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Molecular collisions and reactive scattering in external fields: Are field-induced couplings important at short range?

D. Vieira, 1 R. V. Krems, 1 and T. V. Tscherbul 2
1Department of Chemistry, University of British Columbia, Vancouver, British Columbia V6T 1Z1, Canada
2Department of Physics, University of Nevada, Reno, Nevada 89557, USA

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We use accurate quantum scattering calculations to elucidate the role of short-range molecule-field interactions in atom-molecule inelastic collisions and abstraction chemical reactions at low temperatures. We consider two examples: elastic and inelastic scattering of NH(3Σ) molecules with Mg(1Σ) atoms in a magnetic field; reactive scattering LiF + H → Li + HF in an electric field. Our calculations suggest that, for non-reactive collision systems and abstraction chemical reactions, the molecule-field interactions cannot generally be neglected at short range because the atom-molecule potential passes through zero at short range. An important exception occurs for Zeeman transitions in atom-molecule collisions at magnetic fields ≤1000 G, for which the molecule-field couplings need only be included at large ρ outside the range of the atom-molecule interaction. Our results highlight the importance of an accurate description of ρ-dependent molecule-field interactions in quantum scattering calculations on molecular collisions and chemical reactions at low temperatures. Published by AIP Publishing.

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I. INTRODUCTION

The energy levels of a molecule placed in a DC magnetic or electric field are perturbed due to the Zeeman or Stark effect. The Zeeman/Stark shifts of the energy levels are typically <5 cm⁻¹ for open-shell molecules in strong magnetic fields and for polar molecules with small rotational constants in strong DC electric fields. Although small compared to the kinetic energy of molecules in a thermal gas at ambient temperatures, these energy shifts modify the collision dynamics of molecules at cold (∼1 K) and ultracold (<10⁻³ K) temperatures. The Zeeman and/or Stark energy shifts are used to confine molecules in magnetic or electric traps, a necessary step for creating an ultracold gas with a high phase-space density. The stability of molecules in such traps is limited by inelastic collisions and chemical reactions that lead to trap loss.1 In order to understand the prospect of cooling trapped molecules to ultralow temperatures, many authors have recently studied the effects of external fields on molecular collisions and chemical reactions.2–68,70–88 Pioneering experimental studies explored the dynamics of inelastic spin relaxation of magnetically trapped molecular radicals CaH2,6 and NH3,37 collisions with background He atoms in a cryogenic environment, and more recent experiments observed cold N-NH,4 OH-OH,70 OH-ND3,9 and Rb-ND60 collisions in co-trapped atom-molecule and molecule-molecule ensembles.4 An exothermic chemical reaction has been observed to occur in an ultracold gas of KRB molecules at temperatures below 1 μK.59 It was shown that the reaction rate can be modified by polarizing the reactants with external DC electric fields and confining them in low-dimensional geometries.2,58

Theoretical simulations of atom-molecule and molecule-molecule collisions in external fields have been carried out using a variety of methods. The direct numerical integration of the Schrödinger equation using the close-coupling (CC) method, as reported in Refs. 21–33, provides the most complete information about the collision process. Alternative methods that reduce the complexity of the full quantum scattering problem include statistical theories,12,62–64 quantum threshold models,62 multichannel quantum defect theories (MQDTs),2,13,14 and combinations thereof.7–11 These methods rely on the observation that ultracold collisions are primarily governed by long-range interactions of the colliding species. By separating the entire configuration space into short-range and long-range regions and invoking a statistical description of the reaction complex in the short-range region, these methods allow one to neglect the intricate details of short-range intermolecular interactions and thereby simplify the theoretical description of chemical reactions to a great extent. When applied to the KRB + KRB chemical reaction, these methods predict the reaction rates within a factor of 2-3 of the measured values and explain the experimentally observed electric field modulation of the reaction rates in the ultracold scattering regime.62 Recently, approaches combining the accurate CC calculations at short-range and MQDT at long-range have been developed for an improved analysis of insertion chemical reactions and inelastic scattering of strongly interacting molecular systems.2–11

Much of the previous work on cold molecular collisions was motivated by three main goals: (i) understand the mechanisms of collisions leading to trap loss; (ii) predict the range of molecules amenable to collisional cooling in electromagnetic field traps; (iii) explore the possibility of tuning microscopic reactions and identify the regimes of field-induced interactions that would suppress inelastic and reactive collisions while enhancing elastic scattering necessary for cooling. Despite the rapid progress of the theoretical and experimental work, there are still many open questions. For example, while recent experiments observed evaporative cooling of OH radicals in an electromagnetic trap,70 it is not yet known if polyatomic...
molecules can be cooled by evaporation in a magnetic or electric trap from cold to ultracold temperatures or whether polyatomic molecules are collisionally stable in external field traps.

