. This approach uses a primitive uncoupled basis set to describe the states of the free diatomic molecule in the presence of an external field. This is a simple basis set $\phi_i=\chi_{v,N}(r)|NM_N\rangle|SM_S\rangle$ made of the products of the eigenfunction of the rotational (N^2,N_Z) and electronic spin (S^2,S_Z) angular momenta of the diatomic molecule, where N_Z and S_Z designate the projection of the angular momenta N and S along the direction of the applied field. A completely equivalent approach based on a coupled representation of the wave function of the diatomic molecule can be found in the recent paper of Gonzalez-Martinez and Hutson [7] dedicated to the He-NH collision. As the asymptotical Hamiltonian (1) describing the free molecule in the presence of the field includes the spin-rotation interaction and the interaction of the spin with the magnetic field B, it is not diagonal in the uncoupled basis set ϕ_i which then cannot be used to describe the asymptotic states of the dressed molecule in the presence of the field,

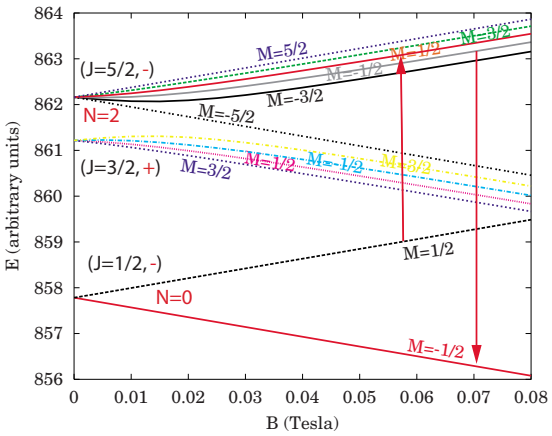

FIG. 2. (Color online) Eigenenergies of the two first Zeeman parastates of the N_2^+ diatomic molecule as a function of the magnetic field strength. The energy units are arbitrary and the rotational spacing between the $N=0$ and $N=2$ states was modified in order to show all of the curves on the same figure.

$$H_{\text{Diatom}}^{\text{Asymp}} = H_{\text{Diatom}}^{\text{Spin Free}} + \gamma\vec{N}\cdot\vec{S} + g\mu_B\vec{B}\cdot\vec{S}, \tag{1}$$

where γ is the spin-rotation constant, g is the g factor for the electron, and μ_B is the Bohr magneton. One uses instead the basis set $\chi_\alpha=\Sigma_i C_{\alpha i}\phi_i$ which diagonalizes this Hamiltonian,

$$\lfloor CH_{\text{Diatom}}^{\text{Asymp}}C^{-1}\rfloor_{\alpha\beta} = \xi_\alpha\delta_{\alpha\beta}. \tag{2}$$

The magnetic field removes the degeneracy in $M_J=M_N+M_S$ and each energy level ξ_α of the dressed diatomic molecule in the presence of the field is associated with a single value of M_J denoted $M_J(\alpha)$. For a given value of the projection of the total angular momentum along the direction of the field M_T and for a given $M_J(\alpha)$, the projection of the relative angular momentum L along the direction of the field basis set is given by $M_L=M_T-M_J(\alpha)$. The basis set describing the collision process is obtained by including the possible values of the quantum number L for each value of α. This basis set

