Basic concepts of the electronic models: $E^{(2)}$ electron-electron interactions,

U and J

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The Hubbard model:
a simple model to treat electron-electron correlation in solids

Extension of a tight-binding model…

electrons can hop between lattice sites with a probability given by the hopping γ

$$\mathcal{H} = -\gamma \sum_{\langle l,m\rangle,\sigma} \left(c^{\dagger}_{l\sigma} c_{m\sigma} + \text{c.c.} \right) + U \sum_{l} n_{l\uparrow} n_{l\downarrow}$$

…plus one additional term

introducing an energy amount U **for each pair of electrons occupying the same lattice site representing Coulomb repulsion**

σ	**Spin**	$n_{l\uparrow}$	**Number of electrons with spin up on site** l
l, m	**Lattice sites**	$n_{l\downarrow}$	**Number of electrons with down up on site** l

The Hubbard model:
a simple model to treat electron-electron correlation in solids

New ingredients appear with respect the standard tight-binding model

$$\mathcal{H} = -\gamma \sum_{\langle l,m \rangle,\sigma} \left(c^{\dagger}_{l\sigma} c_{m\sigma} + \text{c.c.} \right) + U \sum_{l} n_{l\uparrow} n_{l\downarrow}$$

1. **The spin:** the electrons with opposite spin on the same lattice site repel each other via electrostatic forces.

The self-interaction (interaction of one electron with itself, i.e., with the same spin) are not considered

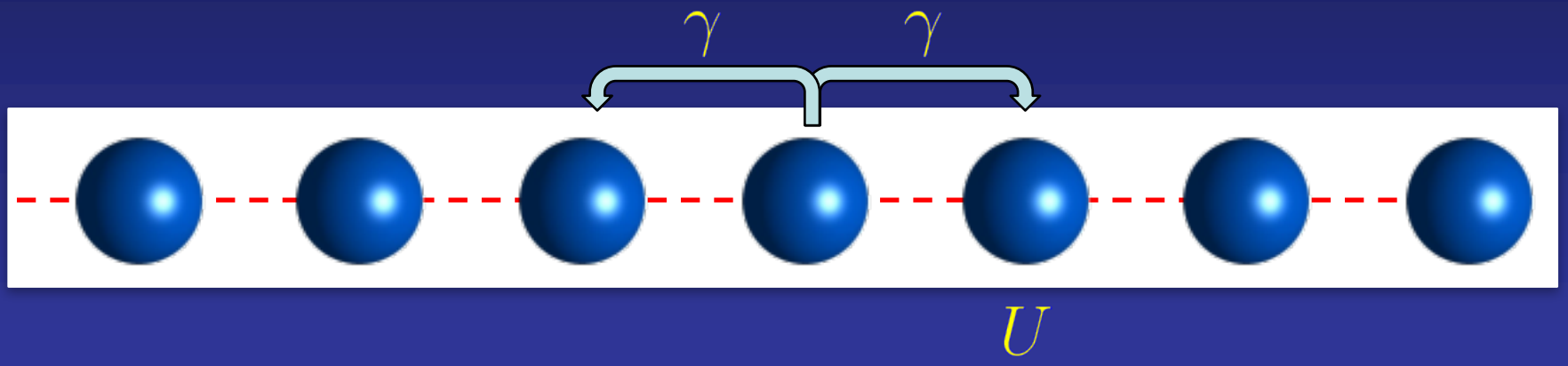
2. **The occupation number for each lattice site**

Assuming the most simple model with one atomic orbital per site,

$$0 \leq n_{l\uparrow} \leq 1$$

$$0 \leq n_{l\downarrow} \leq 1$$

Ground state of a monoatomic chain with one-orbital per site within the Hubbard model



The larger the hopping parameter, the broader the band width, and metallic phase is favoured

The Hubbard term penalizes the occupation of a site with electrons of different spin

If an atom is already occupied with a given density of electrons of a given spin, the electrons with different spin will feel a repulsion to hop there.

The U inhibits the hopping and favours localized states

Relationship between the Hubbard model and the parameters in the SCALE-UP Hamiltonian

The Hubbard parameter couples the number of electrons with different spin in a given lattice site

In the paper, this is called the *antiparallel* U parameter [Eq. (27)]

But these are not the parameters that finally enter in the SCALE-UP Hamiltonian
In its final form, it is written in terms of parameters that couple:

- **The total number of electrons in a given site (sum of the occupation for both spin), U**
- **The difference between electrons with spin up and electrons with spin down I**

$$U^{\text{anti}}_{aba'b'} = \int d^3r \int d^3r' \chi_a(\vec{r})\chi_b(\vec{r})\chi_{a'}(r)\chi_{b'}(r)g(\vec{r},r,\uparrow,\downarrow)$$
$$= \int d^3r \int d^3r' \chi_a(\vec{r})\chi_b(\vec{r})\chi_{a'}(r)\chi_{b'}(r)g(\vec{r},r,\downarrow,\uparrow)$$

In practice,

$$U^{\text{anti}} = U + I$$ **Eq. (34) of the manuscript**

Please, note that the U used in the manuscript is not the U of our Hubbard model

Relationship between the Hubbard model and the parameters in the SCALE-UP Hamiltonian

In its final form, it is written in terms of parameters that couple:

- The total number of electrons in a given site (sum of the occupation of both spin), U

$$U\left(n_{l\uparrow}+n_{l\downarrow}\right)\left(n_{l\uparrow}+n_{l\downarrow}\right)=U\left(n_{l\uparrow}^{2}+n_{l\downarrow}^{2}+2n_{l\uparrow}n_{l}\right)$$

- The difference between electrons with spin up and electrons with spin down, I

$$I\left(n_{l\uparrow}-n_{l\downarrow}\right)\left(n_{l\uparrow}-n_{l\downarrow}\right)=I\left(n_{l\uparrow}^{2}+n_{l\downarrow}^{2}-2n_{l\uparrow}n_{l}\right)$$

To simulate the Hubbard model we need to impose that $U=I$

Then, according to Eq. (39) of the paper, the two body energy term becomes

$$E^{(2)}=\frac{1}{2}\left[U\left(n_{l\uparrow}+n_{l\downarrow}\right)\left(n_{l\uparrow}+n_{l\downarrow}\right)-U\left(n_{l\uparrow}-n_{l\downarrow}\right)\left(n_{l\uparrow}-n_{l\downarrow}\right)\right]=2Un_{l\uparrow}n_{l\downarrow}$$

i.e. the term required by the Hubbard model with an $U^{\text{model}}=2U^{\text{calculation}}$

Relationship between the Hubbard model and the parameters in the SCALE-UP Hamiltonian

