A step back : finding our way in the many-body labyrinth

Lucia Reining and Matteo Gatti
Palaiseau Theoretical Spectroscopy Group
And all of you here present

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→ The many-body marvel

→ The many-body problem

→ Observables

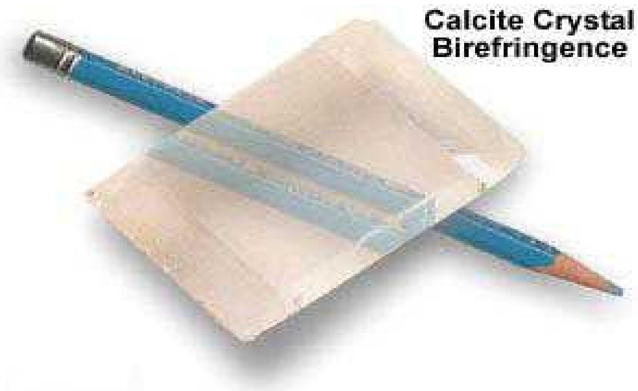
→ Descriptors and density functional theory

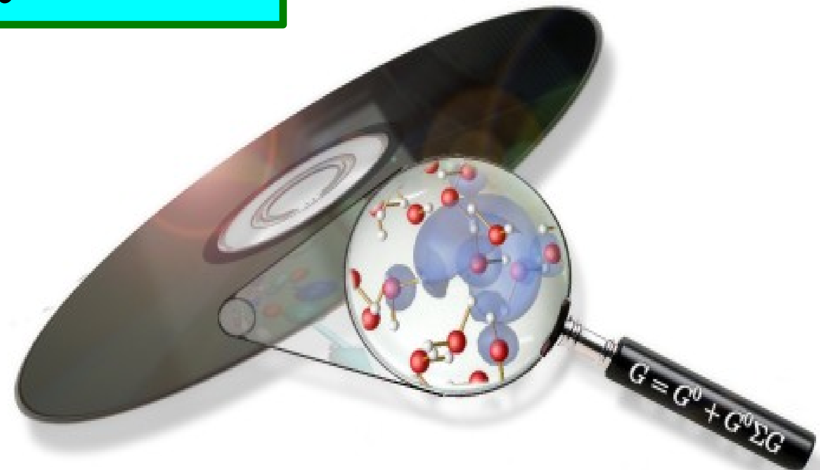
→ Effective worlds and the Kohn-Sham auxiliary system

→ The two fundamental difficulties with KS

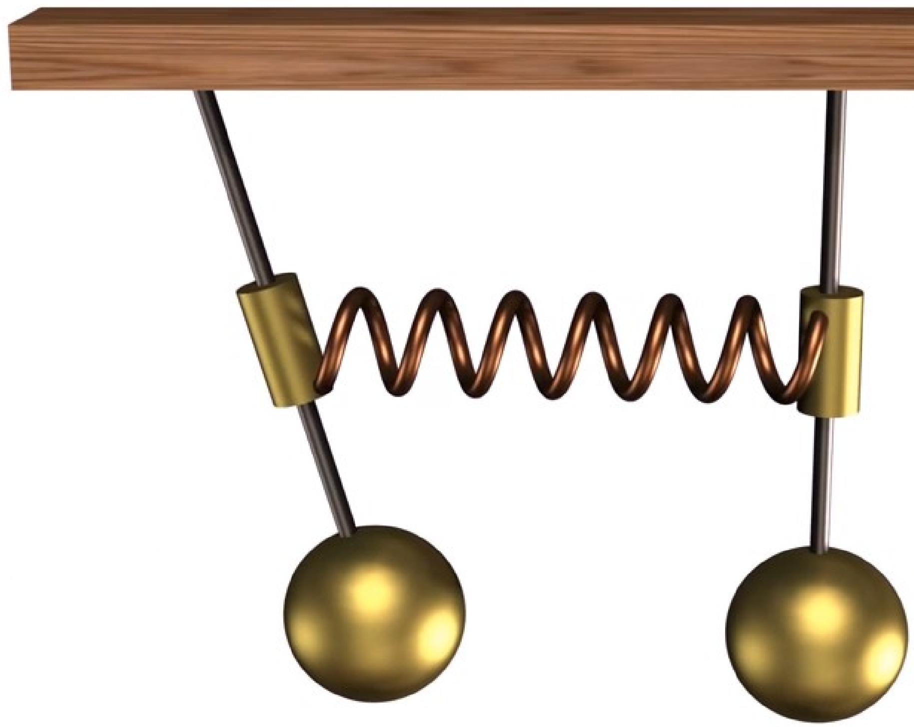
→ More complicated effective worlds: from KS to many-body (meeting on the way: Hartree-Fock, DFT+U, hybrids, GW,...)

