Polar Molecules Colliding in Quasi-2d Traps

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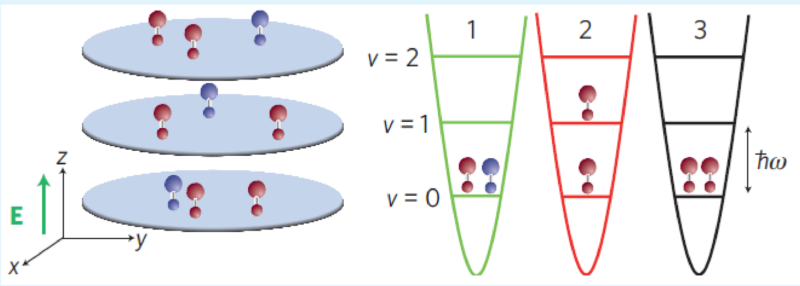
Abstract

We investigate collisions of polar molecules in quasi-2d configuration in the presence of external electric field perpendicular to the collision plane [1]. Our model is characterized by two dimensionless quantum defect parameters: y and s. The former describes probability of reaction, and the latter gives the phase of the wave function at short range. For y close to unity we obtain universal collision rates determined only by the quantum reflection process from the long-range potential, and dependent only on the van der Waals coefficient, dipole-dipole interaction and the trap frequency. At small reaction probabilities the collision rates are not universal and exhibit resonances induced by the confining potential. At high dipole moments we observe the supression of reactive collisions that can stabilize the ultracold gas of polar molecules. The calculations are done by propagating multichannel wavefunction in the spherical basis and then transforming to the cylindrical coordinates at large distances. In this way we can describe collisions of highly polar molecules, e.g. LiCs, NaCs. Successful experimental production of ultracold molecules [2, 3] provides an opportunity for testing presented calculations.

Motivation

Experimental realization of ground-state KRb polar molecules in quasi-2d traps



M. H. G. de Miranda, A. Chotia, B. Neyenhuis, D. Wang, G. Quemener, S. Ospelkaus, J. L. Bohn, J. Ye, and D. S. Jin, Nature Phys. 7, 502-507 (2011)

Basic properties

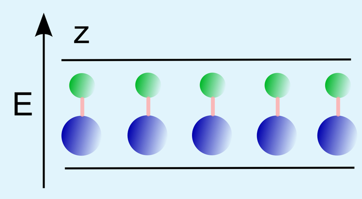
Gas of polar molecules in quasi-2D geometry

$$H = \sum_i \frac{p_i^2}{2m} + \frac{1}{2} m\Omega^2 z_i^2 + \sum_{i<j} V(r_i - r_j)$$

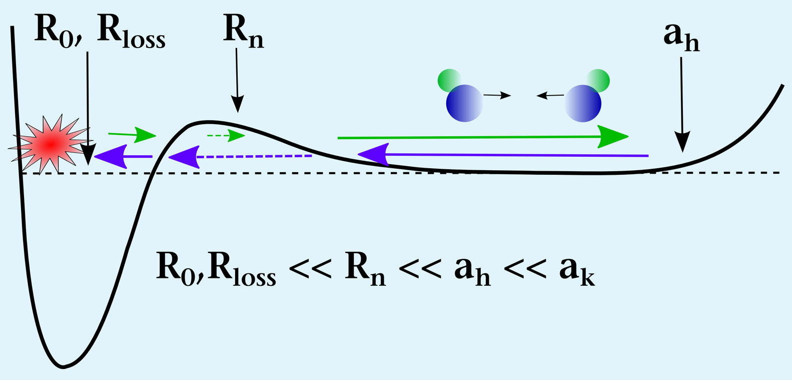
For $r \geq R_0$

$$V(r) = \frac{d^2}{r^3}(1 - 3\cos^2\theta) - \frac{C_6}{r^6}$$

Motion along z is frozen $\mu \ll \hbar\Omega$



Separation of length scales



We define an energy-dependent complex scattering length

$$\tilde{a}_{\ell m}(E) = \tilde{\alpha}_{\ell m}(E) - i\tilde{\beta}_{\ell m}(E) = \frac{1}{ik}\frac{1 - S_{\ell m,\ell m}}{1 + S_{\ell m,\ell m}}.$$