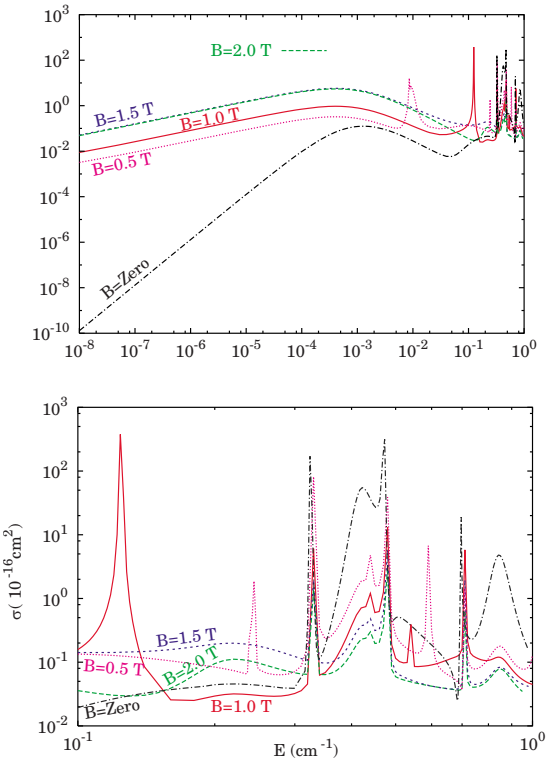

FIG. 3. (Color online) Comparison of the spin-depolarization cross sections of $N_2^+[N=0,\alpha=2,M_J=1/2\rightarrow\alpha=1,M_J(\alpha=1)=-1/2]$ in collisions with ^{4}He as a function of collision energy with and without an applied magnetic field. The values of the magnetic field represented are 0; 0.5; 1; 1.5, and 2 T.

is denoted by the quantum numbers α, M_L, L. In this basis set, the close-coupling equations which must be solved (3) and the asymptotic boundary conditions which must be imposed in order to obtain the scattering matrix, take the form demonstrated in Ref. [4],

$$\left(\frac{d^2}{dR^2}-\frac{L(L+1)}{R^2}+2\mu[E-\xi_\alpha]\right)F_{\alpha,M_L(\alpha),L}(R)$$
$$=2\mu\sum_{\alpha',M_L'(\alpha'),L'}[C^TUC]^{\alpha',M_L'(\alpha'),L'}_{\alpha,M_L(\alpha),L}F_{\alpha',M_L(\alpha'),L'}(R). \tag{3}$$

This system of coupled equations must in principle be solved for each possible value of the total angular momentum projection M_T in order to obtain the transition cross sections (4),

$$\sigma_{\alpha\rightarrow\alpha'}(E_\alpha)=\frac{\pi}{k_\alpha^2}\sum_{M_T}\sum_{M_L}\sum_{L}\sum_{M_L'}\sum_{L'}|T^{M_T}_{\alpha,M_L(\alpha),L;\alpha',M_{L'}(\alpha'),L'}|^2. \tag{4}$$

At ultralow collision energies, it is only necessary to calculate the scattering matrix only for the single value of the projection M_T of the total angular momentum corresponding to the s wave in the incident channel. We found however that in order to reproduce our previous calculations between 10^{-8} cm^{-1} and 1 cm^{-1} that we must include values from $-7/2$ up to $7/2$.

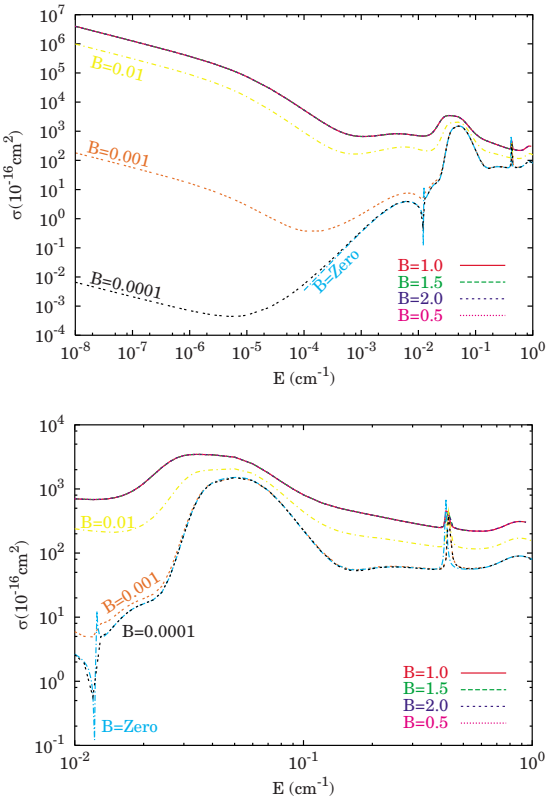

FIG. 4. (Color online) Comparison of the spin-depolarization cross sections of $N_2^+(N=1,\alpha=2,M_J=-1/2\rightarrow\alpha=1,M_J=+1/2)$ in collisions with ^{3}He as a function of collision energy with and without an applied magnetic field. The values of the magnetic field represented are 0, 10^{-4}, 10^{-3}, 10^{-2}, 0.5, 1, 1.5, and 2 T.

