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Variational Calculations for Hydrogen in Introductory Solid State

JAVIER HASBUN, University of West Georgia — Molecular hydrogen is very important in the introductory solid state physics course because it is used as one of the simplest molecular realistic models where bonding and anti-bonding takes place. This system is one of the first examples in which interactions among the ions and the electrons is incorporated realistically. To this end, we approach the system starting from the hydrogen atom. Here we introduce a numerical approach that reproduces the known analytic result for the ground state. The idea is to expand the hydrogenic wavefunction in terms of Gaussians (four of them) with variational parameters. As the parameters are varied the numerical approach stops when the energy is a minimum. The scheme is consistently extended through the ionized hydrogen molecule and the reproduction of its analytically known ground state energy result. We finally culminate with the hydrogen molecule using a variational wavefunction, a la Hartree, and proceed to repeat the process with a particular flavor of a Hartree-Fock wavefunction [1] and finally obtaining a hydrogen molecule total ground state energy of -31.10 eV with a bond length of 1.37 Bohr radius.

[1] "Atomic and Electronic Structure of Solids," Efthimios Kaxiras (Cambridge UP, Cambridge UK, 2003).

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