Introduction to Density Functional Theory

a short PhD course
February 2026
by

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and
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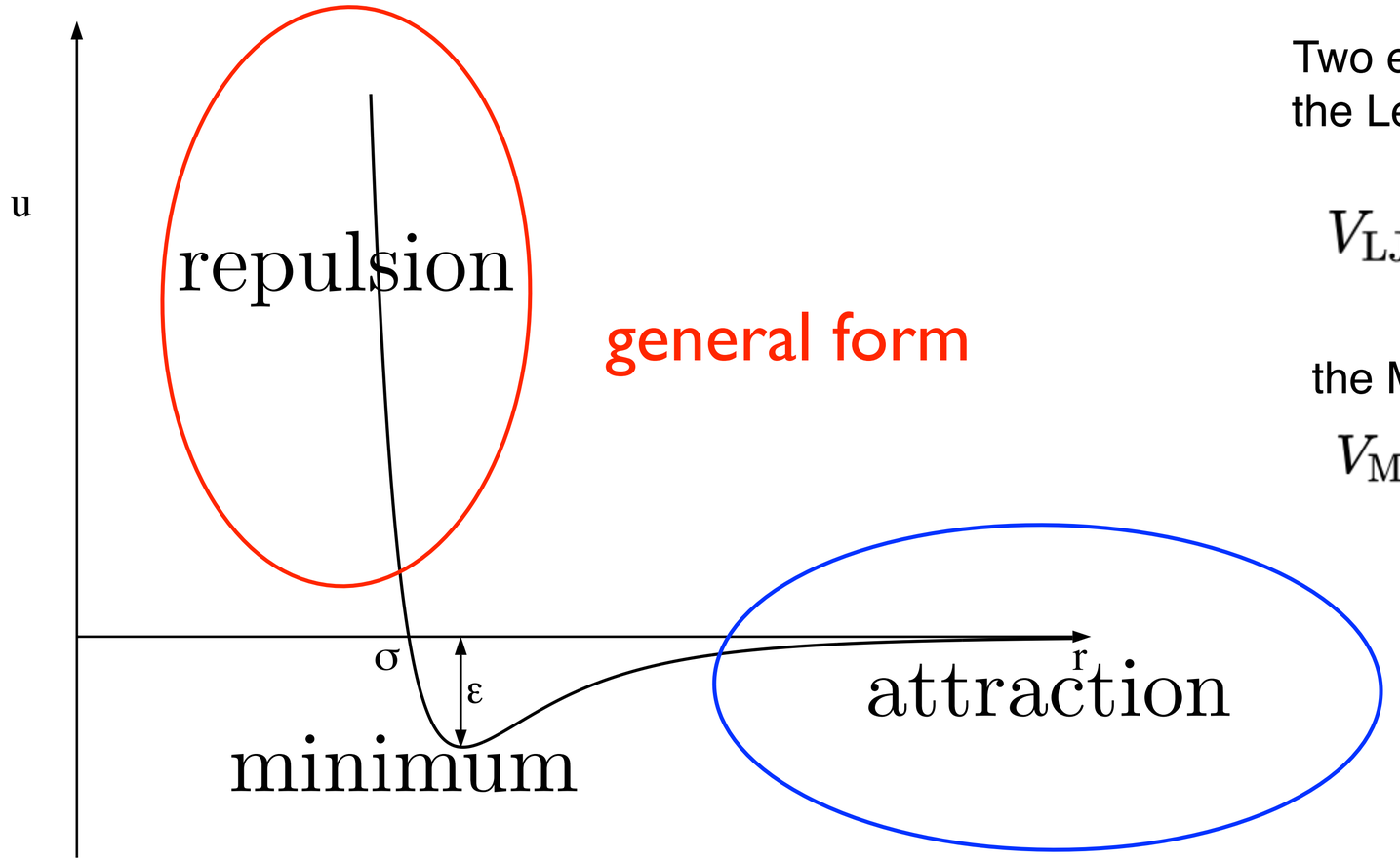
Atomistic approaches

We can describe a molecule, a material, … as a system of **atoms** with given positions in space.

We can think about atoms interacting through **interatomic potentials.**
The **total energy** of the system can be obtained by **summing all the interactions between the atoms** using such potentials**.**

Interatomic potentials can have different **functional forms**.

A typical 2-body effective potential



general form

Two examples of a specific functional form:
the Lennard-Jones potential:

$$V_{\mathrm{LJ}}(r) = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$$

the Morse potential:

$$V_{\mathrm{M}}(r) = D_e(e^{-2a(r-r_e)} - 2e^{-a(r-r_e)})$$

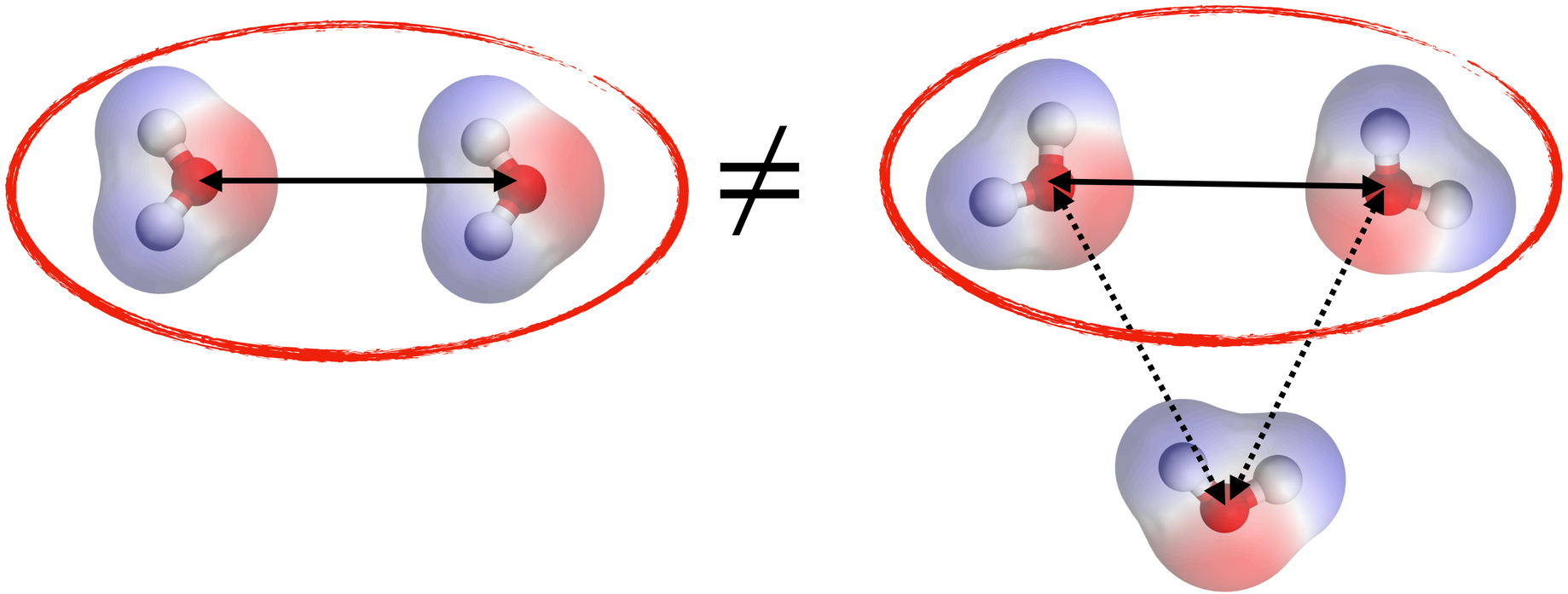
with parameters fitted
from experimental data

a strong repulsion for small r and a weak attraction at large r.

consequence of the Pauli exclusion principle.
`core repulsion`

mutual polarization of each molecule
`van der Waals`

A typical 2-body effective potential



REMARK:

we need a simple form for **u(r)** **=> we use** an **effective** interaction:

it is somehow “phenomenological”, since takes into account the environment;

it is an approximation, since in general, 3-, 4- ... many-body terms are present

Limits of interatomic potentials

interactions between electrons and nuclei and hence interatomic interactions are quantum mechanical in nature =>

we need to describe them => but the “true” interactions cannot be cast into an analytical functional form!
Hence all analytical interatomic potentials are necessarily approximations.

A typical problem of interatomic potentials: **non-trasferability**
(the effective potential in two different environments is different!)

we thus are going to afford
more accurate atomistic simulations that **consider the full quantum mechanical nature of the interaction between electrons and nuclei**
("**ab-initio**" or "**first-principles**" methods,
i.e. no empirical parameters
or fit from experimental data)

From foundations…

- ab-initio methods
- nuclei and electrons
- Born-Oppenheimer approximation
- limits of one-electron scheme
- density functional theory:
  - Hohenberg-Kohn theorem
  - functionals
  - one-electron (Kohn-Sham) equations and self-consistent cycle

… to practical implementation (towards Quantum Espresso suite of codes)

with physical approximation and numerical issues

Ab-initio methods

PURPOSES: to describe and explain material properties at a quantum and atomic level

INGREDIENTS: Electrons / nuclei / interactions; NO external parameters

METHOD: solution of the Schroedinger equation through:

– modeling (physical approximations)

– algorithms for a numerical solution

PECULIARITIES: reliable / predictive power / extensively used in materials of medium complexity and for a wide range of physical properties (mainly related to the ground state; extended with limitations also to excited states -e.g. optical spectra-)

Ab initio simulations

A many-body problem:

$$H_{tot} = \sum_i \frac{\mathbf{p}_i^2}{2m} + \sum_I \frac{\mathbf{P}_I^2}{2M_I} + \sum_i V_{nucl}(\mathbf{r}_i) + \frac{1}{2}\sum_{i \neq j} \frac{e^2}{r_{ij}} + \frac{1}{2}\sum_{I \neq J} \frac{Z_I Z_J e^2}{R_{IJ}}$$

$$V_{nucl}(\mathbf{r}) = -\sum_I \frac{Z_I e^2}{|\mathbf{r} - \mathbf{R}_I|}$$

$$r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$$

$$R_{IJ} = |\mathbf{R}_I - \mathbf{R}_J|$$

Indicating with V the total (e-e, e-nucl., nucl-nucl., ext.) potential...

