Use of the Feshbach-Fano R-matrix approach to the calculation of the discrete state and the coupling for solution of resonance nuclear dynamics in diatomics.

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The Feshbach-Fano (FF) projection-operator formalism represents particularly useful tool for investigation of the resonant phenomena in quantum theory. Within this approach, a single square integrable wave function (the discrete state $|\varphi_d\rangle$) is associated with each resonance. Once the linear functional subspace $\mathcal{Q}$ spanned by the discrete states is defined, the FF formalism provides a detailed and intuitive understanding of the resonant processes. The major drawback of the the formalism is the need for *a priori* definition of the subspace $\mathcal{Q}$. Its choice is usually evident in the case of Feshbach resonances but can be difficult in case of shape resonances.

Nestmann [1] has proposed a systematic approach to determining $\mathcal{Q}$, the Feshbach-Fano R-matrix (FFR) method. The FFR method provides the discrete state, its position and the associated coupling terms to the background continuum. The method has been successfully applied to several molecules in the equilibrium geometry of the ground state (e.g. N_2, C_3H_6 and N_2O). More recently, detailed analysis of the FFR method was done on the ground of potential scattering [2] with the aim to determine the strengths and the limits of the method and to establish it as a general tool for investigation of the resonant phenomena. The FFR method can be applied to any system which can be studied via the R-matrix method. Once the standard R-matrix calculations are done the FFR procedure represents computationally very cheap way how to treat the results and obtain all necessary information about the resonances.

One of the most striking features of the FFR method is that it can be used directly to construct the so-called nonlocal resonance model (NRM) [3] of the nuclear dynamics of the low-energy electron-molecule collisions. Nonlocal resonance theory yields cross sections for vibrational excitation, dissociative electron attachment and associative electron detachment. It was used successfully to describe low-energy collisions of electrons with molecular hydrogen and hydrogen halides. The FFR method was used to provide model for the electron-F_2 scattering [4] and recently also for electron-Cl_2 scattering. Those systems are essential in plasma and laser physics and are also of great atmospheric and environmental interest. It is the lack of accurate data on inelastic electron scattering, both experimental and theoretical, that motivated our study.

References

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