Computational Materials Physics

Center for Molecular Modeling

Department of Materials Science and Engineering

all-electron methods vs. pseudopotential methods

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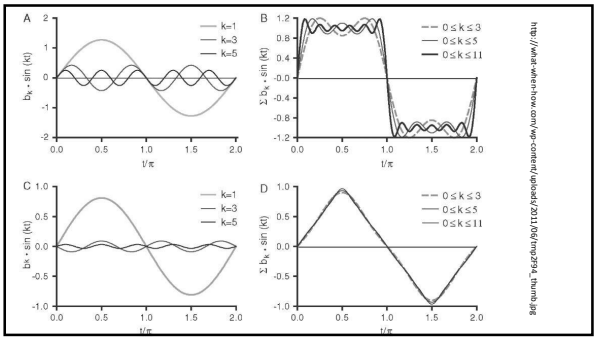
http://molmod.ugent.be
http://www.ugent.be/ea/dmse/en
my talks on Youtube: http://goo.gl/P2b1Hs

lemma 1

decomposition of a function
in a sum over basis functions :

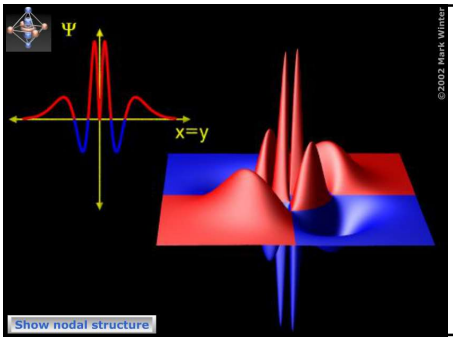
the larger the qualitative difference
between original function and basis functions,
the more basis functions will be needed



lemma 2

the time required to perform a DFT calculation
increases rapidly
with the number of basis functions that are used.

all-electron methods

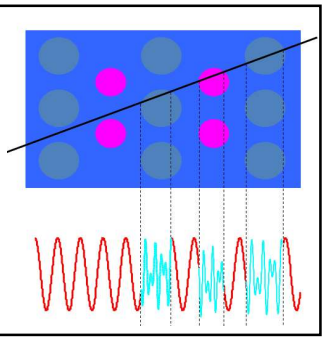


all-electron methods

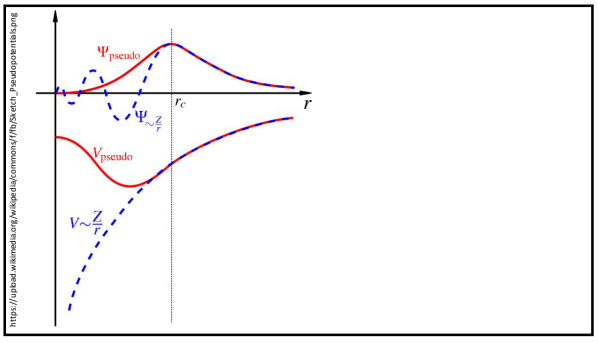
➔ limit the number of basis functions
by selecting basis functions
that look similarly
to how the result will look like

all-electron methods

LAPW
APW+lo
LMTO
(some) local orbitals



pseudopotential methods



pseudopotential methods

➔ limit the number of basis functions by solving a hypothetical crystal that looks like the original one only in interesting regions (=far away from the nuclei)

pseudopotential methods

plane waves
PAW
(some) local orbitals