→ The many-body marvel





NEMO



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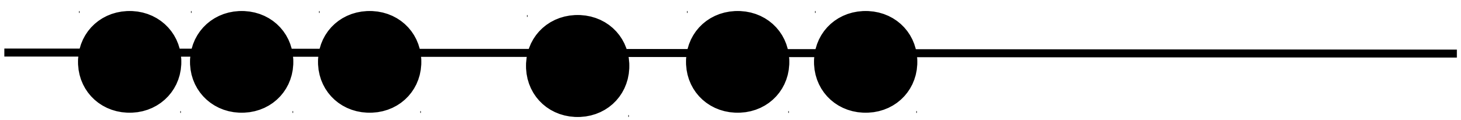
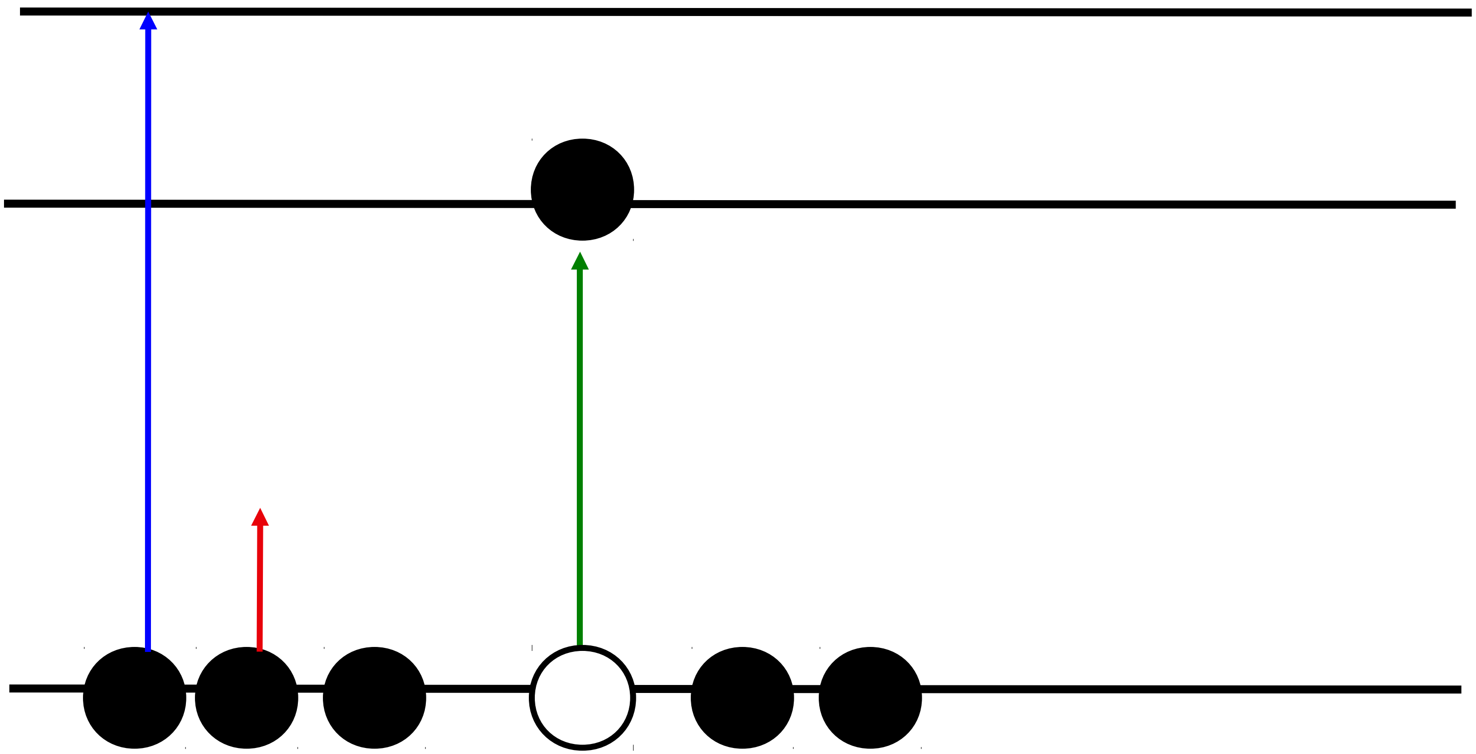