The calculations were performed using the potential energy surface presented in our previous papers [10,16]. The results of the calculations obtained with our new code of propagation were checked, for a magnetic field set equal to zero, to be identical to those presented in our previous paper dedicated to field free spin-flipping transitions for this system. We calculate for the lowest-lying orthostates and parastates of N_2^+, the elastic and spin-depolarization cross sections for collisions involving both ^{3}He and ^{4}He. The cross sections are calculated in the ultracold energy regime between 10^{-8} cm^{-1} and 1 cm^{-1} and over a wide range of field values from 0 up to 1.5 T. As in our previous work dedicated to the field free spin-flipping cross sections we took into account the vibrational dependence of the potential energy surface but only included one vibrational level in the calculations. Results are converged using partial waves, respectively, up to $L=8$ and $L=10$ for collisions involving ^{3}He and ^{4}He and including four rotational states of the diatomic molecules: $N=0,2,4,6$ for para-N_2^+ and $N=1,3,5,7$ for ortho-N_2^+. The maximum numbers of channels that we had to propagate were consequently, respectively, 364 and 476 for the ^{3}He $+N_2^+(N=0)$ and ^{4}He$+N_2^+(N=0)$ collisions whereas they had to be increased up to 588 and 825 for the ^{3}He$+N_2^+(N=1)$ and ^{4}He$+N_2^+(N=1)$ collisions. The maximum value of R to which the coupled-channel equations were propagated was 700 bohr. These parameters assure the cross sections to be converged within less than 1%.

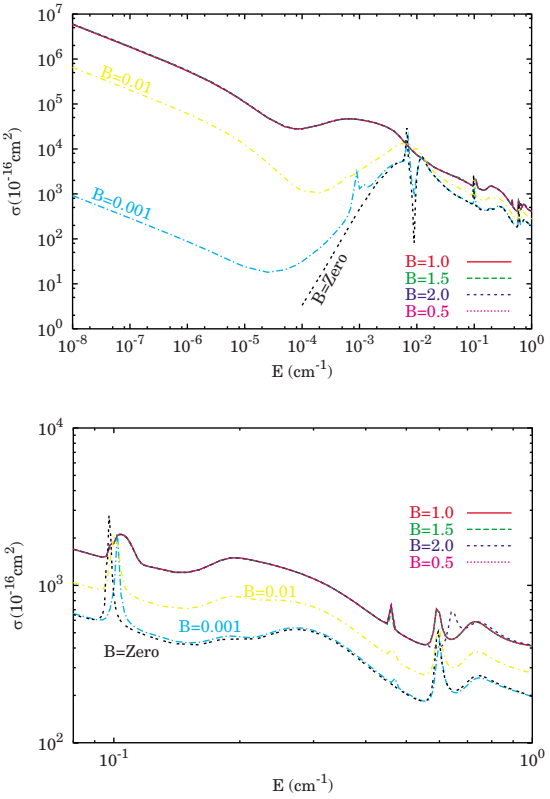

FIG. 5. (Color online) Comparison of the spin-depolarization cross sections of $N_2^+(N=1,\alpha=2,M_J=-1/2\rightarrow\alpha=1,M_J=+1/2)$ in collisions with ^{4}He as a function of collision energy with and without an applied magnetic field. The values of the magnetic field represented are 0, 10^{-3}, 10^{-2}, 0.5, 1, 1.5, and 2 T.

III. RESULTS AND ANALYSIS

A. Zeeman relaxation for the fundamental pararotational level $N=0$ of N_2^+

As the computed elastic cross sections are unchanged when a magnetic field is applied they will not be reported on the figures for the sake of clarity. Each figure of the present paper is made out of two panels, the upper panel showing the full interval of energy of our calculation $[10^{-8};1]$ cm^{-1} and the lower panel screening a close-up of the $[0.1;1]$ cm^{-1} interval. Figure 1 shows the comparison of the cross section for the $(\alpha=2,M_j=1/2)\rightarrow(\alpha=1,M_j=-1/2)$ relaxation of the fundamental parastate $N=0$ of N_2^+ in collisions with ^{3}He computed at different magnetic field strengths, 0.5, 1, 1.5, and 2 T. They can also be compared to the field free cross section for this transition which is also reported on the same figure and was commented in our previous paper dedicated to the calculation of the spin-flipping transition cross sections for this system. The first striking result is the usual progressive removal of the Wigner's law suppression as the field increases in strength in the $[10^{-8};10^{-3}]$ cm^{-1} energy interval. The energy dependence of the cross section changes progressively from $E^{-1/2}$ in the absence of an applied magnetic field to an increasing function of the collision energy. The explanation of this mechanism which was proposed by Tiesinga *et al.* [17] and Volpi and Bohn [3] is based on the removal of the degeneracy of the initial and final channels

