Quasi-1D ultracold rigid-rotor collisions : reactive and non-reactive cases

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We study polar alkali dimer scattering in a quasi-1D geometry for both reactive and non-reactive species. Elastic and reactive rates are computed as a function of the amplitude of a static electric field within a purely long-range model with suitable boundary conditions at shorter range. We describe the diatomic molecules as rigid rotors and results are compared to the fixed-dipole approximation. We show in particular that for molecules with a sufficiently strong induced dipole moment oriented perpendicular to the trap axis, the long-range repulsive interaction leads to the suppression of short-range processes. Such shielding effect occurs for both reactive and non-reactive molecules, preventing two-body reactions as well as losses due to “sticky processes” [Phys. Rev. A 85, 062712 (2012)] from occurring. The present results demonstrate the possibility to suppress loss rates in current ultracold molecule experiments using 1D confinement.
I. INTRODUCTION

Ultracold molecules have added a new twist to the field of cold atoms \[1, 2\]. First groundbreaking experiments were carried out several years ago at JILA, where a dense gas of ultracold fermionic KRb dimers was produced by two photon association \[3\]. This molecular species is reactive, a feature that has been explored in the context of quantum-state controlled chemical reactions \[4\]. However, from the standpoint of many-body studies the reactivity of KRb is in general a drawback leading to fast particle loss from the trap.

More recently, different groups have reported the production of non-reactive ultracold alkali dimers \[5–11\]. Such molecules, if prepared in the absolute single-particle energy state, are strictly stable under two-body collisions. However, in particular for bosonic molecules, there is experimental evidence that even under these favorable conditions inelastic losses still occur at fast pace \[6–8, 11\]. This is true in particular for bosonic molecules, whereas fermionic samples appear to be more stable \[9, 10\]. A mechanism that might explain the observed losses is related to the existence of Fano-Feshbach resonances available with high density at thermal energies even in an ultracold gas. Presence of such resonances increases the collision lifetime of a pair of molecules, creating a tetrameric complex. Such metastable complex can be lost from the trap since it is not necessarily trapped in the optical lattice and can undergo recombination to deeper levels by colliding with a third molecule \[12, 13\].

In order to increase the sample lifetime, it is therefore important to devise strategies to prevent molecules from approaching at short distances, where detrimental inelastic processes take place. Unfortunately, in three dimensions there always exists an attractive head-to-tail reaction path leading to the short range. This circumstance has been shown to result in a strong dependence $\sim d^6$ of the reactive rate on the induced dipole moment $d$ \[14\]. More subtle quantum effects have been proposed to control the reaction dynamics of alkali dimers prepared in rotationally excited states \[15\]. Microwave shielding leading to a dramatic lifetime increase has also been recently theoretically studied \[16\].

The situation is different if molecules are confined in tight traps, for instance by optical means. In fact, confinement can then be easily designed in such a way that molecule pairs will tend to collide in a repulsive side-to-side configuration, the head-to-tail pathway being energetically unfavorable by the confining potential. This approach has been demonstrated both experimentally and theoretically to lead to a drastic increase of the lifetime of reactive polar molecules trapped in one and two spatial dimensions \[17–20\].

Our previous study of reactive collisions in one-dimensional optical tubes has addressed highly reactive species \[20\]. Therein, polar molecules have been simply described as fixed dipoles of magnitude equal to the induced dipole moment $d$. More subtle quantum effects have been proposed to control the reaction dynamics of alkali dimers prepared in rotationally excited states \[15\]. Microwave shielding leading to a dramatic lifetime increase has also been recently theoretically studied \[16\].

The paper is organized as follows. Section II introduces the formalism and our numerical approach. Section III presents the long-range multipolar expansion of the molecule-molecule interaction. Results for different dialkali species and collision energies are presented as a function of an applied electric field in Sec. IV. A short conclusion summarizes this work.

II. FORMALISM

We consider two molecules A and B confined in a quasi one-dimensional geometry by a potential approximated as an harmonic trap. The quadratic nature of the confining potential allows one to separate center-of-mass and relative motion. The rigid-rotor Hamiltonian describing the collision in relative coordinates includes the kinetic energy, the confinement potential, and an interaction term $V_{\text{int}}$ defined below in Eq. (2) which includes inter-molecular forces and the Stark interaction energy with the external electric field. In this work we will describe the dimer molecules as rigid rotors, an approximation valid as long as the intermolecular distance remains large compared to the extent of the internal coordinates.

