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Секция 3. Математическое моделирование в фундаментальных и прикладных исследованиях

RESUMMATION OF DIVERGENT PERTUBATION SERIES. APPLICATION TO CALCULATIONS OF VIBRATIONAL ENERGY SPECTRUM OF DIFFERENT MOLECULES.

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In this research high-order Rayleigh-Schrödinger perturbation theory (RSPT) is applied to the calculation of the vibrational energy spectrum of HDO, H_2O and H_2CO molecule within a simple model of quartic force field. It is well-known that perturbation series generally diverge. Our calculations confirm the rapid divergence of RSPT series. As it is shown on graph 1, 100-th term of RSPT series is approximately equal to 10 raised to power 42.
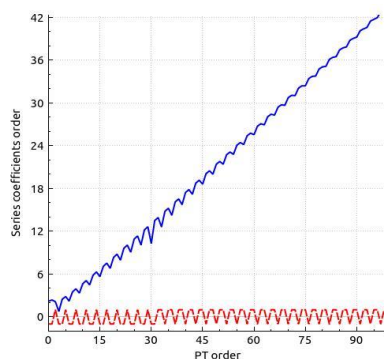

Figure 1. The order of RSPT series. (001110) H_2CO state

Despite the bad behavior of RSPT series, this approach turns out to be promising for studying polyatomic molecules. The RSPT series expansions (even divergent) exhibit hidden properties that indicate at the possibility of their computation by making use of the resummation methods for divergent series such as high-order Hermite-Pade approximants. Graph 2 shows true significant digits of calculated energy level for (001110) H_2CO state.
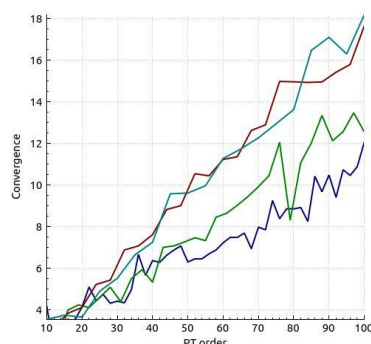

Figure 2. Convergence of Pade-Hermite methods. (001110) H_2CO state

The aim of this study is to probe these methods on the models, which are close to real polyatomic molecules and reflect their specific properties, yet relatively simple for numerical implementation. Numerical analysis of the high-order RSPT series for the H_2CO vibrational states have been performed using high-order Hermite-Pade approximants. All calculations have shown that for convergent and divergent RSPT series Hermite-Pade approximants are in a good agreement with the variational calculations.