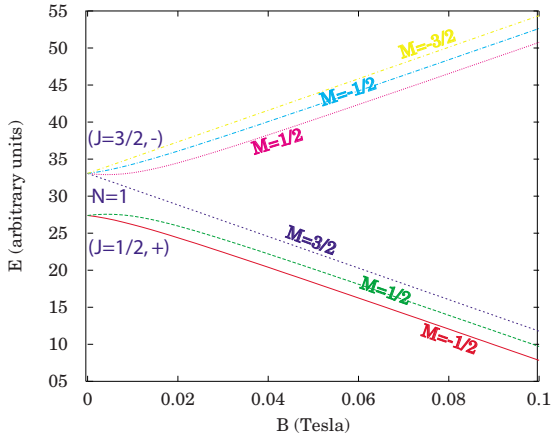

FIG. 6. (Color online) Eigenenergies of the first Zeeman orthostates of the N_2^+ diatomic molecule as a function of the magnetic field strength. The energy units are arbitrary.

when the field is applied. The threshold energy in the exit channel then becomes greater than the centrifugal barrier and explains the increase of the cross section at very low energy when the field is applied. A very low energy upturn of the cross section is even obtained for values of the field larger or equal to 1.5 T whereas it was obtained for lower values of the field for the He-CaH collision [4]. In their presentation dedicated to the field free Zeeman relaxation of CaH in collisions with He, Krems *et al.* [1] showed that these transitions are mediated by the spin-rotation interaction in the excited level $N=1$ as the matrix elements of this operator are zero for the $N=0$ state. Here the rotational spacing between the fundamental and the first excited paralevel $N=2$ of N_2^+ is 11.59 cm^{-1} which is larger than the splitting between the $N=0$ and $N=1$ levels of CaH (8.54 cm^{-1}). This difference and the smaller value of the spin-rotation constant of N_2^+ are the two reasons which make this collision less sensitive to the magnitude of the applied magnetic field. Another interesting feature of this figure is the monotonous lowering of the broad resonance peak around 0.6 cm^{-1} when the strength of the field is increased while its position and width are conserved. This is in fact a general trend of the cross section even in regions which do not exhibit any resonances outside the Wigner regime. It can be understood as a simple consequence of the increase of the splitting between the $N=0$, $\alpha=1$, $\varepsilon=-1$ state and the excited levels $N=2$, $\varepsilon=-1$ state resulting from the application of a growing field and of the resulting decrease of the coupling between these coupled Zeeman levels as illustrated in Fig. 2. We have reported in this figure the parity of the levels as the magnetic field mix states of the same parity [18] and because of the propensity rule to conserve parity which was analyzed by Lengel and Crosley [19] and Alexander and Corey [20] for collisions between a structureless atom and a $^2\Sigma$ diatomic molecule. This effect is amplified around the resonance as the maximum of the peak for $B=2$ T is more than two orders of magnitude smaller than in the absence of a field. For the highest values of the applied field considered in this paper we can also notice new resonances appearing which are the signature of new quasibound states of the field dressed potential. In Fig. 3 the same comparison is represented for the

