Contribution ID: **41** Type: **Talk**

Rovibrational energy levels of the hydrogen molecule and its isotopologues from relativistic nonadiabatic calculations

Wednesday 12 June 2024 16:30 (25 minutes)

The energy of a molecular rovibrational level is theoretically derived from several components, including nonrelativistic, relativistic, quantum electrodynamics, and more. When it comes to a light molecule such as hydrogen or its isotopologue, the nonrelativistic quantum electrodynamics (NRQED) can accurately describe this energy using an expansion in powers of the fine structure constant $E(\alpha) = \sum_{i=2}^{\infty} \alpha^i \, E^{(i)}$.
The component that is least accurate in this expansion is limiting the accuracy of the total energy. Precise predictions for hydrogen molecular levels require the treatment of electrons and nuclei on an equal footing. While nonrelativistic theory has been effectively formulated this way, calculations of relativistic and quantum electrodynamic effects with well-controlled numerical precision are much more challenging. In this communication, we report extending this nonadiabatic method to the relativistic correction term, $E^{(4)}$. The four-body nonadiabatic James-Coolidge wave function is applied to evaluate the expectation value of the Breit-Pauli Hamiltonian. The main obstacle encountered in this approach is the need for a whole class of integrals resulting from combining relativistic operators with exponential basis functions. Such integrals have been successfully evaluated, and new results of the relativistic correction will be reported. The convergence analysis indicates that the numerical uncertainty of this correction is of the order of 10^{-7} cm^{-1}. Similar to the nonrelativistic component, the uncertainty of the relativistic term is negligible enough to eliminate it from the overall uncertainty budget. An essential aspect of the newly developed method is its capability of handling arbitrarily high rotational angular momentum without significant loss in accuracy. With the new relativistic results, the achieved accuracy is limited only by the uncertainty of the quantum electrodynamic effects, $E^{(n)}, n \geq 5$.

Several recent experimental studies have revealed a minor discrepancy between the most precise theoretical and experimental data. This inconsistency offers an opportunity for further advancements in the field. It will be examined in light of new nonadiabatic relativistic calculations, providing insight into further improvements in the current theory.

Authors: KOMASA, Jacek (Adam Mickiewicz University in Poznań, Poland); PACHUCKI, Krzysztof (University of Warsaw)

Presenter: KOMASA, Jacek (Adam Mickiewicz University in Poznań, Poland)

Session Classification: Session 6