

Mechanisms of decoherence, an ab-initio perspective

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Decoherence, i.e. the phenomenon that quantum systems tend to lose their quantumness due to interactions with other degrees of freedom, is ubiquitous. Most prominently, decoherence is responsible for preventing genuine quantum computing at useful scales to this day. It appears desirable to develop a genuine ab-initio theory of decoherence that allows one to make reliable predictions of decoherence times for a given material, and to gain a microscopic understanding of decoherence with the goal to ultimately find ways to control it. For electrons, the principal source of decoherence is the non-adiabatic interaction with nuclear degrees of freedom, i.e. with an “environment” that is strongly coupled to the electronic subsystem. In the paradigm of electronic-structure theory where electrons move in the static Coulomb potential of clamped nuclei, decoherence is absent. In this lecture, a universally applicable approach to the description of decoherence and, in particular, to the prediction of decoherence times will be presented. We start from the exact factorization [1] of the full electron-nuclear wave function into a purely nuclear part and a correlated many-electron wave function which parametrically depends on the nuclear configuration and which has the meaning of a conditional probability amplitude. This gives the exact electron-nuclear wave function an adiabatic-like appearance while decoherence is fully contained in this wave function. The equations of motion for the two factors are then used to calculate measures of decoherence, such as the purity, from first principles, allowing us to identify different mechanisms of decoherence.

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