Antonio J C Varandas, J Laser Opt Photonics 2018, Volume 5
DOI: 10.4172/2469-410X-C3-029

On the born-oppenheimer (BO) approximation and beyond

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The most fundamental approximation in quantum mechanics has been proposed just 90 years ago by Born and Oppenheimer to justify treating separately the motions of the electrons and nuclei in molecular systems. Using four fermions, each one described by a single Gaussian orbital, we have of the BO approximation as a function of their masses. After addressing it, its topological implications are noted and a generalization (GBO) suggested to take them into account. The result of the BO approximation, Schrödinger equations emerge: One describes the motion of the electrons with the nuclei positions kept frozen, the other so obtained. Converged solutions of both equations are then required. Because this implies using unaffordable basis sets or grids, the problem of extrapolating the results obtained with small bases/grids to their limits is next examined. As for the electronic problem, the focus will be on how to extrapolate the energies to the in mind large-sized molecules. Regarding the nuclear counterpart, we will examine how to approximate quantum cross sections and rate constants by extrapolating the quantum reaction probabilities computed for the J=0 case to any value of the total angular momentum J. For this, quasiclassical trajectory calculations will be used for the extrapolation, as justified from the well-established correspondence principle. Amongst illustrative examples, we consider the energetics and dynamics of small carbon clusters. In particular, it will be shown how four conical intersections arising in C3 due to combined Jahn- pseudo-Jahn-Teller interactions can complicate the modeling of its ground-state energy surface. used to tackle also be briefly addressed, other ongoing research. Time permitting, the extrapolation of atom+diatom probabilities calculated with time-dependent code in hyperspherical coordinates will be presented. Prospective remarks conclude the talk.

Biography

Antonio JC Varandas obtained a degree in Chemical Engineering from University of Porto (1971), and a Ph.D. in Theoretical Chemistry from University of Sussex (1976). After graduation, joined the Department of Chemistry of Universidade de Coimbra, where is Full Professor since 1988. He has recently been appointed distinguished Professor at Qufu University (China). Published more than 400 papers, co-authored the first monograph in Molecular Potential Energy Functions (Wiley 1984), and 2 others in Portuguese. Received awards: Prize Artur Malheiros for Physics and Chemistry of Lisbon Academy of Sciences (1985); Prize Silva of Portuguese Chemical Society (2001); Prize Stimulus to Excellence of Portuguese Ministry of Science, Innovation and High Studies (2004). Serves the editorial board of Journal of Theoretical and Computational Chemistry amongst others. recognition abroad. In 2006 was elected a corresponding member of Academia de Ciências de Lisboa and, in 2014, of EU Academy of Sciences.

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