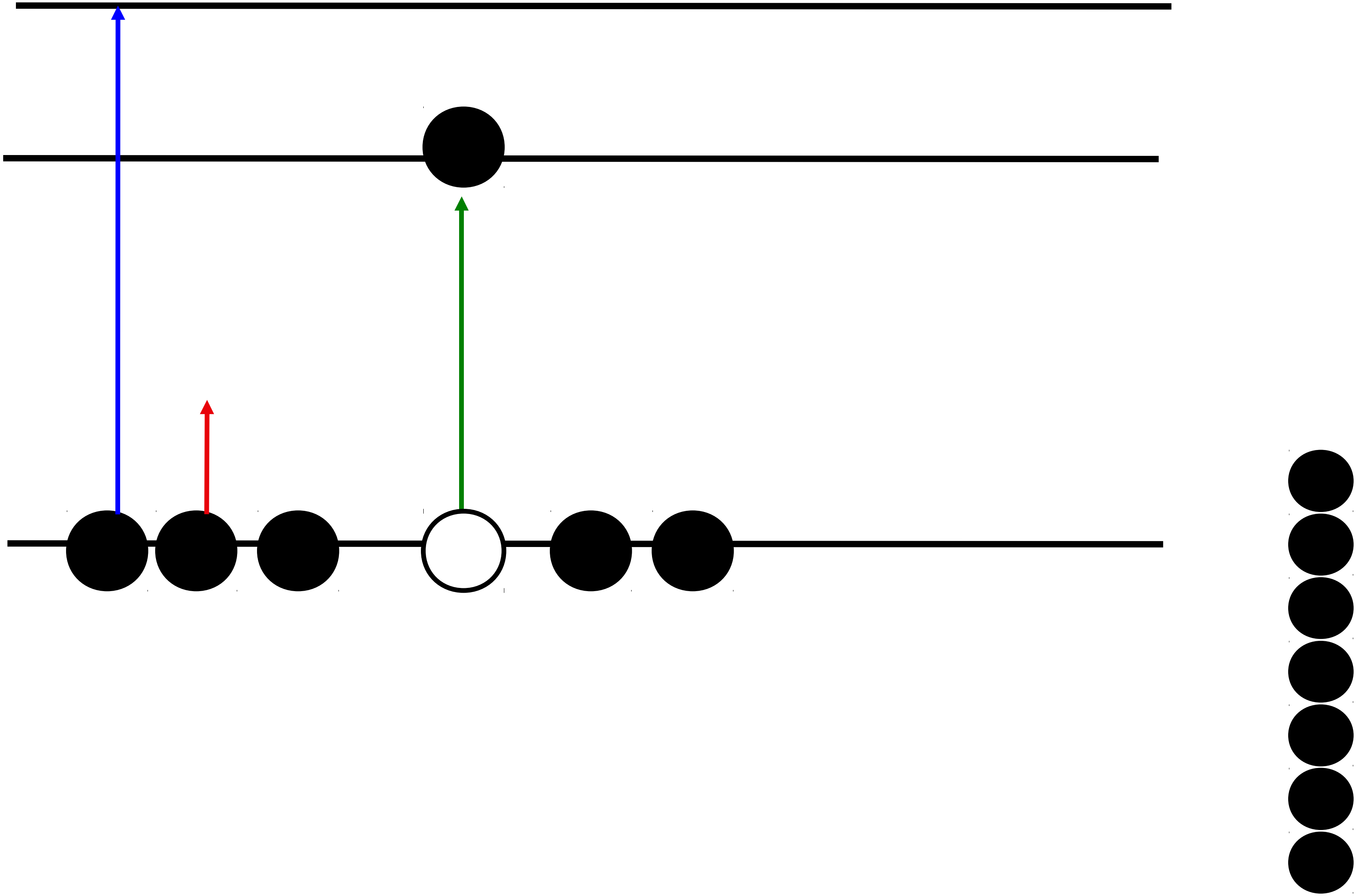
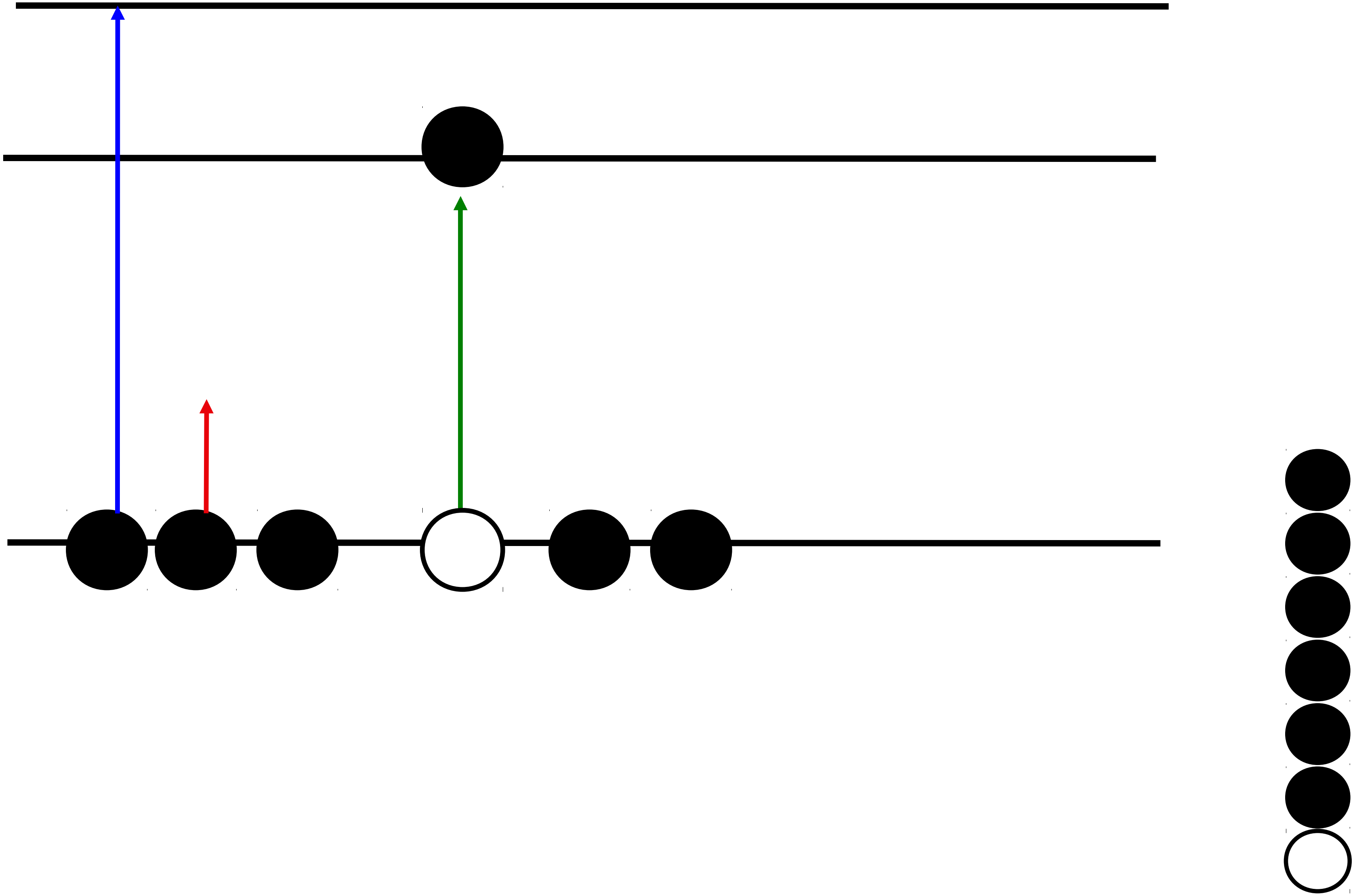
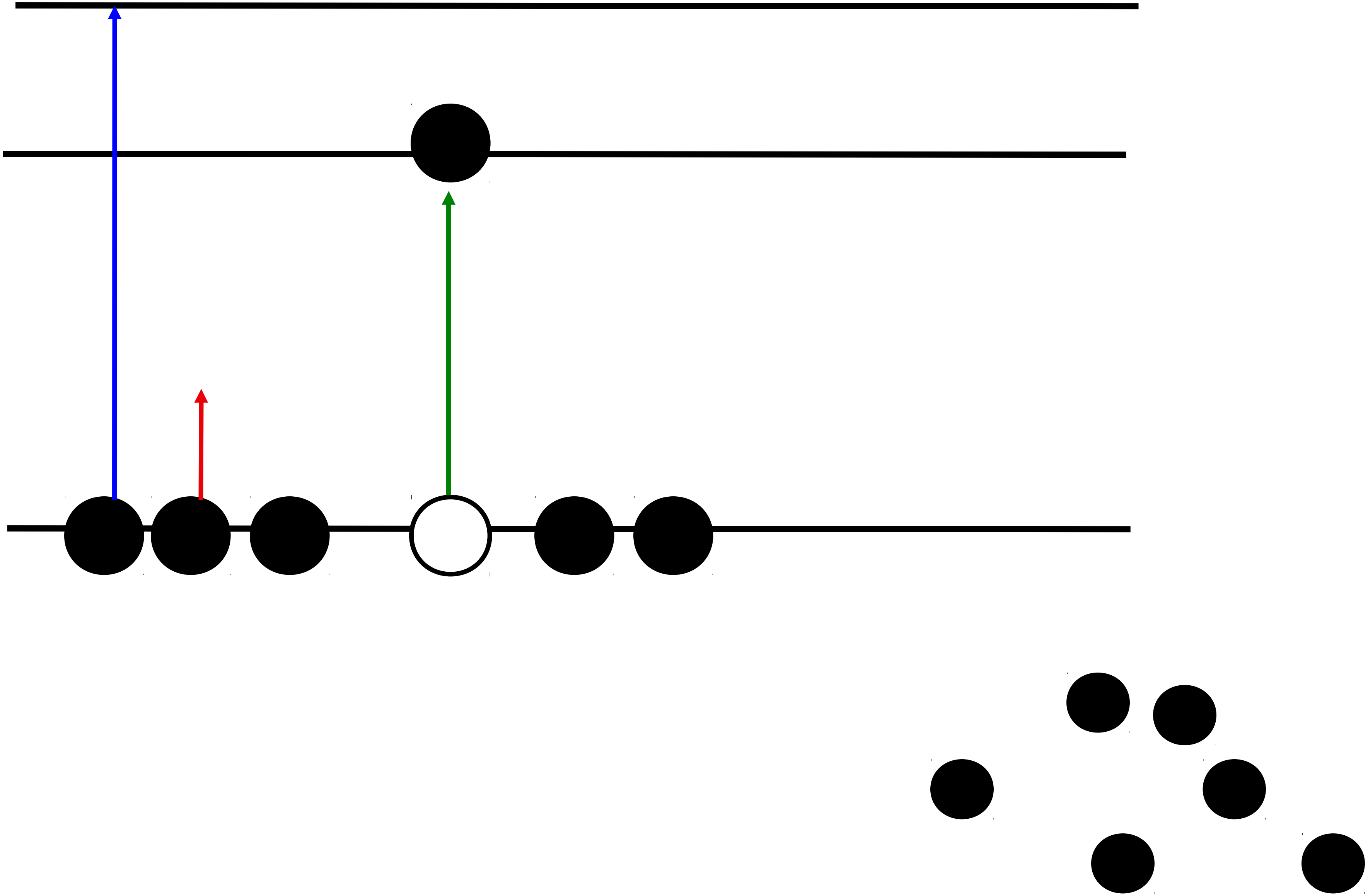
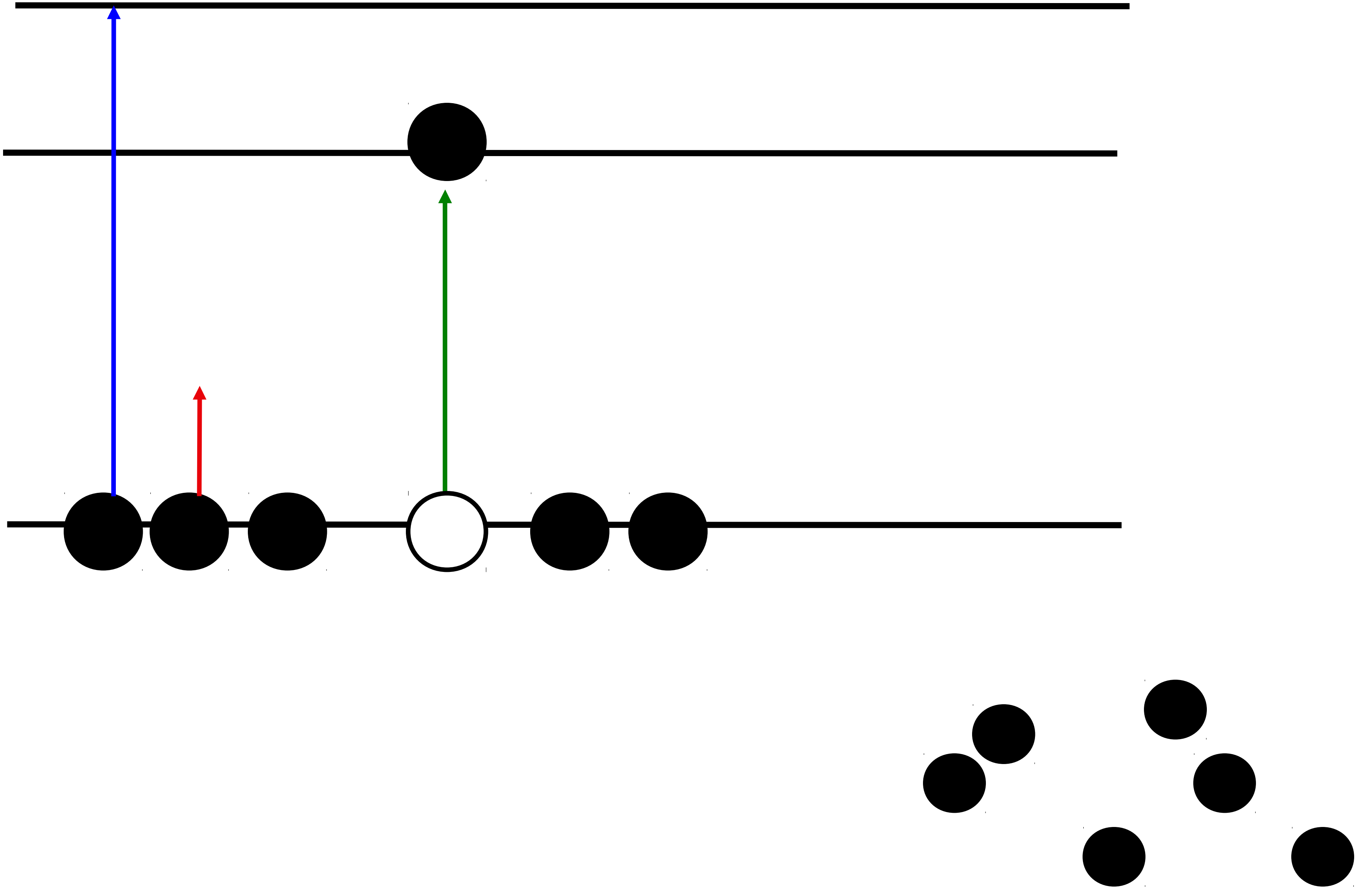