Ab initio simulations

... the time-dependent Schr eq. reads:

$$i\hbar\frac{\partial\Phi(r,R;t)}{\partial t}=\left(-\frac{\hbar^2}{2M}\frac{\partial^2}{\partial R_I^2}-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial r_i^2}+V(r,R)\right)\Phi(r,R;t)$$

A physical approximation: Born-Oppenheimer (adiabatic) (M>>m)

Classic eq. of motion for nuclei fixing electrons -> E (**R**):

$$M\ddot{R}_I=-\frac{\partial E(R)}{\partial R_I}$$

$$\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial r_i^2}+V(r,R)\right)\Psi(r|R)=E(R)\Psi(r|R)$$

electronic Hamiltonian for nuclei fixed in {**R**}

Hartree-Fock method for electrons

- Also the **electronic problem** is a difficult one (**many-body, interacting**) => yet another physical approx. is necessary

- One-electron approx.: interacting but independent electrons (NO correlations):

- the ground-state can be written as an individual Slater determinant (antisymmetrized product of one-electron spin-orbitals)

$$\Psi_0(\mathbf{r}_1\sigma_1, \mathbf{r}_2\sigma_2, \ldots \mathbf{r}_N\sigma_N) = \mathcal{A}\{\psi_1(\mathbf{r}_1\sigma_1)\psi_2(\mathbf{r}_2\sigma_2)\ldots\psi_N(\mathbf{r}_N\sigma_N)\}$$

$$\psi_i(\mathbf{r}\sigma) = \phi_i(\mathbf{r})\chi_i(\sigma)$$

Hartree-Fock method for electrons

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e.g. for 2 electrons (He atom):

$$\Psi(\mathbf{x}_1,\mathbf{x}_2) = \frac{1}{\sqrt{2}}\{\chi_1(\mathbf{x}_1)\chi_2(\mathbf{x}_2) - \chi_1(\mathbf{x}_2)\chi_2(\mathbf{x}_1)\}$$

$$= \frac{1}{\sqrt{2}}\begin{vmatrix} \chi_1(\mathbf{x}_1) & \chi_2(\mathbf{x}_1) \\ \chi_1(\mathbf{x}_2) & \chi_2(\mathbf{x}_2) \end{vmatrix},$$

How to overcome the limits of the Hartree-Fock method?

- better approximations to the many-body wavefunction, for instance:

- use a combination of different Slater determinants (“configuration interaction”, CI)
- …

How to overcome the limits of one-electron methods?

- Instead of looking for better approximations to the many-body wavefunction, let's follow an alternative way:

- Focus on the one-particle electron density n(**r**) which is easier to treat (less degrees of freedom)

- HOENBERG-KOHN THEOREM: correspondence

ground state of a system characterized by n(**r**) <=> external potential

Great idea ! **Walter Kohn:**
Nobel prize in Chemistry, 1998

$$H_e = H_{int} + V_{ext}$$

$H_e, H_{int}, V_{ext}, T, V_{ee}$ are many-body operators

$$H_{int} = T + V_{ee} = \sum_i \frac{\mathbf{p}_i^2}{2m} + \frac{1}{2}\sum_{i\neq j} \frac{e^2}{r_{ij}}$$

$$V_{ext} = \sum_i v_{ext}(\mathbf{r}_i) = \sum_i \int v_{ext}(\mathbf{r})\delta(\mathbf{r} - \mathbf{r}_i)d\mathbf{r}$$

$$v_{ext}(\mathbf{r}) \equiv V_{nucl}(\mathbf{r}) = -\sum_I \frac{Z_I e^2}{|\mathbf{r} - \mathbf{R}_I|} + \frac{1}{2}\sum_{I\neq J} \frac{Z_I Z_J e^2}{R_{IJ}}$$

$\Psi_0(\mathbf{r_1}, \mathbf{r_2}, \ldots, \mathbf{r_N})$: Many-body wfc

$n(\mathbf{r}) = \langle\Psi_0|\sum_i \delta(\mathbf{r} - \mathbf{r}_i)|\Psi_0\rangle$: Single-particle density

$$\langle\Psi_0|V_{ext}|\Psi_0\rangle = \int n(\mathbf{r})v_{ext}(\mathbf{r})d\mathbf{r}$$

(1 PART): V_{ext} => n (**r**) is trivial:

$$v_{ext}(\mathbf{r}) \Longrightarrow \Psi_0[v_{ext}] \Longrightarrow n(\mathbf{r}) \quad \text{i.e.,} \quad \boxed{n(\mathbf{r}) = F[v_{ext}]}$$

(2 PART): V_{ext} <= n (**r**) is NOT trivial: (per absurdum)

$$\boxed{v_{ext} \neq \overline{v}_{ext} \Longrightarrow n(\mathbf{r}) \neq \overline{n}(\mathbf{r})}$$

(and not only for a rigid shift)

i.e.,

$$\boxed{n(\mathbf{r}) \Longrightarrow V_{ext}(\mathbf{r})}$$

Let be: $H = H_{int} + V_{ext}$ with: $\Psi_0,\ E_0$

$\overline{H} = H_{int} + \overline{V}_{ext}$ $\overline{\Psi}_0,\ \overline{E}_0;$

$$\begin{aligned}
\langle \overline{\Psi}_0 | H | \overline{\Psi}_0 \rangle &= \langle \overline{\Psi}_0 | H_{int} + V_{ext} + \overline{V}_{ext} - \overline{V}_{ext} | \overline{\Psi}_0 \rangle \\
&= \overline{E_0} + \langle \overline{\Psi}_0 | V_{ext} - \overline{V}_{ext} | \overline{\Psi}_0 \rangle \\
&= \overline{E_0} + \int \overline{n}(\mathbf{r})[v_{ext}(\mathbf{r}) - \overline{v}_{ext}(\mathbf{r})]d\mathbf{r}
\end{aligned}$$

