Parametrizing ultracold complex-mediated reactions using statistical assumptions

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In the ultracold regime, the influence of long-range (LR) interactions becomes paramount, leading in extreme cases to the paradoxical idea of *universality*: the result of the collision depends exclusively on the LR behaviour and not on the short-range chemical interactions. In this regard, recently proposed LR parametrization procedures are very appealing: from the sole knowledge of the interactions at LR, and by fitting experimental data, these models are able to predict nonmeasured values and to provide some insight into the underlying interactions. In particular, the approach by Jachymski and coworkers[1], based on multichannel quantum-defect theory (MQDT), provides analytical expressions which have been already used to parametrize experimental data in a few systems. Alternatively, and this is the aim of the work I will present, the availability of accurate theoretical scattering calculations may allow to test the MQDT model by fitting the obtained scattering quantities using the formulas of the model. Indeed, in the past few years we have theoretically studied the collisions i) $D^+ + H_2$ (j=0) → $H^+ + HD$ [2] and ii) $S(^1D) + D_2$(j=0) → SD + D [3], which are complex-mediated processes, using a modified hyperspherical quantum reactive scattering method[4]. We have thus obtained abundant scattering data. The considered collision energy ranges from the *ultracold regime*, where only one partial wave is open, up to the *Langevin regime*, where many of them contribute. An overall good agreement (in both systems) is found between the theoretical calculations and the existing experiments in the *Langevin region* (where they are already available). Regarding the behaviour in the *ultracold domain* I will show how the theoretical scattering results, characterized through the definition of the scattering length, can be discussed in terms of the MQDT model.

This has allowed to test the model for two different LR behaviours: $\sim R^{-4}$ in process i) and $\sim R^{-6}$ in process ii). We conclude that, for complex mediated reactions, one of the parameters of the model can be related to a well-known statistical factor. This provides a way to estimate from first principles (and working on the more reliable Langevin energy region) a parameter which characterizes the behaviour at ultracold energies.

References

[1] K. Jachymski, M. Krych , P. S. Julienne and Z. Idziaszek, Phys. Rev. Lett. 110, 213202 (2013); K. Jachymski, M. Krych , P. S. Julienne and Z. Idziaszek, Phys. Rev. A 90, 042705 (2014); Z. Idziaszek and P. S. Julienne, Phys. Rev. Lett. 104, 113202 (2010)

[2] M. Lara, P. G. Jambrina, J.-M. Launay and F. J. Aoiz, Phys. Rev. A 91, 030701(R), Rapid Communication (2015); M. Lara, P. G. Jambrina, J.-M. Launay and F. J. Aoiz, J. Chem. Phys. 143, 204305 (2015)

[3] M. Lara, S. Chefdeville, P. Larregaray, L. Bonnet, J.-M. Launay, M. Costes, C.Naulin and A. Bergeat, J. Phys. Chem. A, D120, 5274 (2016).

[4] M. Lara, F. Dayou, and J. M. Launay, Phys. Chem. Chem. Phys. 13, 8359 (2011)