These questions can be answered by quantum scattering calculations of cross sections (CSs) for elastic, inelastic, and reactive collisions of molecules in external fields. While the formalism for such calculations has been developed,17,20,21,23,27,68 quantum scattering calculations for molecules in external fields are challenging. The interactions of molecules with external fields break the spherical symmetry of the collision problem. As a consequence, the total angular momentum of the collision system is not conserved, which results in a dramatic increase of the Hilbert space needed to represent the scattering states. For reactive scattering calculations performed in hyperspherical coordinates and involving transformations between the Jacobi and hyperspherical coordinates,57 the need to include couplings between states of different total angular momenta further complicates the formalism and the complexity of the numerical calculations.68 In order to simplify quantum scattering calculations for collisions of molecules in external fields, the present work explores the possibility of combining field-free scattering computations at short range ($\rho < \rho^*$) with full scattering calculations involving field-induced interactions at long range ($\rho > \rho^*$) of the radial coordinate $\rho$ describing the separation of the collision partners. For inelastic scattering calculations, $\rho$ is a Jacobi radial coordinate, while for reactive scattering calculations $\rho$ is a hyperradius.

The field-induced interactions have magnitudes <10 cm$^{-1}$ and, typically, a weak dependence on $\rho$. In most calculations to date, the field-induced interactions have been approximated by their asymptotic values. This approximation was tested in rigorous CC calculations and found to be accurate for cold He–ThO collisions in DC electric fields below 200 kV/cm.69 At large $\rho$, the field-induced interactions are much stronger than the inter-molecular interactions. However, at short range, in the region of strong interaction between the colliding molecules, the inter-molecular interaction potential is typically much larger than the field-induced interactions. This suggests that the scattering states can be calculated by solving the Schrödinger equation without the field-induced interactions at short range ($\rho < \rho^*$) and matching the results to the solutions of the field-free Hamiltonian $\hat{H}$.

II. COMPUTATION DETAILS

The calculations of cross sections for inelastic scattering of NH with Mg are performed using the Jacobi coordinates as described in Ref. 20. We employed the potential energy surface for the Mg–NH interaction obtained by Soldan and coworkers.57 The scattering calculations for the H + LiF $\rightarrow$ Li + HF reaction are performed using the Fock-Delves hyperspherical coordinates, as described in Ref. 68 based on an ab initio potential energy surface from Ref. 89. The full Hamiltonian for both systems can be written as

$$\hat{\mathbf{H}} = \hat{\mathbf{H}}_0(\rho) + \hat{\mathbf{V}}_{\text{field}},$$

where $\rho$ is used to represent the Jacobi distance between the center of mass of the NH molecules and the He atom or the hyperradius describing the reaction complex Li–H–F. The field-free Hamiltonian $\hat{\mathbf{H}}_0(\rho)$ includes the kinetic energy of the relative motion and the potential energy of the atom-molecule interaction. The term $\hat{\mathbf{V}}_{\text{field}}$ describes the interaction with an external field assumed to be independent of $\rho$.