For the variational principle:

$$\langle \Psi_0 | H | \Psi_0 \rangle < \langle \overline{\Psi}_0 | H | \overline{\Psi}_0 \rangle$$

i.e.:

$$E_0 < \overline{E}_0 + \int \overline{n}(\mathbf{r})[v_{ext}(\mathbf{r}) - \overline{v}_{ext}(\mathbf{r})]d\mathbf{r}$$

Similarly:

$$\overline{E}_0 < E_0 + \int n(\mathbf{r})[\overline{v}_{ext}(\mathbf{r}) - v_{ext}(\mathbf{r})]d\mathbf{r}$$

Combining the two we must exclude that

$$n = \overline{n}$$

Ok, $n(\mathbf{r})$ is a fundamental quantity...

But what will we do in practice to solve the Schr. eq.?
How to reduce the number of variables from 3N to 3 ?

The path:

From HK theorem
to single electron (Kohn-Sham) eqs.

mapping the interacting system into a non-interacting one

(that can thus be cast into a **one-electron problem**)

with the same density n(r)

next lecture

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From HK theorem
to single electron (Kohn-Sham) eqs.

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(that can thus be cast into a **one-electron problem**)

with the same density n(r)

now we jump to this one-electron problem

HK theorem and functionals

Consequence of the HK theorem:

E is a functional $E[n(\mathbf{r})]$ of $n(\mathbf{r})$

interacting el. potential ↓ U ; external potential ↓ V

$$E[n(\mathbf{r})] = \langle \Psi | T + U + V | \Psi \rangle = \langle \Psi | T + U | \Psi \rangle + \langle \Psi | V | \Psi \rangle$$
$$= F[n(\mathbf{r})] + \int n(\mathbf{r}) V(\mathbf{r}) d\mathbf{r}$$

$F[n(\mathbf{r})]$ is a universal functional of $n(\mathbf{r})$ (and not of V)

(unknown!)

next lecture

Problem: determine $n(\mathbf{r})$ which minimizes $E[n(\mathbf{r})]$

Kohn-Sham equations (I)

The system of interacting electrons is mapped on to a non-interacting electrons having the same density $n(\mathbf{r})$
For non-interacting electrons:

$$n(\mathbf{r}) = \sum_i |\psi_i(\mathbf{r})|^2$$

(for all the fully occupied orbitals;
otherwise, insert an occupation factor)

<= link between *n(**r**)* and single-electron wavefunctions

with $\psi_i(\mathbf{r})$ one-electron orthonormal orbitals (Kohn-Sham orbitals) satisfying:

next lecture

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + \underbrace{V(\mathbf{r}) + V_H[n(\mathbf{r})] + V_{xc}[n(\mathbf{r})]}_{= V_{KS}[n(\mathbf{r})]} \right) \psi_i(\mathbf{r}) = \epsilon_i \psi_i(\mathbf{r})$$

in practice, this is V_{nucl}

Kohn-Sham equations (II)

recover the expression for the energy:

$$E[n(\mathbf{r})] = F[n(\mathbf{r})] + \int n(\mathbf{r})V(\mathbf{r})d\mathbf{r}$$

From the mapping on to a non-interacting system:

$$F[n(\mathbf{r})] = T_s[n(\mathbf{r})] + E_H[n(\mathbf{r})] + E_{xc}[n(\mathbf{r})]$$

with:

$$T_s[n(\mathbf{r})] = -\frac{\hbar^2}{2m}\sum_i \int \Psi_i^*(\mathbf{r})\nabla^2\Psi_i(\mathbf{r})d\mathbf{r}$$ kinetic energy of non-inte electrons

$$E_H[n(\mathbf{r})] = \frac{e^2}{2}\int \frac{n(\mathbf{r})n(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}d\mathbf{r}d\mathbf{r}'$$ Hartree energy:
electrostatic energy o acting electrons

next lecture

$E_{xc}[n(\mathbf{r})]$ exchange-correlation energy:

contains all the remaining terms!!! (unknown)

let’s recap…

Ab-initio simulations

To summarize up to here:

- need of **transferable methods**
- **at the atomistic level**
- giving **results with predictive capabilities**

=> ab-initio methods:

- ingredients: nuclei, electrons, interactions

how to solve the many-body Schroedinger equation?

How to solve the many-body Schr. eq.?

A first physical approximation

- the adiabatic (Born-Oppenheimer) approx. (M>>m): decouples electronic and nuclear problems

Density Functional Theory (DFT) for the electronic problem: from a many-body wave function (3N variables) to the electron density n(**r**) (3 variables):

- use of the variational principle: ok for occupied states (not excited)
- map the interacting system into a non-interacting system and factorize =>
- **one-electron** Scr. eq.

How to solve the one-electron Schr. eq.?

