Published in final edited form as:

Phys Rev A. 2012 February ; 85(2): . doi:10.1103/PhysRevA.85.022703.

Resonant control of polar molecules in individual sites of an optical lattice

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Abstract

We study the resonant control of two nonreactive polar molecules in an optical lattice site, focusing on the example of RbCs. Collisional control can be achieved by tuning bound states of the intermolecular dipolar potential by varying the applied electric field or trap frequency. We consider a wide range of electric fields and trapping geometries, showing that a three-dimensional optical lattice allows significantly wider avoided crossings than free space or quasi-two dimensional geometries. Furthermore, we find that dipolar confinement-induced resonances can be created with reasonable trapping frequencies and electric fields, and have widths that will enable useful control in forthcoming experiments.

I. INTRODUCTION

Ultracold gases of polar molecules are of interest for their long-range dipolar interactions, which give them unique applications in areas such as many-body phases [1], quantum information [2], and precision measurement [3–5]. Cold gases of LiCs [6] and RbCs [7] have been formed with temperatures $T \lesssim 1$ mK, and work continues to produce degenerate gases [8,9]. A near-degenerate gas of $^{40}\text{K}^{87}\text{Rb}$ with $T \lesssim 1$ μK has been produced [10], since then a number of studies have elucidated its collisional properties [11–14]. Two colliding KRb molecules have exothermic reactions producing $\text{K}_2 + \text{Rb}_2$, which occur with almost unit probability when the two molecules are sufficiently close. This allows a simple description of the collision properties in terms of universal physics [15–22]. Such techniques should also apply to other species with reactive collisions, and to the quenching of any vibrationally excited molecule. For many studies it is therefore desirable to keep molecules separated, for example, by confining the gas in a three-dimensional (3D) lattice [23], in a quasi-two-dimensional (2D) geometry with the molecules polarized perpendicular to the plane (side-by-side) [14–17,24,26], or in a quasi-one-dimensional (1D) geometry [25]. This reduces the likelihood of molecules approaching each other along the attractive “head-to-tail” path which is available in 3D.

In contrast to reactive molecules such as KRb, ground-state NaK, NaRb, NaCs, KCs, and RbCs are not reactive, and so are available for experiments on longer time scales and at higher densities where control of elastic collisions is useful. The long-range dipole-dipole

interaction between two molecules produces an anisotropic potential which is capable of supporting bound states [27]. Tuning these bound states around a collision threshold with an electric field allows resonant control of the interactions [18,28,29], in analogy to the magnetic and optical control that has been so useful for neutral atoms [30]. Because three-body recombination can still occur [31], isolating a pair of molecules in an optical lattice site provides an ideal, loss-free environment for studying the two-body energy spectrum. Such a scenario is analogous to several experiments performed on atom pairs [32–35]. Optical lattices have also been used to tune atomic collisions through confinement-induced resonances [36–41] (CIRs), which depend on the scattering length being comparable to the characteristic length of the confinement. With the interactions of polar molecules having an even longer range, we will show that it is reasonable to anticipate the existence of CIRs as well.

In this paper we study the states and control possibilities of two polar molecules isolated in an optical lattice site, focusing on the specific example of RbCs. We examine in detail the effects of tuning the lattice parameters and electric field. We show that the optical lattice can be used to increase the resonance width past what is possible in free space or 2D geometries. We compare the eigenenergies obtained for a quasi-2D lattice site to scattering calculations for a system with confinement in only one direction. Locations of resonances in the scattering calculations accurately reproduce those of avoided crossings between eigenenergies. In addition, we show their utility for resonant control. Our studies show that tuning the confinement has a significant effect on the collisional and bound-state properties of the pair of molecules, allowing the creation of useful CIRs.

II. MODEL

We consider two ground state $^{87}\text{Rb}^{133}\text{Cs}$ molecules in a cylindrically symmetric optical lattice site. In Table I we list length scales relevant to ultracoldmolecular collisions and give representative values for the parameter regimes used in this work. Typical van der Waals coefficients for polar molecules are of order $10^5 E_h a_0^6$ to $10^7 E_h a_0^6$, much larger than those for pairs of alkali atoms ($10^3 E_h a_0^6$ to $10^4 E_h a_0^6$). However, the mean scattering length scales as $\bar{a} \propto C_6^{1/4}$, giving a similar characteristic length to the van der Waals part of the potential. We take the dipole moment $\mu = \langle \hat{\mu} \rangle_z$ to be the expectation value of the electric dipole operator $\hat{\mu}$ for the molecular ground state in the electric field direction. We calculate this electric-field-dependent quantity according to the method of Ref. [42]. The dipole length, tunable with an electric field, is typically the largest length scale in the problem. For a trapping frequency $\omega/2\pi = 50$ kHz, $a_\mu = \ell_{\text{ho}}$ for $\mu = 0.16$ D. We note that the use of a strong dipole moment takes us beyond the region of validity of pseudopotential approaches such as those of Refs. [43,44].

