Reactive Collisions of Ultracold Polar Molecules in Quasi-1D Geometry

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Abstract

Quantum-defect model gives analytic expressions for elastic and reactive collision rates of ultracold polar molecules interacting by a van der Waals potential [1].
Quasi-two-dimensional and quasi-one-dimensional collisions may be described as well [2]. When the molecules are highly reactive, the rate constants behave universally. When dipole-dipole interaction occurs, numerical methods, such as the adiabatic potentials method, become useful.

Introduction

- we consider ultracold ($T \leq 1\mu K$) $^{40}K^{87}Rb$ molecules (fermionic) in rovibrational and electronic ground state
- at long range, they interact via van der Waals potential
- turning the electric field on polarizes the molecules, causing dipole-dipole interactions; dipole moment d may be controlled by the value of $\vec{E}$
- the molecules are put in external harmonic trap, which may be highly asymmetric and change the geometry of the system;
- they are reactive; chemical reaction introduces losses
- the full hamiltonian of the system confined in two dimensions by the trap:

$$H = -\frac{\hbar^2}{2\mu r}\frac{\partial^2}{\partial r^2}r - \frac{\hbar^2}{2\mu}\hat{L}^2 + \frac{1}{2}\mu\omega r^2\left(\sin^2\theta\sin^2\phi + \cos^2\theta\right) - \frac{C_6}{r^6} + \frac{d^2}{r^3}\left(1 - 3\cos^2\theta\right) + V_{sh}$$

- different partial waves are coupled by this potential
- V_{sh} describes short range physics; the quantum-defect theory parametrizes it by a single parameter $0 \leq y \leq 1$ – probability of chemical reaction
- universal regime: $y \rightarrow 1$, no flux is reflected at short range
- information on reactive and elastic scattering for channel α is provided by the diagonal elements $S_{\alpha\alpha}$ of the S matrix where $S_{\alpha\alpha} = e^{i\delta_\alpha}$, $\delta_\alpha \in \mathbb{C}$
- knowing S, we may calculate the elastic and inelastic rate constants in different dimensions; in 1D

$$K_\alpha^{1D\,el}(k) = g_\alpha\frac{\hbar k}{2\mu}\|1 - S_{\alpha\alpha}\|^2$$

$$K_\alpha^{1D\,re}(k) = g_\alpha\frac{\hbar k}{2\mu}(1 - \|S_{\alpha\alpha}\|)^2$$

where g_α is 1 except for identical particles, where it becomes 2 (this is the case here)
- $K^{1D\,el/re}(n_{1D})^2$ gives us the number of elastic and inelastic scattering acts per unit of time and volume

Adiabatic potentials method

- diagonalise the hamiltonian in spherical harmonics basis, with possibly large L_{max} ($L_{min} = 1$, fermions)
- obtain the equation with effective potential $\lambda(r)$

$$\left(-\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial r^2} + \lambda_n(r)\right)R_n(r) = ER_n(r)$$

- solve it and find the S matrix
- assume that taking the lowest lying curve is sufficient (single channel approximation)

Typical experimental parameters

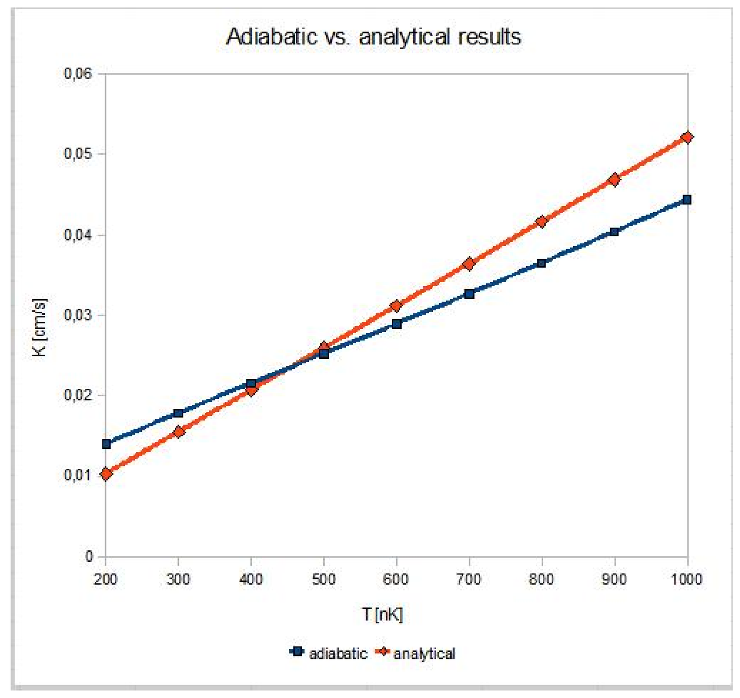
- trap frequency $\omega \approx 2\pi \times 50\,kHz$
- atomic density $n_{3D} \approx 10^{10-12}\,cm^{-3}$; corresponding 1D density $n_{1D} \approx 1-100\,cm^{-1}$
- temperature $T \approx 100 - 1000\,nK$
- KRb dipole moment $d_{perm} = 0,566$ Debye
- KRb van der Waals interaction strength $C_6 = 16130\,a.u.$
- characteristic van der Waals length $R_6 = \frac{2\mu C_6}{\hbar^2}$