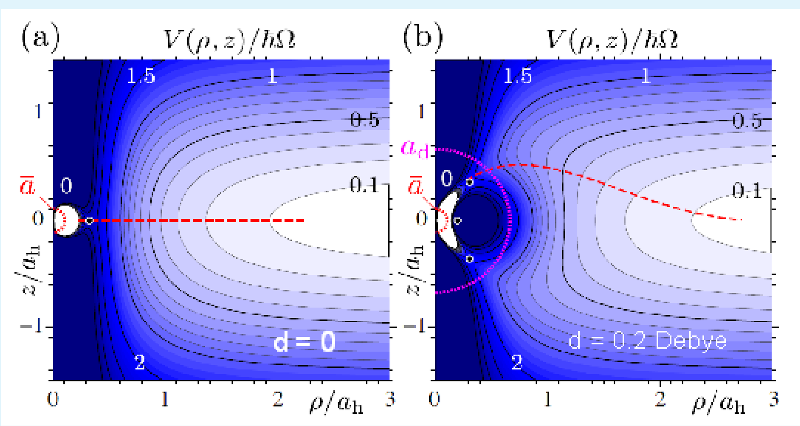
defined in terms of the diagonal elements of S matrix. The elastic $\mathcal{K}^{\rm el}$ and the reactive $\mathcal{K}^{\rm re}$ rate constants can be expressed as

$$\mathcal{K}^{\rm el}_{\ell m}(E) = g\frac{\pi\hbar}{\mu k}\left|1 - S_{\ell m,\ell m}(E)\right|^2 = 2g\frac{hk}{\mu}|\tilde{a}_{\ell m}(k)|^2 f_{\ell m}(k)\,,$$

$$\mathcal{K}^{\rm re}_{\ell m}(E) = g\frac{\pi\hbar}{\mu k}\left(1 - |S_{\ell m,\ell m}(E)|^2\right) = 2g\frac{h}{\mu}\tilde{\beta}_{\ell m}(k) f_{\ell m}(k)\,.$$

Reactive collisions - semiclassical analysis

P-wave centrifugal barrier with and without the electric field



A.Micheli et al., PRL 105, 073202 (2010)

Short and long-range parameters

- Short range WKB approximation

$$\Psi(r) \propto \frac{exp[-i\int^r k(x)dx - i\varphi]}{\sqrt{(k(r))}} - \frac{1-y}{1+y}\frac{exp[i\int^r k(x)dx + i\varphi]}{\sqrt{(k(r))}}$$

- Zero energy solution in the presence of the van der Waals interaction

$$\sqrt{r}R^{(1)}_\ell(r > r_0, E = 0) = J_{2l+1/4}(x)$$

$$\sqrt{r}R^{(2)}_\ell(r > r_0, E = 0) = Y_{2l+1/4}(x)$$

- Expansion around zero connects $s = a/\bar{a}$ with φ

$$s = \sqrt{2}\frac{\cos(\varphi - \pi/8)}{\sin(\varphi + \pi/8)}$$

Collision rate per particle in N dimensions

Reaction rates weakly change across dimensions assuming the same equivalent 3D density.

$$\Gamma^{re}_j \approx \frac{4\pi\hbar}{\mu} g_j L_j(\kappa) \frac{\rho}{a_h^{3-N}}$$