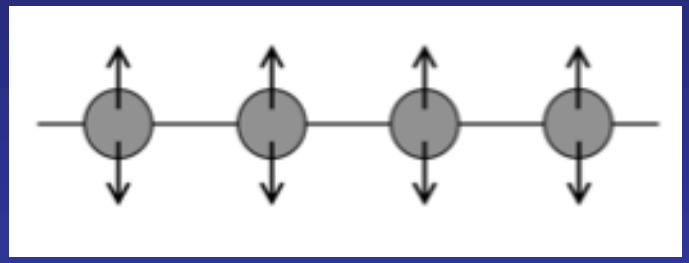
In summary: to simulate the Hubbard model with SCALE-UP:

$$U_{aba'b'} = I_{aba'b'}$$

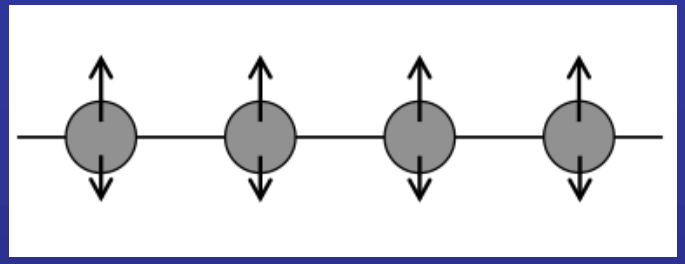
Even more, since in the Hubbard model we include only the on-site interactions, the previous parameters must be totally diagonal

$$U_{aba'b'} = U\delta_{ab}\delta_{aa'}\delta_{ab'} = U_{aaaa}$$

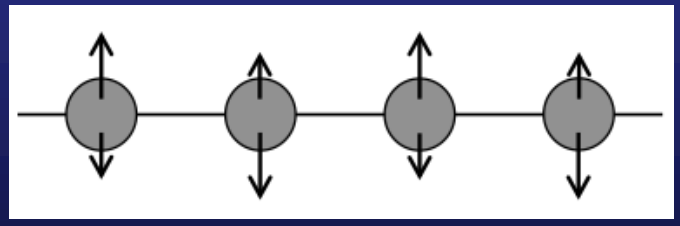
Ground state of a monoatomic chain with one-orbital per site within the Hubbard model



Diamagnetic:
Same amount of occupation for both spin channels



Ferromagnetic:
One spin component is more occupied than the other
The majority spin channel is the same from atom to atom



Antiferromagnetic:
One spin component is more occupied than the other
The majority spin channel changes from atom to atom

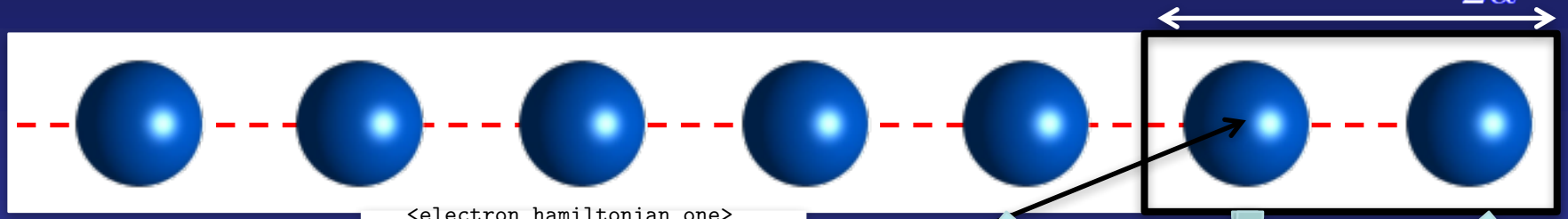
Linear chain of s-orbitals: The input file of SCALE-UP

```
%block Supercell
 1 1 2
%endblock Supercell

Magnetic

MaximumSCFiter   1000
SCFthreshold     0.00000001
SCFmixing        0.10
StartPulay       10000
ForceSCF
```

To account for all possible **magnetic solutions** (ferro, antiferro and diamagnetic), we need at least a **supercell** made up from the repetion of two unit cells

Very stringent conditions required in the convergence to avoid ending in a local metastable phase.
For the time being, we deactivate the Pulay mixing

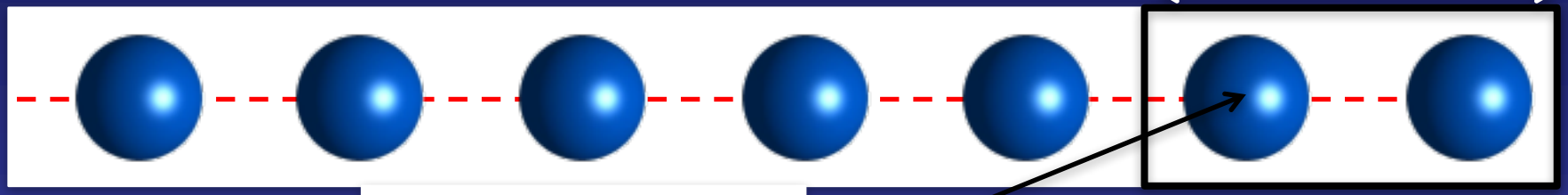
Linear chain of s-orbitals: How to introduce the parameters of the hamiltonian to run SCALE-UP



The one-electron terms as before

```
<electron_hamiltonian_one>
   <interaction_gm
        orbital_1="1"
        orbital_2="1"
        hopa="0"
        hopb="0"
        hopc="0"
        gamma="0.0000"
        rx="0.000"
        ry="0.000"
        rz="0.000">
   </interaction_gm>
   <interaction_gm
        orbital_1="1"
        orbital_2="1"
        hopa="0"
        hopb="0"
        hopc="-1"
        gamma="2.0000"
        rx="0.000"
        ry="0.000"
        rz="0.000">
   </interaction_gm>
   <interaction_gm
        orbital_1="1"
        orbital_2="1"
        hopa="0"
        hopb="0"
        hopc="1"
        gamma="2.0000"
        rx="0.000"
        ry="0.000"
        rz="0.000">
   </interaction_gm>
</electron_hamiltonian_one>
```

Linear chain of s-orbitals: How to introduce the parameters of the hamiltonian to run SCALE-UP



The two-electron terms refer for the indexing to the one-electron terms

```
<electron_hamiltonian_two>
   <interaction_ee
      gamma_1="1"
      gamma_2="1"
      hopa="0"
      hopb="0"
      hopc="0"
      hubbard="0.5000"
      stoner="0.5000">
   </interaction_ee>
</electron_hamiltonian_two>
```

$$U_{aba'b'} = U\delta_{ab}\delta_{aa'}\delta_{ab'} = U_{aaaa}$$

The term gamma_1 is between a and a

The term gamma_2 is between a and a

So the term introduced here is totally diagonal

$$U_{aba'b'} = I_{aba'b'}$$

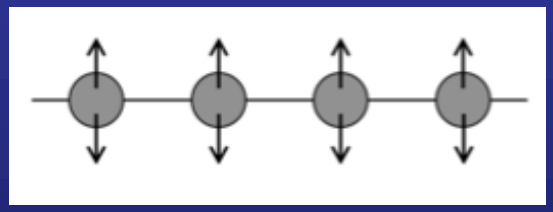
And the Hubbard and Stoner parameters are equal, as required to simulate our Hubbard model

