**How to make the Born-Oppenheimer approximation exact: A fresh look at potential energy surfaces and Berry phases**

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The Born-Oppenheimer approximation is among the most fundamental ingredients of modern Theoretical Chemistry and Condensed-Matter Physics. This approximation not only makes calculations feasible, it also provides us with an intuitive picture of chemical reactions. Yet it is an approximation, and some of the most fascinating phenomena, such as the process of vision, photovoltaic dynamics, as well as phonon-driven superconductivity occur in the regime where the Born-Oppenheimer approximation breaks down. To tackle such situations one has to face the full Hamiltonian of the complete system of electrons and nuclei. We deduce an exact factorization of the full electron-nuclear wavefunction into a purely nuclear part and a many-electron wavefunction which parametrically depends on the nuclear configuration and which has the meaning of a conditional probability amplitude. The equations of motion for these wavefunctions lead to a unique definition of *exact* potential energy surfaces as well as *exact* geometric phases [1], both in the time-dependent and in the static case. We discuss a case where the exact Berry phase vanishes although there is a non-trivial Berry phase for the same system in Born-Oppenheimer approximation, implying that in this particular case the Born-Oppenheimer Berry phase is an artifact [2]. In the time-domain, whenever there is a splitting of the nuclear wavepacket in the vicinity of an avoided crossing, the exact time-dependent surface shows a nearly discontinuous step [3]. This makes the classical force on the nuclei jump from one to another adiabatic surface, reminiscent of Tully surface hopping algorithms. Based on this observation, we propose novel mixed-quantum-classical algorithms [4] which provide a rather accurate description of decoherence.

[1] A. Abedi, N.T. Maitra, E.K.U. Gross, Phys. Rev. Lett. **105**, 123002 (2010).

[2] S.K. Min, A. Abedi, K.S. Kim, E.K.U. Gross, Phys. Rev. Lett. **113**, 263004 (2014).

[3] A. Abedi, F. Agostini,Y. Suzuki, E.K.U. Gross, Phys. Rev. Lett. **110**, 263001 (2013).

[4] S.K. Min, F. Agostini, E.K.U. Gross, Phys. Rev. Lett. **115**, 073001 (2015).