Collision dynamics of molecules and rotational excitons in an ultracold gas confined by an optical lattice

Roman Krems
University of British Columbia

Sergey Alyabyshev
Chris Hemming
Felipe Herrera
Zhiying Li
Marina Litinskaya
Timur Tscherbul
Erik Abrahamsson

UBC Physics

UBC Physics

Harvard University

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Outline

I. Inelastic collisions of molecules confined by an optical lattice in quasi-2D geometry
   • Effects of laser forces on reactive collisions

II. Controlled dynamics of rotational excitons in an array of molecules on an optical lattice
   • System with tunable exciton-impurity interactions
   • Scattering resonances in exciton-impurity collisions
   • Controlled localization/delocalization of excitons

III. Tuning ultracold molecules by microwave fields
   • Collision-induced absorption of non-resonant microwave photons near Feshbach resonances
Quantum Gases in Confined Geometries

Inelastic collisions

\[ \psi_{sc}^{\alpha' \neq \alpha} = - \sum_{\alpha' \neq \alpha} \sum_{l'} \sum_{m'_l} \nu^{-\frac{1}{2}} \nu r^{-1} S_{\alpha' l' m'_l \leftarrow \alpha 0 0} \frac{i 2 \pi}{k_\alpha} Y_{00}^* (\hat{r}_i) e^{i (k_{\alpha'} r - l' \pi / 2)} \phi_{\alpha'} Y_{l m'_l} (\hat{r}) \]

Couplings occur in 3D collision core

The confined and unconfined channels can be treated separately.

The asymptotic wave function for inelastic collisions:

\[ \psi_{sc}^{\alpha' \neq \alpha} = \sum_{\alpha' \neq \alpha} \nu^{-\frac{1}{2}} f_{\alpha' \leftarrow \alpha} \frac{e^{i k_{\alpha'} r}}{r} \phi_{\alpha'} \]

Z. Li and RK, PRA 79, 050701 (2009)
6.7. Numerical results

Figure 6: The ratios of inelastic and elastic cross sections for wave collisions of $^6\text{Li}$ and $^{87}\text{Rb}$ atoms as functions of $l_0$ for $|a| = \text{uw}$. The initial states are $|1,2\rangle \otimes |u,t\rangle$. The collision energy is $u - 8 \text{cm}^{-1}$.

The ratios are always smaller than one which means that both elastic and inelastic collisions are suppressed when the geometry changes from qwD to quasi-qD while the inelastic collisions are suppressed much more significantly than the elastic scattering. An other interesting observation: the magnitude of the cross section for both elastic and inelastic collisions increases as the strength of the confinement increases. This happens because the extension of the wave function $l_0$ decreases with the increase of the confinement potential $V_r$ which leads to a higher probability to detect scattering atoms and molecules. Yet the suppression of inelastic collisions when the geometry changes from qwD to quasi-qD is due to the modification of the wave function.

The formalism presented in this Chapter can be applied to describe chemical reactions in an ultracold molecular gas under laser confinement. The index $\alpha'$ in Eq. 6 must then include outgoing channels in different chemical arrangements. To explore the effects of laser confinement on chemical interactions of ultracold molecules, we consider an illustrative example of the reaction $^7\text{Li} + ^6\text{Li} \rightarrow ^{13}\text{Li} + ^{16}\text{O}$. The cross sections for elastic scattering and the $\omega^\lambda Z$. Li and R.V. Krems, Phys. Rev. A 79,050701(R) (2009)
Rotational Excitons in Optical Lattices with Polar Molecules

Scattering of molecular excitons by tunable impurities

Felipe Herrera, Marina Litinskaya and RK,
arXiv:1003.3048
Optical lattice with polar molecules

Ground: \( |J = 0, M_J = 0\rangle \)

Excited: \( |J = 1, M_J = \{-1,0,1\}\rangle \)

LiCs molecules
Dispersion Curves

\[ E(k) \text{ (in units of } 10^{-6} B) \]

\[ m_* < 0 \]
Impurities

One impurity:

\[ H = \sum_{n \neq 0} E_0 B_n^\dagger B_n + E_{\text{imp}} B_{n=0}^\dagger B_{n=0} + \sum_{n} J_{mn} B_m^\dagger B_n \]