The kinetic energy of the dimer+dimer complex will be decomposed into a sum of three independent terms depending respectively on the relative distance $R$ between the two centers of mass, the internal coordinate of the dimer A and the internal coordinate of dimer B \[21\]. Furthermore, we will assume that the dimers remain in their vibrational ground level reducing the dimer contribution to the kinetic energy to a purely rotational term.
Putting together all the terms, the total Hamiltonian reads:

\[ H = T_R + T_{\text{rot}} + V_{\text{trap}} + V_{\text{int}} = -\frac{\hbar^2}{2\mu} \frac{d^2}{dR^2} + \frac{\ell^2}{2\mu R^2} + \frac{1}{2}\mu\omega_\perp^2 \rho^2 + B_v J_A' + B_v J_B' + V_{\text{int}}(R). \]  

(1)

Here \( \ell \) is the orbital angular momentum of the relative motion, \( J_A \) and \( J_B \) are the angular momenta of A and B with rotational constant \( B_v \), \( \omega_\perp = 2\pi\nu_\perp \) is the trap frequency and \( \rho \) the distance to the trap axis \( z \). We use for each molecule the spectroscopically determined rotational constant \( B_v \) of the ground level \( X^1\Sigma^+; v = 0 \). Values and reference of the spectroscopic study can be found in [22].

The transverse oscillator length characterizing the trap size will be defined as \( a_{\text{ho}} = \sqrt{\hbar/(\mu\omega_\perp)} \). As demonstrated in three spatial dimensions, hyperfine interactions would greatly increase the complexity of the problem [12, 13]. However, we do not expect such added complexity to bring novel qualitative features to the main effects we wish to demonstrate and hyperfine interactions will be neglected in this work.

We will now extend to rigid rotors the computational approach developed for fixed dipoles in our previous work [20]. Our method to construct the scattering wavefunction consists in a simultaneous expansion of the angular part of the solution in a suitable internal basis whereas the radial coordinate is discretized on a grid of points. The radial discretization is detailed in Sec. II A. The angular basis comprises the orbital angular coordinate \( \vec{R} \) as well as any internal degree of freedom of the diatomic, as described in Sec. II B.

### A. Radial discretization

The radial discretization is performed according to the spectral element approach [23, 24]. Briefly, we choose a minimum \( r_c \) and a maximum \( r_{\text{max}} \) radial distance and define a solution interval \( I = [r_c, r_{\text{max}}] \) which is in turn partitioned into a set of \( N \) non-overlapping sectors. A number of grid points and a basis set of Gauss-Lobatto cardinal functions associated with those points are assigned to each sector. The wavefunction is represented on the discrete basis and continuity of the wavefunction and of its radial derivative is enforced at the connection points between sectors. This strategy results in a highly sparse matrix in the grid indices. It should be remarked that our method allows different angular bases to be used in each sector. With the basis over all coordinates defined, we can rewrite the Schrödinger equation as a linear system that can be solved for a matrix solution \( \Psi \) in the interval \( I \) provided boundary conditions are assigned at the endpoints \( r_c \) and \( r_{\text{max}} \).

At the right endpoint we impose \( \Psi'(r_{\text{max}}) = I \), the matrix solution at \( r_{\text{max}} \) becomes then equal to the \( R \)-matrix defined as \( R = \Psi(\Psi')^{-1} \). From \( R \) one can then extract the scattering matrix and hence all physical observables such as the elastic and reactive collision rates [17, 20].

