

Non-universal reactive collisions of polar molecules 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



Reactive collisions - semiclassical analysis

P-wave centrifugal barrier with and without the electric field



Full quantum dynamics for y=1



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)

Interactions of ground-state polar molecules

Van der Waals interaction - isotropic for molecules in a rovibrational ground state



Dipole-dipole interaction - long range and anisotropic



Dipole moment induced by an external 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

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

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

• 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.

Results

Real and imaginary parts of the complex scattering length



Reactive and elastic collision rates - s-dependence





haps and length scales

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



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

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

N	3D	2D	1D	N	3D	2D	1D
$\begin{array}{c} g_0 \\ g_1 \end{array}$	$rac{1/\pi}{1/\pi}$	$2/\pi$ $4/\pi$	$\begin{array}{c} 2\\ 6\end{array}$	$ \begin{array}{c} L_0 \\ L_1 \end{array} $	$\frac{\bar{a}}{\left(k\bar{a}\right)^{2}\bar{a}_{1}}$	$\frac{\sqrt{\pi}\bar{a}}{(3\sqrt{\pi}/2)(q\bar{a})^2\bar{a}_1}$	$\frac{2\bar{a}}{6(p\bar{a})^2\bar{a}_1}$

Complex scattering length

Real and imaginary parts of complex scattering length



Z.I., P.S. Julienne, PRL 104, 113202 (2010)

Reactive and elastic collision rates - trap confinement dependence



Reactive collision rates - energy dependence



$R_0, R_{loss} << R_n << a_h << a_k$

Wave funtion

Real part of the wave function for two bosonic molecules





- Strongest losses for small reaction probability
- Top of the circles: near-treshold bound states for $s = \infty$ (s-wave) and s = 2 (p-wave) resnances

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).

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