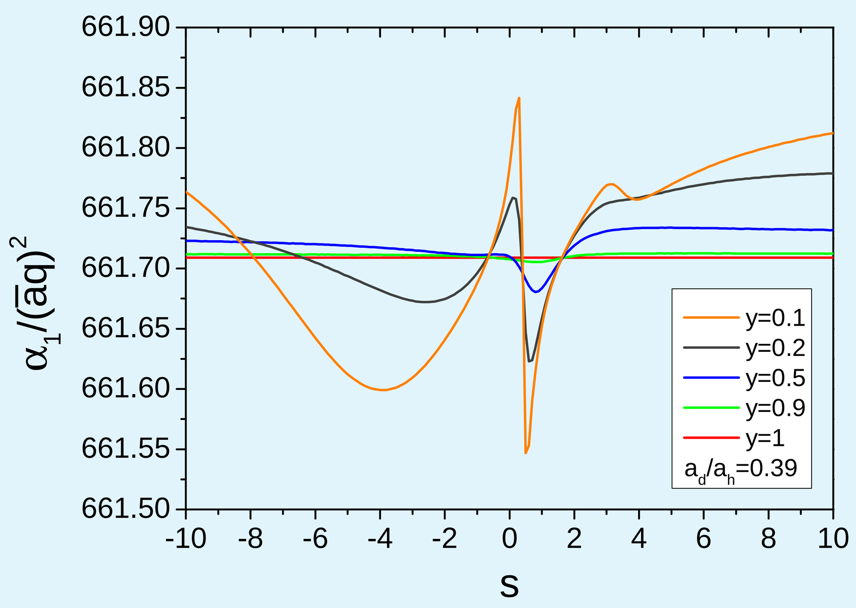
- $j = 0$ ($j = 1$) for even (odd) partial waves
- g - dimensionality, sum over m
- $\frac{\rho}{a_h^{3-N}}$ - equivalent 3D density of a gas (units of cm^{-3})
- $L_j(\kappa)$ - length parameter

N	3D	2D	1D
g_0	$1/\pi$	$2/\pi$	2
g_1	$1/\pi$	$4/\pi$	6

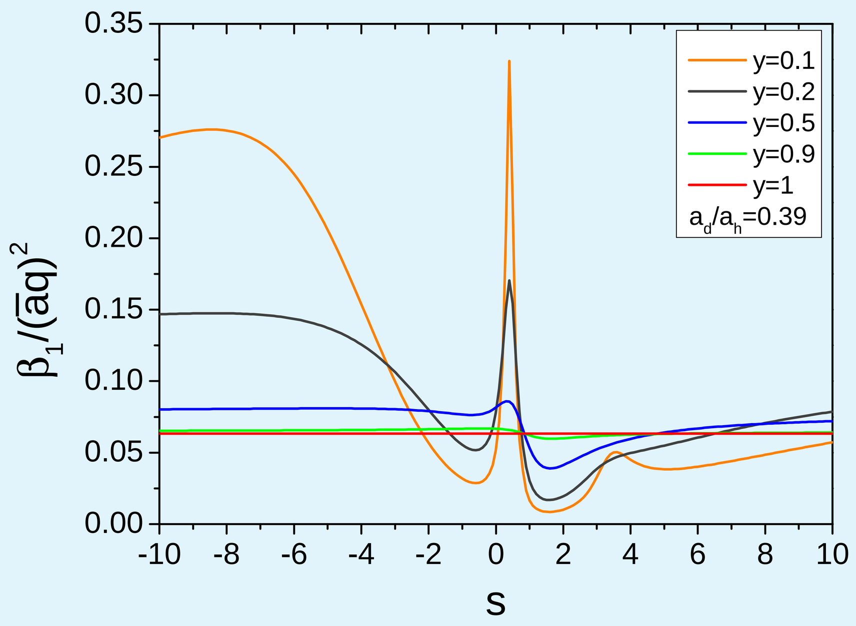
N	3D	2D	1D
L_0	$\bar{a}$	$\sqrt{\pi}\bar{a}$	$2\bar{a}$
L_1	$(k\bar{a})^2\bar{a}_1$	$(3\sqrt{\pi}/2)(q\bar{a})^2\bar{a}_1$	$6(p\bar{a})^2\bar{a}_1$