Linear chain of s-orbitals: How to introduce the occupation to run SCALE-UP


```
<orbital
   name="cond_s"
   ref_occ_up="0.5000"
   ref_occ_dn="0.5000"
   ini_occ_up="1.0000"
   ini_occ_dn="0.0000">
</orbital>
```

These numbers refer to the occupation matrix $d^{(0)}_{ab}$ that defines the reference electron density [Eq. (18) of the manuscript]

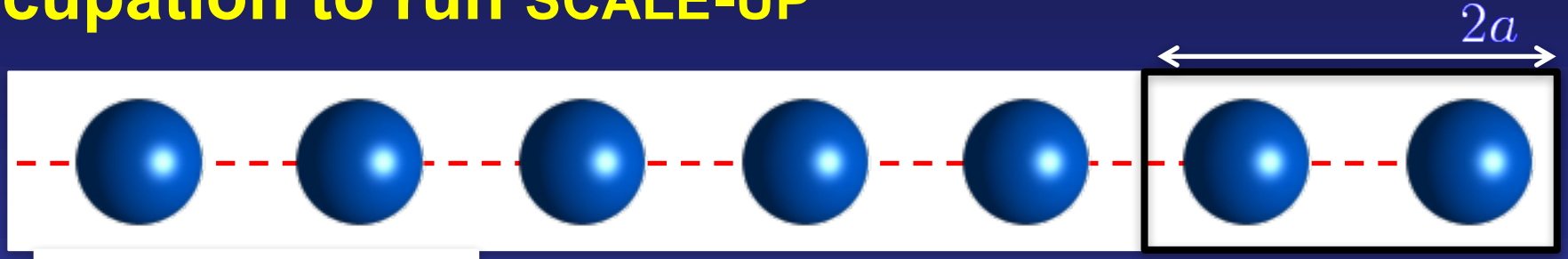
In these case, a diamagnetic configuration with the same number of electrons up and down per site



All the energies will be referred to the energy of this configuration, $E^{(0)}$

And the numbers for the density matrix written in files like _DENMATOLD refer to deformation occupation matrices, i.e. Changes with respect this reference occupation matrix, Eq. (19) in the paper.

Linear chain of s-orbitals: How to introduce the occupation to run SCALE-UP




```
<orbital
   name="cond_s"
   ref_occ_up="0.5000"
   ref_occ_dn="0.5000"
   ini_occ_up="1.0000"
   ini_occ_dn="0.0000">
</orbital>
```

These numbers refer to the occupation matrix that defines the initial density [Eq. (16) of the manuscript]

In these case, a completely polarized ferromagnetic configuration where only the up component of the spin is polarized

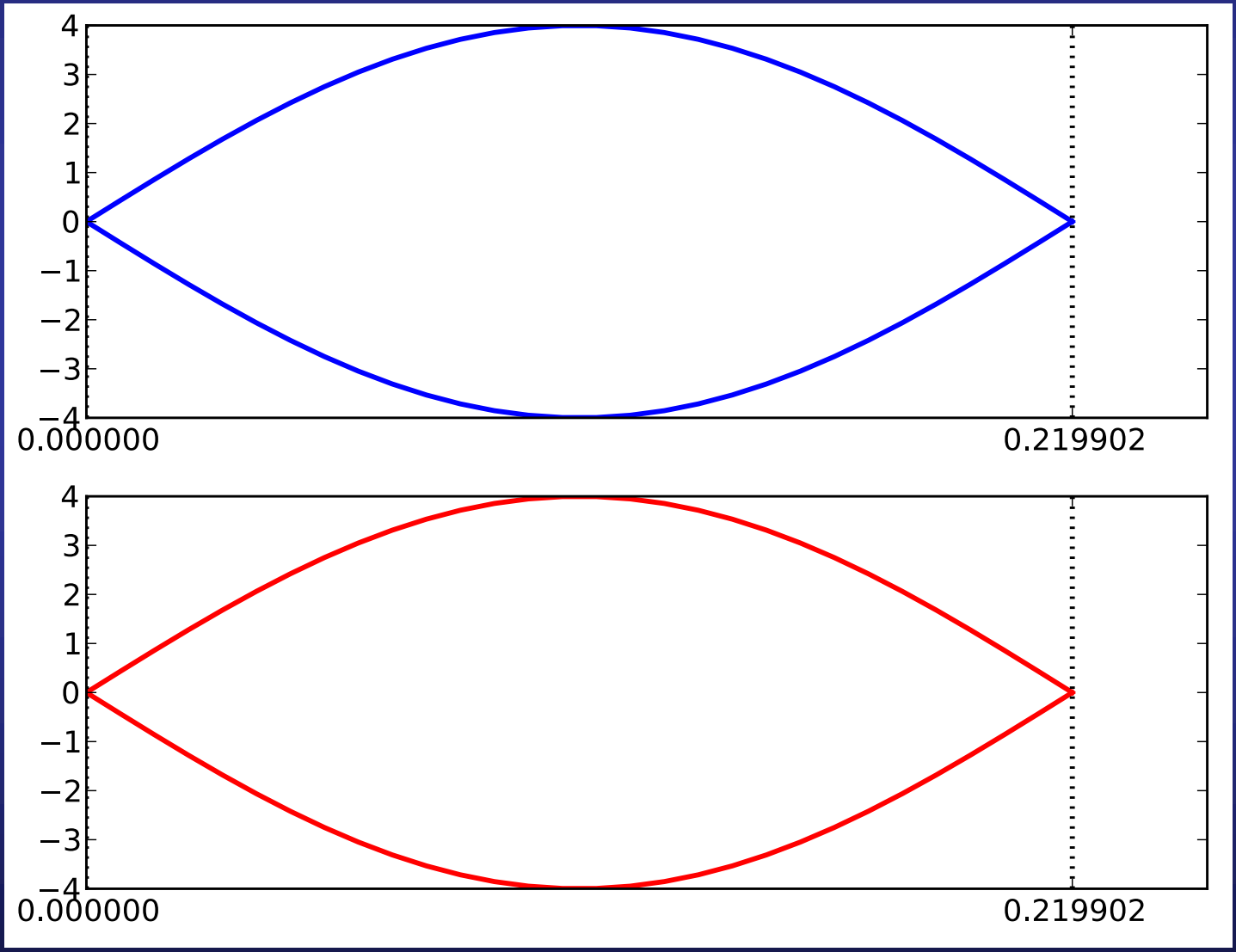
Obviously, in this example we are running a half-filled system, with one electron per atom

