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"Perturbations in vibrational diatomic spectra: Exact factorization of the wave function"

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The Born-Oppenheimer (BO) approximation is an essential tool in the study of Molecular processes. The wave function is written as a product of an electronic factor (the wave function of the electrons with frozen nuclei) and a factor describing the nuclear motion with the nuclear-dependent electronic energy as a potential. However a condition is necessary for the scheme to be valid: The electronic energies must be well separated. Many situations do not fulfill this condition. For instance if two electronic potentials cover the same energy range, this may affect the positions of the vibrational energies calculated separately for the two states. The BO method consists in writing the total wave function as a combination of Born-Oppenheimer products. An example is the study of the perturbations in the N_2 vibrational spectrum. It has been suggested recently [1,2] that even in cases where the traditional BO approach is failing, the exact molecular wave function can still be written as the product of an electronic wave function depending parametrically on nuclear positions by a nuclear factor. We use the supposedly exact wave function for the treatment of the perturbations in N_2 to determine the ingredients necessary to write the wave function of the new scheme, that is with a single product [3]. One should insist here that this does not mean solving the basic equations of the "exact" BO scheme. However this proves the existence of this function. We then use these functions to build the potentials which determine the vibrational states. The wave equation with these potentials is solved to show that we recover the correct energies.

References

- [1] L. S. Cederbaum, J. Chem. Phys. 138, 224110 (2013).
- [2] N. I. Gidopoulos and E. K. U. Gross, Phil. Trans. R. Soc. A372, 20130059 (2014).
- [3] R. Lefebvre, J. Chem. Phys. 142, 074106 (2015).

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