EULER SERIES TRANSFORMATION METHOD IN THE TRIATOMIC MOLECULES VR ENERGY LEVEL CALCULATIONS

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The Effective Hamiltonian (EH) method is accurate and efficient when applied to the ground or low energy vibration molecular states. But in the case of highly excited states it can not be used because of the strong divergence of series involved in the EH. Early there was several papers dealing with this problem, the papers [1-3] are only examples.

The Generalized Euler Transformation (GET) is known to be efficient method for summing of slowly convergent or divergent series, it was already used for solving of several quantum problems [4]. The GET allows one to use easy the additional information about the energy levels the series to be sum to. In the case of molecule vibration – rotation states this additional information can be obtained from solutions of the model problems.

In this contribution the results of application of the GET to the series summation in the EH method are presented. It is shown that original series can be transformed to form of functional series that is equivalent to its partial summation. The exactly solvable Pöshle – Teller and Kratcer oscillator were used as approximants for the case of diatomic and $XY_2(C_{2V})$ - type molecules. It is also shown that transformed series has the butter convergent properties, than the initial ones. Also the GET for the series of two variables is derived.

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[3]. V.I.Starikov, S.A.Tashkun, Vl.G.Tuyterev Description of Vibration-Rotation Energies of Nonrigid Triatomic Molecules Using the Generating Function Method // J.Mol.Spectrosc. 1992, v.151 p.130-147
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