Linear chain of s-orbitals: How to run SCALE-UP

```
$ <your_path_to_scale_up_dir>/bin/scaleup.x < 1d_hubbard.fdf > 1d_hubbard.out
```

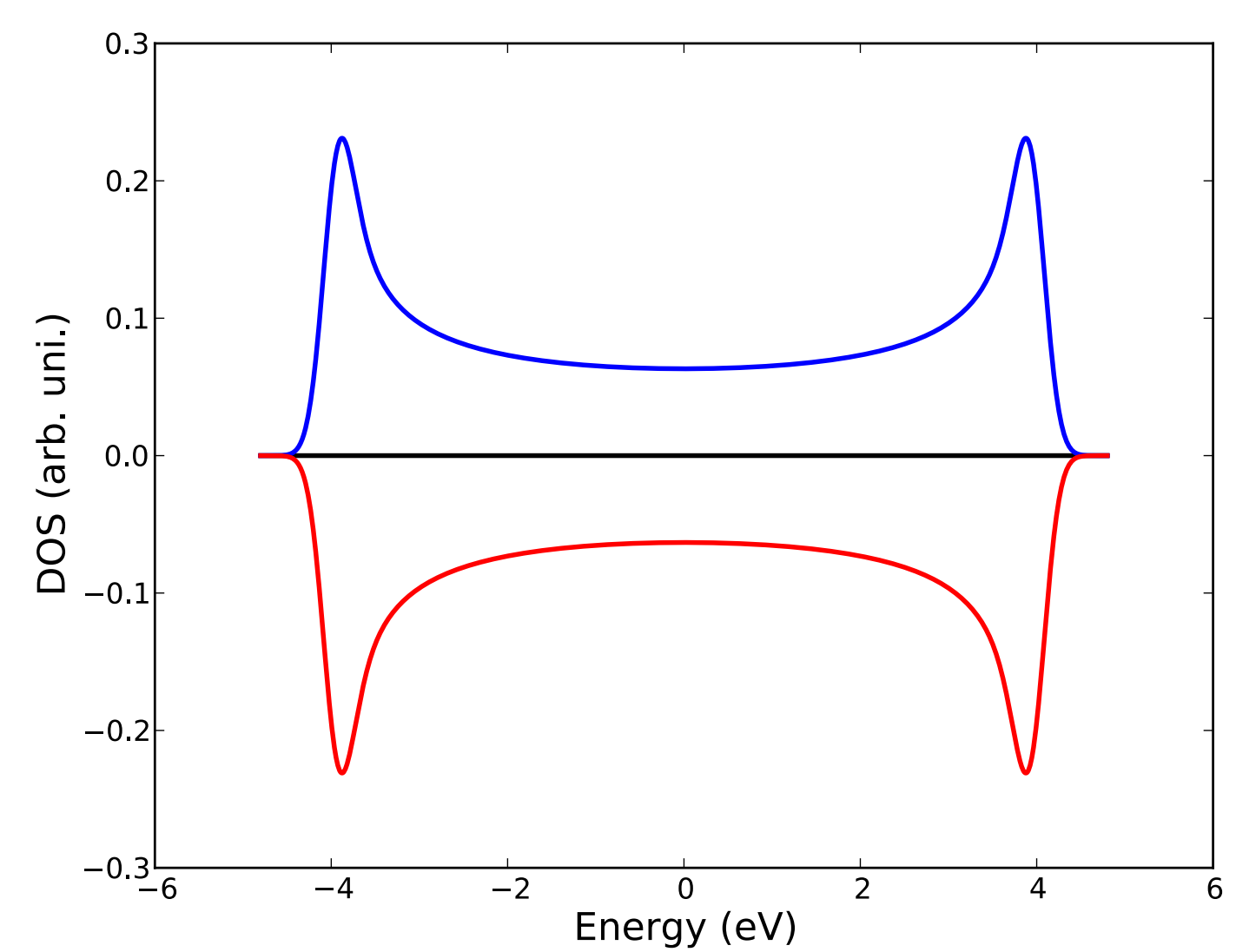
Linear chain of s-orbitals: How to plot the band structure with SCALE-UP

```
$ python  <your_path_to_scale_up_dir>/scripts/scaleup_utils.py -bands -file _1d_hubbard_FINAL.bands
```



Linear chain of s-orbitals: How to plot the density of states with SCALE-UP

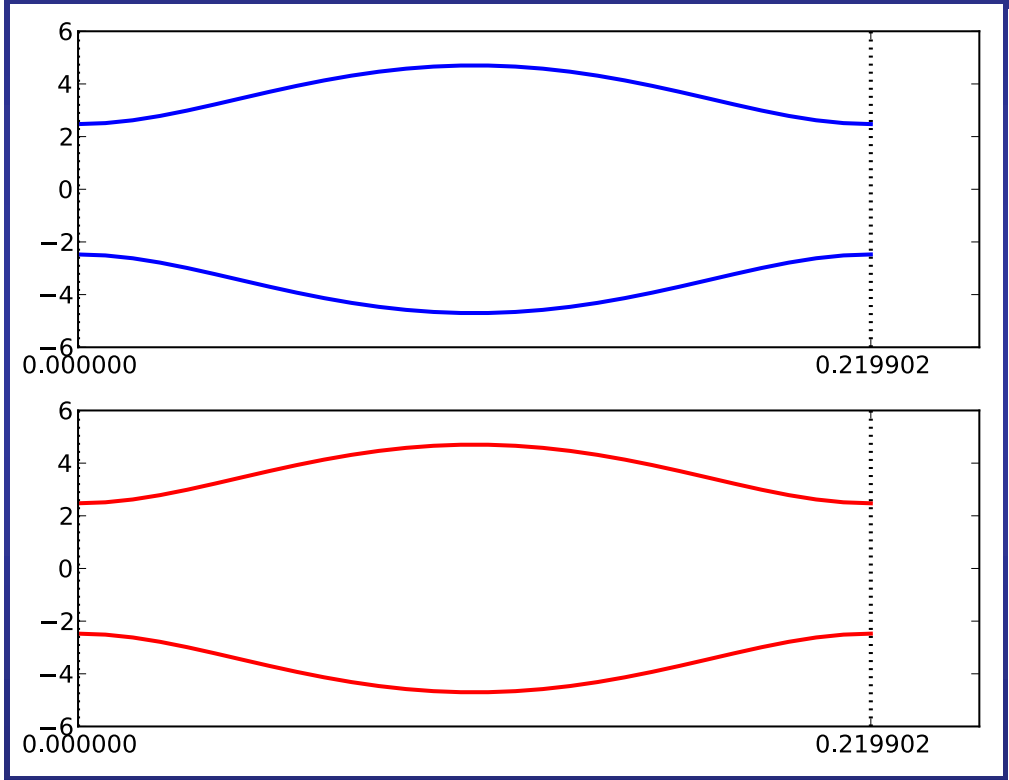
```
$ python  <your_path_to_scale_up_dir>/scripts/scaleup_utils.py -dos -file _1d_hubbard_FINAL.ener
```



