

Quantum Physics, Course KFY/7KVAF

WS 2022/2023

Theme 9: Born-Oppenheimer approximation

1. Derive the Schrödinger equation for nuclei motion if you assume the Born-Oppenheimer approximation. [Hint: assume a known solution of the electronic Schrödinger equation, expand the total wavefunction using the basis of the electronic Hamiltonian wavefunction, use that expansion in the global Schrödinger equation, and neglect the terms including the change of electronic wavefunction.]
2. Show the difference in dissociation energies of homonuclear molecules H_2 , HD, and D_2 . Calculate differences in dissociation energies if the wavenumber of 4395 cm^{-1} corresponds to H_2 vibration. [Hint: Assume you know the solution of the electronic Schrödinger equation and consider that the electronic contribution of molecular energy is given just by electrostatic interaction and therefore is independent of isotope mass.]