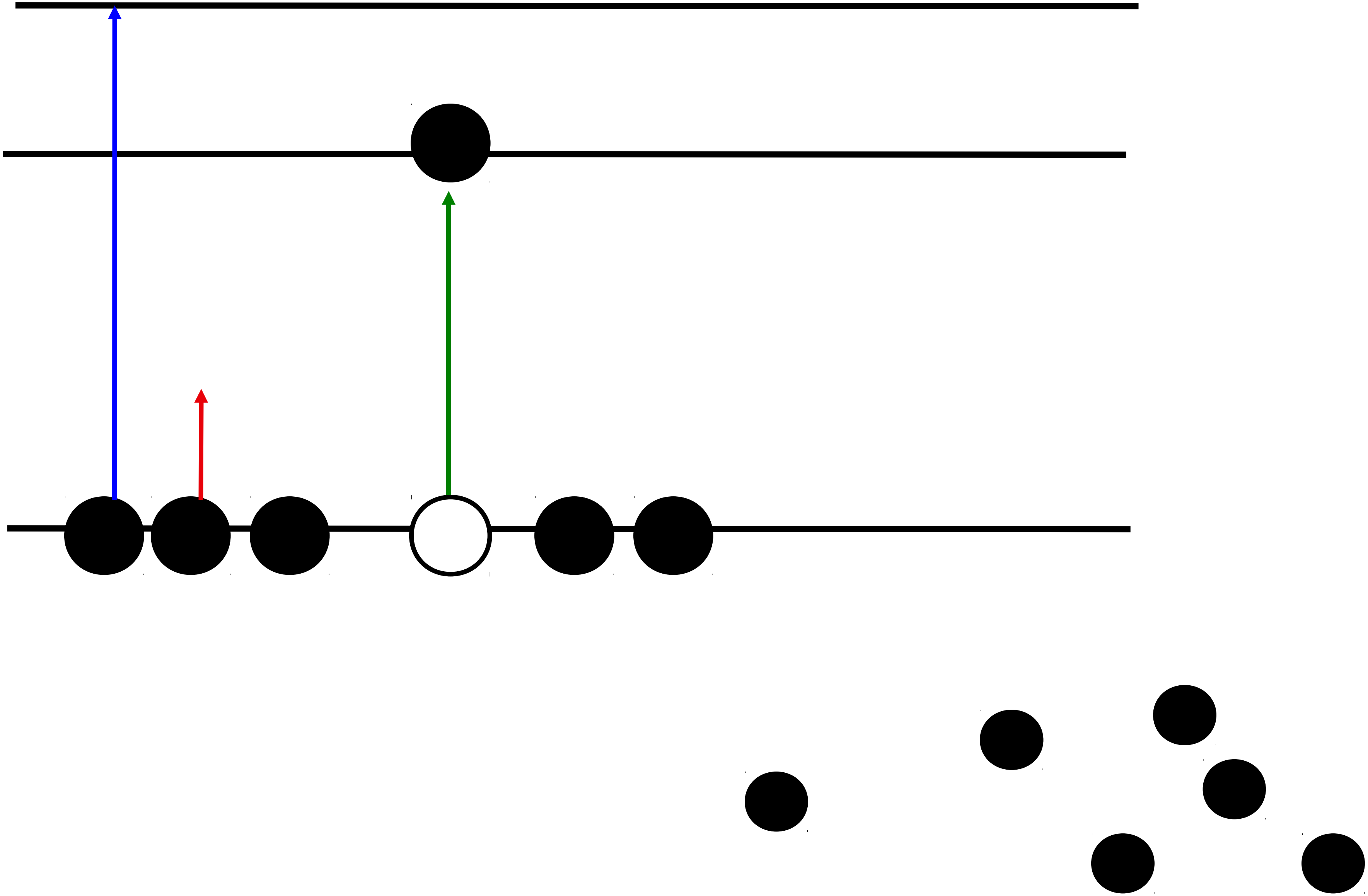


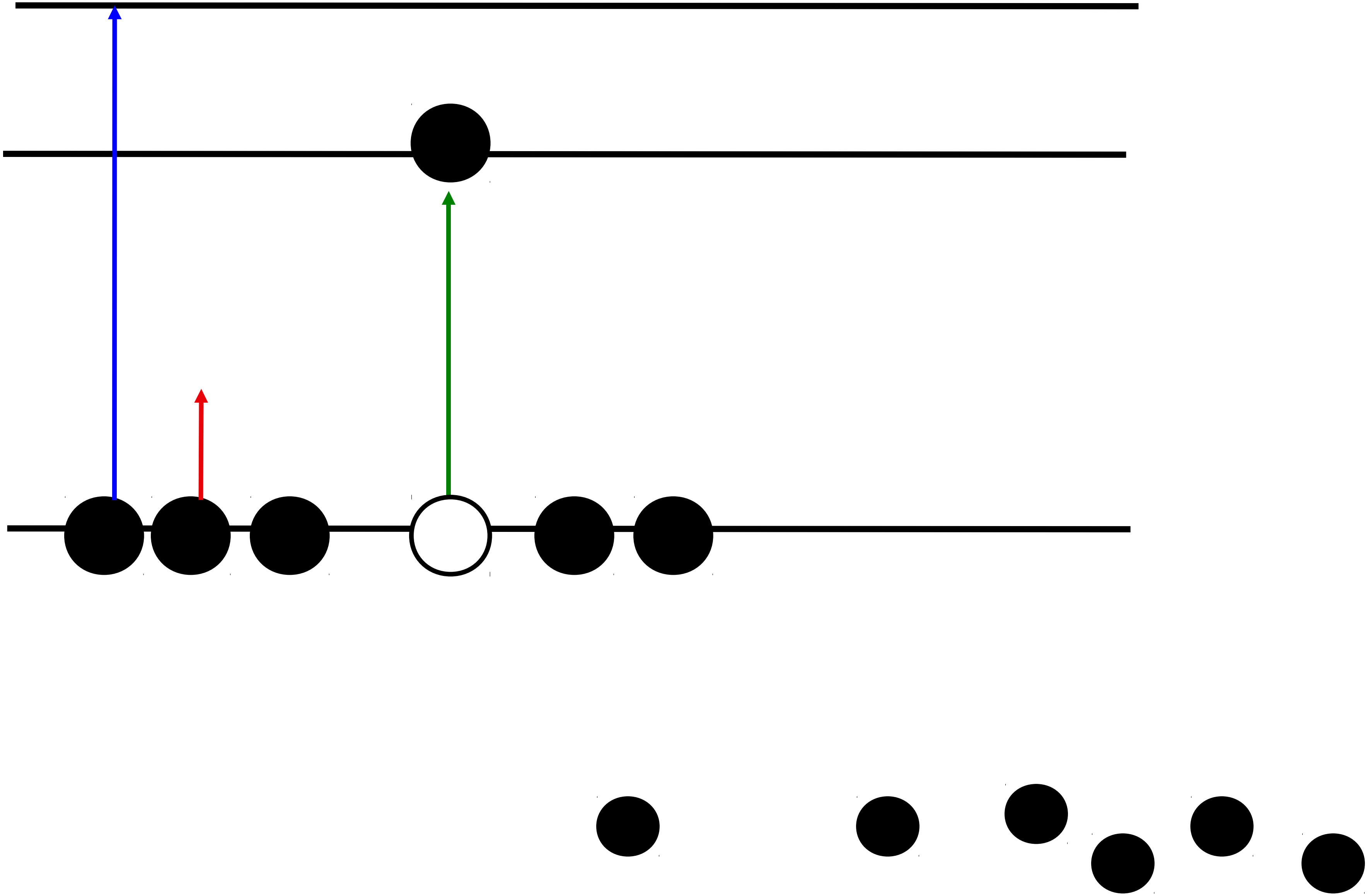


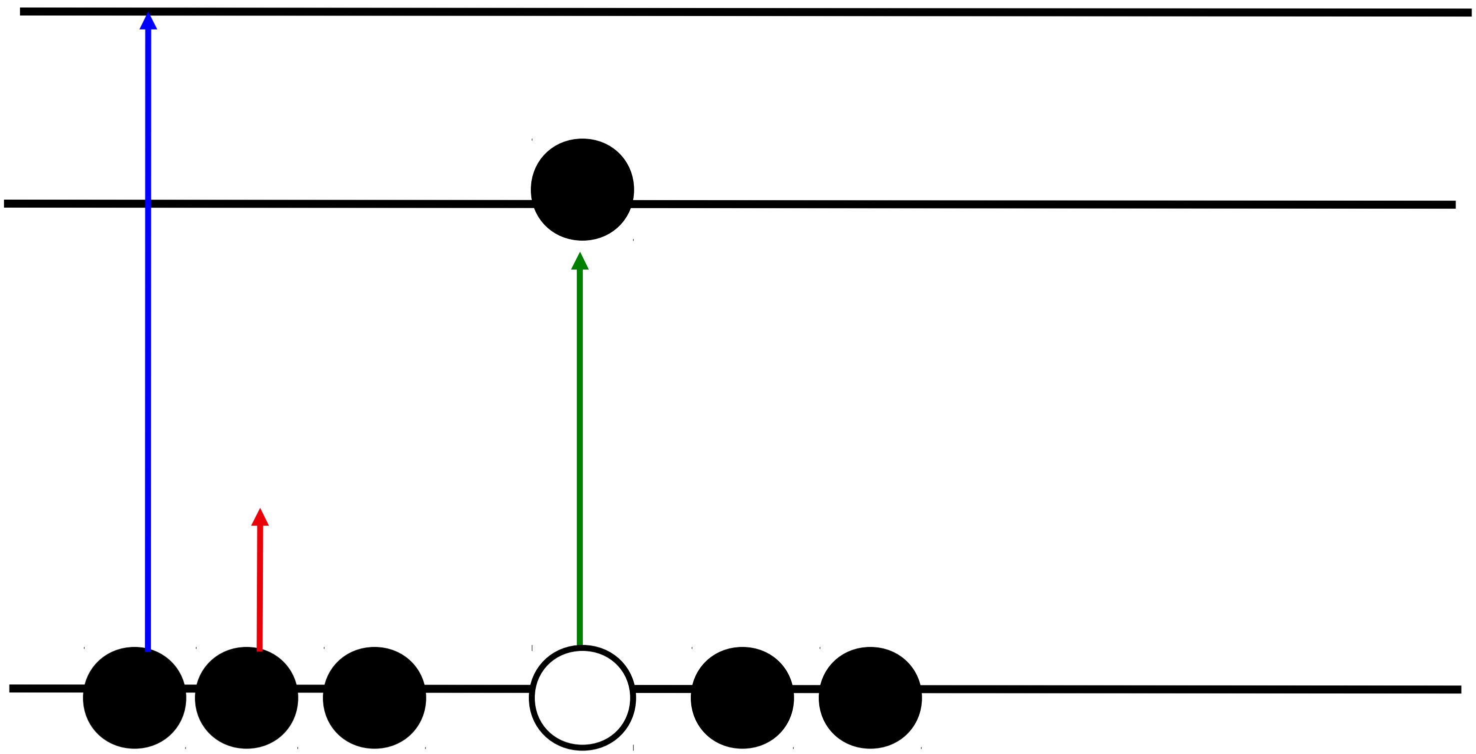




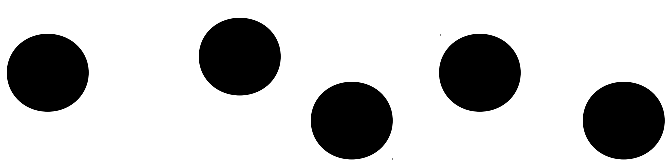




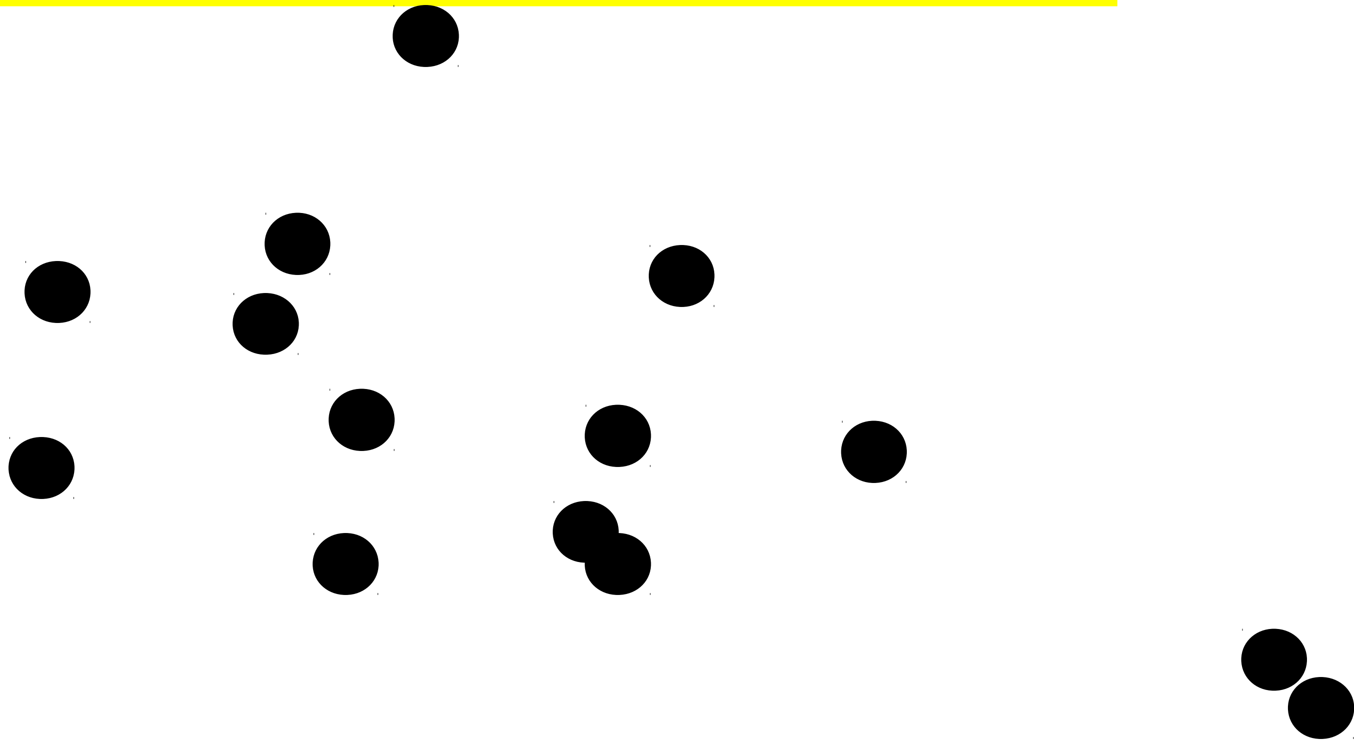




Electrons are interacting !!!



12 g of diamond:
3600000000000000000000000 electrons



12 g of diamond:
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$$\hat{H} = -\frac{\hbar^2}{2m_e}\sum_i \nabla_i^2 + \sum_i v_{\mathrm{ext}}(\mathbf{r}_i) + \frac{1}{2}\sum_{i\neq j}\frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|}$$

$$\hat{H}(\mathbf{r}_1, \mathbf{r}_2, \ldots.\mathbf{r}_N)\Psi_\lambda(x_1, x_2, \ldots..x_N) = E_\lambda \Psi_\lambda(x_1, x_2, \ldots..x_N)$$

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A tale of many particles

One particle

$$\phi(r)$$

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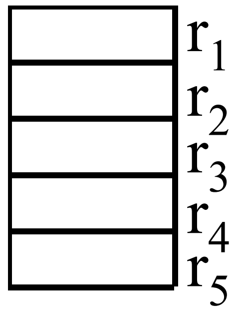
One particle