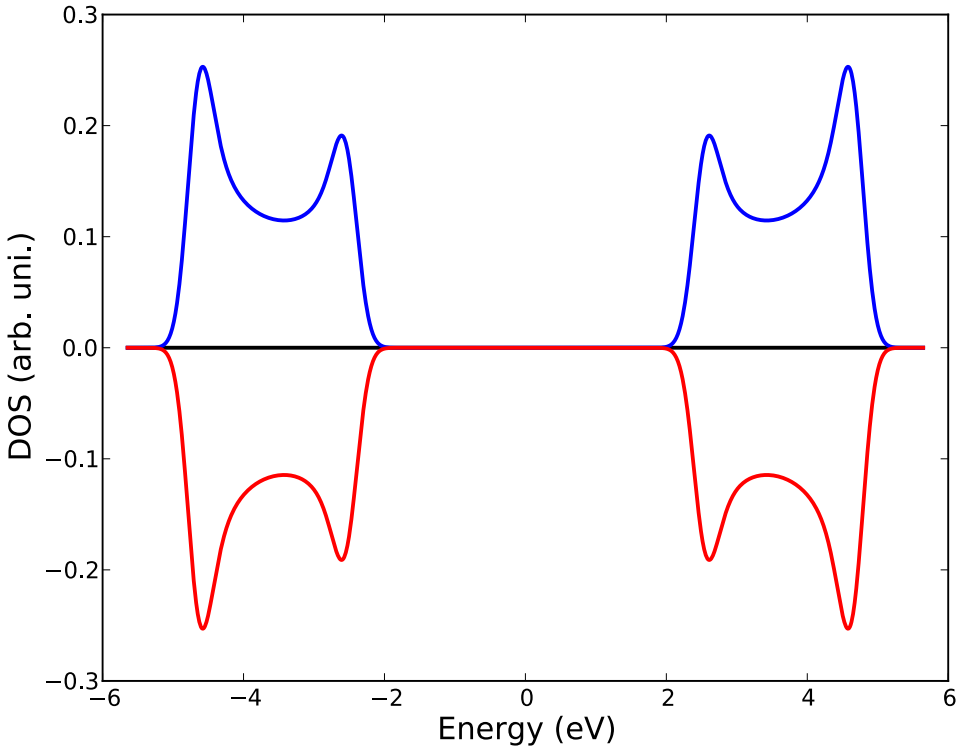
Increasing the value of U, we observe a phase transition to an antiferromagnetic state

$$U = I = 3.5\text{eV} \qquad \gamma = 2.0\text{eV}$$

Band structure



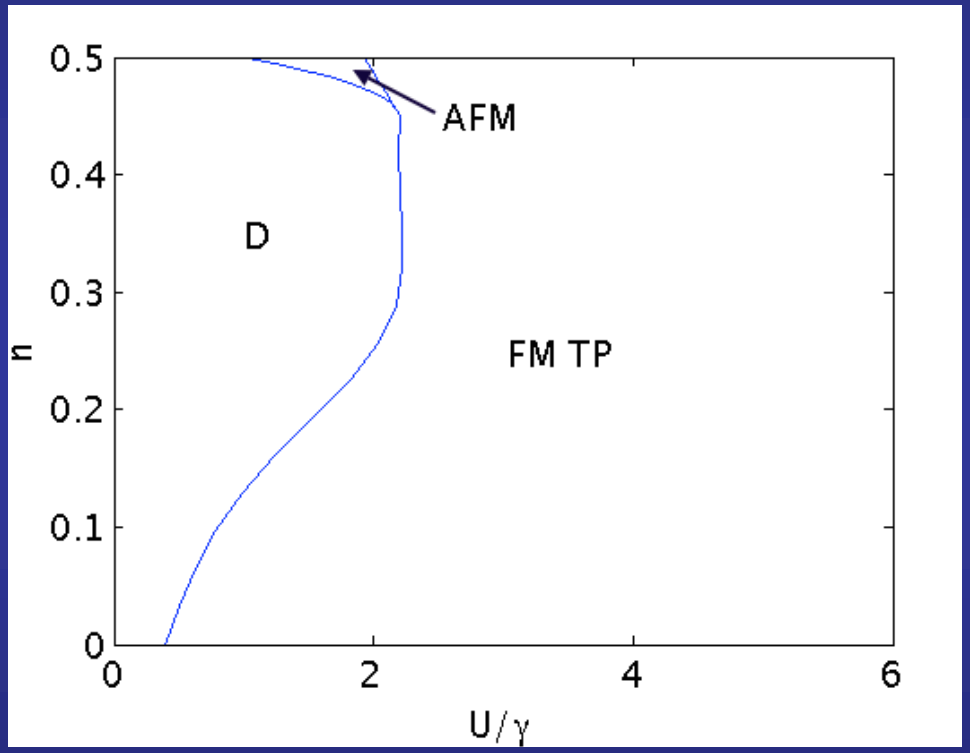
Density of states



Although the initial state was ferromagnetic, the code finds that the ground state is antiferromagnetic

To arrive to this conclusion, tight conditions on the SCF must be impossed

Phase diagram for the monoatomic chain with only one orbital per site



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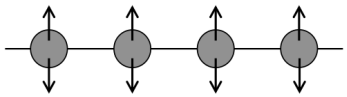
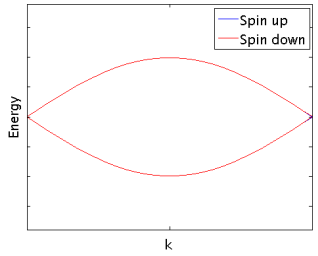
trabajo fin de grado, UC, 2017

Phase diagram for the monoatomic chain with only one orbital per site

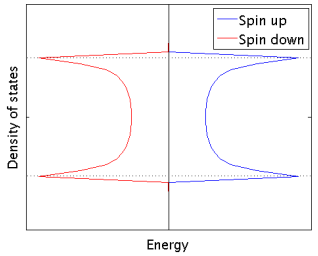
(a) Sketch diamagnetic.



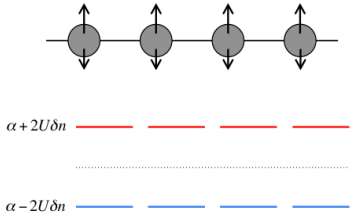
(b) Bands diamagnetic.