Resonances

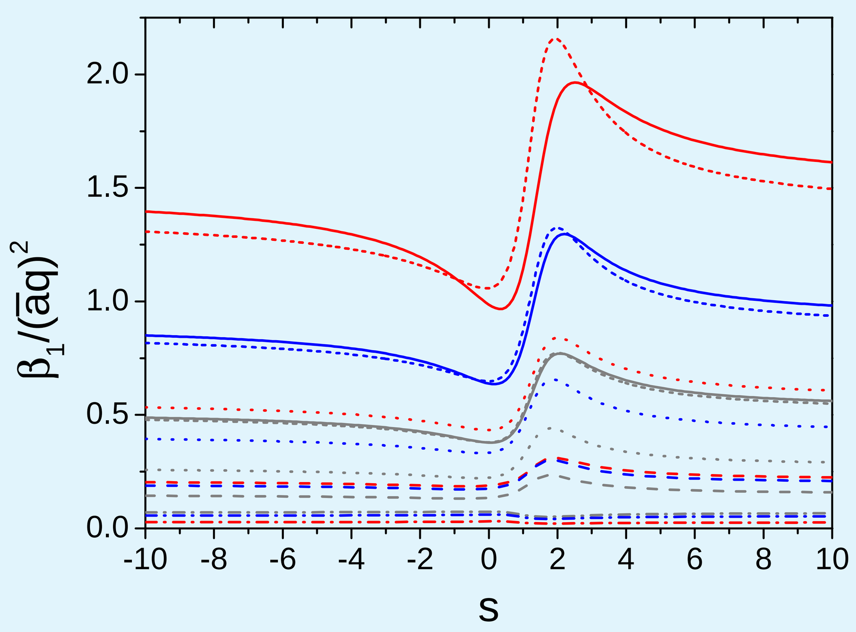
Real part of the complex scattering length for different reaction probabilities and nonzero induced dipole moment



Imaginary part of the complex scattering length for different reaction probabilities and nonzero induced dipole moment



Imaginary part of the complex scattering length for different induced dipole moments and confinement strengths



Red: $a_{HO}/\bar{a} = 1.7$, blue: $a_{HO}/\bar{a} = 3.0$, grey: $a_{HO}/\bar{a} = 5.2$, short dash: analytical approximation for $a_d/\bar{a} = 0$, solid: numerical calculations for $a_d/\bar{a} = 0$, dots: $a_d/\bar{a} = 0.32$, dash: $a_d/\bar{a} = 0.73$, dot-dash: $a_d/\bar{a} = 2.02$.

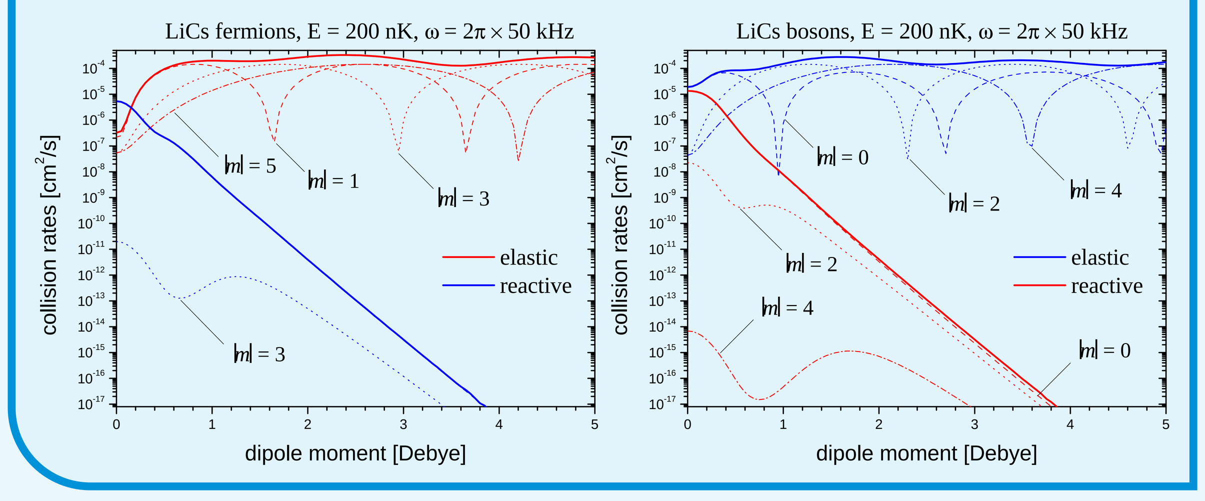
References

[1] A. Micheli, Z. Idziaszek, G. Pupillo, M.A. Baranov, P. Zoller, P.S. Julienne, Phys. Rev. Lett. **105**, pp. 073202 (2010).

[2] K.K. Ni, S. Ospelkaus, M.H.G. de Miranda, A. Pe'er, B. Neyenhuis, J. J. Zirbel, S. Kotochigova, P. S. Julienne, D. S. Jin, and J. Ye, Science **322**, pp. 231 (2008).