Scatterer with the strength = difference in transition energies:

\[ H = \left( \sum_{n} E_0 B_n^\dagger B_n + \sum_{n} J_{mn} B_m^\dagger B_n \right) + (E_{\text{imp}} - E_0) B_{n=0}^\dagger B_{n=0} \]

Breaks translational symmetry \( \rightarrow \) Mixes states with different \( k \)

\[ H = \sum_{k} E(k) B_k^\dagger B(k) + \frac{V_0}{N} \sum_{k,q} B_k^\dagger(k) B(q) \]
Tunable impurities

\[
\Delta E_{eg} \text{ (} \times 10^4 \text{ MHz)}
\]

- CsF
- LiCs
- LiRb

\[
E (\text{kV/cm})
\]
0 1 2 3 4

\[
\Delta E_{eg}
\]

- LiCs
- LiRb

\[
\sigma_{2D} (\text{Å})
\]

- \(k=10^{-8} \text{ Å}^{-1}\)
- \(k=10^{-6} \text{ Å}^{-1}\)
- \(k=10^{-5} \text{ Å}^{-1}\)
Tunable impurities

Quantum simulations:

Tune exciton-impurity interactions
by an external electric field
Vary impurity distributions and concentrations
Exciton - impurity Hamiltonian matrix

\[ \langle \hat{H}_0 \rangle_{q,k} = E(k) \delta_{k,q}, \]

\[ \langle \hat{W} \rangle_{q,k} = \frac{2 \Delta J(a)}{N_{\text{mol}}} (\cos q \cdot a + \cos k \cdot a) \sum_{i_n=1}^{N_i} e^{i(q-k) \cdot i_n} \]

Off-diagonal disorder

Diagonal disorder

\[ \langle \hat{V} \rangle_{q,k} = \frac{V_0}{N_{\text{mol}}} \sum_{i_n=1}^{N_i} e^{i(q-k) \cdot i_n} \]
\[ |\Psi(x)|^2 \left( \frac{1}{N_{\text{mol}}} \right) \]

- **No diagonal disorder**
- **Diagonal disorder \sim off-diagonal disorder**
- **Large diagonal disorder**
Dynamical Multiple Impurity Problem

\[ i\hbar \frac{\partial}{\partial t} \left| \Psi(t) \right\rangle = \left( H_0 + V(t) \right) \left| \Psi(t) \right\rangle \]

\[ \psi_k(r) = \sum_k C(k,t) \varphi_k(r,t) \]

\[ \frac{\partial C(k,t)}{\partial t} = \sum_q D(k,q;t) C(q,t) \]

\[ D(k,q;t) = \frac{i f(t)}{\hbar N} e^{i(E_k-E_q)t/\hbar} \sum_{\text{impurities}} e^{-i(k-q)r_{imp}} \]

Wave packet formation and dynamics,

\[ k \text{-space distribution} \ldots \]
\[ |\Psi(x)|^2 \left( \frac{1}{N_{\text{mol}}} \right) \]

Diagram showing the wave function \( |\Psi(x)|^2 \) with time instances:
- \( t = 0 \)
- \( t = 0.4 \text{ ms} \)
- \( t = 0.8 \text{ ms} \)

The graph plots \( x \) (\( a \)) against \( |\Psi(x)|^2 \left( \frac{1}{N_{\text{mol}}} \right) \) for different time points.
\[ |\Psi(x)|^2 \left( \frac{1}{N_{\text{mol}}} \right) \]

\[ |C(k)|^2 \]

Inset graph:

\[ f(t) \]

VS:

\[ t (\mu s) \]

Graphs show the behavior of \(|\Psi(x)|^2\) and \(|C(k)|^2\) as functions of \(x\) and \(ka\) respectively.
Tuning ultracold molecules with microwave fields

S. V. Alyabyshev, T. V. Tscherbul and RK, PRA 79, 060703(R) (2009)
S. V. Alyabyshev and RK, PRA 80, 033419 (2009).
S. V. Alyabyshev and RK, submitted.
Polar molecules in a microwave cavity

Molecular Hamiltonian: \( H_{\text{mol}} = B N^2 \)