We will impose two different boundary conditions at \( r_c \). The first assumes that at short distance the molecules react with unit probability. We thus require that the spherical surface \( R = r_c \) is totally absorbing, i.e. across the surface we only have incoming flux and no reflected outgoing flux. In practice we first define local adiabatic channels \( |\alpha\rangle \) and corresponding energies \( E_\alpha \) by diagonalizing the angular Hamiltonian \( T_{\text{rot}} + V_{\text{int}} \) at distance \( R = r_c \). Next, we assume that the wavefunction can be described by a pure incoming spherical wave in each channel \( \alpha \) for \( R \approx r_c \)

The logarithmic derivative \( Z(r_c) \equiv \Psi'(r_c)\Psi^{-1}(r_c) \) is therefore diagonal with elements \((-ik_\alpha - \frac{1}{2}k'_\alpha k_\alpha^{-1/2})\), where \( k_\alpha = \sqrt{2\mu(E_{\text{coll}} - E_\alpha)/\hbar^2} \) is the channel wave vector and the derivative is taken with respect to \( R \). This method has been shown to give accurate prediction for diatomic reactive species [25].

Our second approach amounts to the Dirichlet boundary condition \( \Psi = 0 \), i.e. the wavefunction is required to have a nodal surface for \( R = r_c \). In this description we can observe resonances between the incoming open channel with collision energy \( E_{\text{coll}} \) and bound levels of closed channels with energy close to \( E_{\text{coll}} \). Since the radius \( r_c \) is chosen arbitrarily and there is \textit{a-priori} no reason for the wavefunction to have a nodal surface for \( R = r_c \), we cannot predict the location of the resonances in terms of the amplitude of the electric field. As a matter of fact, the short-range collision parameters (more precisely, the quantum defects, see [12, 13]) can be considered as stochastic variables arising from the extremely complex four-body dynamics taking place inside \( r_c \). In this view, our specific Dirichlet condition can be considered as one possible realization of such complex process.

The specific value \( r_c = 40 \, a_0 \) has been chosen so to satisfy the following criteria. Firstly, the rigid rotor model is expected to be accurate in the external region \( R > r_c \). Second, motion is semiclassical near \( r_c \) for the adsorbing model of Ref. [25] to apply. Finally, since we are interested in resonance spectra, the density of states near threshold must be the same for the Dirichlet “truncated potential” as for the full one. We have checked that for our choice of \( r_c \) this holds true up to energies on the order of 1 K in the case of a single deep potential well with van der Waals tail.

The present approach can therefore expected to give useful insight into the collisions dynamics and it allow us to compare on an equal footing different approaches, namely the fixed-dipole and the rigid-rotor descriptions. Finally,
note that for the sake of comparison we will use the non-reactive Dirichlet condition even for intrinsically reactive species such as LiCs or LiRb.

B. Angular basis

The angular part of the wavefunction in the rigid-rotor model is expanded in the so-called decoupled basis $|J_A M_A J_B M_B l M_l\rangle$, representation defined by the operators $J_A^2, J_B^2, \ell^2$ with eigenvalues $\hbar^2 J_A(J_A+1)$, $\hbar^2 J_B(J_B+1)$, and $\hbar^2 l(l+1)$ as well as by their projections on the laboratory axis with eigenvalues $M_A, M_B$ and $M_l$. The laboratory axis is taken as the axis of the confining optical tube. In parallel configuration where the electric field axis is aligned along the laboratory axis, the projection of the total angular momentum $M \equiv M_A + M_B + M_l$ is conserved, allowing us to work with a smaller basis set. For non-parallel configurations one has to take into account couplings between different $M$ due to the electric field.

The interaction potential matrix included in Eq. (1)

$$V_{\text{int}}(R) = \frac{C_3}{R^3} + \frac{C_6}{R^6} + V_{\text{Stark},A} + V_{\text{Stark},B}$$

(2)

comprises the dipole-dipole interaction $C_3/R^3$, the van der Walls interaction $C_6/R^6$, and the Stark term arising from the interaction between the molecular dipoles $d_{A,B}$ and the electric field. The matrix elements of $C_3$ and $C_6$ depend on the angular momenta $J_A, J_B$ and $l$ as well as their projection on the laboratory axis. They are obtained using Wigner-Eckart theorem, their expression in the space fixed frame can be found in [26–29].