Given the one-electron Schroedinger equation (i.e., the Kohn-Sham eq.) how to proceed to really solve it?

$$H_{KS}\psi_i \equiv \left(T + V + V_H[n] + V_{xc}[n]\right)\psi_i = \epsilon_i \psi_i$$

where

- $n(\mathbf{r}) = \sum_i f_i |\psi_i(\mathbf{r})|^2$ is the charge density, f_i are occupation numbers
- V is the nuclear (pseudo-)potential acting on electrons
- $V_H[n]$ is the Hartree potential, $V_H(\mathbf{r}) = e^2 \int \frac{n(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r}'$
- $V_{xc}[n]$ is the exchange-correlation potential. (what is it??? we'll be back later on that...)

Now let's focus on this issue:

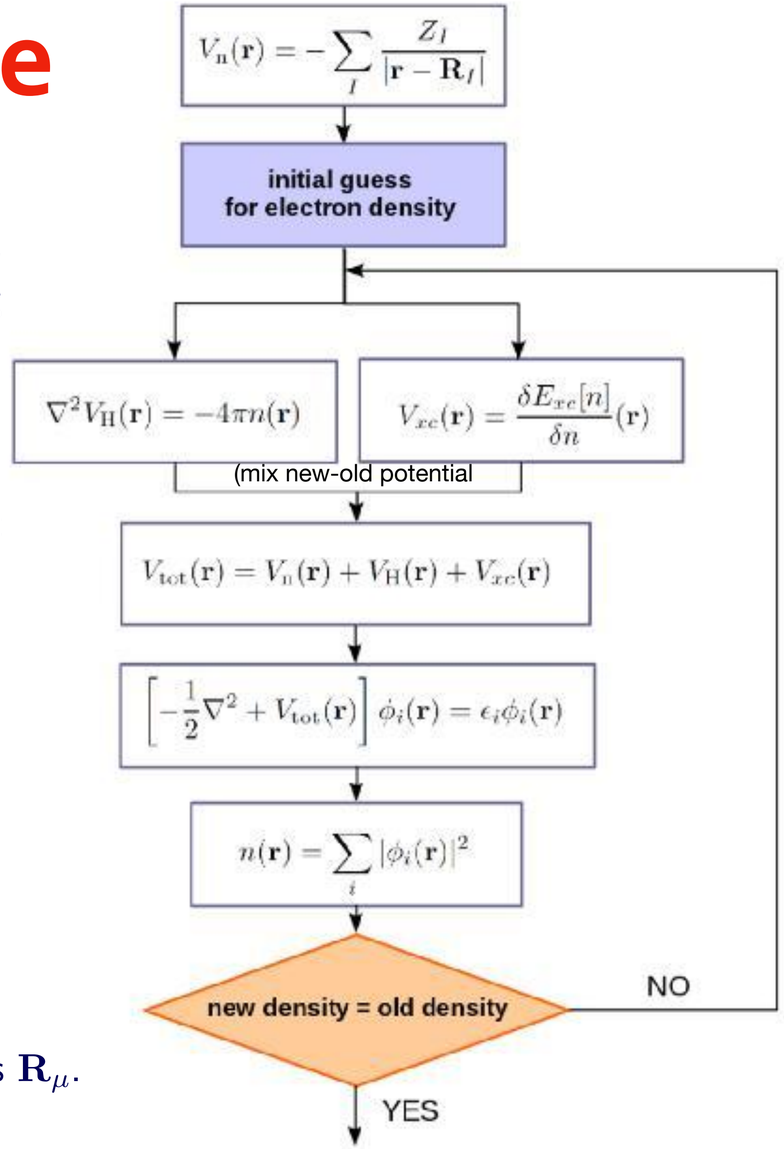
the potential depends on the solution itself!

How to solve the one-electron Schr. eq.?

Self-consistent cycle

In a self-consistent approach, we need to find the self-consistent charge density (or potential), performing the following operations:

- Calculate the potential from the charge density
- Solve (*diagonalize*) the Kohn-Sham equations at fixed potential
- Calculate the charge density from Kohn-Sham orbitals



The total energy depends upon all atomic positions $\mathbf{R}_\mu$.

How to solve the one-electron Schr. eq.?

Other issues:

The formal derivation of the KS equations is exact, but approximations are necessary for the practical implementation of the theory:

- how to describe ψ ?
- how to describe V_{nucl} ?
- how to describe V_{xc} ?
- how to perform the integrations?

How to solve the <u>one-electron</u> Schr. eq.?

- how to describe ψ ?

The solution of the Kohn-Sham problem $H_{KS}\psi = \epsilon\psi$ at fixed potential is (usually) the toughest problem. How to proceed? By expanding ψ into some suitable **basis set** $\{\phi_i\}$ as

$$\psi(\mathbf{r}) = \sum_i c_i \phi_i(\mathbf{r}).$$

If we expand the unknown ψ onto a basis set, we transform the problem into one of linear algebr