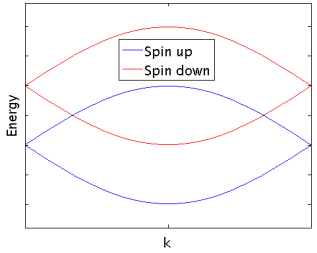
(c) DOS diamagnetic.



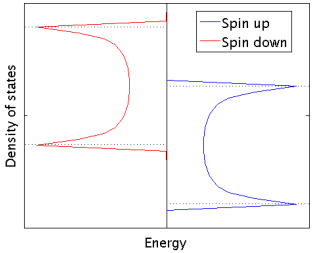
(d) Sketch ferromagnetic.



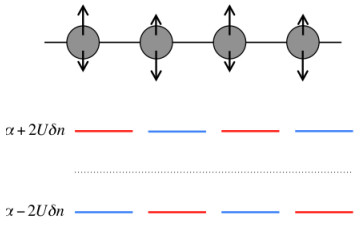
(e) Bands ferromagnetic.



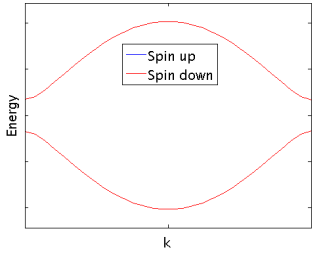
(f) DOS ferromagnetic.



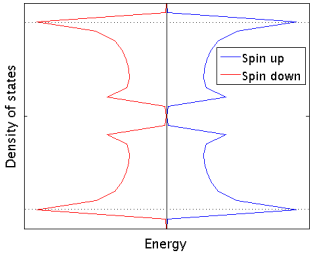
(g) Sketch antiferromagnetic.



(h) Bands antiferromagnetic.



(i) DOS antiferromagnetic.



Interestingly, this metallic phase is never obtained as the ground state of our simulations.

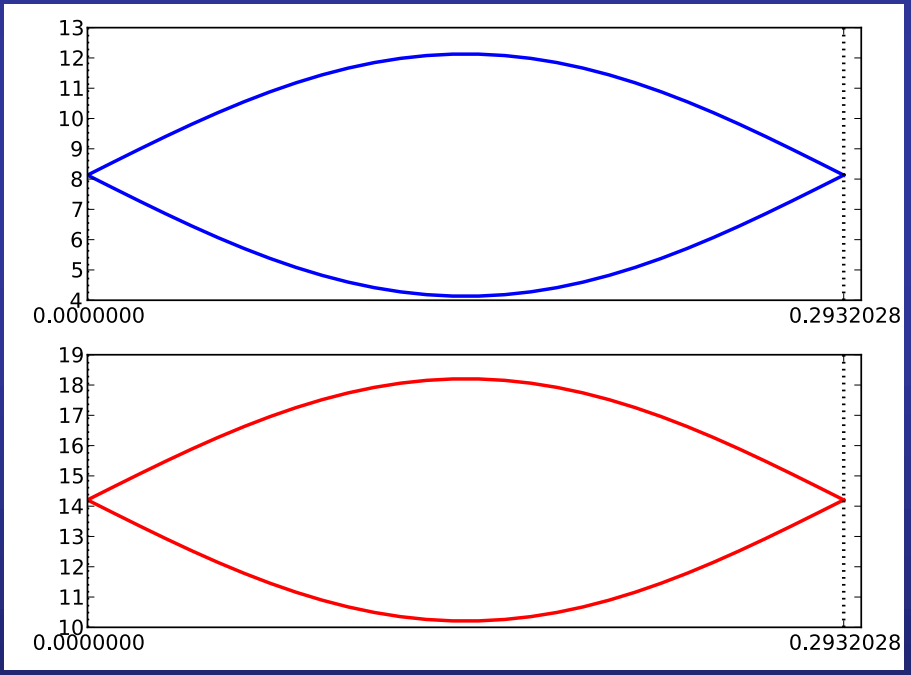
The ferromagnetic phase is stabilized only with large values of U/γ , with one spin band totally filled and the other totally empty

Marta Saiz de la Maza Cantero, trabajo fin de grado, UC, 2017

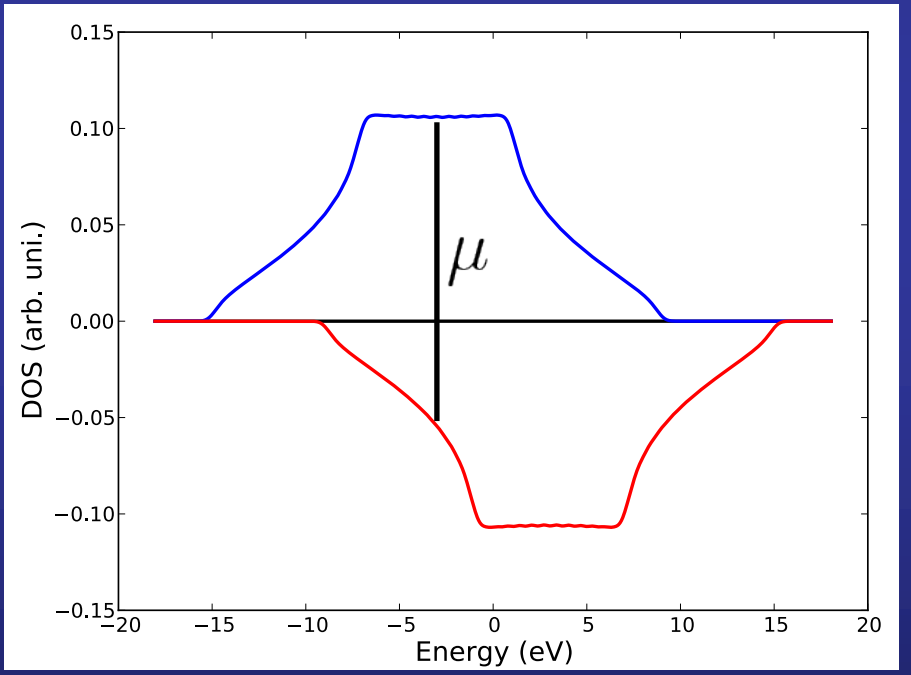
Phase transition to a ferromagnetic metallic ground state in 3D

```
$ <your_path_to_scale_up_dir>/bin/scaleup.x < < 3d_hubbard.fm.fdf > 3d_hubbard.fm.out

$ python  <your_path_to_scale_up_dir>/scripts/scaleup_utils.py -bands -file _3d_hubbard_fm_FINAL.bands

$ python  <your_path_to_scale_up_dir>/scripts/scaleup_utils.py -dos -file _3d_hubbard_fm_FINAL.ener -width 0.035
```

Bands



DOS



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Question: what does happen in 2D for half filling, where there is a logarithmic divergence at the center of the band width