Few additional points must be taken into consideration. First, since we focus on collisions of identical diatomics we need to use symmetrized wavefunctions

$$|\tilde{\Psi}_{J_A M_A J_B M_B J_l M_l}\rangle = \frac{|\tilde{\Psi}_{J_A M_A J_B M_B J_l M_l}\rangle + (-1)^l |\tilde{\Psi}_{J_B M_B J_A M_A J_l M_l}\rangle}{\sqrt{2(1 + \delta_{J_A J_B} \delta_{M_A M_B})}}.$$  

(3)

For the perpendicular electric field configuration, the Hamiltonian is also symmetric with respect to reflection across the plane orthogonal to the trap axis and containing the origin. We can construct a symmetrized wavefunction

$$|\tilde{\Psi}_{J_A M_A J_B M_B J_l M_l}\rangle = \frac{|\tilde{\Psi}_{J_A M_A J_B M_B J_l M_l}\rangle + (-1)^{M_A+M_B+M_l} |\tilde{\Psi}_{-J_A M_A -J_B M_B -J_l M_l}\rangle}{\sqrt{2(1 + \delta_{M_A 0} \delta_{M_B 0} \delta_{M_l 0})}}.$$  

(4)

Lastly, while the decoupled basis is useful in the weak electric field regime, for higher amplitudes, different J levels are heavily mixed by the field, the system is better described in a dressed basis set [30, 31]. To obtain this basis we numerically diagonalize for each field amplitude the diatomic potential $B_x J_x^2 + V_{\text{Stark},X} (X = A, B)$. We thus get the eigenfunctions $|\tilde{J} M_l\rangle = \sum J \alpha_{J} |J M_J\rangle$ which are in turn combined into the tetrameric wavefunction $|\tilde{J}_A \tilde{M}_A \tilde{J}_B \tilde{M}_B J_l M_l\rangle$. In order to compute the total potential matrix we first evaluate the matrix elements in the decoupled basis and then we numerically evaluate

$$\langle \tilde{J}_A \tilde{J}_B J_l l' | H | \tilde{J}_A \tilde{J}_B J_l \rangle = \sum_{J_A J_B J_{l'}} \alpha_{J_A} \alpha_{J_B} \alpha_{J_A} \alpha_{J_B} \langle J_A' J_B' | J_A J_B \rangle |H| J_A J_B J_{l'},$$

(5)

where the magnetic quantum numbers have been suppressed for notational convenience.

The rigid-rotor description is only used between $R = 40 a_0$, chosen as the $r_c$ boundary value in this work, and $R = 200 a_0$. For intermediate distances above $R = 200 a_0$, dipole-dipole interaction between different rotational level is weak compared to the energy gap of those level. One can thus focus on the rotational ground level with $\tilde{J}_A = 0$ and $\tilde{J}_B = 0$, using perturbation theory to take into account excited levels; see Sec. III. Spherical harmonics $|l M_l\rangle$ are still used to represent orbital motion.

Finally, in the long-range domain, typically $R > 10^4 a_0$, the cylindrical confining potential of the 2D-trap overcomes the molecule-molecule interaction, limiting $R$ to a small angular region around the pole. A development in spherical harmonic becomes increasingly inefficient, and we use cylindrical grid basis functions projected on the spherical surface that stay localized near the pole as $R$ varies. As an order of magnitude, few hundreds spherical harmonics are needed to enforce continuity at the connection point between the intermediate and the long-range regions.

We will compare the rates obtained with the current approach to results from our previous model where fixed dipoles were used instead of rigid-rotors [20]. In the latter, the interaction between the molecule in its rotational ground level and the Stark field is described as a point particle with a given induced permanent dipole moment. All
rotational effects factor into a unique $C_6$ long-range coefficient. The total angular wavefunction is expanded on a basis of orbital spherical harmonics and the Hamiltonian only contains the orbital kinetic energy, the confinement potential and the interaction potential $V_{\text{int}}$. Such point-particle model is equivalent to our intermediate-range rigid-rotor model where we include only the rotational ground state, though the correction to the $C_6$ coefficient needs to be taken the same in both models; See Sec. III.

### III. INDUCED DIPOLE MOMENT INTERACTION

Some care must be taken in the definition of the $C_6$ matrix coefficient in order to have a correct description of the Van der Waals interaction. Two different approaches are used in this work.