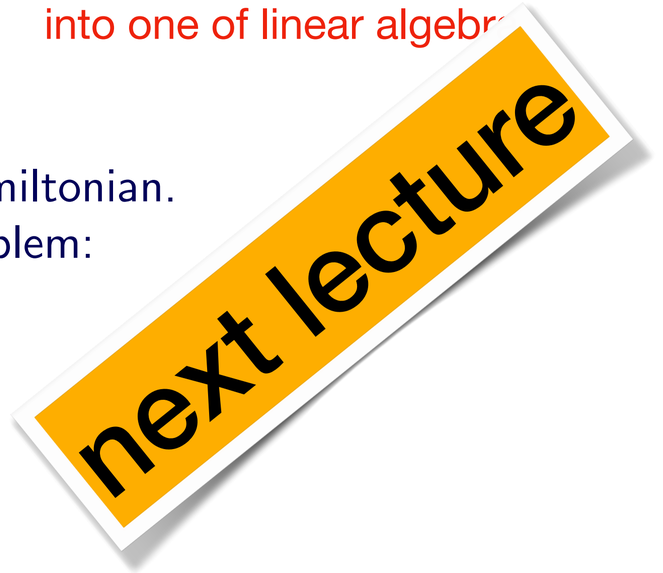
For an orthonormal basis set, we solve the secular equations

$$\sum_j (H_{ij} - \epsilon\delta_{ij})c_j = 0$$

where $H_{ij} = \langle\phi_i|H_{KS}|\phi_j\rangle$ are the *matrix elements* of the Hamiltonian.
For a non-orthonormal basis set, we solve the generalized problem:

$$\sum_j (H_{ij} - \epsilon S_{ij})c_j = 0$$

where $S_{ij} = \langle\phi_i|\phi_j\rangle$ is the *overlap matrix*.



Diagonalization algorithms are well known in linear algebra, but in practice, one has to resort to smarter *iterative* algorithms, allowing *not* to store those matrices.

Plane-wave basis set - 1

A PW basis set for states of wave vector $\mathbf{k}$ is defined as

$$\phi_{\mathbf{k+G}}(\mathbf{r}) = \langle \mathbf{r}|\mathbf{k}+\mathbf{G}\rangle = \frac{1}{\sqrt{\mathcal{N}\Omega}} e^{i(\mathbf{k}+\mathbf{G})\cdot\mathbf{r}}, \quad \frac{\hbar^2}{2m}|\mathbf{k}+\mathbf{G}|^2 \leq E_{cut}$$

$\Omega =$ unit cell volume, $\mathcal{N}\Omega =$ crystal volume, $E_{cut} =$ cutoff on the kinetic energy of PWs (in order to have a finite number of PWs!). The PW basis set is *complete* for $E_{cut} \to \infty$ and *orthonormal*: $\langle \mathbf{k}+\mathbf{G}|\mathbf{k}+\mathbf{G}'\rangle = \delta_{\mathbf{G}\mathbf{G}'}$

In a PW basis set one works with *Fourier components* ($c_{i,\mathbf{k+G}}$ below):

$$|\psi_i\rangle = \sum_{\mathbf{G}} c_{i,\mathbf{k}+\mathbf{G}} |\mathbf{k}+\mathbf{G}\rangle$$

$$c_{i,\mathbf{k}+\mathbf{G}} = \langle \mathbf{k}+\mathbf{G}|\psi_i\rangle = \frac{1}{\sqrt{\mathcal{N}\Omega}} \int \psi_i(\mathbf{r}) e^{-i(\mathbf{k}+\mathbf{G})\cdot\mathbf{r}} d\mathbf{r} = \widetilde{\psi}_i(\mathbf{k}+\mathbf{G}).$$

Real-space quantities can be obtained on a grid using Fast Fourier Transform.

Plane-wave basis set - 2

- Plane Waves:
  - slow convergence with respect to basis set size (many more PWs than localized functions needed)
  - require periodicity: in finite systems, *supercells* must be introduced
  + easy to evaluate convergence quality (just increase a single parameter, the *cutoff*)
  + easy to use (Fourier transform)

Periodicity needed !

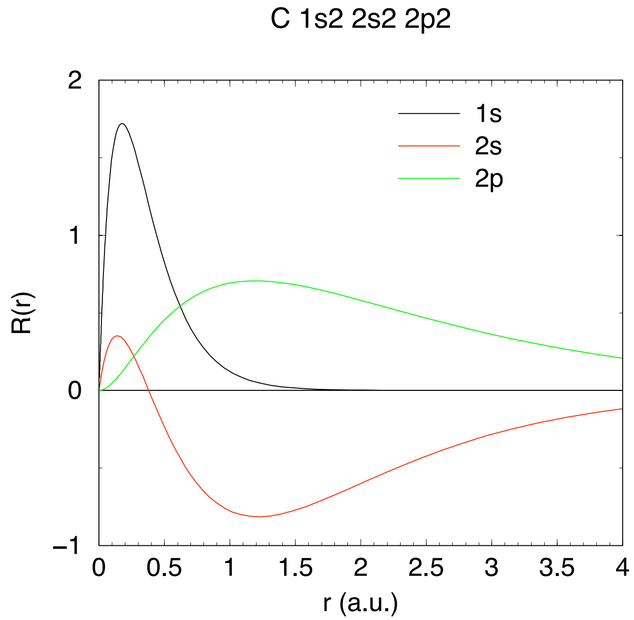
Pseudopotentials - o

- how to describe V_{nucl} ?

From simple Fourier analysis: length scale $\delta \longrightarrow$ Fourier components up to $q \sim 2\pi/\delta$. In a solid, this means $\sim 4\pi(2\pi/\delta)^3/3\Omega_{BZ}$ PWs (volume of the sphere of radius q divided by $\Omega_{BZ} = 8\pi^3/\Omega$, volume of the Brillouin Zone).