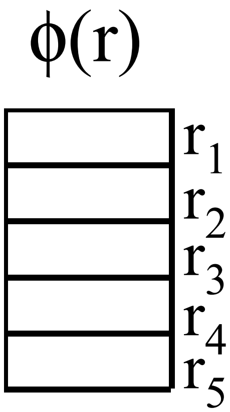
$$\phi(r)$$



5 points → 5 entries

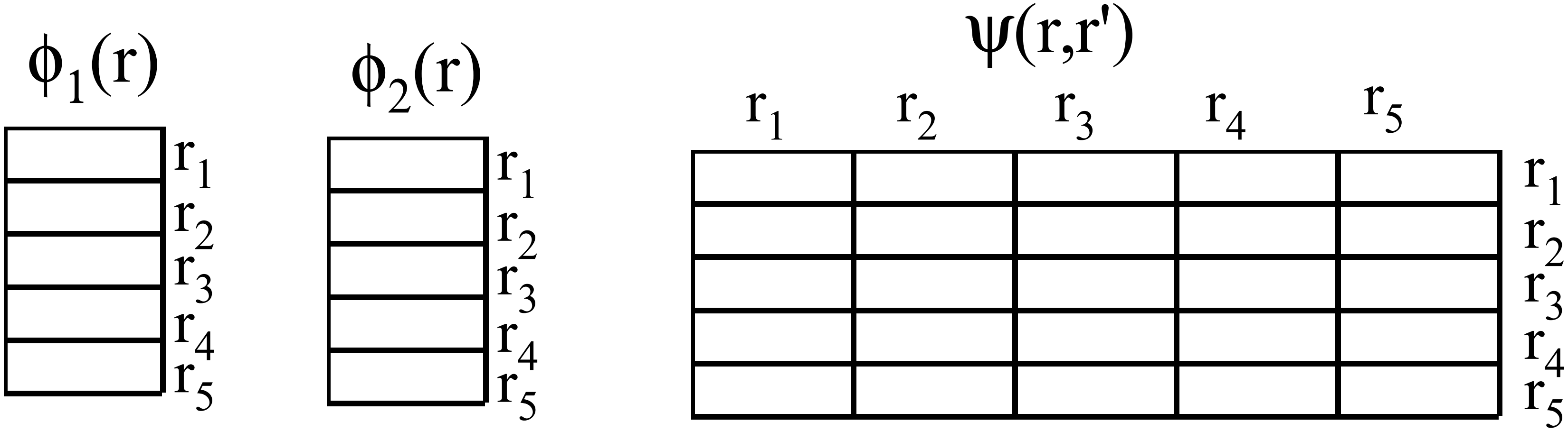
A tale of many particles

One particle



5 points → 5 entries

Two particles



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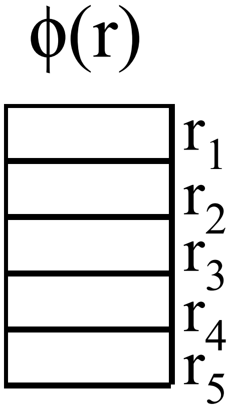

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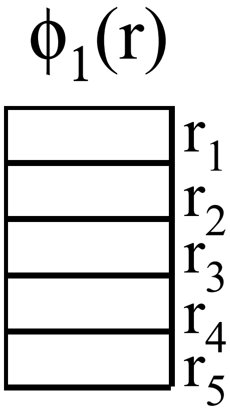
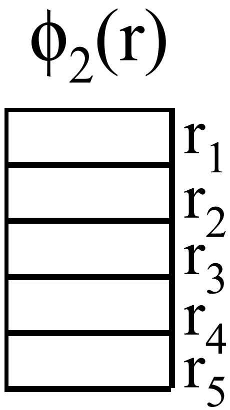
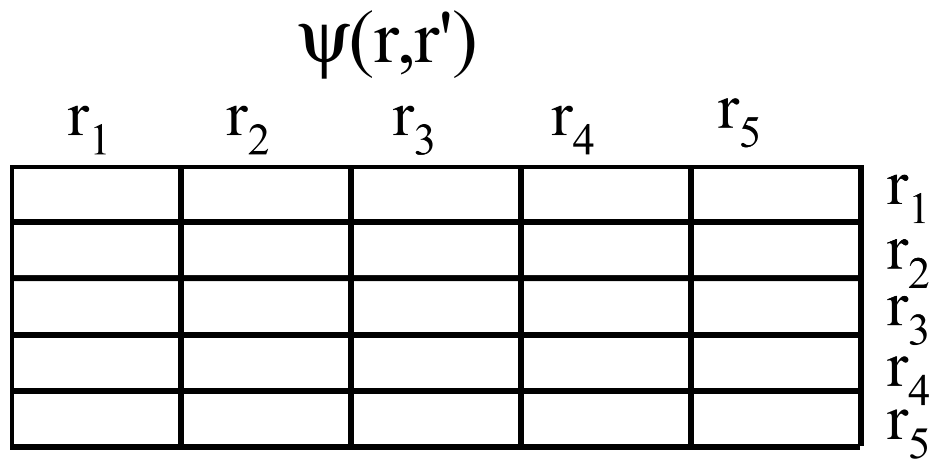




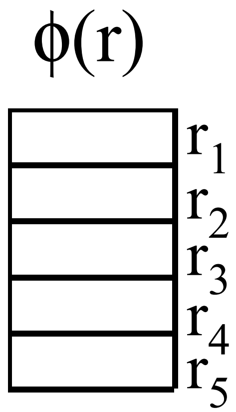
5 x 2 = 10 entries



5^2 = 25 entries

A tale of many particles

One particle

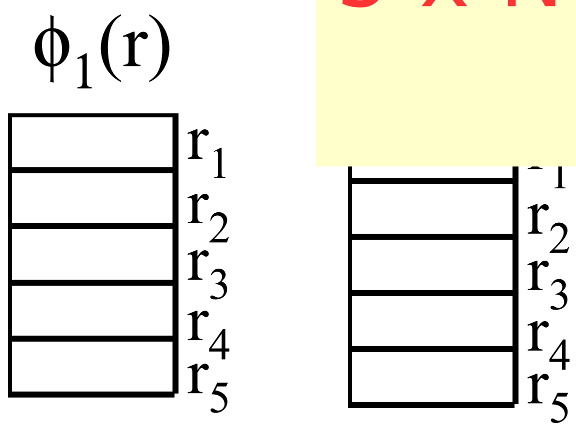


5 points → 5 entries

N particles ?

5 x N entries or 5^N entries ???

Two particles



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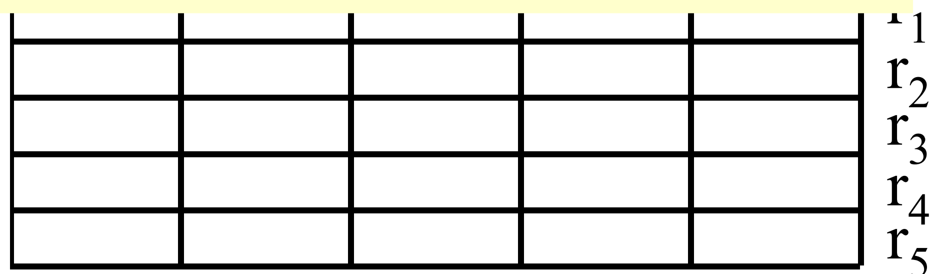

5^2 = 25 entries

Do we have to work with this monster???

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$\boxed{\text{→ Observables}}$

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→ Observables

$$\Psi(x_1, x_2, \ldots\ldots, x_N)$$

"If electron 1 is in position 1 and if electron 2 is in position 2 and..."

$$O = \langle \hat{O} \rangle$$

Observables are **expectation values**...........

$$O = \int \ldots \int dx_1 \ldots dx_N \, \Psi^*(x_1, \ldots . x_N) \sum_{i,j,\ldots} O(x_i, x_j, \ldots) \Psi(x_1, \ldots x_N)$$

…..............they do not care about each single situation!!!

Calculate only what you want,.....so that you can understand!

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What describes our system???

$$\Psi(x_1, x_2, \ldots\ldots, x_N)$$

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What describes our system???

$$O = O[\Psi] \qquad \tilde{O}[v_{\text{ext}}]$$

$$\cancel{\Psi(x_1, x_2, \ldots\ldots x_N)}$$

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What describes our system???

$$O = O[\Psi] \qquad \tilde{O}[v_{\mathrm{ext}}] \longrightarrow \boxed{O = \tilde{O}[n]}$$

→ Descriptors and density functional theory

$$\cancel{\Psi(x_1, x_2, \ldots\ldots, x_N)}$$

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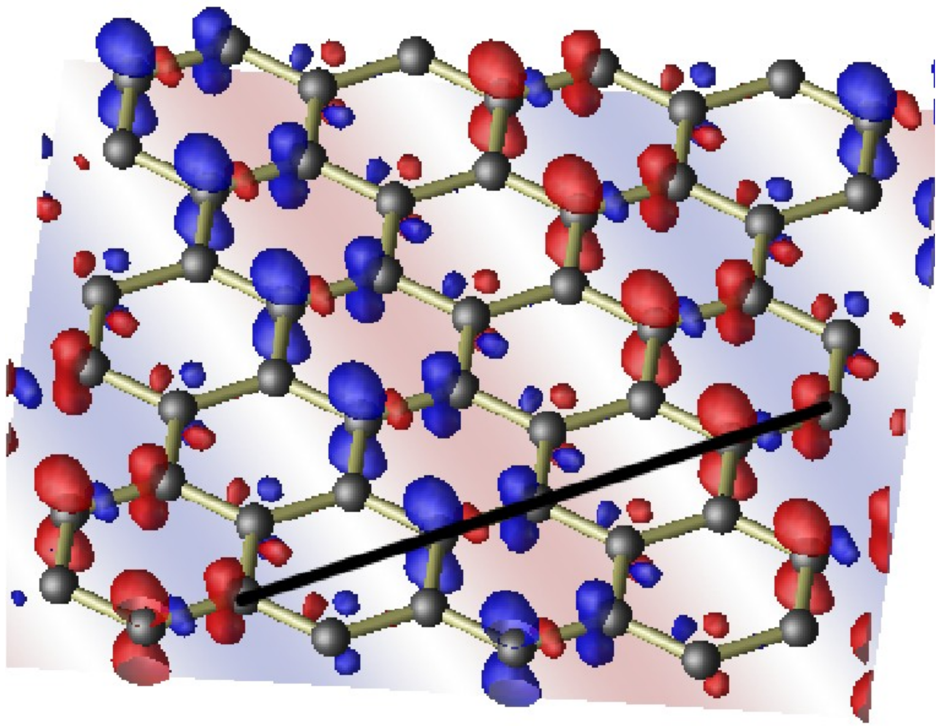
$$O = O[\Psi] \longrightarrow \boxed{O = \tilde{O}[n]}$$

→ Use a simpler descriptor,
such as the density *n(r)*

Good descriptor: density *n(r)*

"Density Functional Theory"



P. Hohenberg and W. Kohn, Phys. Rev. 136B 864 (1964)

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→ Effective worlds and the Kohn-Sham auxiliary system

$$O = \tilde{O}[n]$$

Problem 1: how to write e.g. *E[n]*?