In the first one, used for the intermediate range domain or for the point particle model, excited rotational states are not explicitly included in the basis. Resulting from a second order perturbation treatment, the $C_6$ coefficient is thus written as a sum over all excited rotational, vibrational and electronic levels of both molecules. Following Refs. [22, 32] the $C_6$ can be decomposed into the sum of two contributions, a term $C_6^e$ including the electronic transitions contribution and one $C_6^r$ including the rotational transition contribution. Pure vibrational transitions as well as cross terms have been shown to be negligible [22]. Values of the $C_6^e$ are taken from [22]. The $C_6^r$ term is described in more detail in Sec. III A.

In the second approach, used for the short range domain, the rotational states are explicitly included in the basis. The second order term is thus coming only from the electronic transitions $C_6^e$. An additional corrective term is however needed to prevent the appearance of unphysical levels see Sec. III B.

Note that in both cases we take the $C_6^r$ as a purely isotropic term. In fact, the anisotropic contribution has been taken into account for the study of KRb+KRb and found to give negligible corrections to the computed scattering observables.

#### A. Rotational transition contribution

Due to the competition between the electric field and the rotational Hamiltonian, the rotational spectrum is heavily perturbed. A field free $C_6^r$ value would thus not be appropriate [33].

In more detail the expression of the rotational contribution is

$$C_6^r = \sum_{(J_A, J_B) \neq (0,0)} \frac{\left| \langle \tilde{J}_A, \tilde{J}_B | d_A d_B | 0, 0 \rangle \right|^2}{\Delta E_A + \Delta E_B}$$

(6)

$\Delta E_A$ (resp. $\Delta E_B$) being the energy difference between the ground and the excited $J_A$ (resp. $J_B$) level. Dependence on the space-fixed projections $M_A$ and $M_B$ of the excited rotational levels are omitted in the formula for ease of reading. For the field free case $\tilde{J} \equiv J$ and the only non-zero transition is from $J = 0$ to $J = 1$. We then obtain the expression for two identical molecules

$$C_6^r(C = 0) = \frac{d_{\text{perm}}^6}{4B_v}$$

(7)

with $d_{\text{perm}}$ the permanent dipole moment of the diatomic, expressed in its own molecular frame.

To obtain more accurate results for the collision rate we compute an improved $C_6^r$ value using Eq. (6) at each electric field amplitude. We note that for a non-zero field the heteronuclear molecules present an induced permanent dipole moment in the laboratory frame. In this case the contribution of matrix elements like $\langle 0, 1 | d_A d_B | 0, 0 \rangle$ is non negligible. Those transition terms with one molecule in the ground level and the other in an excited one are related to the induction interaction $C_6^\text{ind}$. While the remaining transitions involving two rotationally excited molecules added to the electronic $C_6^e$ form the dispersion coefficient $C_6^\text{disp}$.

Rotational contributions have been shown to be small for heteronuclear molecules LiNa and KRb due to their weak permanent dipole moment [22]. However for a molecule like LiCs they are by far the dominant term. In Fig. 1 we show the difference in $C_6$ coefficients for LiCs-LiCs interactions depending on the model used. Calculation were performed with a single $C_6^e$ term, a fixed field-free $C_6$ term, a field-dependent $C_6^\text{disp}$ term and finally a field-dependant $C_6^\text{disp} + C_6^\text{ind}$ term. At weak fields the difference between the values obtained at the different levels of approximation is small and the collision rate is essentially the same for each model. At higher fields the dominant term is the $C_3$ dipole-dipole interaction and modifications of the $C_6$ coefficient have no major impact on our results. However the
$C_6$ interaction is still relevant at short intermolecular distances. In particular the energy density of bound states decreases as the van der Waals interaction decreases. Top panel in Fig. 1 shows the elastic collision rate computed using the Dirichlet boundary condition. It is apparent that for strong electric field the density of quasi-bound states is severely underestimated if one omits the induction interaction.