Field Hamiltonian: \( H_f = \hbar \omega (\hat{a} \hat{a}^\dagger - \bar{N}) \)

Molecule - Field Interaction: \( H_{\text{mol},f} = -\frac{d\epsilon_0}{2\sqrt{N}} \left( \hat{a} + \hat{a}^\dagger \right) \cos \chi \)

Basis set: \( |NM_N\rangle |\bar{N} + n\rangle \)

The matrix elements:

\[
\langle \bar{N} + n | H_{\text{mol},f} | N'M'_N \rangle |\bar{N} + n'\rangle \sim \langle NM_N | \cos \chi | N'M'_N \rangle \times \\
\times \left( \delta_{n,n'+1} + \delta_{n,n'-1} \right)
\]

\[
\langle NM_N | \cos \chi | N'M'_N \rangle \sim \delta_{M_N,M'_N} \left( \delta_{N,N'+1} + \delta_{N,N'-1} \right)
\]
the field-dressed basis \(|NM_N\rangle|\bar{N} + n\rangle\), where \(M_N\) is the projection of \(\bar{N}\) on the space-fixed quantization axis, and \(|\bar{N} + n\rangle\) are the photon number states. For the microwave trap proposed in [12], \(n \ll \bar{N}\) and the matrix elements of Eq. (3) are independent of \(N\). Diagonalization of the molecule-field Hamiltonian (2) yields

\[
|\nu K\rangle = \sum_{N,M_N} \sum_{n=-n_{\text{max}}}^{n_{\text{max}}} C_{NM_N \nu K} |NM_N\rangle|\bar{N} + n\rangle, \tag{4}
\]

where the indices \(\nu\) and \(K\) label the field-dressed states and the coefficients \(C_{NM_N \nu K}\) depend on \(\Omega_R\) and \(\omega\). The total wave function of the collision complex is expanded in the products of field-dressed wave functions (4) and spherical harmonics \(|\ell m\ell\rangle\). The probabilities for collision-induced transitions between the microwave field-dressed states (4) are obtained from the solution of the multichannel Schrödinger equation [9, 10].

Figure 1(a) shows the energy levels of CaH in a microwave field as functions of the Rabi frequency at \(\omega/B_e = 1.57\). The field-dressed levels are arranged in manifolds separated by multiples of the photon energy \(\omega\). We label the states by \(|\nu K\rangle\), where \(\nu\) denotes the state of the molecule within a photon manifold, and \(K\) labels the photon manifold. We consider collisions of CaH molecules in the strong-field-seeking state \(|\nu = \alpha, K = 0\rangle\), which correlates with the ground rotational state \(N = 0\) of CaH at zero field. The states of different \(K\) may interact when \(\Omega_R \geq 3B_e\). In this work, we consider moderate Rabi frequencies \(0 < \Omega_R < B_e\) suitable for a microwave trapping experiment [12].

Figure 2 shows the cross sections for elastic scattering and inelastic relaxation in CaH–He collisions as functions of \(\Omega_R\) at a collision energy of 0.3 \(\text{cm}^{-1}\). The probabilities for inelastic collisions increase with decreasing the detuning from resonance \(\Delta = 2B_e - \omega\). For the off-resonant microwave frequencies of 0.01 and 1.1 \(B_e\), the inelastic cross sections increase monotonically with increasing \(\Omega_R\). At a near-resonant frequency of 1.9 \(B_e\), the cross sections increase by a factor of \(\sim 50\) and show broad oscillations. The difference between the cross sections corresponding to different microwave frequencies becomes smaller with increasing the field strength.

In order to elucidate the propensities for collision-induced transitions in a microwave field, we present in Fig. 3 the state-resolved cross sections for inelastic transitions to various final field-dressed states. As our initial state is the ground state in the \(K = 0\) manifold, inelastic relaxation involves transitions between different photon manifolds. Figure 3 shows that the total relaxation probability is determined by two major transitions: \(|\alpha, K = 0\rangle \rightarrow |\alpha, K' = -1\rangle\) and \(|\alpha, K = 0\rangle \rightarrow |\xi, K = -1\rangle\).