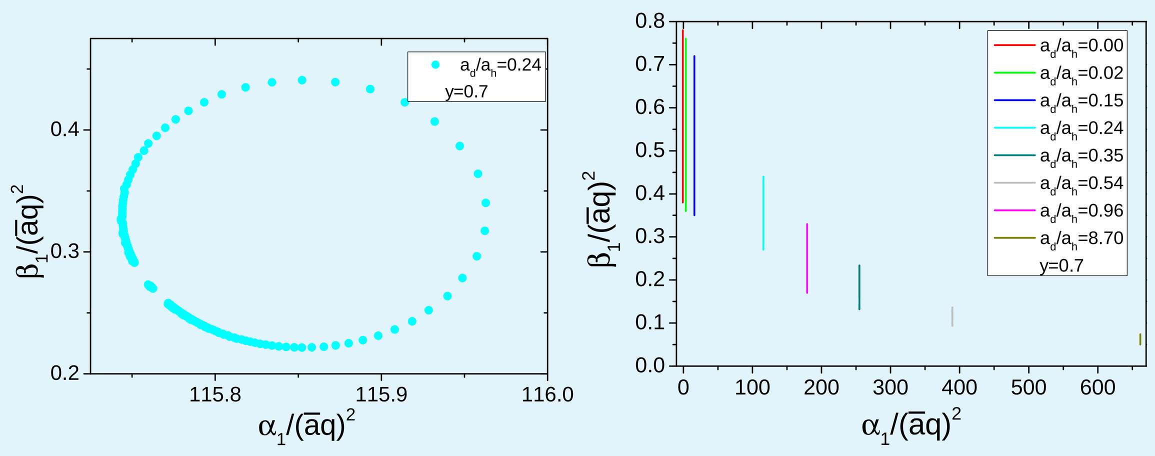
[3] J.G. Danzl, M. J. Mark, E. Haller, M. Gustavsson, R. Hart, J. Aldegunde, J. M. Hutson, H.-Ch. Nägerl, Nature Phys. **6**, 265 (2010).