B. Unphysical states

When neglecting the rotation in the point-particle model we still need to compute a corrective $C_6$ term, which means that the modification of the rotational structure must be taken into account in the model in second order perturbation theory. In a similar fashion, the use of the rigid-rotor basis mentioned in Sec. II B leads to unphysical states if no correction is made [34, 35]. Indeed due to computational limitations one has to truncate the basis, neglecting all the levels with $J > J_{\text{max}}$. In particular all the coupling matrix element of the type $\langle \tilde{J}_A'\tilde{J}_B'\mid V\mid \tilde{J}_A\tilde{J}_B \rangle$ with either $J_A'$ or $J_B'$ above the angular momenta $J_{\text{max}}$ are cut off. Rotational levels with $J = J_{\text{max}}$ are the most affected by this truncation [34, 35]. To reduce the effect of this approximation on the ground state, and thus on the collision rate, one can simply increase the size of the basis.

Another approach is to use second order perturbation theory. In this approximation, the omitted couplings are assumed to be a perturbation to the levels included in our basis, giving rise to a corrective term $V_{\text{corr}}$ to be added to the Hamiltonian. This term is diagonal with matrix elements

$$
\langle \tilde{J}_A\tilde{J}_B\mid V_{\text{corr}}\mid \tilde{J}_A\tilde{J}_B \rangle = \sum_{J_A'J_B' > J} \frac{|\langle \tilde{J}_A'\tilde{J}_B'\mid V\mid \tilde{J}_A\tilde{J}_B \rangle|^2}{\Delta E_A + \Delta E_B} \tag{8}
$$

where the sum is over every level above the cutoff angular momentum and $V$ is the dominant coupling term, the dipole-dipole interaction $C_6/R^6$ in our case. The square of the matrix element on the rhs leads to a $R^{-6}$ correction to the $C_6$ coefficient. In this work we take $J_{\text{max}}$ equal to either 1 or 2, and the sum is carried out up to $J = 7$. The energy gap $\Delta E$ is taken as the diatomic energy gap, thus neglecting the molecule-molecule interaction.

IV. RESULTS

We perform calculations for different bosonic species under various trapping conditions, collision energy and electric field. Table I resumes the relevant characteristic physical parameters relevant for our calculations. The van der Waals length $\bar{a} = (2\mu C_6/\hbar^2)^{1/4}/2$ given in the table represents the average scattering length for collisions in a pure $C_6/R^6$ potential and can be interpreted as the range of such potential [36]. We focus here on an intermediate confinement regime, which we define following Ref. [37] as $\bar{a}_{\text{int}} = 10 \bar{a}$. The collision energy of the identical heteronuclear molecules will be fixed in most calculations to 50 nK. With reference to the table one can remark that for a heavy molecule such as LiCs such collision energy can be considered as “hot” in terms of the trap level spacing. In fact, the gap with the first excited energy level of the transverse harmonic oscillator is only slightly larger than twice the collision energy.

| Species | $\bar{a}$ (a.u.) | $a_{\text{int}}$ (a.u.) | $v_\perp$ (kHz) | $E_{\text{coll}}/\hbar\omega_{\text{perp}}$ | $d_{\text{perm}}$ (a.u.) | $B_e$ (GHz) |
|--------|----------------|----------------|----------------|---------------------------------|----------------|-----------|
| $^{39}$K-$^{87}$Rb | 117 | 955 | 10 | 1.6[-2] | 0.242 | 1.13 |
| $^{7}$Li-$^{85}$K | 224 | 2236 | 5 | 3.3[-2] | 1.410 | 7.69 |
| $^{7}$Li-$^{87}$Rb | 325 | 2473 | 2 | 8.3[-2] | 1.645 | 6.46 |
| strong | - | 341 | 100 | 1.6[-3] | - | - |
| $^{7}$Li-$^{133}$Cs | 497 | 6408 | 0.2 | 8.3[-1] | 2.201 | 5.62 |
| $^{23}$Na-$^{87}$Rb | 355 | 2286 | 2 | 8.3[-2] | 1.304 | 2.09 |

TABLE I. Relevant numerical parameters used in our calculation, as defined in the text. The reference collision energy $E_{\text{coll}}$ is 50 nK. Two confinement strengths, intermediate and strong, are indicated for the LiRb dimer.

