

Institutsseminar

Path Integral Simulations

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Statistical mechanics of many-body quantum systems is fundamental to our understanding of physical reality and of central importance for emerging quantum technologies. In this context, Feynman's imaginary time path integral (PI) has proven to be a powerful tool by providing a framework for calculating thermal properties of molecules within the canonical ensemble from a purely classical system. In my talk, I will review how this mapping from the original quantum system to the classical one, described by a so-called classical isomorphic Hamiltonian, is achieved.

Further, I will demonstrate how electronic degrees of freedom, which are typically neglected in this classical isomorphic Hamiltonian, can be included, thus allowing for the description of molecular systems where multiple thermally accessible low-lying excited states are present.

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16:15 Uhr

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