Abstract

Description of the first principle of the hydrogen molecule: dynamical and statistical properties and interaction with the environment

In my dissertation, I analyzed the physical properties of a diatomic molecule, which is the simplest possible, but non-trivial physical system that can be very accurately described. I determined the dynamic and statistical properties as well as the interaction of the molecule with its environment.

In the first part of the dissertation, I used ions for the analysis, which could consist of two identical or diferent atoms, where the nuclei of atoms together with the electrons of the inner shells were atomic cores with an effective charge, and the bonding in the ions was carried out via one electron. The electron Hamiltonian energy parameters were calculated using the variation method. Chaotic behavior was observed in the system with an appropriately selected input. The charge distribution of the cores and their mass did not qualitatively affect the value of the Lapunov exponents in the amplitude-frequency parameter space.

During further research, I used a hydrogen molecule. In the Hubbard Hamiltonian, which is used to determine the energy states of a molecule, I included all two-body interactions. In order to analyze the statistical properties of the system of hydrogen molecules, I used the molecular diluted gas model. I determined the entropy, total energy and specific heat of systems that contain more than three molecules. I made the calculations using non-extensive statistics. After the analysis, it turned out that a noticeable deviation of the results from classical statistical physics occurs for a system containing more than a thousand molecules.

In the last part of the work, I analyzed the electronic properties of the hydrogen bridge in molecular nanojunctions with platinum, gold and copper electrodes. To describe the electronic system of the bridge, I used the non-Hermitian Hamiltonian invariant to the PT-symmetry, which allowed me to analyze the inuence of the electrodes on the interesting physical properties of the bridge. I determined the values of the force acting on the molecule in each of the examined nanojunctions, the energetic parameters of the Hamiltonian as well as the electronic states of the bridge and its energetic structure.

Domagalska