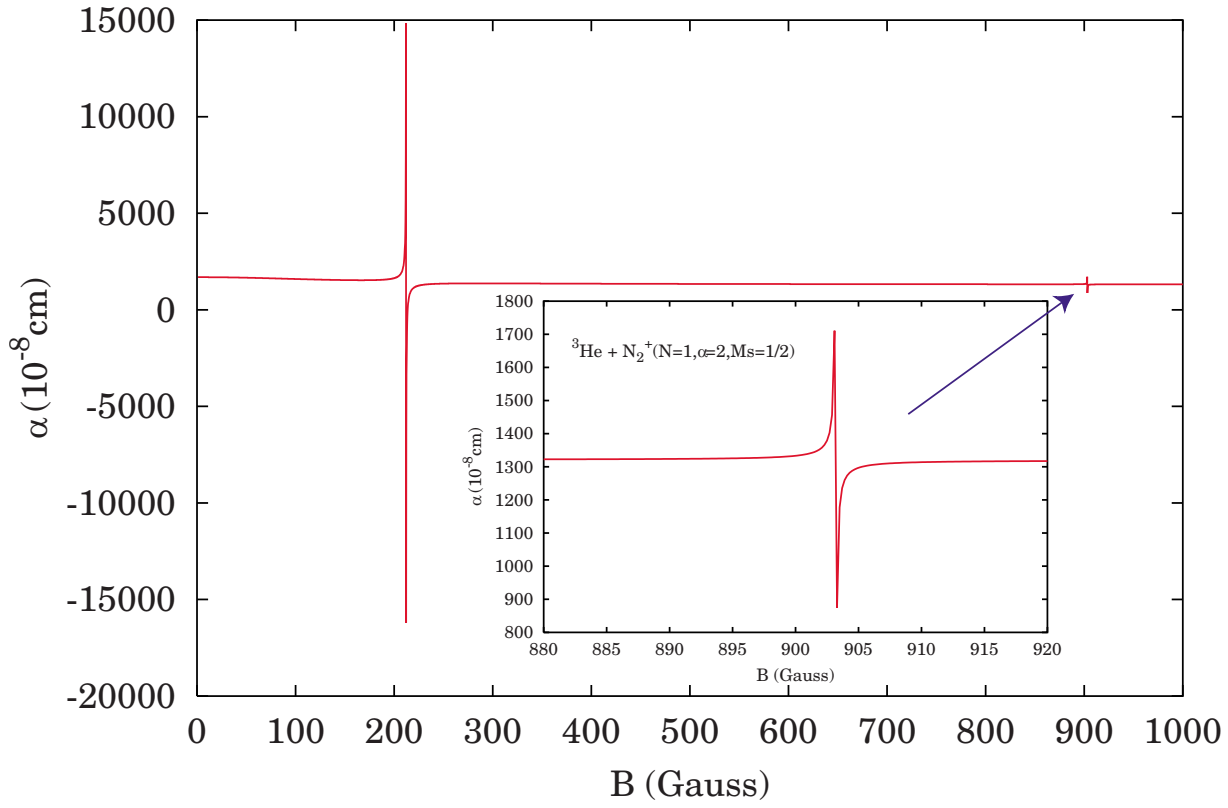

FIG. 7. (Color online) Real part of the scattering length for the elastic $^3He+N_2^+(N=1,\alpha=2,M_J=1/2)$ collision as a function of the magnetic field from calculations at a kinetic energy of 10^{-8} cm^{-1}.

$^4He+N_2^+$ collisions. The same general behavior is observed when the field is increased with a progressive increase of the magnitude of the cross section, the conservation of the energy position, and of the general profile of the shape resonances and the apparition of new resonances. However, the change of relative mass of the system makes the collision less responsive to the applied magnetic field as this figure does not show any very low energy upturn of the cross section even for the highest value of the field considered ($B=2$ T).

B. Zeeman relaxation for the fundamental orthorotational level $N=1$ of N_2^+

The same comparison is presented in Figs. 4 and 5 for the $(\alpha=2,M_j=-1/2)\rightarrow(\alpha=1,M_j=1/2)$ transition originating from the fundamental $N=1$ orthorotational state of N_2^+ again, respectively, in collisions with ^3He and ^4He. In order to reproduce the field free curves that we obtained in our previous study we had to include five rotational levels instead of four which increases dramatically the size of the matrix that we had to propagate. The spin-rotation interaction acts directly on this level and we can clearly see that it is more responsive to the applied magnetic field. A field of 1 G is enough to change drastically the Wigner law for the ^4He-N_2^+ collision while a field of 10 G produces a new resonance around 10^{-3} cm^{-1} for the ^3He-N_2^+ collision. The position and width of the shape resonances again are conserved but for the highest value of the field considered ($B=2$ T) the position of the shape resonance around 0.6 cm^{-1} is shifted to higher energy for the collision involving ^4He. Conversely, the Feshbach resonance around 0.01 cm^{-1} which was shown in our previous work [10] to be associated with the opening of the negative parity level of the $N=1$ doublet and is represented in Figs. 4 and 5 is strongly modified even by small values of the field. It even completely disappears when the field is larger or equal to 1000 G. However, the increase of the magnitude of the cross section when the field increases is the most striking difference with the figure dedicated to the fundamental paralevel ($N=0$) which is a consequence of the direct mechanism of the Zeeman relaxation for the fundamental ortholevel ($N=1$). This is again the result of the removal of the degeneracy of the initial and exit channels which explains the general increase of the cross section when the field is applied. If some new resonances appear (see the lower panel of Fig. 5), the magnitudes of the cross sections however do not keep increasing for values of the field approximately larger than 0.02 T. This can be understood by looking at Fig. 6 where the splitting between the initial and exit orthochannel appears to first increase and become constant for values of the field larger than 0.02 T. In Figs. 7 and 8 we represented the real part of the scattering length for the elastic collisions of $N_2^+(N=1,\alpha=2,M_J=1/2)$ with ^3He and ^4He as a function of the applied magnetic field. These figures illustrate the great sensitivity of the collision involving the orthostates of N_2^+ to the applied magnetic field as we can clearly identify Feshbach resonances arising already for values of the field as small as 50 G. This is in contrast with a system such as He-NH which for the first resonance is found

