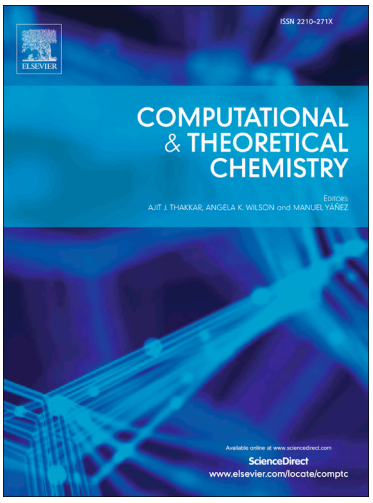

Analytic calculation of ground state splitting in symmetric double well potential

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PII: S2210-271X(18)30209-3
DOI: https://doi.org/10.1016/j.comptc.2018.05.021
Reference: COMPTC 2807

To appear in: *Computational & Theoretical Chemistry*

Received Date: 24 May 2018
Revised Date: 30 May 2018
Accepted Date: 31 May 2018

Please cite this article as: A.E. Sitnitsky, Analytic calculation of ground state splitting in symmetric double well potential, *Computational & Theoretical Chemistry* (2018), doi: https://doi.org/10.1016/j.comptc.2018.05.021

Analytic calculation of ground state splitting in symmetric double well potential

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Abstract

The exact solution of the one-dimensional Schrödinger equation with symmetric trigonometric double-well potential (DWP) is obtained via angular oblate spheroidal function. The results of stringent analytic calculation for the ground state splitting of ring-puckering vibration in the 1,3-dioxole (as an example of the case when the ground state tunneling doublet is well below the potential barrier top) and 2,3-dihydrofuran (as an example of the case when the ground state tunneling doublet is close to the potential barrier top) are compared with several variants of approximate semiclassical (WKB) ones. This enables us to verify the accuracy of various WKB formulas suggested in the literature: 1. ordinary WKB, i.e., the formula from the Landau and Lifshitz textbook; 2. Garg's formula; 3. instanton approach. We show that for the former case all three variants of WKB provide good accuracy while for the latter one they are very inaccurate. The results obtained provide a new theoretical tool for describing relevant experimental data on IR spectroscopy of ring-puckering vibrations.

Key words: Schrödinger equation, confluent Heun's function, Coulomb spheroidal function.

1 Introduction

Quantum particle transfer in a double-well potential (DWP) is one of the main processes in reaction rate theory. Proton transfer in hydrogen bonds is a notable example of the above general case. The latter takes place in the most important biological molecules such as proteins (participating in some enzymatic reactions [1], [2]) and DNA (arguably participating in the occurrence of

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