Full quantum dynamics for y=1

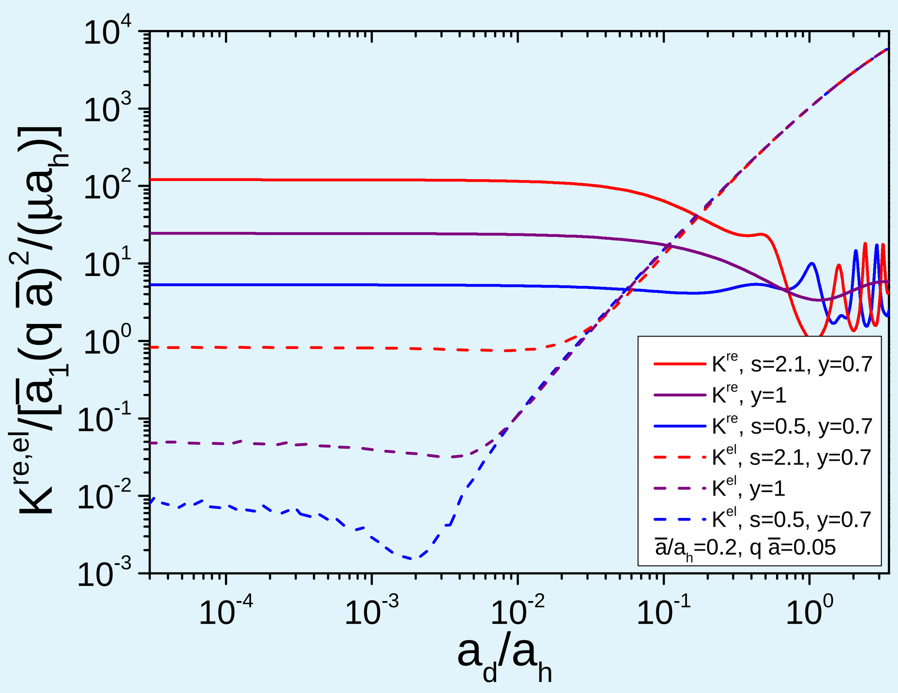


Reactive and elastic rates

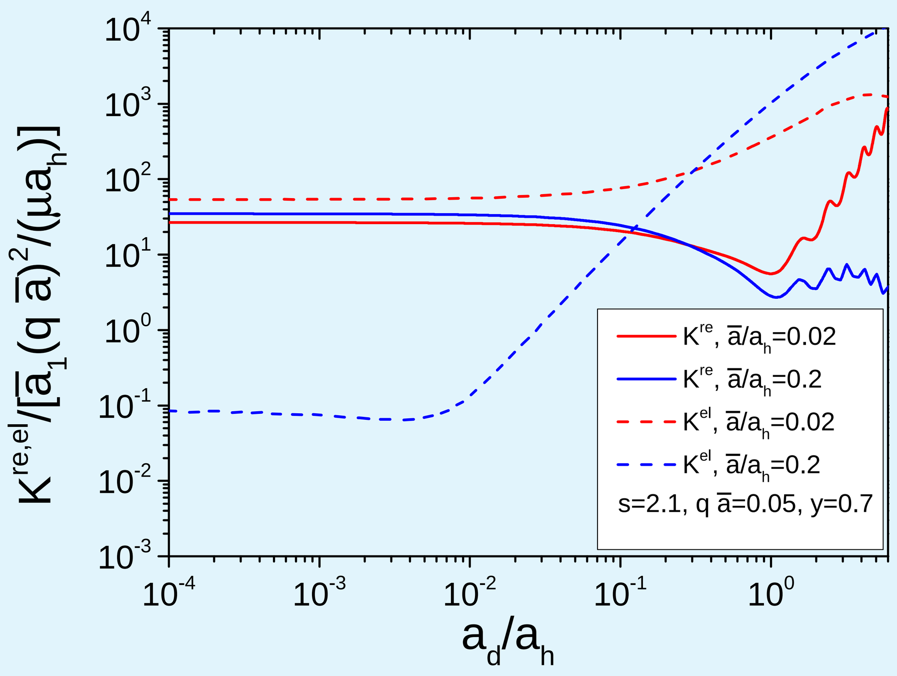
Real and imaginary parts of the complex scattering length



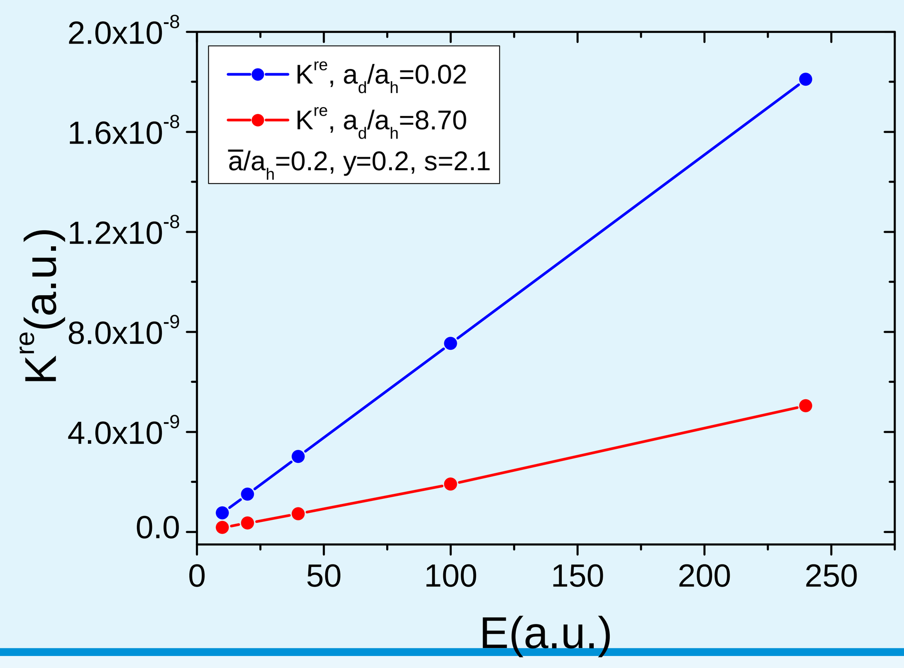
Reactive and elastic collision rates - s-dependence



Reactive and elastic collision rates - trap confinement dependence



Reactive collision rates - energy dependence



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