



Center for
Molecular
Modeling

Computational Materials Physics



Department of
Materials Science
and Engineering

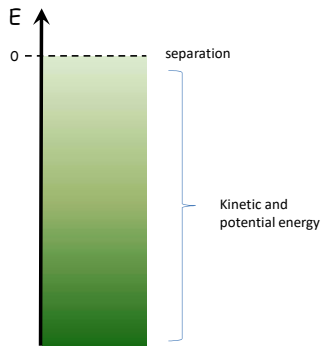
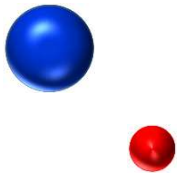
quantum numbers and the state of a system

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<http://molmod.ugent.be>
<http://www.ugent.be/ea/dmse/en>
my talks on Youtube: <http://goo.gl/P2b1Hs>

Quantum numbers

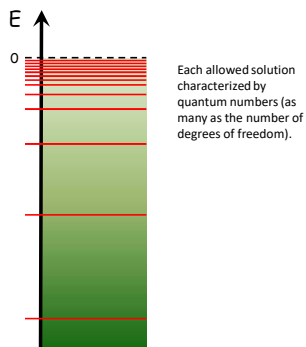
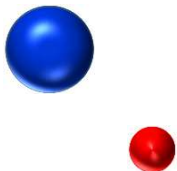
H-atom (classical)



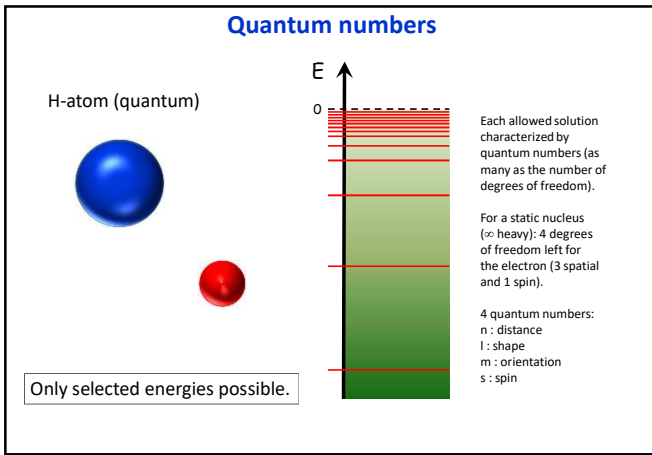
All energies possible.

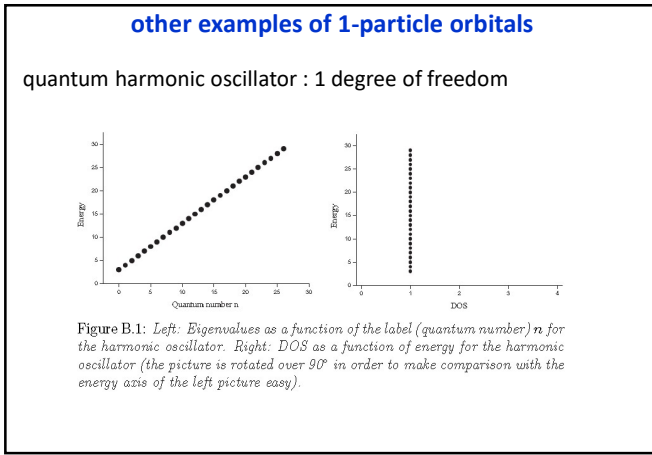
Quantum numbers

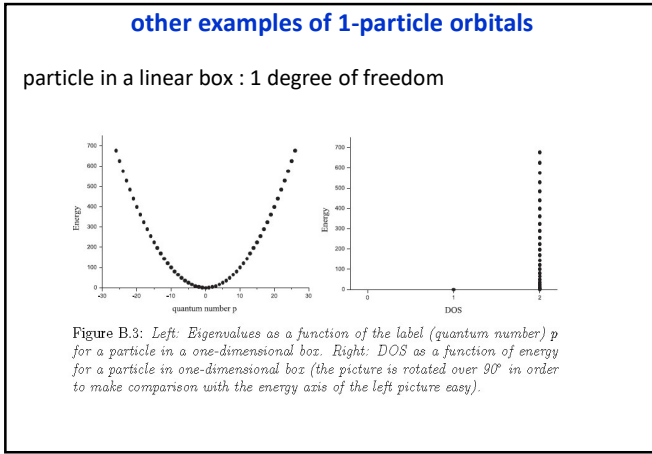
H-atom (quantum)



Only selected energies possible.







other examples of 1-particle orbitals

H-atom : 3(+1) degrees of freedom

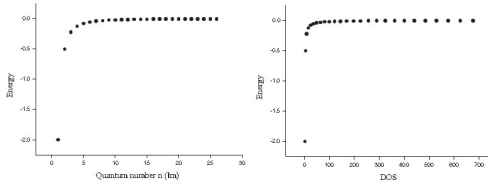
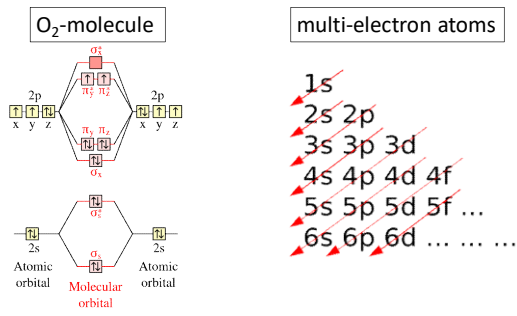


Figure B.2: Left: Eigenvalues as a function of the label (quantum number) n for a free one-electron atom (states with the same n but a different l and m are degenerate). Right: DOS as a function of energy for a free one-electron atom (the picture is rotated over 90° in order to make comparison with the energy axis of the left picture easy).

more electrons and/or more nuclei

often the picture of electrons (with spin) that gradually fill single particle orbitals (with 3 quantum numbers) remains valid :



more electrons and/or more nuclei

crystal ?