The calculations are performed by representing the full wave function of the collision system as a basis expansion over the eigenstates $|JM\rangle$ of $\mathbf{J}^2$ and $\mathbf{J}_z$, where $\mathbf{J}$ is the total angular momentum of the collision system and $\mathbf{J}_z$ is the component of the total angular momentum along the field axis.22,23 The full Hamiltonian is diagonal in $M$, but the blocks of states corresponding to $J$ and $J' = J \pm 1$ are coupled by the matrix elements of $\hat{\mathbf{V}}_{\text{field}}$. This basis set expansion, when substituted into the Schrödinger equation, leads to a system of coupled differential equations. The full calculations are performed by integrating these equations on a grid of $\rho$ with different $J$-blocks simultaneously. Asymptotically, the solutions are transformed to the eigenbasis of the full Hamiltonian (1), as described in previous work.20,22,23

For the approximate calculations, we separate the grid of $\rho$ into two regions. For $\rho < \rho^*$, we neglect the couplings induced by $\hat{\mathbf{V}}_{\text{field}}$. At these values of $\rho$, the Hamiltonian is...
The field-induced couplings are introduced at \( \rho > \rho^* \). We refer to this approximation as the truncated field-induced couplings (TFICs) approach. The results of the TFIC calculations are examined as a function of \( \rho^* \) and compared with the full calculations including the field-induced couplings at all values of \( \rho \).

The Mg–NH scattering calculations are performed for collisions of molecules initially in the lowest rotational state and the Zeeman state with the projection of the electron spin on the magnetic field axis \( M_S = +1 \). The ground rotational state of the NH molecule in a magnetic field is characterized by the triplet of the Zeeman states corresponding to \( M_S = 0, \pm 1 \). We report the elastic scattering cross sections preserving the Zeeman state in Mg–NH collisions and the inelastic scattering cross sections obtained by summing the cross sections for the \( M_S = 1 \rightarrow M_S = 0 \) and \( M_S = 1 \rightarrow M_S = -1 \) transitions.

The reactive scattering calculations are performed for collisions of \( H \) atoms with LiF molecules initially in the lowest Stark sublevel of the rotationally ground state of the first vibrationally excited state (\( v = 1 \)). We report the elastic scattering cross sections that describe non-reactive collisions of \( H \) with LiF and the total scattering cross sections for the reaction \( H + LiF \rightarrow Li + HF \). The reactive scattering cross sections are summed over cross sections for the production of LiF in all energetically accessible states.

III. RESULTS

A. Mg–NH scattering

In this section, we consider an example representative of weakly interacting atom-molecule and molecule-molecule scattering systems which do not chemically react. Scattering calculations on such systems in external magnetic and/or electric fields are important for understanding the feasibility of buffer gas cooling experiments, aiming to reduce the temperature of trapped molecules by momentum-transfer collisions with cold buffer gas atoms. Weakly interacting molecule-molecule systems must be considered for the analysis of evaporative cooling of molecules in magnetic traps. Magnetic trapping orients the magnetic moment of open-shell molecules so interactions of molecules in a magnetic trap are often characterized by the PESs of the maximum possible electronic spin, which normally prohibit chemical reactions and have rather shallow minima.

Figure 1 presents the cross sections for elastic collisions and inelastic scattering of NH with Mg as functions of \( \rho^* \) at a collision energy \( 10^{-3} \text{ cm}^{-1} \). The results show that the magnetic-field induced couplings at short range \( \rho < 10 \) bohrs affect the elastic scattering cross sections at magnetic fields \( >1000 \) G. For collisions in a magnetic field \( B = 10 \, 000 \) G, it is necessary to include the magnetic-field induced couplings at \( \rho > 5 \) bohrs. By contrast, the cross sections for inelastic scattering are much less sensitive to magnetic-field induced couplings at short range. This must be the result of the kinetic energy gain induced by inelastic collisions. The elastic collisions are sensitive to interferences of the incoming and outgoing scattering waves. The results of Figure 1 show that perturbing the Hamiltonian at short-range by neglecting field-induced interactions disturbs these interferences significantly. For inelastic collisions, the incoming and outgoing scattering waves have significantly different energies. The outgoing waves propagate with increased energy determined by the Hamiltonian at \( \rho = \infty \) and are thus less perturbed by weak magnetic-field couplings.