Quasi-1D pure van der Waals potential

- to check the accuracy of the method we may apply it to $d = 0$ case
- for $d = 0$ analytic expressions for the rate constants are given [2]:

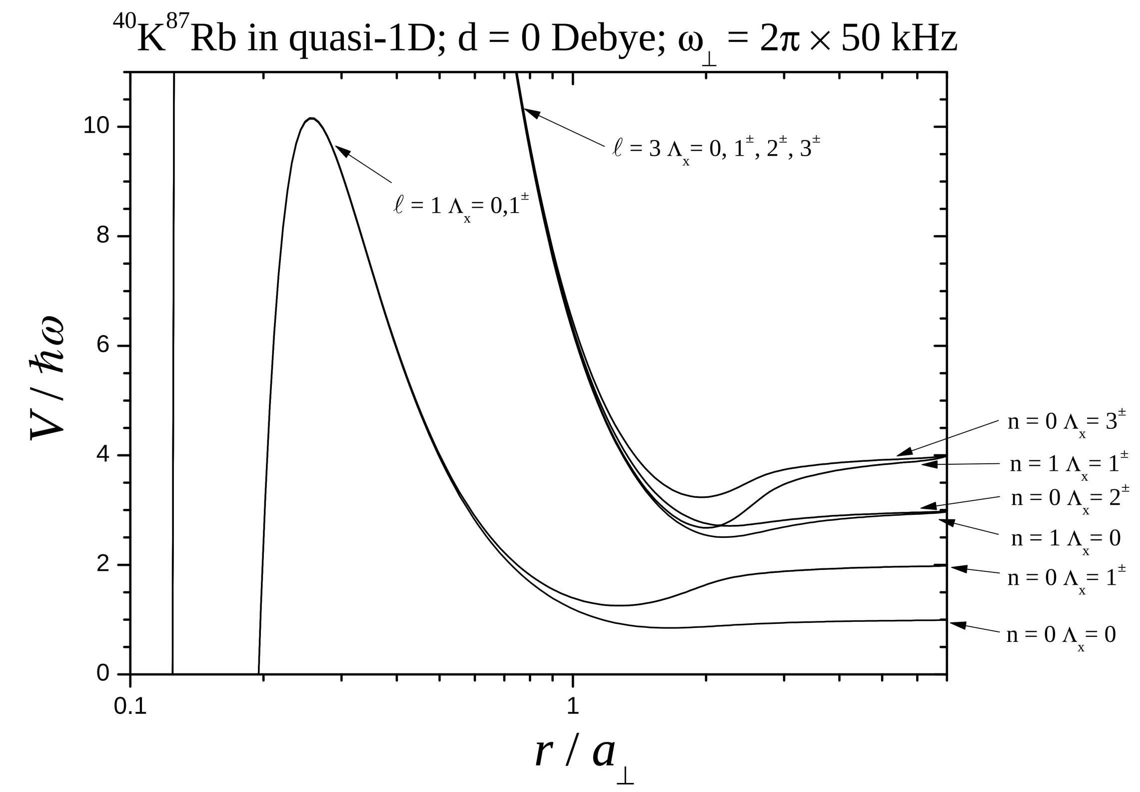
$$K^{re\,1D}(k) = \frac{4\pi\hbar}{\mu}g_1 L_1(k) f_1(k)\frac{1}{a_{HO}^2}$$