The molecules are assumed to be rigid rotors, aligned in the axial direction by an applied electric field. We approximate the lattice site with a harmonic trap and consider only the relative motion of the molecules. The combined interaction and trapping potential is given by

$$V(\rho, z) = \frac{\mu^2}{r^3} \left(1 - \frac{3z^2}{r^2} \right) + \frac{C_{12}}{r^{12}} - \frac{C_6}{r^6} + \frac{\hbar^2}{2m_r} \frac{m^2}{\rho^2} + \frac{1}{2} m_r (\omega_\rho^2 \rho^2 + \omega_z^2 z^2). \quad (1)$$

Here, ρ and z are the relative radial and axial coordinates, respectively. Also, $\omega_{\rho, z} = 2\pi f_{\rho, z}$, where $f_{\rho, z}$ are the corresponding trapping frequencies. The intermolecular separation is given by $r = \sqrt{\rho^2 + z^2}$, and the projection of the relative motion along the axis of symmetry is given by m . We impose a repulsive short-range potential, C_{12}/r^{12} , setting the C_{12} coefficient such that the potential $C_{12}/r^{12} - C_6/r^6$ contains six bound states and gives a scattering length of $100a_0$. We neglect the anisotropic C_6 coefficient. While arbitrary, setting the short-range part of the potential in this way allows us to conveniently study the important long-range effects. We have performed simulations, not reported here, for different scattering lengths. They show bound-state spectra as well as rate coefficients as a function of dipole moment and trap frequencies that are similar to the figures shown in this paper. The locations of resonances change. Their density of states and trends in resonance widths, however, do not.

Although the collisions under consideration involve four atoms, the approach described above is justified by the separation in energy scale between the chemical bonds within the ground-state dimers ($\sim$ THz) and the collision energy or bond between them ($\lesssim$ MHz). We also note that the van der Waals coefficient between polar molecules has contributions from the rotation of the molecules as well as the induced dipole moments of the electron clouds. An electric field polarizes the molecules and changes the rotational contribution. We have calculated the extent of this change and checked that it does not noticeably change the results presented here, as was the case in Ref. [22]. Consequently, we neglect this effect. Because we confine ourselves to a single collision channel, the resonances we find correspond to shape resonances [30], in which the potential experienced by a colliding pair supports a near-degenerate quasi-bound state. We note that Feshbach resonances, in which a colliding pair is coupled to a near-degenerate bound state of a different spin configuration, are possible for the general case of coupling between states of different molecular spin and rotational quantum number.

We first study the two-body energy spectrum. We solve for eigenstates and eigenvalues of the Hamiltonian with the potential of Eq. (1) using PHAML version 1.8.0 [45,46], a parallel two-dimensional finite-element code for elliptic boundary value and eigenvalue problems. PHAML features adaptive grid refinement of the discretized spatial coordinates to concentrate the grid in areas where the wave function varies rapidly, and high-order elements to obtain an accurate solution. For these computations we used eighth degree elements. Within PHAML, ARPACK [47] was used to solve the discrete eigenvalue problem, using the shift-and-invert spectral transformation to compute interior eigenvalues, and MUMPS [48] to solve the resulting linear system of equations. The parallel computations were performed on two nodes of a LINUX cluster. A particular advantage of the two-dimensional solver is its ability to readily account for the anisotropic interaction and trapping potential. By contrast, an expansion in spherical harmonics or noninteracting trap states will struggle to accurately

resolve the wave function without a very large basis set. However, for analysis of the wave functions we calculate projections onto these functions. We solve for the function $R(\rho, z)$, where the full wave function is given by $\psi(\rho, z, \phi) = R(\rho, z)e^{im\phi}$. Our bound-state calculations consider only $m = 0$, but in the scattering calculations described below we will consider the effects of nonzero m . We study spherically symmetric ($\omega_z = \omega_\rho$) and quasi-2D ($\omega_z \gg \omega_\rho$) geometries, with the dipoles always aligned along the z axis.

