Controlling 3-body collisions of ultracold dipolar molecules using an electric field

Théomol
Théorie des molécules froides : structure, dynamique, réactivité

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1. Introduction

Nowadays, one of the main goal in ultracold molecular physics is to create quantum degenerate gases of dipolar molecules such as Bose-Einstein condensates or degenerate Fermi gases. Unfortunately, when the molecules start to collide, whether they are chemically reactive or not, a lot of them are lost in the process [1,2,3] in the short range domain. During the last decade, some methods have been developed to reduce those 2-body short-range losses [4,5,6,7]. However, during the evaporative cooling, some 3-body collisions can occur.

## 2. Two-body shielding and simplifications

a) Physical idea of the shielding

If we apply a static electric field on a sample of molecules prepared in their first rotational excited state, we can engineer a long-range potential barrier using the dipole-dipole interaction [5,6,7]. Therefore, the molecules can't come close to each others and quenching collisions (loss + inelastic) highly drop.
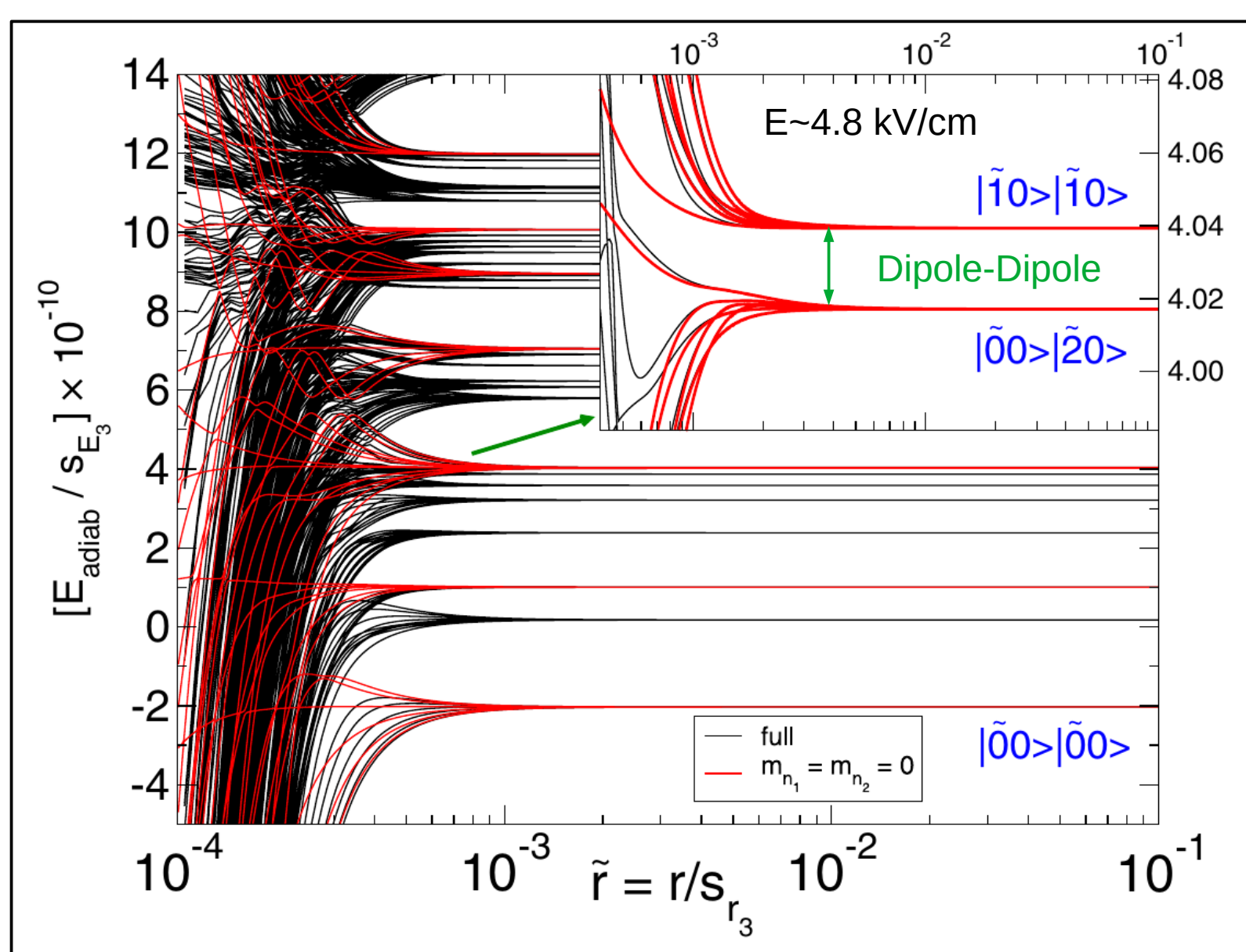
b) Shielding of two-body losses

