Variational approaches to quantum crystals

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Variational approaches to describe the ground state wave functions of quantum liquids and solids [1] have become a powerful tool to obtain a quantitative description of condensed matter systems fully ab-initio, e.g. without any external fitting paramters. Hydrogen at high pressure and low temperatures [2] provides an ideal playground to explore a very rich phase diagram in a system where the Hamiltonian is exactly known and experiments are difficult: electrons and protons, interacting among each other only via the bare Coulomb forces. Within the last years, deep neural network and iterative backflow ansätze have provided the most accurate description in the electron gas model [3]. There, the protonic charge is uniformly smeared out over the system focusing the description on pure electronic quantum and correlation effects. In this thesis, we want to extend this variational description based on machine-learning methods on hydrogen beyond the Born-Oppenheimer approximation to provide an accurate description of the anharmonic quantum crystal formed by the hydrogen atoms or molecules.

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