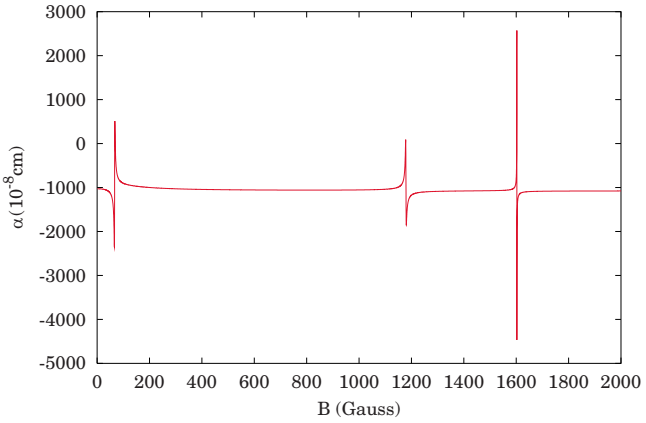

FIG. 8. (Color online) Real part of the scattering length for the elastic $^4He+N_2^+(N=1,\alpha=2,M_J=-1/2)$ collision as a function of the magnetic field from calculations at a kinetic energy of 10^{-8} cm^{-1}.

at $B=7200$ G. We also performed the same calculations for the elastic collisions of the fundamental $(N=0,\alpha=2,M_J=1/2)$ parastate N_2^+ with ^{3}He and ^{4}He as a function of an applied magnetic field varying between 0 and 20 000 G by steps of 0.2 G and did not find any resonance. This result again illustrates the important differences between the collisional behaviors of the two spin isomers of N_2^+. The origin of these resonances is illustrated in Fig. 2 where the energy splitting of the rotational levels of the diatomic molecule as a function of the applied field strength is reported. We can see in this figure that some of the channels energy thresholds decrease when the magnetic field increases. A resonance appears whenever a channel energy threshold becomes equal to one of the field dressed bound states energies. Their positions can also be located by performing bound states calculations as a function of the field as illustrated by the team of Huston for the He NH collision [7].

IV. CONCLUSION

The spin-depolarization cross sections of the two lowest-lying ortho-$(N=1)$ and para-$(N=0)$ states of a homonuclear molecule such as N_2^+ are found to respond quite differently to the application of a magnetic field. One needs to apply values of the field larger or equal to 1.5 T to observe the very low energy upturn of the cross section for the fundamental parastate whereas it is obtained for values of the field as small as 1 G for the fundamental orthostate. When the applied magnetic field increases, the spin-depolarization cross sections are found to monotonously decrease for the fundamental paralevel $N=0$ of N_2^+ whereas they monotonously increase for the fundamental ortholevel $N=1$ of N_2^+. This effect which is found to be amplified around the resonances is a consequence of the fact that the mechanism for spin-flipping transitions in the fundamental rotational state $(N=0)$ are induced through the coupling to the excited rotational levels whereas Zeeman relaxation of the $N=1$ levels follow a direct mechanism. When the field increases, the decrease of the coupling between the $N=0$, $\alpha=1$, $\varepsilon=-1$ and the $N=2$, $\varepsilon=-1$ Zeeman paralevels appears to be a simple consequence of the increase of the splitting between these states. Conversely, for the fundamental ortholevel, it is the removal of the degeneracy of the initial and final channels which explains the general increase of the cross section when the field is applied as the energy available in the output channel increases as a function of the applied field.

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