Very recently, an experimental study at JILA revealed the shielding for KRb molecules in a strong electric field (E=12.67 kV/cm) [8], in very good agreement with previous theoretical predictions [6]. This shielding is also predicted to work for many molecules [7].
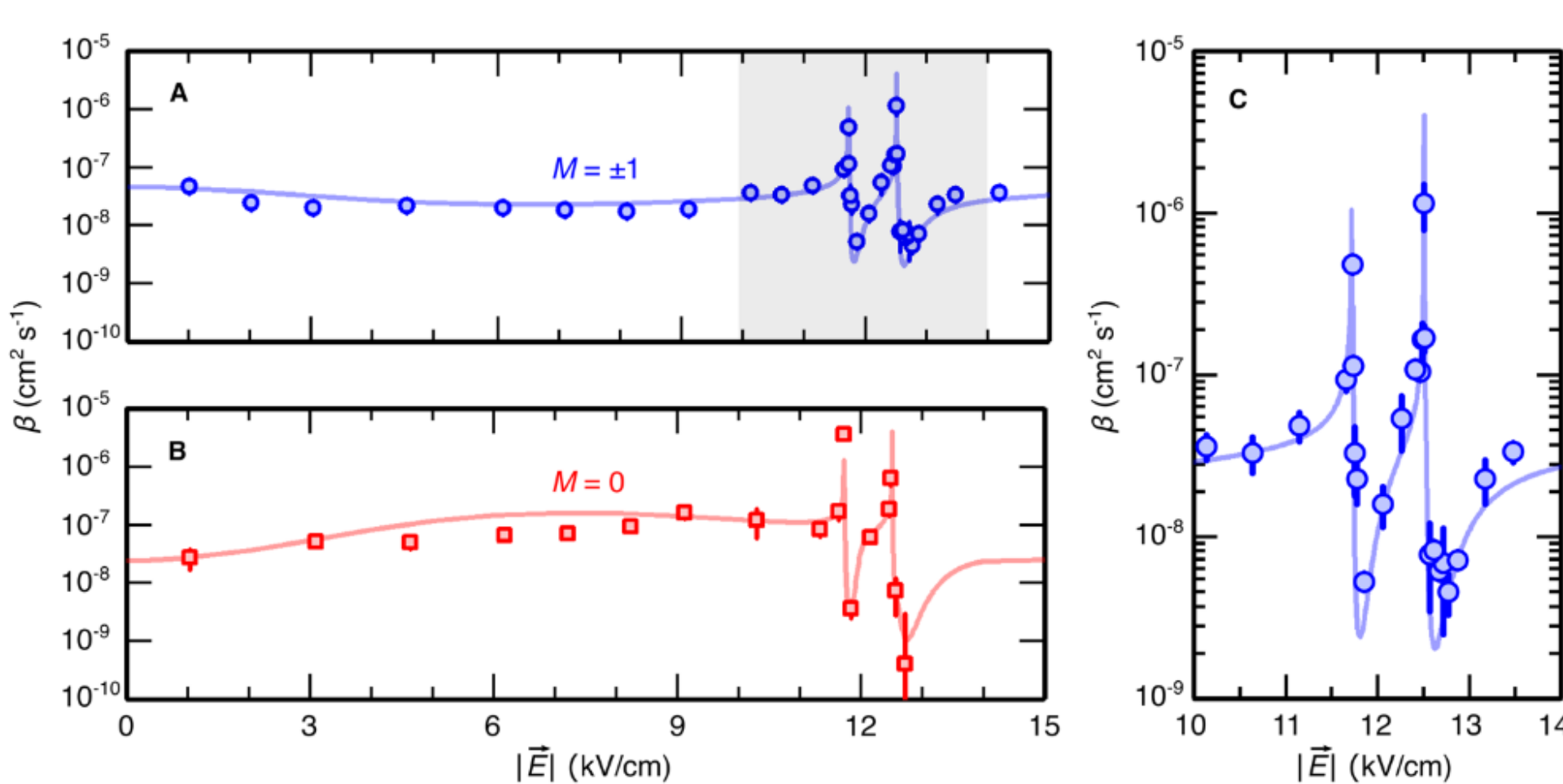
taken from:
K. Matsuda, L. De Marco, J.-R. Li, W. G. Tobias, G. Valtolina, G. Quéméner, J. Ye, arXiv 2009.07461 (2020), accepted to Science