In order to illustrate quantitatively the effect of the field-induced couplings on elastic and inelastic scattering, we plot in Figure 2 the values of \( \rho^* \) corresponding to the deviation of the approximate cross sections from the accurate values in Figure 1. We have chosen the values \( \rho^* \) for Figure 2 such that neglecting field-induced couplings at \( \rho < \rho^* \) modifies the cross sections by less than 5%. The results illustrate that the

FIG. 1. The cross sections for elastic (upper panel) and inelastic (lower panel) scattering of NH(\( \Sigma^+ \), \( N = 0 \), \( M_S = 1 \)) molecules with Mg atoms in a magnetic field as functions of \( \rho^* \) computed at the collision energy \( E = 10^{-3} \text{ cm}^{-1} \). The horizontal lines indicate the values of the cross sections obtained from the full calculations with field-induced couplings included at all values of \( \rho \).

FIG. 2. The value of \( \rho^* \) yielding the cross sections (CSs) for elastic and inelastic scattering of NH(\( \Sigma^+ \), \( N = 0 \), \( M_S = 1 \)) molecules with Mg atoms within 5% of the value obtained from the accurate calculation as a function of the magnetic field.
increasing the PES strength generally allows for larger sections accurate to within 5% computed with the Mg–NH magnitude of the external field. For the scaled interaction potential (magnetic) dipole moment of the molecule and nature of the adiabatic potential, the value of $\rho$ determines the interaction potential while keeping fixed the electric field magnitude. For example, assuming that the interaction potential scales as $V(\rho) = -C_n/\rho^n$ at large $\rho$ with $n = 2$–6 depending on the nature of the adiabatic potential, the value of $\rho^*$ is obtained from $|W(\rho^*)| = |\mu F|$, where $\mu$ is the permanent electric (or magnetic) dipole moment of the molecule and $F$ is the magnitude of the external field. For the scaled interaction potential $\lambda V(\rho)$, we find $\rho^* = (\lambda C_n/|\mu F|)^{1/n}$ increasing monotonically with $\lambda$.

**B. LiF + H reaction**

In this section, we analyze the accuracy of the TFIC approximation for the computation of cross sections for reactive and elastic scattering using an example of a strongly interacting LiF + H collision system in an electric field. This is an example of an abstraction chemical reaction occurring at low temperatures by tunnelling under a reaction barrier at short range. Figure 4 shows the cross sections for reactive collisions as functions of $\rho^*$ at different strengths of the external electric field. For electric fields $>10$ kV/cm, the cross sections become inaccurate at small values of $\rho^* \approx 7$ bohrs. At the same time, the cross sections at all values of the electric field exhibit a maximum at $\rho^* \approx 8$–10 bohrs, cross the accurate values at $\rho^* \approx 10$–15 bohrs, and precipitously decrease for larger values of $\rho^*$. We have found that these peaks arise at $\rho^*$ near the values of $\rho$, where the potential energy crosses the asymptotic energy threshold, thus becoming negligible compared to the field-induced couplings. One can observe the similar behaviour of the cross sections in Figure 1, although the peaks appear to be significantly suppressed in the case of magnetic-field induced interactions.

Figure 4 shows that the cross sections for the LiF + H $\rightarrow$ Li + HF chemical reaction can be computed accurately without field-induced couplings at $\rho^* < 10$–15 bohrs, provided $\rho^*$ is chosen to be at the intersection point of the approximate cross sections with the horizontal lines representing the accurate values of the cross sections on the right side of the peaks. One could envisage an approach based on computing the $\rho^*$-dependence of the cross sections with a small basis and using the intersection point thus defined in a computation with an extended basis. However, we have found that the intersection point varies with both the basis set and the collision energy, and it is not immediately clear how the right side of the peaks can be exploited to accelerate the computations of the reactive scattering cross sections. At the same time, the value of $\rho^*$, where the approximate cross sections become inaccurate on the left side of the peaks, can be identified non-ambiguously. For example, one can find the optimal value of $\rho^*$ in a computation with a high electric field, and use the same value of $\rho^*$ for all computations with lower magnitudes of the electric field.
To qualitatively understand the results shown in Fig. 4, we observe that there are two optimum ranges of $\rho^*$ where the exact cross sections agree well with the TFIC results. The first range ($\rho^* < 5 \ a_0$) corresponds to the region of configuration space where the atom-molecule interaction potential is strongly repulsive and much larger than the field-induced couplings. We expect this range of $\rho^*$ to be universal since the atom-molecule interactions will eventually become repulsive at very small $\rho^*$. However, the different reaction arrangements remain strongly coupled in this range, and no simplification of reactive scattering computations is possible.