(this the problem of finding a formula)

→ Effective worlds and the Kohn-Sham auxiliary system

$$O = \tilde{O}[n]$$

Problem 1: how to write e.g. *E[n]*?

$$O = \tilde{O}[n]$$

Problem 2: how to calculate *n*?

(this is the problem of finding the input values in our formula)

→ How do we think ?

Build an effective world

Image from pixabay:
www.noft-traders.com/establish-zero-gravity-zones-with-supply-and-demand/

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1. Good descriptor: density *n(r)*

So, first we have to calculate the density → DFT

2. Auxiliary system → Kohn-Sham system

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$$v_{\text{eff}}(\mathbf{r}) = v_{\text{ext}}(\mathbf{r}) + v_{\text{H}}([n],\mathbf{r}) + v_{\text{xc}}([n],\mathbf{r})$$

W. Kohn and L. J. Sham, Phys. Rev. 140A 1133 (1965)

Much simpler than $\hat{H}\Psi_\lambda(x_1, x_2, \ldots.., x_N) = E_\lambda\Psi_\lambda(x_1, x_2, \ldots.., x_N)$

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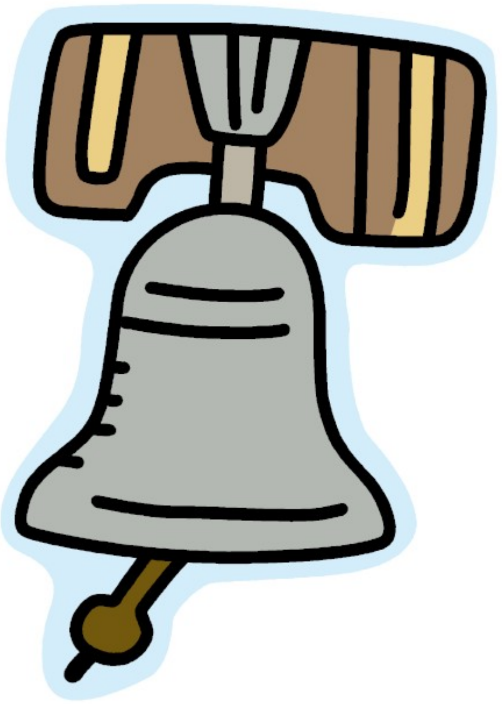
This non-interacting world simulates correctly the density

What about other observables?

Spectroscopy



Spectroscopy

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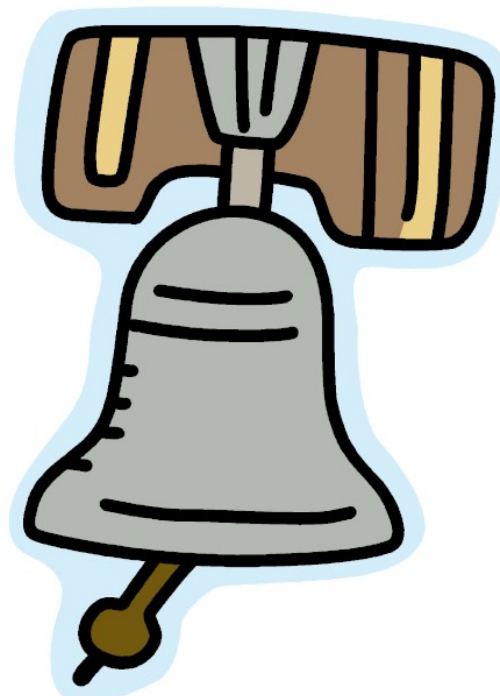
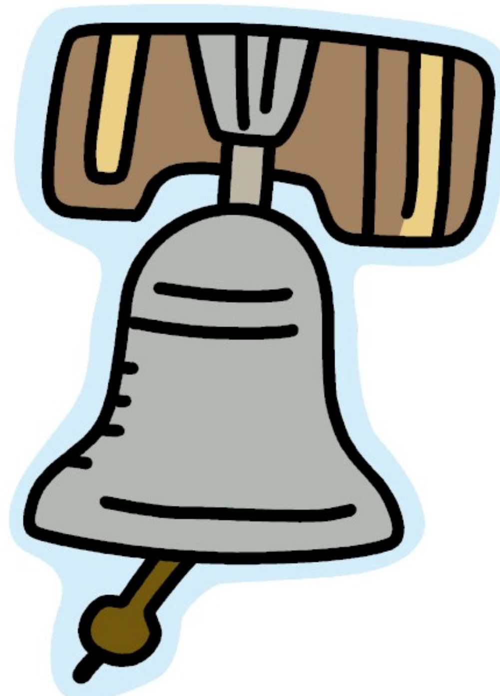


Spectroscopy

Perturbation



Excitation

Response

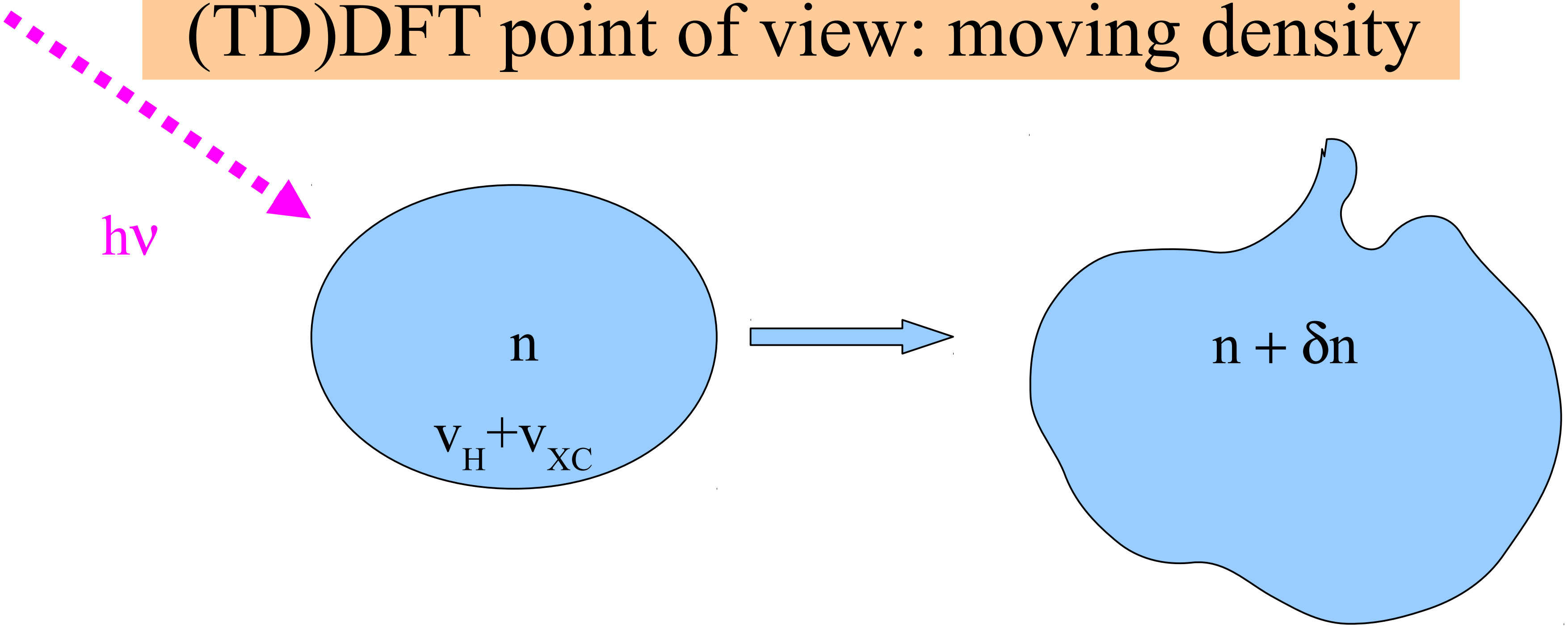
→ Go time dependent!!!

1. Good descriptor: density *n(r)* **[or *n(r,t)*]**

So, first we have to calculate the density → DFT

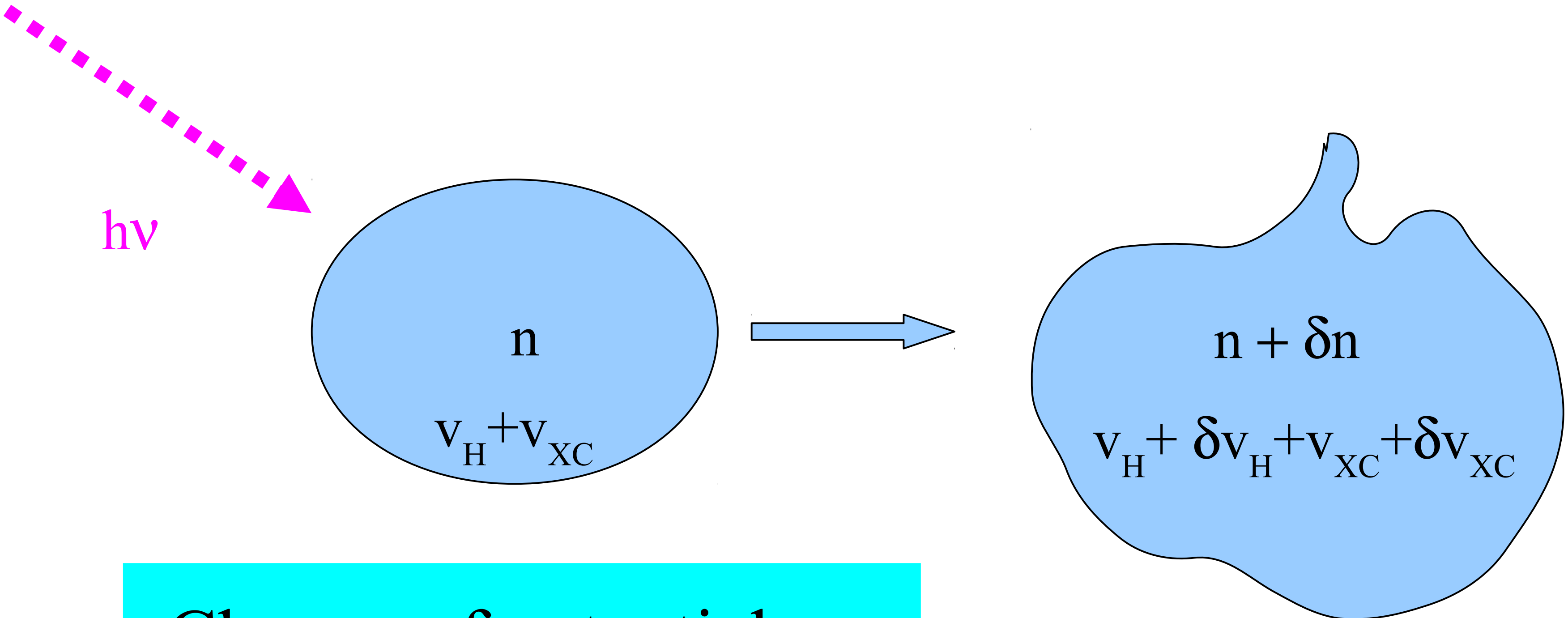
Making it time-dependent:

(TD)DFT point of view: moving density



Excitation ?