c) Simplification of the problem

We have also demonstrated that we can obtain the same results in the vicinity of the shielding E field if :

(i) We work only with the projection of the rotationnal quantum number m_j=0.
(ii) We work only with the two states $|\tilde{1},\tilde{1}>$ and $|\tilde{2},\tilde{0}>$ where the notations stand for $|\tilde{j}_1, \tilde{j}_2>$.

Then, we don't need to include the full rotational structure, we can reduce the problem to two levels only.

3. Three-body formalism

a) Hyperspherical coordinates

The three-body Hamiltonan in symmetrized hyperspherical coordinates is given by:

Hyper-angle n°1 Form of the triangle
Internal structure 2-level system

$$\hat{H} = -\frac{\hbar^2}{2\mu\rho^5}\frac{\partial}{\partial\rho}\rho^5\frac{\partial}{\partial\rho} + \frac{\hat{\Lambda}^2}{2\mu\rho^2} + V(\rho,\theta,\phi,\alpha,\beta,\gamma,\vec{\rho_1},\vec{\rho_2},\vec{\rho_3})$$

Hyper-radius Size of the triangle
Grand angular momentum operator
Hyper-angle n°2 Arrangements

The main difficulty in using symmetrized hyperspherical coordinates lies in the fact that the grand angular momentum operator contains singularties (also called Eckart singularties) :

$$\frac{\hat{\Lambda}^2}{2\mu\rho^2} = \frac{-8\hbar^2}{\mu\rho^2}\left[\frac{\partial^2}{\partial\tilde{\theta}^2} + \cot\tilde{\theta}\frac{\partial}{\partial\tilde{\theta}} + \frac{1}{2(1+\cos\tilde{\theta})}\frac{\partial^2}{\partial\phi^2}\right]$$
$$+ \frac{1}{\mu\rho^2}\left[\frac{J_x^2}{(1-\cos\tilde{\theta}/2)} + \frac{J_y^2}{(1+\cos\tilde{\theta}/2)}\right]$$
$$+ \frac{J_z^2}{(1+\cos\tilde{\theta})}\right] + \frac{4\sin\tilde{\theta}/2}{\mu\rho^2(1+\cos\tilde{\theta})}J_z\frac{\hbar}{i}\frac{\partial}{\partial\phi}. \quad (5)$$

To threat carefully those singularties, we follow the procedure developed by B.Kendrick et al. [9] and adapt it for 3 identical particules. Therefore, we expand the 5D surface functions in terms of an adapted orthonormal basis functions given by :

$$\Phi_t^{JMp}(\omega;\rho_\xi) = \frac{1}{\sqrt{2\pi}}\sum_{l=\mu}^{l_{max}}\sum_{m=-m_{max}}^{m_{max}}\sum_{\Omega=-\Omega_{max}}^{\Omega_{max}} b_t^{lm\Omega}$$
$$\times d_{\mu,\nu}^l(\tilde{\theta})e^{im\phi}\tilde{D}_{\Omega M}^J(\alpha,\beta,\gamma),$$