The second optimum range ($7 < \rho^* < 13 \ a_0$) arises as the atom-molecule interaction changes sign from repulsive to attractive, and its magnitude becomes large again compared to the field-induced couplings. This range of $\rho^*$ can be used to simplify quantum reactive scattering calculations by neglecting the field effects at $\rho < \rho^*$ as discussed below because at $\rho > 7 \ a_0$ the reaction arrangements are completely uncoupled. However, it is not universal because the values of $\rho^*$ where the potential couplings change sign and become asymptotically small depends on both the chemical reaction under consideration and the magnitude of the external field.

Figure 5 shows the $\rho^*$-dependence of the cross sections for elastic LiF + H scattering. Unlike in the case of Mg–NH scattering, the elastic cross sections for the reactive LiF + H system appear to be less sensitive to the external-field couplings at short range than the reactive cross sections. As can be seen in Figure 5, accurate cross sections for elastic LiF + H scattering can be computed without field-induced couplings at $\rho < 11$ bohrs, even for collisions in an electric field of 150 kV/cm.

At short range, different chemical arrangements of the reaction H + LiF $\rightarrow$ Li + HF are coupled by the matrix elements of the atom-molecule potential energy. Figure 6 depicts the $\rho^*$-dependence of the largest matrix element coupling different chemical arrangements. When this matrix element vanishes, the scattering problem can be transformed to the Jacobi coordinates and the Schrödinger equation can be solved using a basis of a single chemical arrangement of interest, a much easier task than solving the full reactive scattering problem in hyperspherical coordinates. As follows from Figure 6, all couplings between the Li + HF and LiF + H chemical arrangements vanish at the value $\rho^* \approx 6.8$ bohrs. Not surprisingly, this value of $\rho^*$ is close to the value of $\rho^*$, where the TFIC calculations start to deviate from the accurate results, on the left side of the peaks in Figure 4. At this value of $\rho^*$, the atom-molecule potential undergoes a transition from the short-range repulsive interaction to the attractive potential well. The results in Figures 4 and 6 suggest that the cross sections for the Li + HF $\rightarrow$ LiF + H chemical reaction in an external electric field can be computed by combining the numerical solution of the field-free Schrödinger equation in the hyperspherical coordinates at $0 < \rho < 6.8$ bohrs and the integration of the CC equations in the Jacobi basis of a single chemical arrangement including couplings with the external fields at $\rho > 6.8$ bohrs. As argued above, we expect that the optimal ranges of $\rho^*$ shown in Fig. 5 are a general feature of chemical reactions with a potential barrier. Additional calculations are needed to explore the optimal range of $\rho^*$ for other abstraction reactions, as well as for the insertion reactions without a potential barrier.

IV. CONCLUSIONS AND OUTLOOK

In this work, we compare the results of rigorous CC calculations of cross sections for elastic and inelastic scattering of NH($^3\Sigma$) molecules with Mg atoms in a magnetic field and elastic and reactive scattering of LiF molecules with H atoms in an electric field with the results of the approximate TFIC calculations, where the field-induced couplings are neglected at short atom-molecule separations $\rho < \rho^*$.

By analyzing the accuracy of the calculations as a function of $\rho^*$, we have arrived at the following conclusions:

(i) In general, the couplings induced by strong DC fields cannot be neglected at short range. This may appear surprising because the atom-molecule interaction potential is usually much stronger than the field-induced couplings at short atom-molecule separations. However, the atom-molecule interaction potential necessarily passes through zero (i.e., its asymptotic value), as $\rho$ increases from very short range, where the potential
is strongly repulsive, to long range, where the potential is attractive. This happens at a value of \( \rho \) classically accessible even at ultralow collision energies. The field-induced couplings at this value of \( \rho \) dominate over the matrix elements of the atom-molecule interaction potential. Our computations show that neglecting the field-induced couplings at these values of \( \rho \) can result in large errors in the calculated cross sections.

(ii) As a consequence of (i), the calculation error has a characteristic dependence on \( \rho^* \) passing through a maximum at short range and through zero at a large value \( \rho^* = \rho' \). Thus, a calculation without field-induced couplings at \( \rho < \rho' \) is accurate. However, it remains to be seen whether the value of \( \rho^* \) can be determined without solving the full-fledged quantum scattering problem.

