Invited talk

Quantum resonances in cold collisions

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Quantum resonances in low-energy collisions are a sensitive probe of the intermolecular forces. They dominate the final quantum state distribution even for strong and highly anisotropic interactions, as recently observed for Feshbach resonances populated by Penning ionization of dihydrogen colliding with a metastable rare gas atom[1]. For such a small collision complex, full quantum scattering calculations can be carried out[1]. The theoretical predictions for the cross section involve then only the approximations made when constructing the potential energy surface (PES). Changes in the shape of the PES thus translate directly into modifications of the cross sections. This can be used to to improve calculated PES, starting from the experimental data[2]. Conversely, one can also ask by how much the experimental resolution of measured cross sections must improve in order to unambiguously discriminate predictions derived from different levels of advanced ab initio electronic structure theory[3]. Such discrimination is equivalent to resolving the intermediate resonances governing the reaction dynamics, on top of the initial and final states.

[1] Margulis et al., Science **380**, 77 (2023)
[2] Horn *et al., Science Advances* **10**, eadi6462 (2024)
[3] Horn *et al.*, arXiv:2408.13197