We first consider the configuration where the electric field is parallel to the confinement axis. In this case, molecules tend to be in attractive head-to-tail configuration and to react at the cutoff radius $r_c$. In fact, for molecules of bosonic character the lowest adiabatic potential curve shows no barrier to reaction; see Fig. 2. The rotational structure of the molecules plays a minor role in the short-range dynamics as can be seen in the upper panel of Fig. 3. When taking the Dirichlet boundary condition, shown in the lower panel, we note however an increase in the density of features
**FIG. 1.** (color online) Upper panel: van der Waals $C_6$ coefficient for LiCs-LiCs interaction. The electric field is parallel to the trap axis. Four different models were used: an electronic $C_6^e$ (full black curve at 7407 a.u.) added to a rotational field-free $C_6^r$ term (dashed red curve) or a field dependent $C_6^r$ (dot-dashed green curve) added to the induction coefficient $C_6^{\text{ind}}$ (full blue curve). Lower panel: elastic collision rate at $E_{\text{coll}} = 50$ nK imposing the Dirichlet boundary condition at short range computed for van der Waals coefficient $C_6^r$ (full line) or $C_6^r + C_6^{\text{ind}}$ (dashed line).
arising from the presence of quasi-bound states embedded in the continuum. Such resonances can arise either due to coupling with closed channels in the optical waveguide in the same rotational state or to potential curves correlating to rotationally excited molecules.

We now focus on a system where the electric field is perpendicular to the trap axis. It can be expected that in this configuration and with a strong enough induced permanent dipole moment the diatomic molecules will repel each other at long range [37] and can be protected against short-range reactive collisions. Figure 4 shows the calculated elastic and reactive collision rates for LiK molecules. Results obtained in the fixed-dipole approximation are virtually indistinguishable from the rigid-rotor model. In particular, the reactive rate is suppressed by about three orders of magnitude in the considered range of \( E \), confirming that shielding is robust versus rotation.

For some molecules however the dipole moment and thus repulsion is not strong enough to suppress reactive paths. With trapping parameters from Tab. I corresponding to intermediate confinement, we find that LiNa and KRb do not have a strong enough permanent dipole moment to obtain a significant shielding effect.

We now consider non-reactive species, taking the NaRb dimer as an example. The long range adiabatic curves of the NaRb-NaRb tetrameric taken for different amplitudes of the static electric field are shown in Fig. 5. Each adiabatic potential correlates asymptotically with an energy level \( \hbar \omega_{n,\perp} (n + 1) \) of the isotropic transverse harmonic oscillator with principal quantum number \( n \) and degeneracy \( (n + 1) \). At shorter distance, the dipolar interaction becomes significant and breaks the isotropy of oscillator. The dipolar interaction contributes for instance an energy of \( d^2/R^3 \) for molecules oscillating in the plane perpendicular to the dipoles and \( d^2/R^3 \left[ 1 - 3 \cos^2(\theta) \right] \) for molecules in the plane containing the dipoles and the trap axis, with \( \theta \) the angle between \( R \) and \( d \). This leads to the lifting of the asymptotic degeneracy clearly visible in the three panels of the figure as the intermolecular distance decreases.

Moreover, as expected at perpendicular configuration, a barrier to reaction is formed in the lowest adiabatic potential as the amplitude of the field increases. To experience a significant short-range dynamics the molecules would need to tunnel through this barrier, which for instance at 5 kV/cm has height of 510 nK; See rightmost panel of Fig. 5. Under this field-induced shield it is interesting to compare the dynamics of a collision with a collision energy well below the maximum of the barrier (50 nK), and slightly over the top of the adiabatic potential barrier (600 nK).

Figure 6 shows the results of calculations performed with the Dirichlet boundary condition. Main feature of collisions at the largest considered energy is that the coupling between the incoming channel and closed channels, either correlating with the trap or with rotationally excited level, gives rise to a dense spectrum of overlapping resonances. As conjectured in [12, 13] resonant population of these quasi-bound states increases the collision lifetime along with the probability of loss of the untrapped complex and of inelastic recombination via collision with a third body. These phenomena are suspected to be a significant limiting mechanism to the lifetime of ultracold quantum gases [6–8]. In contrast, at low collision energy resonance effects tend to be washed out, in particular in a strong field when the adiabatic barrier becomes high and broad. Confinement combined with a static electric field should thus allow one to shield non-reactive molecules from sticky collisions in addition of shielding reactive molecules.