(iii) There are two optimum ranges of \( \rho^* \) where the exact cross sections agree well with the TFIC results (see Fig. 4). The first range corresponds to the region of configuration space where the atom-molecule interaction potential is strongly repulsive (\( \rho < 5 a_0 \)). The second optimum range (\( 7 < \rho^* < 13 a_0 \)) arises in the region of \( \rho \) where the atom-molecule interaction becomes strongly attractive, e.g., near the van der Waals wells in the entrance and exit reaction channels. As the couplings between the different reaction arrangements vanish beyond \( \rho = 7.6 a_0 \) (see Fig. 6), the second optimum range of \( \rho^* \) is of great computational utility. However, we find that the position of the second optimum range depends on the details of the atom-molecule interaction potential and the strength of the molecule-field coupling.

(iv) The effect of short-range couplings induced by magnetic fields with the strength <1000 G can be neglected in light and weakly anisotropic collision systems such as Mg–NH (see Fig. 2). As illustrated by Fig. 3, increasing the strength of the atom-molecule interaction generally makes the calculations with a fixed value of \( \rho^* \) more accurate. Therefore, we expect that this conclusion will apply to all atom-molecule and molecule-molecule scattering systems with the interaction potential strength exceeding that of Mg + NH.

(v) The effect of short-range couplings induced by strong magnetic fields on atom-molecule scattering is generally weaker than the effect of couplings induced by strong DC electric fields. We have illustrated this by comparing the quantum dynamics of a weakly interacting van der Waals collision system Mg–NH in a magnetic field with that of a strongly interacting chemically reactive complex LiHF in a DC electric field.

Thus far, all quantum scattering calculations of molecular collisions in external fields were performed with the molecule-field couplings included at all values of \( \rho \). Neglecting the effects of external fields at short range could potentially lead to a dramatic simplification of the scattering calculations, since field-free collisions can be treated within the much more numerically efficient total angular momentum representation. Further, in the long-range region, the effects of external fields can be taken into account using MQDT. Our conclusions above indicate that these effects can be neglected for weakly anisotropic atom-molecule collisions in a magnetic field. It would be interesting to explore whether the promising results obtained here for Mg–NH would generalize to heavier atom-molecule complexes such as Li–CaH, Li–SrF, or Rb–SrF which are relevant for ongoing sympathetic cooling experiments.

The majority of quantum scattering calculations carried out to date\(^{69}\) assume that the molecule-field couplings are independent of \( \rho \) and equal to their asymptotic values at \( \rho = \infty \). The present results suggest, however, that the variation of the short-range couplings with \( \rho \) could affect the value of \( \rho \) where the matrix elements of the interaction potential become equal to those of the molecule-field interaction, shifting the positions of the maxima in Fig. 4. As a result, the \( \rho \)-dependence of the molecule-field interaction could have a strong effect on low-temperature scattering observables. This should be particularly important for reactive scattering of polar molecules in electric fields (at least for the abstraction reactions similar to LiF + H → Li + HF) where the dipole moment of the reaction complex is expected to vary strongly with \( \rho \).\(^{89}\) Our conclusions thus motivate further studies of atom-molecule reactive scattering with an accurate description of \( \rho \)-dependent molecule-field interactions.

The LiF + H → LiF + H reaction is a representative example of a chemical reaction with a barrier. Thus, we expect the idea of combining the field-free propagation at short range with a separate-arrangement propagation at long range may allow for a simplification of quantum scattering calculations on similar abstraction reactions such as F + H\(_2\) → HF + H or OH + H\(_2\) → H\(_2\)O + H in the presence of external fields.

Unlike the abstraction chemical reactions, barrierless “insertion” reactions are typically determined by strongly attractive interaction potentials throughout the entire configuration space. These potentials are not expected to pass through zero (except at very short \( \rho \)) unless a long-range angular momentum barrier is present. As a result, the peaks shown in Fig. 4 may not be present for the insertion reactions and larger \( \rho^* \) values may be possible, allowing for a more efficient decoupling of reaction arrangements.

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