The field-dressed states \(|\alpha, K = 0\rangle\) and \(|\alpha, K' = -1\rangle\) differ exactly by one quantum of microwave field energy. Therefore, the transition \(|\alpha, K = 0\rangle \rightarrow |\alpha, K' = -1\rangle\) may be interpreted as a collision process accompanied by absorption of a microwave photon. The molecule-field interaction (2) couples the product states with \(\Delta N = \pm 1\) and \(\Delta n = \mp 1\), so the strongest couplings occur between the field-dressed states in the adjacent photon manifolds \((\Delta K = \pm 1)\). Figure 3 shows that the transitions with the minimal change of \(K\) are the most probable, and that the transition probabilities decrease rapidly with increasing.
Polar molecule in a microwave cavity
In order to elucidate the propensities for collisions-induced transitions in a microwave cavity, we consider moderate Rabi frequencies \( \Omega \). The inelastic cross sections increase with decreasing the detuning from resonance \( \Delta \). The fields-dressed states in the adjacent photon manifolds correlate with the ground rotational state in the field. We present in Figure x the states-resolved cross sections for inelastic transitions to various final fields-dressed states.

The collisions-induced transitions are determined by the matrix elements of the electric dipole moment. The interaction between the molecule and the microwave field is described by the Hamiltonian:

\[
\hat{H} = \hbar \Omega_R \hat{a}^\dagger \hat{a} \hat{N} - \hbar \Delta \hat{N} \\hat{N} - \hbar \omega \hat{N} \\hat{N} + \hbar \omega \hat{N} \\hat{N}.
\]

Here, \( \Omega_R \) is the Rabi frequency, \( \Delta \) is the detuning, \( \omega \) is the field frequency, and \( \hat{N} \) is the number operator. The transitions are given by:

\[
a_0|N = 0, \bar{N}\rangle + a_1|N = 1, \bar{N} - 1\rangle,
\]

\[
a_0|N = 0, \bar{N} - 1\rangle + a_1|N = 1, \bar{N} - 2\rangle.
\]

\( \|a_0\|^2 \) and \( \|a_1\|^2 \) correspond to the inelastic cross sections for different microwave frequencies. In the limit of small Rabi frequency, the initial and final fields are uncoupled. The total relaxation probability is determined by two major transitions:

- Inelastic relaxation involves transitions between different microwave frequencies.
- Elastic scattering involves transitions to the ground state.

The strongest couplings occur between the fields in the adjacent photon manifolds. There is no absolute ground state in the microwave cavity.
Cross section (Å$^2$)

(a)  

no mw field  
$h\omega/B_e = 0.7$; $\Omega/B_e = 0.02$

Cross section (Å$^2$)

(b)
$h\omega/B = 0.7$
$\Omega/B_e = 0.02$

$h\omega/B = 0.7$
$\Omega/B_e = 0.2$

$h\omega/B = 1.9$
$\Omega/B_e = 0.02$
Cross section (Å²)

\[ \frac{\hbar \omega}{B_e} = 0.7 \]

\[ \frac{\hbar \omega}{B_e} = 0.1 \]
Summary

Inelastic/Reactive collisions in quasi-2D geometry are suppressed

\[ \frac{\sigma_{3D\text{ reactive}}}{\sigma_{3D\text{ elastic}}} = \gamma \frac{\sigma_{\text{quasi-2D reactive}}}{\sigma_{\text{quasi-2D elastic}}} \]

\[ \gamma = \sqrt{\frac{2E}{\pi \hbar \omega_0}}; \quad \frac{E}{\hbar \omega_0} \ll 1 \]

Z. Li and RK, PRA 79, 050701(R) (2009).
Summary

Mixture of polar molecules on an optical lattice
=> rotational excitons with tunable impurities

• Tunable scattering resonances for exciton – impurity interactions

• Tunable disorder => quantum simulation of localization

• Localization/delocalization of excitons can be tuned by an electric field

• Possibility to study finite-size and geometry effects on dynamics of excitons

F. Herrera, M. Litinskaya and RK, arXiv1003.3048
Collisions of ultracold molecules lead to absorption of far-detuned, non-resonant microwave photons.

- Non-resonant field absorption is dramatically enhanced near a Feshbach resonance.
- This can be used for detecting Feshbach resonances and tuning scattering properties of ultracold molecules.

S. V. Alyabyshev and RK, to be published