With :
- J the total angular momentum in the BF
- Ω the projection of J along the BF z axis
- M the projection of J along the SF Z axis
- p the parity quantum number

The $d_{\mu,\nu}^l(\tilde{\theta})$ functions can be expressed in terms of Jacobi polynomials and the indices (μ,ν) are carefully selected to treat the singularities.

4. Numerical procedure

a) Hybrid method

For the θ operators :

We use the DVR (discrete variable representation) method. The quadrature points θ_i and weights w_i are obtained via a Gauss-Legendre quadrature.

For the φ operators :

We use the FBR (finite basis representation) for the Φ operators. The 1D numerical quadrature :

$$^{ab}\bar{V}_{mm'}^{ii'} \equiv \int_{-\pi}^{+\pi}\frac{d\phi}{2\pi}e^{-im_a\phi}V(\rho,\theta,\phi,\alpha,\beta,\gamma)e^{im_b'\phi}\delta_{ii'}$$

are obtained using a Fourier quadrature.

b) Sequential diagonalization truncation

To reduce the total size of the Hamiltonian, we perform a SDT [9] (Sequential diagonalization truncation). The SDT is crucial for keeping the total matrix size reasonable.

The idea is to solve for each value of θ_i a 1D Hamiltonian (in Φ) and to keep only the 1D eigenvector Q_n^i for which the associated eigenvalues E_i satisfy an energy cutoff condition. Finally, each block (i,i') of the 5D Hamiltonian in the 1D representation is reduced using the transformation :

$$^{5D}\hat{\mathbf{H}}_{\Omega\Omega'ii'}^{jMp} = (\mathbf{Q}^i)^T {}^{5D}\bar{\mathbf{H}}_{\Omega\Omega'ii'}^{jMp}\mathbf{Q}^{i'}$$

c) Identical particle permutation

To treat properly the Eckart singularties, we cannot symmetrize our basis functions before the diagonalization.

In order to obtain solutions which are either symmetric or antisymmetric under the permutations we have constructed and used the operator $\sigma_\pm$:

$$\sigma_\pm = \frac{1}{6}(1 \pm \mathcal{P}_{12} + {}^\pm\mathcal{P}_{23} + {}^\pm\mathcal{P}_{31} \pm \mathcal{P}_{123} \pm \mathcal{P}_{321})$$
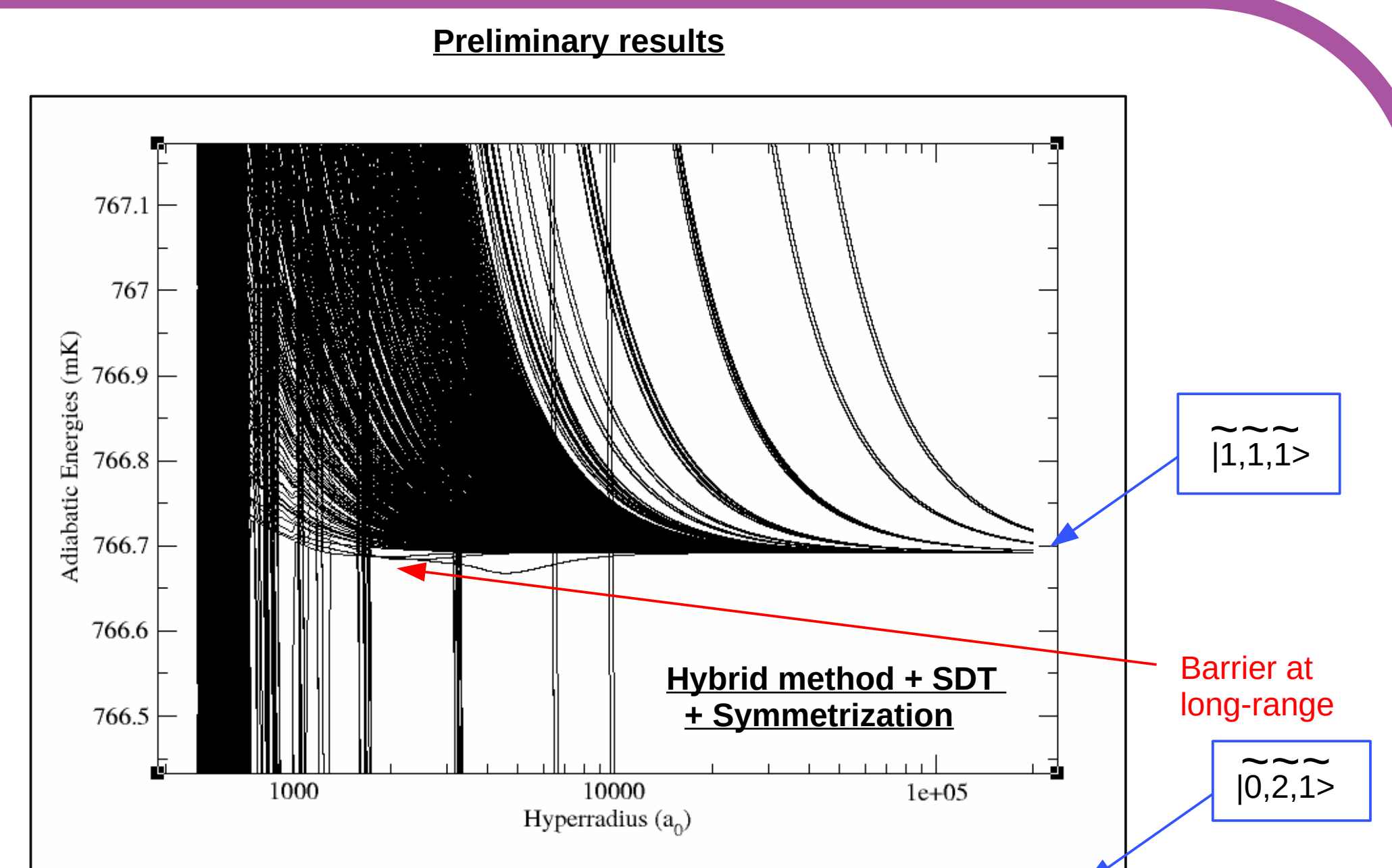
5. Adiabatic energies

To obtain the different observables (cross section, rate coefficient), we must solve the usual set of coupled equations given by :

$$\left[\frac{\partial^2}{\partial\rho^2} + \frac{2\mu}{\hbar^2}E\right]\psi_{it}^{ipq}(\rho)$$
$$= \frac{2\mu}{\hbar^2}\sum_{t'}\langle\Phi_t^{Mpq}|H_c|\Phi_{t'}^{Mpq}\rangle\psi_{it'}^{pq}(\rho)$$

The angular 5D surface functions are obtained by solving :

$$\left[\frac{\hat{\Lambda}^2}{2\mu\rho_\xi^2} + \frac{15\hbar^2}{8\mu\rho_\xi^2} + V(\rho_\xi,\tilde{\theta},\phi)\right]\Phi_t^{Mpq}(\omega;\rho_\xi)$$
$$= \mathcal{E}_t^{pq}\Phi_t^{JMpq}(\omega;\rho_\xi).$$

Adiabatic energy

Preliminary results

Due to the dipole-dipole-dipole interaction, the states $|\tilde{1},\tilde{1},\tilde{1}>$ and $|\tilde{0},\tilde{2},\tilde{1}>$ are highly coupled. The usual attractive s-wave is in this case repulsive at large distance. Then, we expect that the 3B short-range losses must be reduced.

More investigations are under way to complete our study.

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