→ Induced potentials



Change of potentials

Excitation ?

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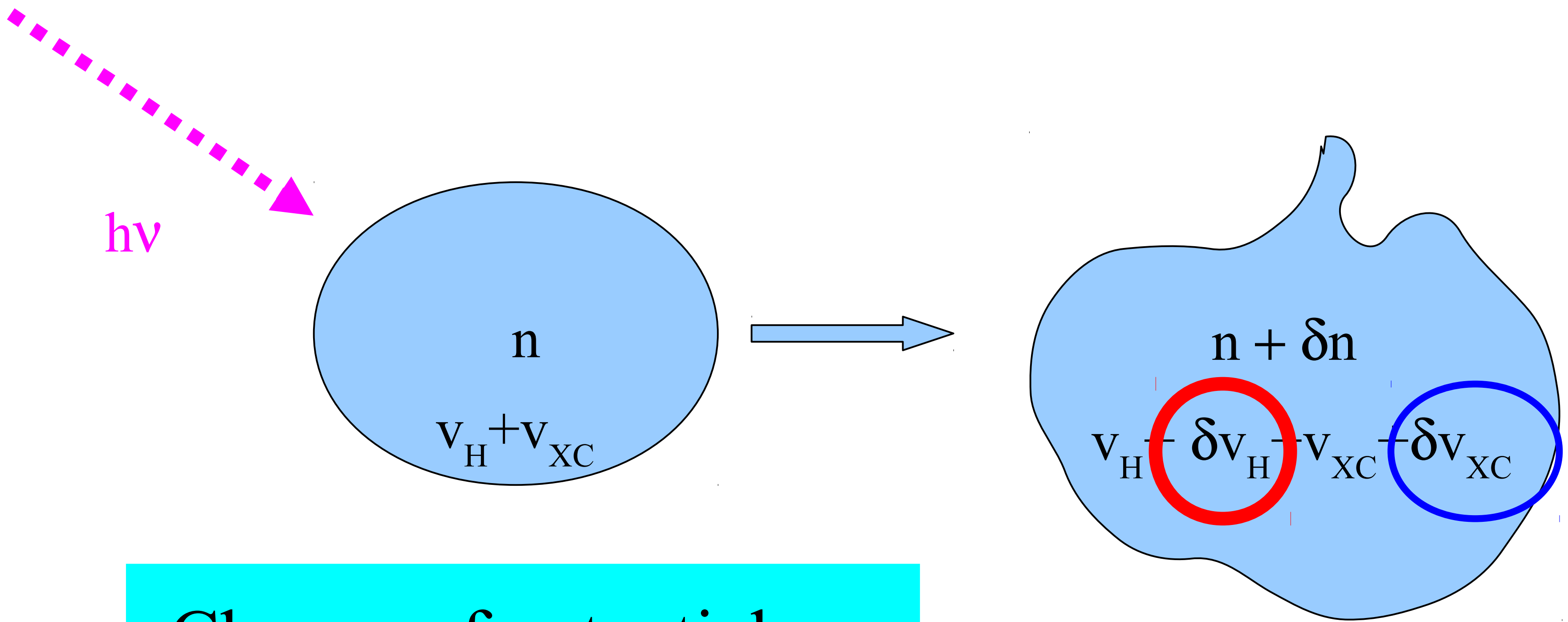

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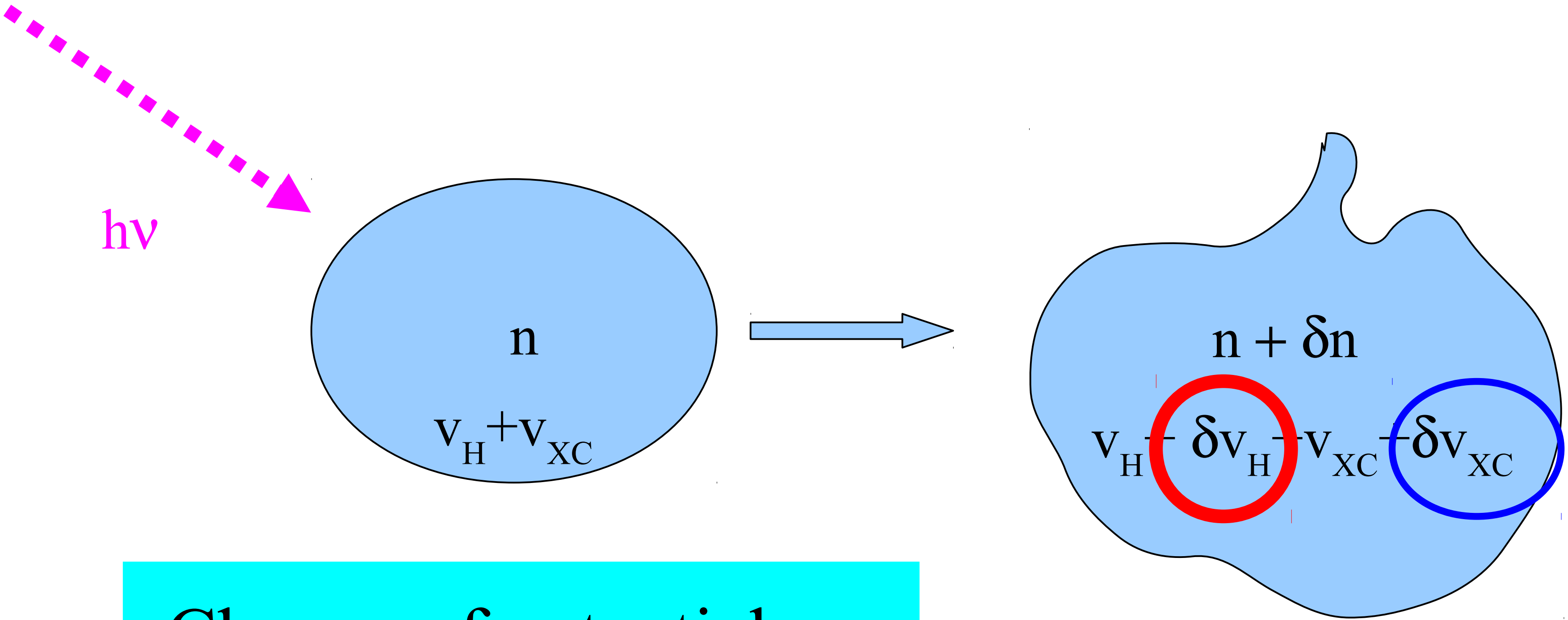


Change of potentials

RPA

ALDA, ...

Approximations

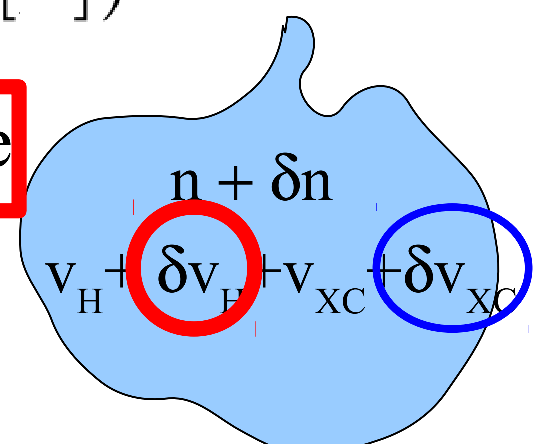
$$\frac{\delta v_H(\mathbf{r},t;[n])}{\delta n(\mathbf{r}',t')} = \frac{\delta \int d\mathbf{x}\, v_c(\mathbf{r}-\mathbf{x})n(\mathbf{x},t)}{\delta n(\mathbf{r}',t')} = v_c(\mathbf{r}-\mathbf{r}')$$

$$\frac{\delta v_{\mathrm{xc}}(\mathbf{r},t;[n])}{\delta n(\mathbf{r}',t')} \equiv f_{\mathrm{xc}}(\mathbf{r},\mathbf{r}',t,t';[n])$$

Memory!

$$f_{\mathrm{xc}}(\mathbf{r},\mathbf{r}',t-t';[n]) \rightarrow f_{\mathrm{xc}}(\mathbf{r},\mathbf{r}',\omega;[n])$$

In equilibrium: memory $\rightarrow \omega$ - dependence



→ ...and even if we just want the density:

1. Good descriptor: density *n(r)* [or *n(r,t)*]

So, first we have to calculate the density → DFT

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The KS auxiliary world is very simple ("local potential").

→ Excursion: what do we mean by "local"?