The U in the Hubbard model modifies the values of the on-site terms of the Hamiltonian in real space

$$h^s_{ab} = \gamma_{ab} + \sum_{a'b'} \left[\left(D^s_{a'b'} + D^{-s}_{a'b'} \right) U_{aba'b'} - \left(D^s_{a'b'} - D^{-s}_{a'b'} \right) I_{aba'b'} \right] .$$

Eq. (71) of the paper

If we remember than in our model

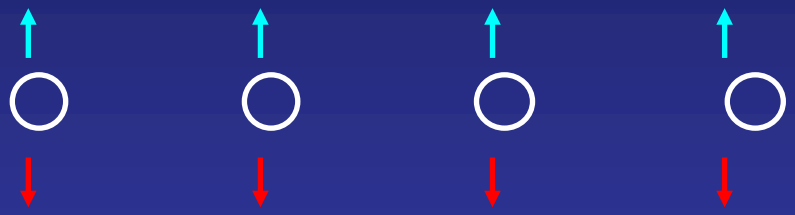
$$U_{aba'b'} = U \delta_{ab} \delta_{aa'} \delta_{ab'} = U_{aaaa} \qquad U_{aba'b'} = I_{aba'b'}$$

Then

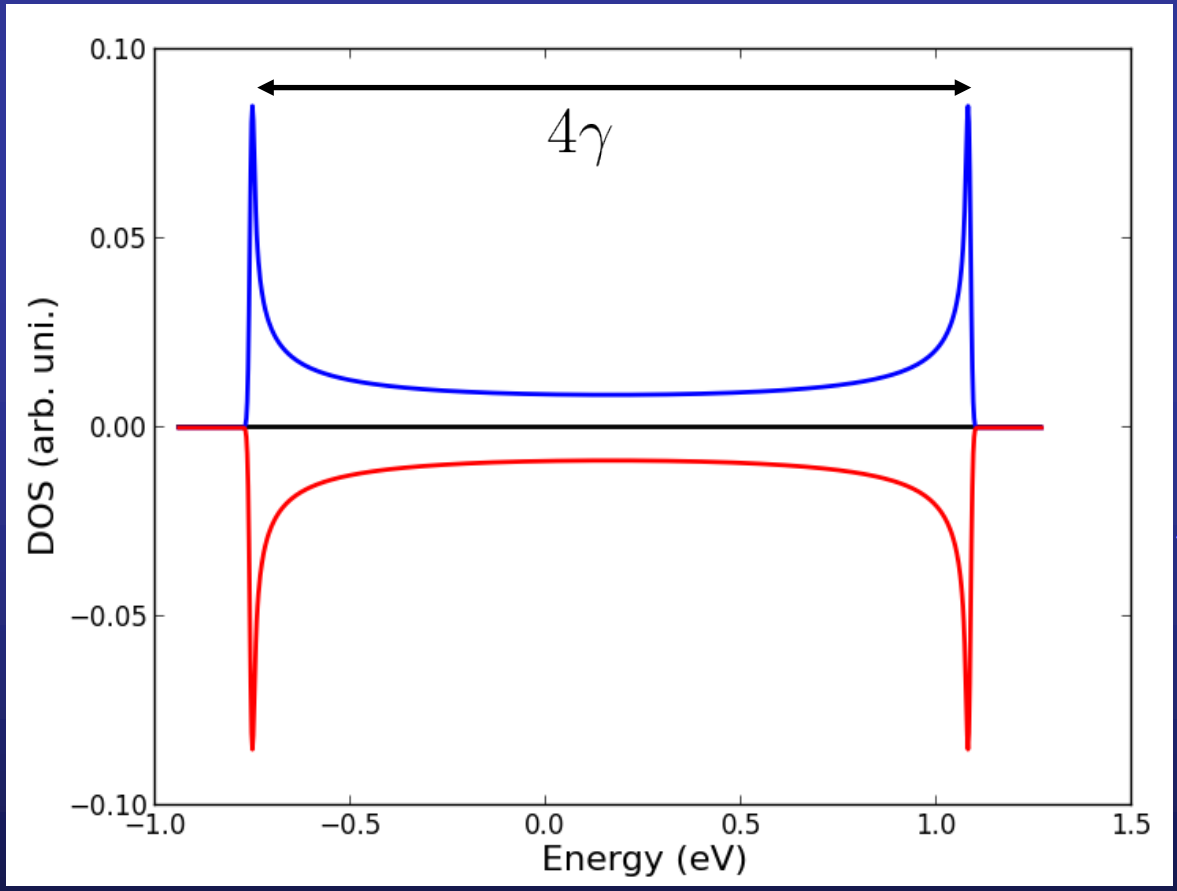
$$h^s_{aa} = \gamma_{aa} + 2 D^{-s}_{aa} U$$

D^{-s}_{aa} **is the diagonal component of the deformation density matrix: how many electrons are there at the Wannier function** χ_a **in excess or defect with respect the reference configuration**

The U in the Hubbard model modifies the values of the on-site terms of the Hamiltonian in real space



Reference configuration:
Diamagnetic
Same population for spin up and spin down on every atom

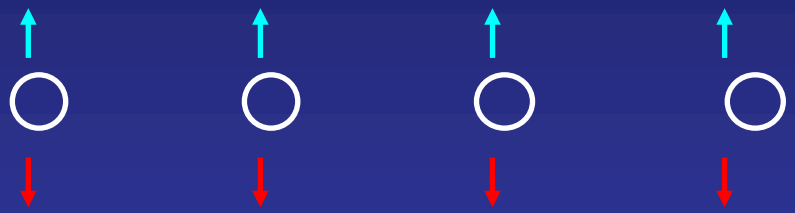


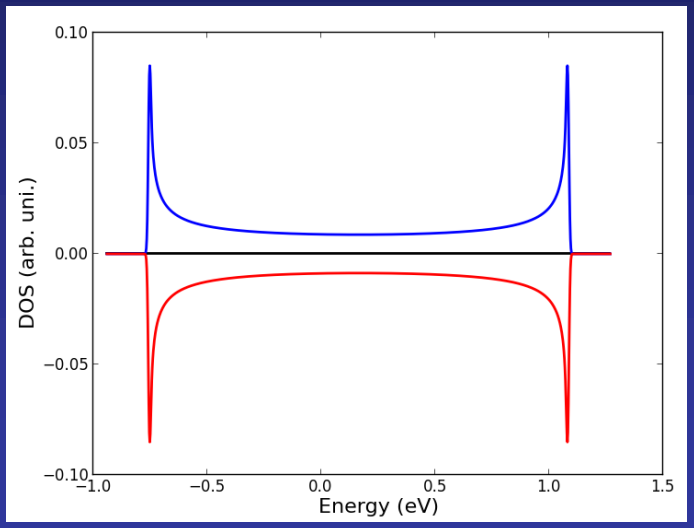
$\alpha = 0.164$ eV

$\gamma = 0.460$ eV

$n_0^{\text{atom}} = 0.8$ e

The U in the Hubbard model modifies the values of the on-site terms of the Hamiltonian in real space