III. RESULTS

The eigenenergies of two RbCs molecules in a spherically symmetric lattice site with $f_z = f_\rho = 25$ kHz are shown as a function of dipole moment in Fig. 1(a). We use the term bound states to refer to those that are bound when the trap is adiabatically turned off. States close to the noninteracting trap level energies, $(n_z + 1/2)\hbar\omega_z + (2n_\rho + |m| + 1)\hbar\omega_\rho$, are called trap states. Here, Bose symmetry allows the trap-state quantum numbers to be $n_z = 0, 2, 4, \dots, n_\rho = 0, 1, 2, \dots$, and $m = 0, \pm 2, \pm 4, \dots$. At zero dipole moment, the trap-state energies are affected by the van der Waals interactions. Dipole moments above approximately 0.1 D cause a significant change to these energies. A large number of avoided crossings occur as trap states are brought into the potential by the increasing dipolar attraction. All crossings are avoided, although some are too narrow to be visible on the scale shown. States of different ℓ are mixed by the dipolar interactions, with the broadest crossings occurring between states of low ℓ . For example, the first two trap levels converted to bound states as μ is increased are primarily of mixed s - and d -wave symmetry, whereas the steeply descending state with a series of narrow crossings near $\mu = 0.31$ D is concentrated in $\ell = 10$. Figures 1(b) and 1(c) illustrate the wave function near $E/\hbar = -50$ kHz for dipole moments of $\mu = 0.17$ and $\mu = 0.498$ D, respectively. We plot the function $\rho|\psi|^2$, to more clearly illustrate both short and large length scales. For the state at $\mu = 0.17$ D, vibrational nodes of the bound states of the van der Waals potential can be seen as rings of constant $r < 0.25\ell_{ho}^z$. A d -wave component at longer range, $r > 0.25\ell_{ho}^z$, provides the head-to-tail configuration, with the wave function concentrated in the region $\rho < |z|$ where the dipole-dipole interaction is attractive. This makes E decrease as μ increases. The state at $\mu = 0.498$ D is much more strongly coupled between partial waves, and has a correspondingly more complicated configuration.

We now compare these results to the case of a quasi-2D optical lattice site, with $f_z = 50$ kHz and $f_\rho = 1$ kHz, where we have significantly weakened the ρ confinement while keeping the trap along z nearly the same. Eigenvalues are plotted as a function of μ in the lower panel of Fig. 2. A quasi-continuum of radial trap levels is found, spaced by $2f_\rho$, instead of the strongly mixed states of Fig. 1. Only the $n_z = 0$ trap state is within the energy range shown, although some bound states have substantial admixture in higher z states, as indicated in the lower panel of Fig. 2. The quasi-2D configuration has the effect of making the avoided crossings narrower than in the 3D lattice case.

An intuitive explanation [49] of the narrowing of the avoided crossings in quasi-2D geometries follows from the realization that the mixing is between a side-by-side trap-state configuration, with a typical volume V_{ho} on the order of $\ell_{ho}^z(\ell_{ho}^\rho)^2$, and an attractive head-to-tail configuration, whose volume is determined by the dipole-dipole potential. When the

latter volume is much smaller than V_{ho} their overlap scales as $1/\sqrt{V_{ho}}$. Hence, the width of the avoided crossings, which is related to this overlap, is reduced both in the limit of a quasi-2D trap and in the limit of free space $\omega_z, \omega_\rho \rightarrow 0$. For the bound-state wave functions shown in Fig. 1, the binding energy is small enough that the trapping potential cannot be neglected. In particular, that of Fig. 1(c) shows the effects of the avoided crossing between states of the dipole-dipole and trapping potentials.

It is desirable to attach meaningful quantum numbers to describe the states that are observed. This is made difficult at large μ by the strong anisotropic interactions; however, some approximate quantum numbers can be used. States can be described by their projections onto the noninteracting trap levels with quantum numbers n_z and n_ρ , although both van der Waals and dipole-dipole interactions mix these levels. We indicate in Fig. 2 the states which are concentrated in higher z trap levels. As we discuss below, it is these states that provide the possibility of creating CIRs. States can also be described by their vibrational quantum number and projections onto spherical harmonics described by the orbital angular momentum ℓ . Both quantum numbers are exact for isotropic traps in the zero-dipole limit. Different ℓ become strongly mixed at sufficient $\mu > 0$, as discussed above for the states shown in Fig. 1.