Similar conclusion that coupling to the quasi-bound states is suppressed by an electric field is reached for the non-reactive LiRb model shown in Fig. 7. In other terms, the resonance width strongly decreases with \( E \) such that resonances first become isolated and their effect on the cross section finally essentially vanishes. The figure also shows comparison with the fixed-dipole approximation. Note that as expected the density of resonant features is larger for the rigid-rotor model due to the additional rotational degrees of freedom of the dimers. Shielding becomes otherwise effective at comparable values of the electric field at each considered collision energy.

As demonstrated in Ref. [37] and expected on physical grounds, for dipoles perpendicular to the axis stronger transverse confinement should further help suppressing head-to-tail collisions. Rotation does not seem to change this general conclusion. For instance, Fig. 8 shows the elastic collision rate for a non-reactive LiRb + LiRb collision model and in a strong confinement regime. The resonance spectrum appears relatively sparse even at relatively low electric fields, meaning again that coupling between the open channel and quasi-bound states is weak since particles are prevented from reaching the short-range region where couplings occur.

Overall, finding optimal conditions for stabilizing the gas against inelastic processes requires a suitable balance between low temperatures, confinement and electric field intensity.

V. CONCLUSIONS

We have presented a rigid-rotor model to study identical polar molecule collisions in a quasi-1D optical trap. Collisions of reactive molecules in the rotational ground state are well described in the fixed-dipole approximation. The present calculation confirms that for sufficiently strong induced dipole moments electrostatic repulsion between dipoles perpendicular to the trap axis leads to suppression of the reactive rates. For non-reactive molecules, the rotational degrees of freedom result in an increased density of Fano-Feshbach resonances. We demonstrate that the resonance widths decrease and resonance spectra become less congested for increasing induced electric dipole moment.
FIG. 2. Adiabatic potential curves for KRb + KRb system. Left panel shows the short range intermolecular-distance domain, right panel the intermediate range distance domain. Transition from a dipolar-dominated system to a 1D confined system is indicated by the “ridge” visible at intermediate distances in the right panel.
FIG. 3. (color online) Elastic collisions rate between two KRb molecules, described as rigid rotor (full line) or fixed dipole (dashed line), in a quasi-1D geometry as a function of the amplitude of the electric field, oriented parallel to the trap axis. Upper panel: rates computed with a unitary loss at short-range. Bottom panel: rates computed using the Dirichlet boundary condition.
FIG. 4. (color online) Elastic (full line) and reactive (dashed line) collisions rate between two LiRb molecules in a quasi-1D geometry as a function of the amplitude of the electric field, oriented perpendicular to the trap axis. Results are for a rigid rotor model, indistinguishable on the figure scale from the ones for fixed dipoles (not shown).
FIG. 5. Adiabatic potential curves for NaRb + NaRb system. Left panel with a weak static electric field of 0.5 kV/cm, middle panel with a field of 1 kV/cm and right panel with a strong field of 5 kV/cm.
FIG. 6. (color online) Elastic collision rate for NaRb + NaRb collisions as a function of the amplitude of the electric field, perpendicular to the trap axis. Collision energy is 50 and 600 nK for lower and upper panel, respectively. Dirichlet boundary condition is imposed at short range.
FIG. 7. (color online) Same as Fig. 6 but for LiRb + LiRb collisions. Solid black lines corresponds to the rigid rotor model, red dashed lines to the fixed dipole one. Plot is for transverse confinement $\nu_{\text{perp}} = 2$ kHz and Dirichlet boundary condition.
FIG. 8. Elastic collision rate for LiRb + LiRb collisions as a function of the electric field amplitude for the rigid rotor model. Plot is for tight transverse confinement with $\nu_{\text{perp}} = 100$ kHz and Dirichlet boundary condition.
of the molecules. This effect can be used to increase the lifetime of the resonance complex and possibly to suppress harmful “sticky collision” processes.

In perspective, it can be interesting to model experiments where collision dynamics has been studied in the presence of an additional optical lattice along the axis of the tube [19]. This computational task could be accomplished for instance by combining the present 3D solution strategy and the asymptotic reference Bloch functions constructed in [38]. The effect of hyperfine interactions could also be included in the model to various levels of approximation.

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