practical considerations on DFT

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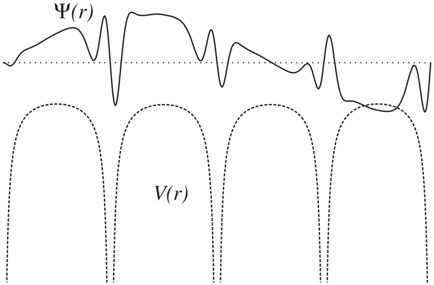
1. Basis functions

2. PAW formalism

Basis functions

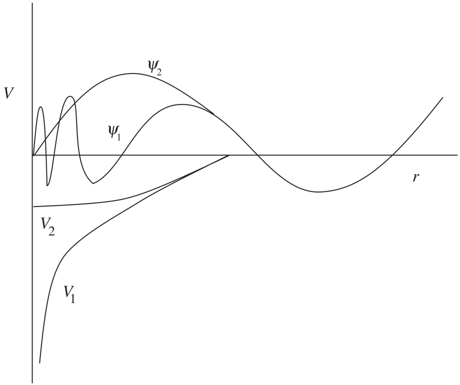
- For solving the SGL we have to choose basis states in which we write down the Bloch Hamiltonian. These can, e.g., be atom-centered/localized or plane waves.
- Plane waves have the advantage that evaluating the matrix is extremely easy.
- complete and orthogonal.
- **But** due to rapidly oscillating wavefunctions close to the cores we need too many wave function: impractical!



: from Jos Thijssen, Computational Physics

Pseudo potentials

- Introduce pseudo potential V_2, which differs from the real potential V_1 close to the cores.
- Smoother wavefunctions means less plane waves needed!



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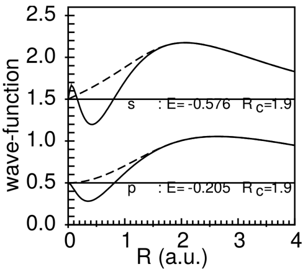
PAW formalism

- Linear transform from rapidly oscillating wavefunctions to smooth pseudo wavefunctions



$$|\Psi\rangle = \mathcal{T}\,|\tilde{\Psi}\rangle = \left(1 + \sum_i \tau_i\right)|\tilde{\Psi}\rangle = |\tilde{\Psi}\rangle + \sum_i (|\phi_i\rangle - |\tilde{\phi}_i\rangle)\langle\tilde{p}_i|\tilde{\Psi}\rangle$$

$\mathcal{T}$: Transformation different from identity only inside augmentation sphere.
$|\tilde{\Psi}\rangle$: pseudo wavefunction.
i: sum over atomic sites, angular momentum, augmentation channels (reference energy ε_i).
$|\phi_i\rangle$: physical partial waves (solution of Schrödinger equation for isolated atom).
$|\tilde{\phi}_i\rangle$: pseudo partial waves matching $|\phi\rangle$ outside augmentation sphere. smooth and differentiable.
$|\tilde{p}_i\rangle$: projector functions $\langle\tilde{p}_i|\tilde{\phi}_j\rangle = \delta_{ij}$.