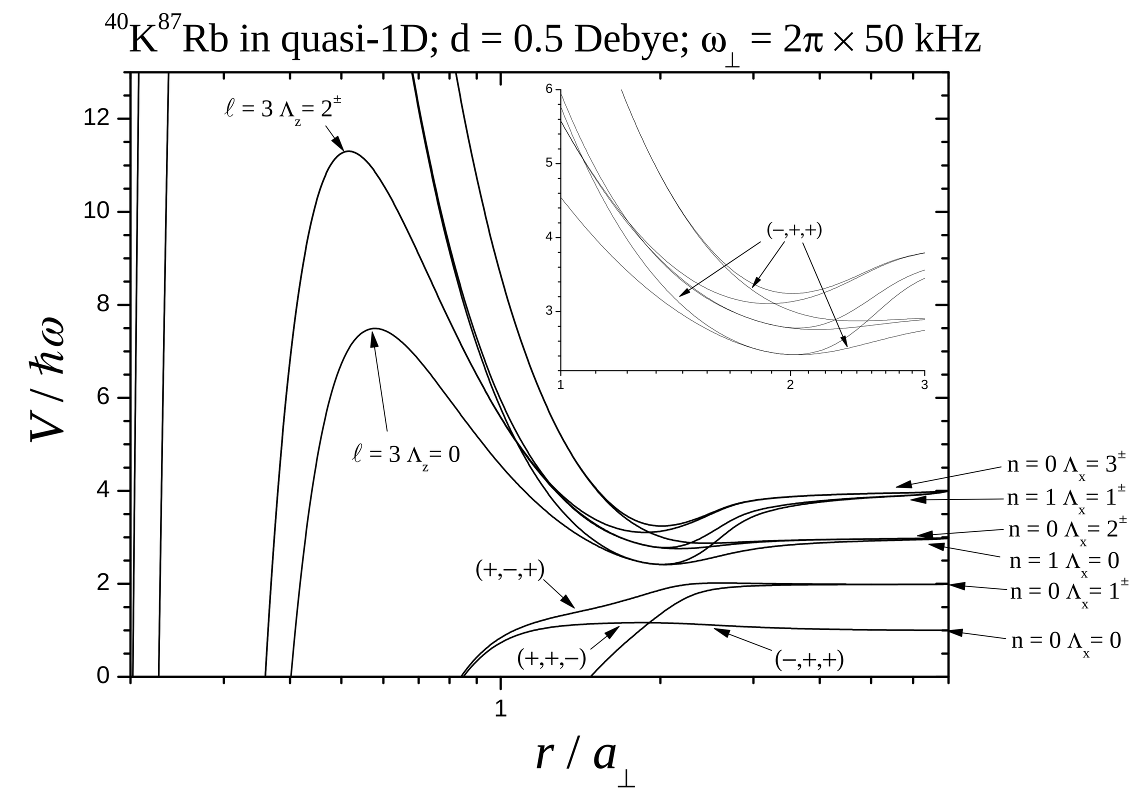
where for quasi-1D $L_1(k) = 6(k\bar{a})^2\bar{a}_1$, $\bar{a}$ and $\bar{a}_1$ being the s-wave and p-wave van der Waals scattering lengths
- this method can be improved by noticing that it works best at temperatures $T \approx 4-5\mu K$ and the rate constants should be linear with respect to T



Adiabatic curves for quasi-1D KRb collisions

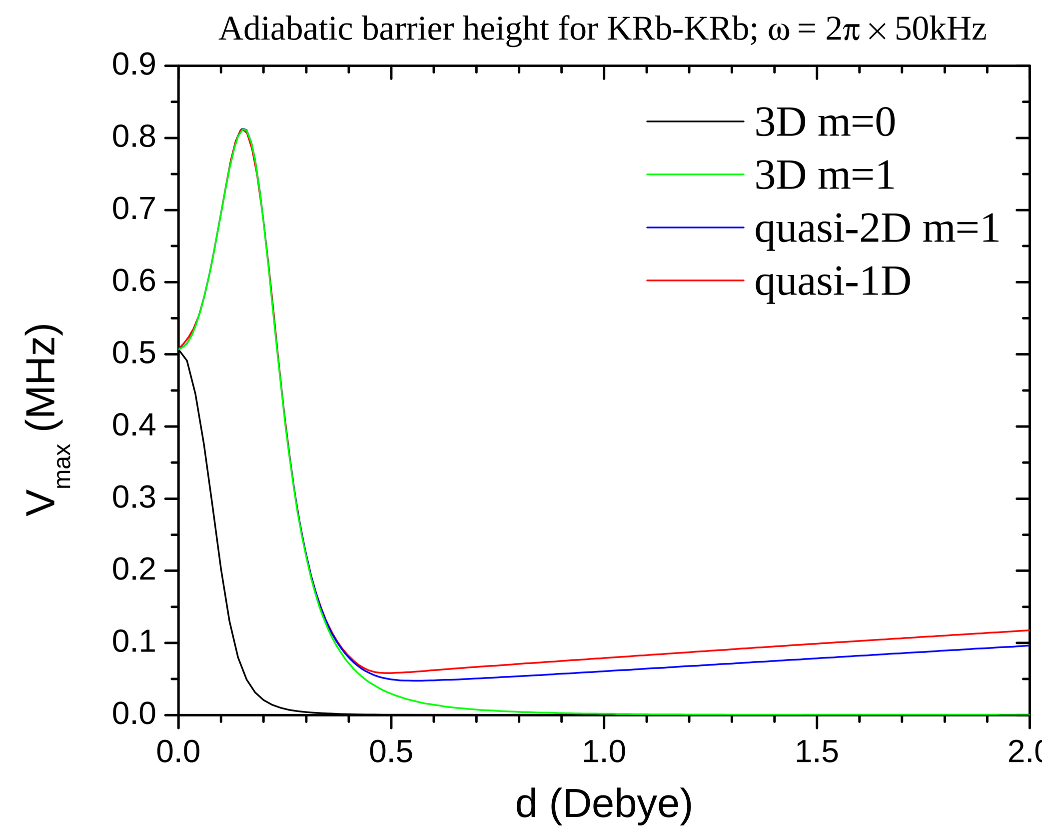
- at short range van de Waals potential dominates
- at long range the harmonic oscillator potential dominates - characteristic ladder structure
- the system exhibits different symmetries at short and long range - at short range the electric field direction is important, at long range the trap direction
- different quantum numbers are valid at different distances:
  - n represents the oscillator levels
  - l represents angular momentum
  - Λ_x and Λ_z stand for the projection of the angular momentum on the x and z axis
- behavior under inversion with respect to x, y and z axis is shown by $+$ and $-$ sign