Estimate for diamond: $1s$ wavefunction has $\delta \simeq 0.1$ a.u., $\Omega = (2\pi)^3/(a_0^3/4)$ with lattice parameter $a_0 = 6.74$ a.u. $\longrightarrow 250,000$ PWs! We need to:

- get rid of core states
- get rid of orthogonality wiggles close to the nucleus



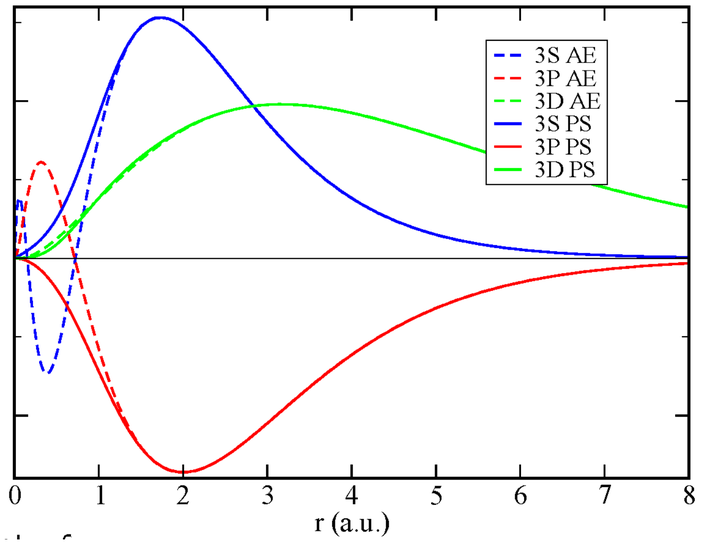
Solution: **Pseudopotentials** (PP). A smooth effective potential that reproduces the effect of the nucleus plus core electrons on valence electrons.

Pseudopotentials - 1

Norm-Conserving Pseudopotentials

Electron-ionic core interactions are typically represented by a nonlocal *Norm-Conserving Pseudopotential* (NCPP): a soft potential, no core states, no orthonormality wiggles.

r ψ**(r)**



AE="all electron"
(i.e. calculations including also core electrons)

PS="pseudopotential"

One pseudo potential for each angular momentum :

$$V_l^{ps} = V_{loc}(r) + V_l(r)P_l = V(r) + \sum_m Y_{lm}(\mathbf{r})V(r)\delta(r-r')Y^*_{lm}(\mathbf{r}')$$

with $V_{loc}(r) = -Z_v e^2 / r$

In many systems, NCPP's allow accurate calculations with moderate-size ($E_c \sim 10-20Ry$) plane-wave basis sets (explained in the following)

Pseudopotentials - 2

Norm-Conserving Pseudopotentials (continued)

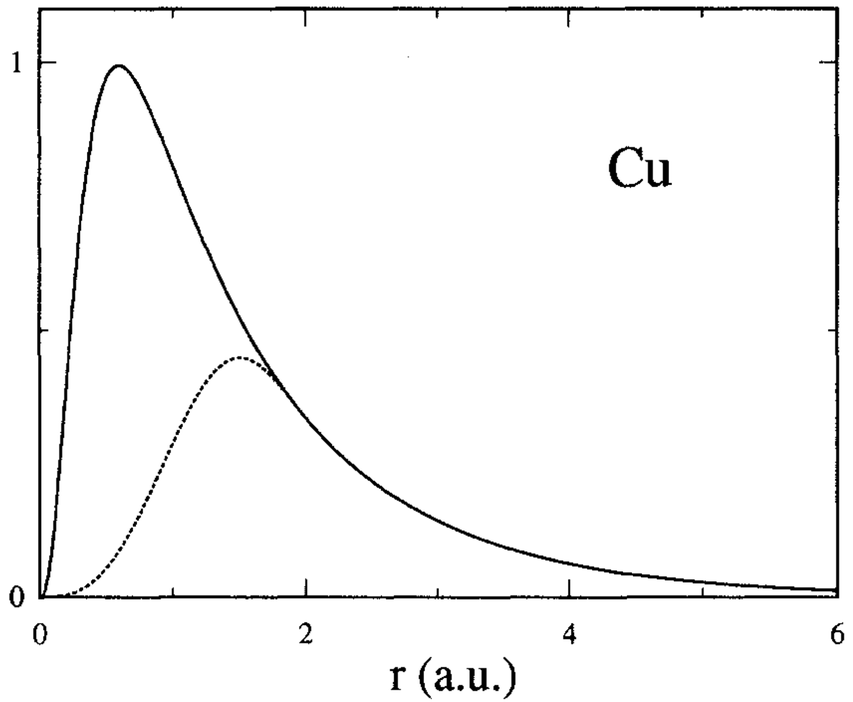
NCPP's based on atomic DFT calculations, were introduced by Hamann, Schlüter, Chiang in 1979. For a given reference atomic configuration, they must meet the following conditions:

- $\epsilon_l^{ps} = \epsilon_l^{ae}$ **<= atomic energy levels must be reproduced**
- $\phi_l^{ps}(r)$ is nodeless
- $\phi_l^{ps}(r) = \phi_l^{ae}(r)$ for $r > r_c$ **<= coincidence between the "true" and "pseudo" wfc in the external region**
- $\int_{r<r_c} |\phi_l^{ps}(r)|^2 r^2 dr = \int_{r<r_c} |\phi_l^{ae}(r)|^2 r^2 dr$ **<= norm-conserving**

where $\phi_l^{ae}(r)$ is the radial part of the atomic valence wavefunction with l angular momentum, ϵ_l^{ae} its orbital energy. The *core radius* r_c is approximately at the outermost maximum of the wavefunction.