We now make the link between our calculated bound-state energies and scattering properties in a quasi-2D system. Our scattering calculations use the coupled channels technique discussed in [22], adapted for elastic boundary conditions at short range. We use the potential of Eq. (1) with ω_ρ set to 0, and propagate the scattering matrix in a basis of spherical harmonics to a value of r large enough to match onto the $n_z = 0$ trap state. The chosen collision energy of $k_B \times 200$ nK, corresponding to $h \times 4$ kHz, is such that higher z trap states are not significantly populated at this separation. Here, k_B is the Boltzmann constant. We then propagate outward in ρ , extracting the scattering properties at long range using the conventional tools of scattering theory [50]. The results are shown in the upper panel of Fig. 2, and agree well with the bound-state calculations. The resonances at low dipole moment are widest and most isolated from other features, making them the most useful for resonant control. Contributions to the elastic collision rate coefficient from collisions with higher m make the resonance minima nonzero.

Optical lattices have been used to control scattering lengths in neutral gases [39,41] by making a state corresponding to an excited trap level near degenerate with the colliding atoms. This depends on the scattering length being of the same order as the characteristic length scale of the confinement. With the large dipole length characteristic of interactions between polar molecules, it is reasonable to expect that similar confinement-induced effects should occur. In the lower panel of Fig. 3 we show this effect for RbCs molecules, calculating eigenenergies as a function of f_z while maintaining $f_\rho = 1$ kHz. We assume $\mu = 0.3048$ D, corresponding to an easily accessible electric field of 0.67 kV/cm. The figure shows seven levels, six trap levels with $n_z = 0$ and $n_\rho = 0, 1, \dots, 5$, and a single bound state crossing these levels. As shown in Fig. 2, this bound state has substantial admixture in higher z trap states. The energy of the bound state therefore increases with f_z faster than the trap levels.

We have perturbatively calculated the change δE in an eigenenergy from changing ω_z to $\omega_z + \delta\omega_z$ which results in

$$\delta E = \frac{1}{2} \left\langle \left(\frac{z}{\ell_{ho}^z} \right)^2 \right\rangle \hbar \delta\omega_z. \quad (2)$$

Here $\langle \dots \rangle$ indicates calculating the expectation value with respect to the selected wave function. The result for the bound state of Fig. 3, evaluated with the numerically obtained wave function at $f_z = 40$ kHz, is shown as a green dashed line. The red dotted lines correspond to the energy of a noninteracting pair of molecules in the ground trap state, with $k_B \times 1$ nK and $k_B \times 200$ nK of relative kinetic energy. The points at which these cross the perturbative calculation correspond well with the scattering resonances shown in the upper panel of Fig. 3. For a relative kinetic energy of $k_B \times 200$ nK, the feature has a width with respect to f_z variation of approximately 5 kHz, although accurate electric field control will be necessary due to the resonance location being strongly dependent on the dipole moment. This is shown by the dashed line in the top panel, for a dipole moment of 0.3058 D, which corresponds to a change in the applied electric field of approximately 2.5 V/cm. The temperature is also of significance, as shown by the calculations for collision energies of $k_B \times 100$ nK and $k_B \times 1$ nK, which produce narrower peaks at lower trapping frequencies. The asymmetric Fano line shape at $k_B \times 1$ nK differs significantly from those at higher collision energies, indicating a changing interference between direct scattering in the 2D continuum and scattering mediated by the single bound state. A fit of the rate coefficient to a Fano line profile as a function of f_z shows that to good approximation the resonance location depends linearly on collision energy E_{rel} , while its width increases as E_{rel}^γ with a power γ between 0.5 and 1.0. For collision energies above $k_B \times 1$ nK we are not in the Wigner threshold limit of scattering from a two-dimensional $1/\rho^3$ potential. [The dipole-dipole energy scale $\hbar^2/(m_r a_\mu^2)$ is $k_B \times 1.1$ nK for RbCs with a dipole moment of 1.0 D.] Consequently, threshold scaling laws do not apply even at rather cold collision energies of $k_B \times 1$ nK. We plan to investigate this threshold behavior in the near future. Nevertheless, our current results illustrate that the location and properties of the resonances can be controlled by manipulating both the electric field and the confinement.

