THEORIEKOLLOQUIUM &
Sonderkolloquium SFB 1242

Freitag, den 05.07.19 um 12:00 in MC 351

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MPI Halle

Potential Energy Surfaces and Berry Phases beyond the Born-Oppenheimer Approximation

Some of the most fascinating phenomena in physics and chemistry, such as the process of vision, exciton dynamics in photovoltaic systems, as well as phonon-driven superconductivity occur in the so-called non-adiabatic regime where the coupled motion of electrons and nuclei beyond the Born-Oppenheimer approximation is essential. The Born-Oppenheimer approximation is among the most fundamental ingredients of condensed-matter theory. It not only makes computations feasible, it also provides us with an intuitive picture of chemical reactions. Yet it is an approximation. To go beyond it is notoriously difficult because one has to start from scratch, i.e. from the complete Hamiltonian of interacting electrons and nuclei. We deduce an exact factorization of the full electron-nuclear wave function into a purely nuclear part and a many-electron wave function which parametrically depends on the nuclear configuration and which has the meaning of a conditional probability amplitude. The equations of motion for these two wave functions provide an ideal starting point to study non-adiabatic phenomena: Light-induced isomerization, the appearance of decoherence, and the molecular Berry phase without invoking the Born-Oppenheimer approximation have been described very successfully. To tackle non-adiabatic phenomena in solids, such as laser-induced phase transitions, the equations of motion of the exact factorization are “density-functionalized”, leading to a set of Kohn-Sham equations for electrons and phonons.

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