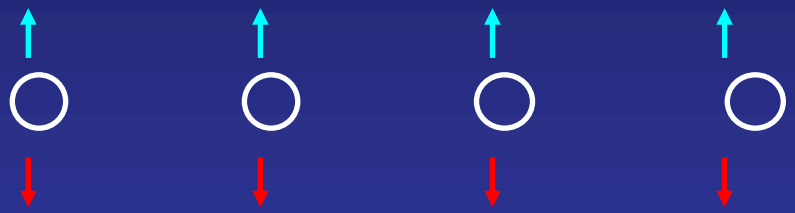
Initial configuration:
Ferromagnetic
Only spin up electrons.
Spin down channel is empty

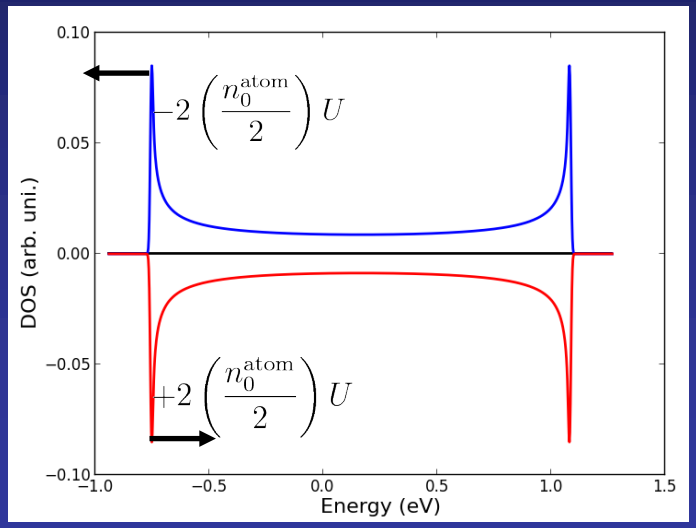
$$D_{aa}^{\uparrow} = \frac{n_0^{\text{atom}}}{2}$$

Diagonal terms of the deformation charge densities

$$D_{aa}^{\downarrow} = -\frac{n_0^{\text{atom}}}{2}$$

The U in the Hubbard model modifies the values of the on-site terms of the Hamiltonian in real space





Initial configuration:
Ferromagnetic
Only spin up electrons.
Spin down channel is empty

$$D_{aa}^{\uparrow} = \frac{n_0^{\text{atom}}}{2}$$

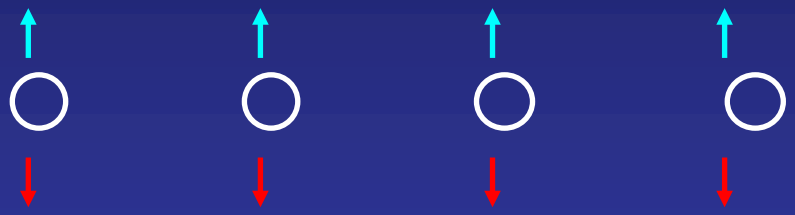
$$D_{aa}^{\downarrow} = -\frac{n_0^{\text{atom}}}{2}$$

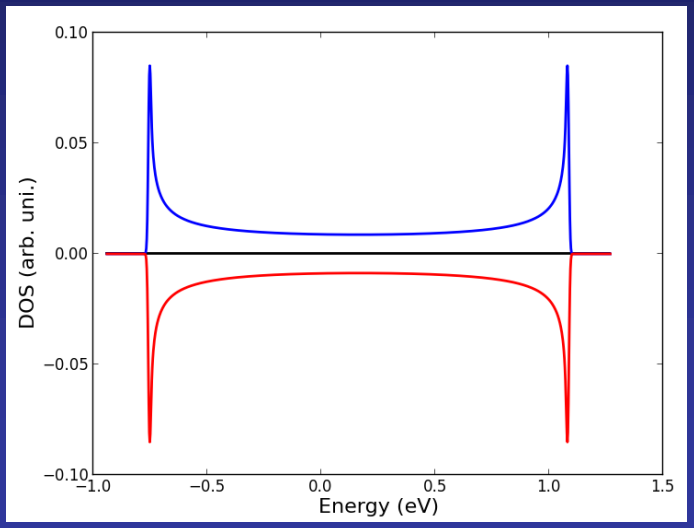
$\Longrightarrow$ **Change in the on-site term of the real space Hamiltonian** $\Longrightarrow$

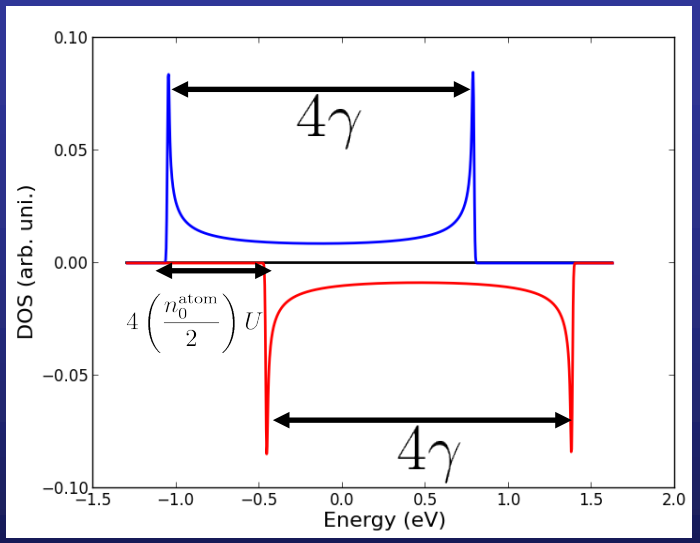
$$h_{aa}^{\uparrow} = \gamma_{aa} + 2D_{aa}^{\downarrow}U = \gamma_{aa} - 2\left(\frac{n_0^{\text{atom}}}{2}\right)U$$

$$h_{aa}^{\downarrow} = \gamma_{aa} + 2D_{aa}^{\uparrow}U = \gamma_{aa} + 2\left(\frac{n_0^{\text{atom}}}{2}\right)U$$

The U in the Hubbard model modifies the values of the on-site terms of the Hamiltonian in real space







$$h_{aa}^{\uparrow} = \gamma_{aa} + 2D_{aa}^{\downarrow}U = \gamma_{aa} - 2\left(\frac{n_0^{\mathrm{atom}}}{2}\right)U$$

$$h_{aa}^{\downarrow} = \gamma_{aa} + 2D_{aa}^{\uparrow}U = \gamma_{aa} + 2\left(\frac{n_0^{\mathrm{atom}}}{2}\right)U$$

$$U = 0.37 \text{ eV}$$