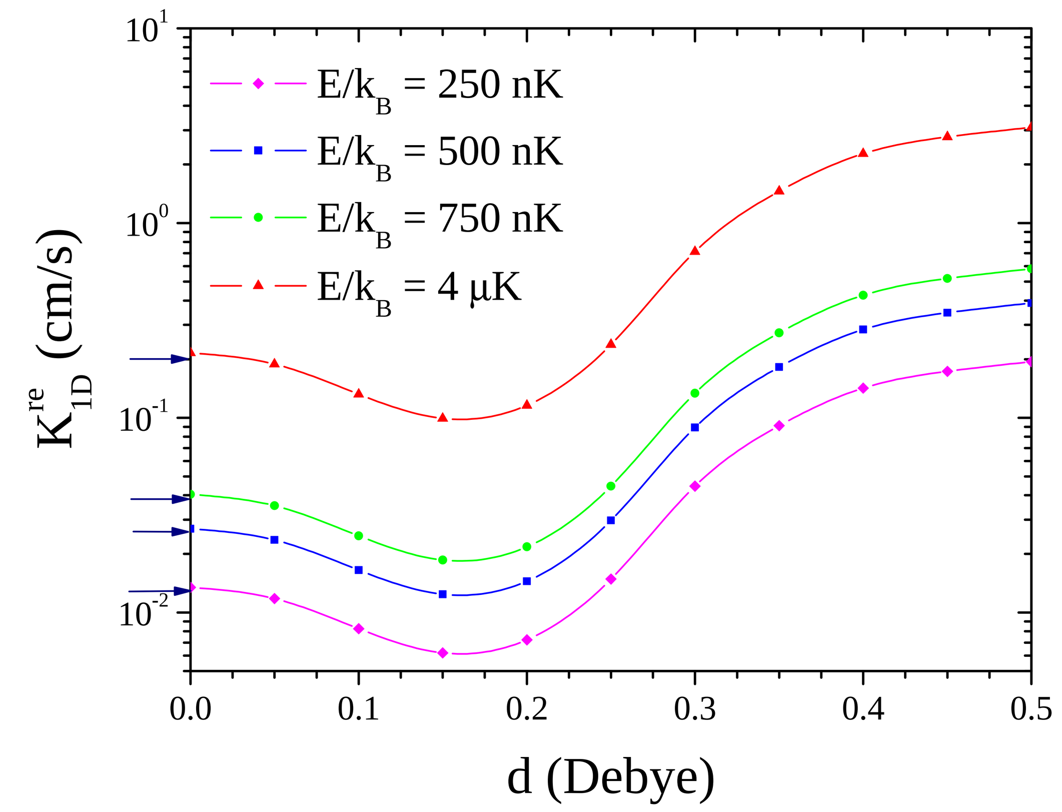
Barrier heights in different dimensions

- it is interesting to compare the barrier heights obtained for systems with different geometries
- it turns out that for low values of d the kind of trap is not so important; the collision is effectively 3D
- this results from domination of van der Waals potential at short range



Loss rate constants for quasi-1D KRb collisions

- arrows point at analytic results for no dipole moment
- for low dipole moment the barrier increases (see the barier heights), so the loss rate decreases



Conclusions and further plans

- quantum-defect theory enables us to get rid of the details of short-range interaction
- adiabatic potentials may provide an estimate for the rate constants possible to be checked experimentally
- aim: full numerical treatment, such as adiabatic bisector method
- aim: multichannel computations

References

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