Pseudopotentials - 3

“soft” or “ultrasoft” pseudopotentials: release the condition of norm-conserving =>
Smoother potentials => smoother wfc => less plane waves to describe them (see later)



running the pw.x code:

In the input:

```
…
/
&electrons
   …
   mixing_beta      =  0.5
   conv_thr         =  1D-10
   electron_maxstep =  100
/
```

In the output:

```
Self-consistent Calculation

iteration #  1     ecut=    50.00 Ry     beta= 0.50
Davidson diagonalization with overlap
ethr =  1.00E-02,  avg # of iterations =  2.2

total cpu time spent up to now is       20.0 secs

total energy              =    -202.68145378 Ry
estimated scf accuracy    <       0.45007650 Ry

iteration #  2     ecut=    50.00 Ry     beta= 0.50
….
….

End of self-consistent calculation

convergence has been achieved in  13 iterations
```

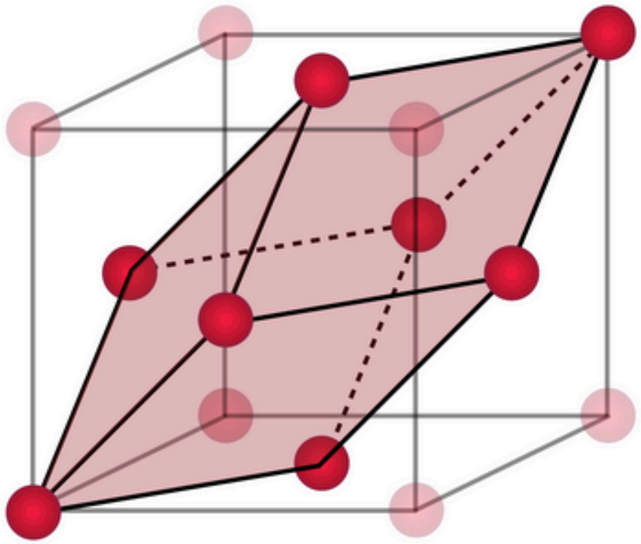
running the pw.x code:

In the input:

```
…
/
&system
    ibrav= 2, celldm(1) = 7.5,
    ntyp= 1,
    nat= 1
    ….
/
….
ATOMIC_SPECIES
 Al     26.98     Al.pz-vbc.UPF

ATOMIC_POSITIONS alat
Al       0.    0.    0.    0   0   0
….
```

fcc Bravais lattice



describe the lattice vectors
of a periodically repeated cell
(or indicate in an alternative way
which is the Bravais lattice and
which is the lattice parameter)
and the internal atomic positions

https://www.quantum-espresso.org/Doc/INPUT_PW.html

Input File Description

Program: pw.x / PWscf / Quantum ESPRESSO (version: 7.2)

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INTRODUCTION

&CONTROL

calculation | title | verbosity | restart_mode | wf_collect | nstep | iprint | tstress | tprnfor | dt | outdir | wfcdir | prefix | lkpoint_dir | max_seconds | etot_conv_thr | forc_conv_thr | disk_io | pseudo_dir | tefield | dipfield | lelfield | nberrycyc | lorbm | lberry | gdir | nppstr | gate | twochem | lfcp | trism

&SYSTEM

ibrav | celldm | A | B | C | cosAB | cosAC | cosBC | nat | ntyp | nbnd | nbnd_cond | tot_charge | starting_charge | tot_magnetization | starting_magnetization | ecutwfc | ecutrho | ecutfock | nr1 | nr2 | nr3 | nr1s | nr2s | nr3s | nosym | nosym_evc | noinv | no_t_rev | force_symmorphic | use_all_frac | occupations | one_atom_occupations | starting_spin_angle | degauss_cond | nelec_cond | degauss | smearing | nspin | sic_gamma | pol_type | sic_energy | sci_vb | sci_cb | noncolin | ecfixed | qcutz | q2sigma | input_dft | ace | ...

...

&ELECTRONS

electron_maxstep | exx_maxstep | scf_must_converge | conv_thr | adaptive_thr | conv_thr_init | conv_thr_multi | mixing_mode | mixing_beta | mixing_ndim | mixing_fixed_ns | diagonalization | diago_thr_init | diago_cg_maxiter | diago_ppcg_maxiter | diago_david_ndim | diago_rmm_ndim | diago_rmm_conv | diago_gs_nblock | diago_full_acc | efield | efield_cart | efield_phase | startingpot | startingwfc | tqr | real_space

...

ATOMIC_SPECIES

X | Mass_X | PseudoPot_X

ATOMIC_POSITIONS

X | x | y | z | if_pos(1) | if_pos(2) | if_pos(3)

K_POINTS

nks | xk_x | xk_y | xk_z | wk | nk1 | nk2 | nk3 | sk1 | sk2 | sk3