IV. CONCLUSIONS

We have studied the role that an optical lattice can play in controlling the collisional properties of nonreactive polar molecules. We have shown that tight confinement allows for much broader avoided crossings, giving a greater resonance width than is available in free space. We have also shown that confinement-induced resonances can be easily created, with the caveat that their location is sensitive to the dipole moment. Measurements of resonance locations would constrain the short-range potential, for which we studied just one example with a scattering length of $100a_0$. However, models with other scattering lengths should not significantly alter the density of states or our finding that RbCs will have several accessible resonances for dipole moments less than 0.5 D and trapping frequencies on the order of tens

of kHz. These results will therefore be of significance for upcoming experiments using nonreactive polar molecules.

Acknowledgments

We acknowledge funding from an AFOSR MURI on ultracold molecules (T.M.H. and P.S.J.) and partial funding from the ONR (P.S.J.). We thank Z. Idziaszek for stimulating discussions.

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FIG. 1.

(Color online) (a) Eigenenergies for two RbCs molecules in an optical lattice site with $f_z = f_\rho = 25$ kHz. Trap states are adiabatically converted to bound states as the dipolar interaction is increased. Points marked 'b' and 'c' correspond to the wave functions shown in the lower panels, which illustrate the head-to-tail configuration at two different dipole moments. For the three lowest energy trap states, the partial wave at $\mu = 0$ is indicated. We also give the partial waves into which these states have a significant projection after being converted to bound states as μ is increased. Red crosses indicate the noninteracting trap-state energies. In

(b) and (c), we plot $\rho|\psi|^2$, and scale all lengths by the confinement length in the z direction, ℓ_{ho}^z .

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FIG. 2.

(Color online) Elastic collision rate as a function of μ for a trapping frequency of $f_z = 50$ kHz and collision energy of $k_B \times 200$ nK, showing the contributions of the $m = 0, \pm 2$, and ± 4 partial waves (upper panel), and the corresponding $m = 0$ bound-state calculation with $f_z = 50$ kHz and $f_\rho = 1$ kHz (lower panel). The z trap states with a substantial admixture are indicated for each bound state not concentrated solely in $n_z = 0$.

FIG. 3.

(Color online) Confinement-induced resonances for a quasi-2D trap as function of f_z . The top panel shows the elastic collision rate, where we have summed the contributions of partial waves from $m = 0$ to $|m| = 4$. Solid lines correspond to $\mu = 0.3048$ D and collision energies of $k_B \times 1$ nK, $k_B \times 100$ nK, and $k_B \times 200$ nK, as labeled. The dashed line ($\mu = 0.3058$ D) shows the sensitivity of the resonance location to electric field variation. The bottom panel shows the eigenenergies of the Schrödinger equation with the potential of Eq. (1), using $\mu = 0.3048$ D and trapping frequencies of $f_z = 50$ kHz and $f_\rho = 1$ kHz. The dashed green line shows the perturbative result of Eq. (2). Dotted red lines correspond to the energy of a

noninteracting pair of molecules in the ground trap state with $k_B \times 1$ nK and $k_B \times 200$ nK of relative kinetic energy. Arrows show the intersections of this calculation with scattering states of the given kinetic energies. These intersections agree well with the calculated resonance locations of the upper panel.

TABLE I

Characteristic length scales for the interaction of ultracold molecules in an optical lattice, with values given for RbCs in parameter regimes used in the present work. For the van der Waals coefficient, we use $C_6 = 142129 E_h a_0^6$ [20], where $E_h = 4.3597 \times 10^{-18}$ J is the Hartree energy and $a_0 = 52.918$ pm is the Bohr radius. We give the confinement length for optical lattice sites with frequencies $\omega/2\pi = 1$ kHz and 50 kHz. The dipole length is given for RbCs molecules with a dipole moment of $\mu = 1.0$ D, where $D = 0.39343 e a_0 = 3.336 \times 10^{-30}$ Cm is the debye and e is the charge of an electron. Here, m_r is the reduced mass.

Quantity	Definition	Value (a_0)
Mean scattering length	$\bar{a} = \frac{2\pi}{[\Gamma(1/4)]^2} (2m_r C_6 / \hbar^2)^{1/4}$	233.5
Confinement length	$\ell_{ho} = \sqrt{\hbar / (2m_r \omega)}$	
$\omega/2\pi = 1$ kHz		5728
$\omega/2\pi = 50$ kHz		810.5
Dipole length	$a_\mu = m_r \mu^2 / \hbar^2$	3.1×10^4