Local potential

$$v_{xc}\left([n],\mathbf{r}\right)\varphi(\mathbf{r})$$

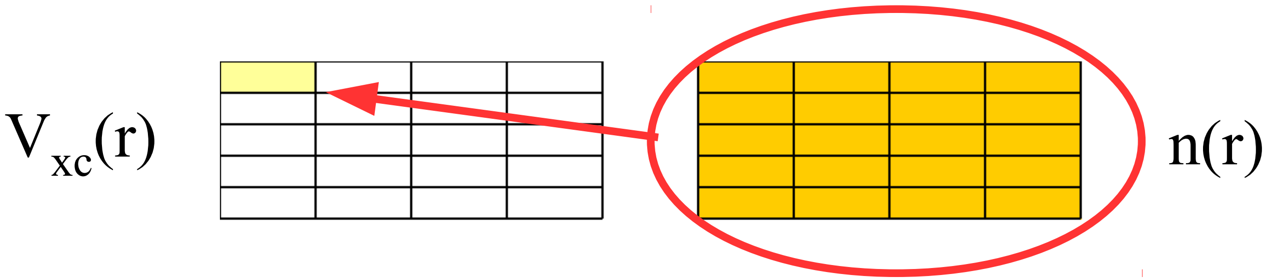
Non-local potential

$$\int d\mathbf{r}' V(\mathbf{r},\mathbf{r}')\varphi(\mathbf{r}')$$

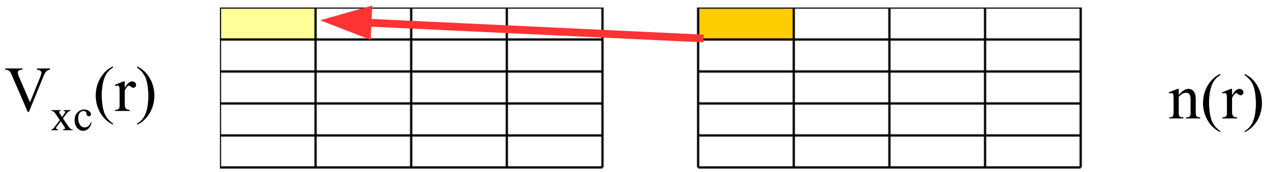
→ Excursion: what do we mean by "local"?

Local potential	Non-local potential
$v_{xc}([n], \mathbf{r})\,\varphi(\mathbf{r})$	$\int d\mathbf{r}' V(\mathbf{r}, \mathbf{r}')\varphi(\mathbf{r}')$

Non-local functional



Local functional



→ ...and even if we just want the density:

1. Good descriptor: density *n(r)* [or *n(r,t)*]

The design of the effective world
versus the way to approximate the design

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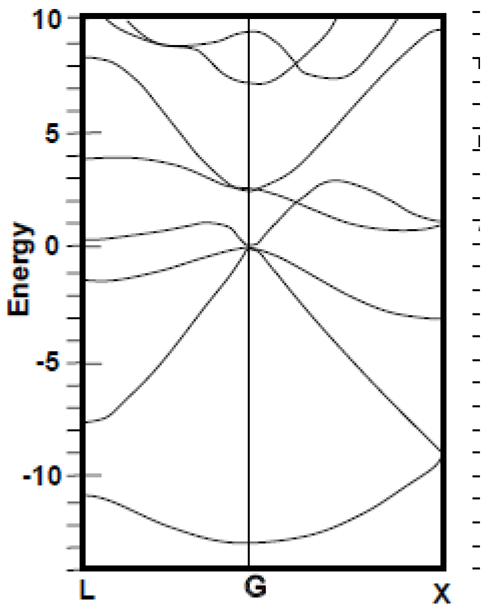
→ More complicated effective worlds

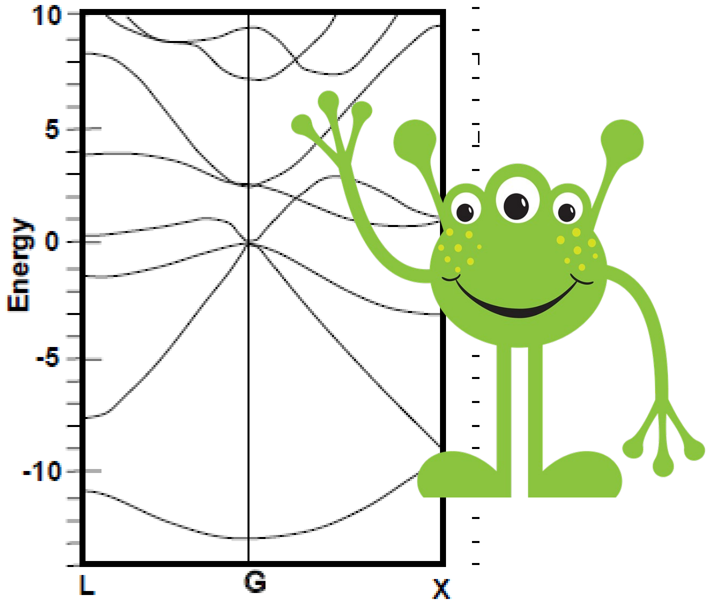
LDA



Bandstructure of germanium, theory versus experiment

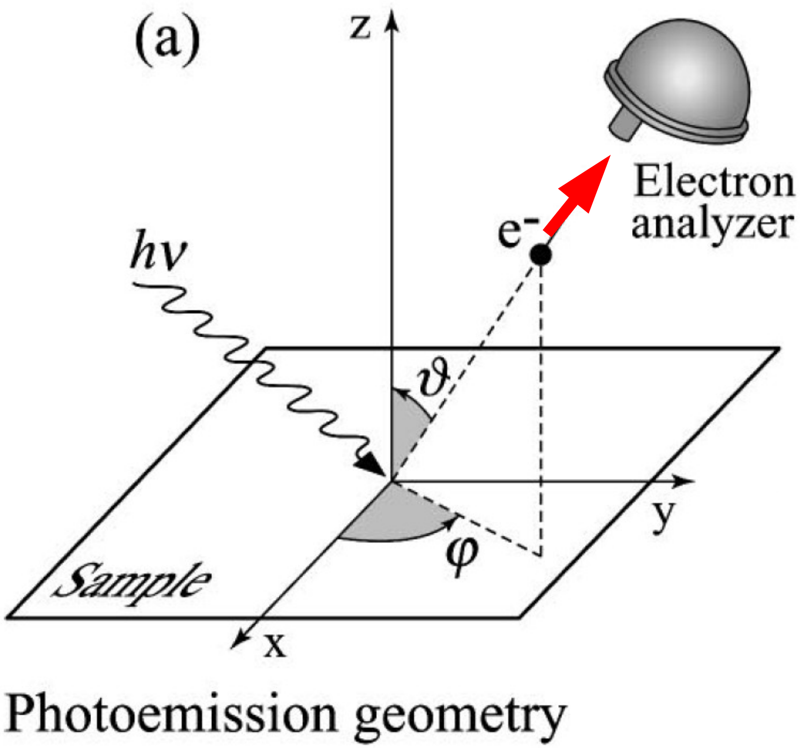
→ More complicated effective worlds

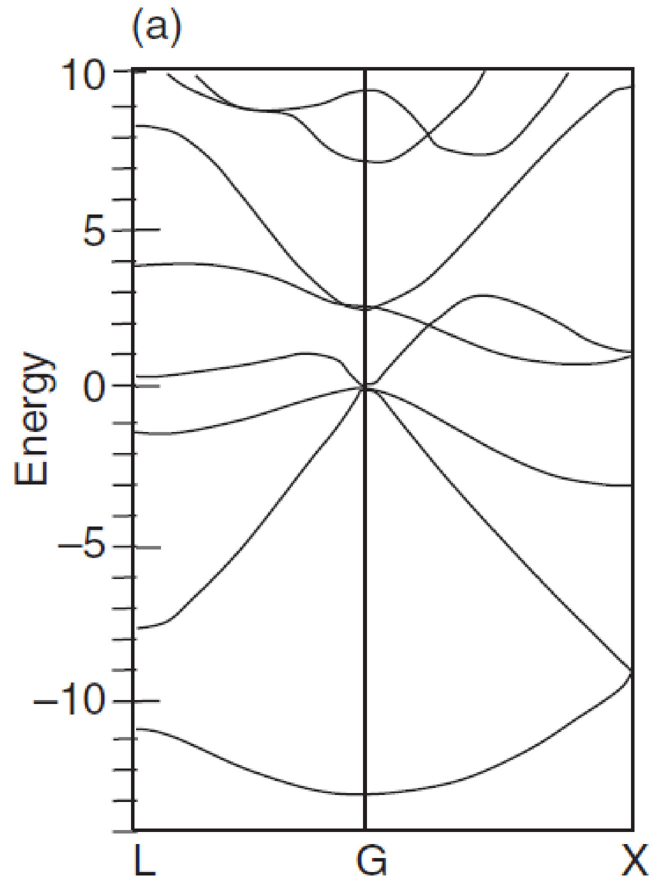
LDA



Bandstructure of germanium, theory versus experiment

→ From functionals to applications: photoemission

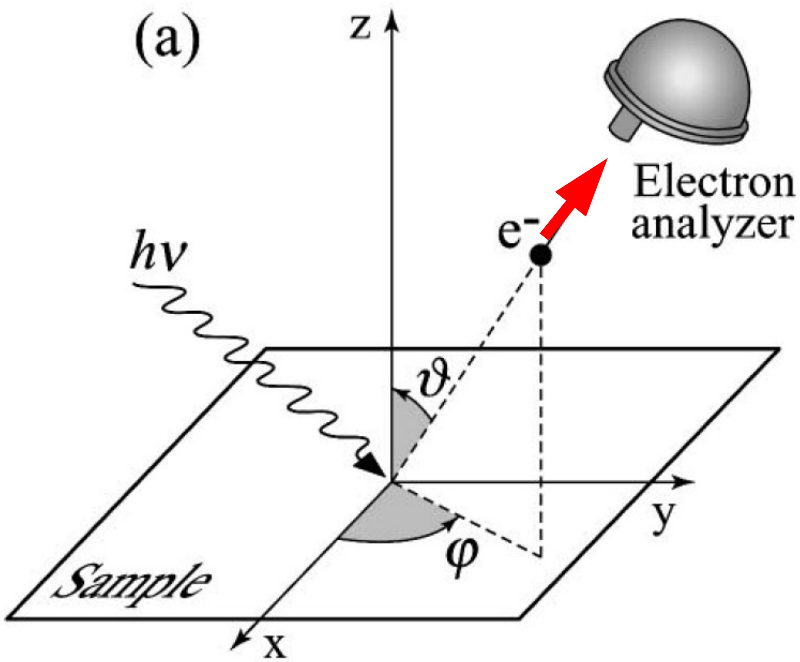




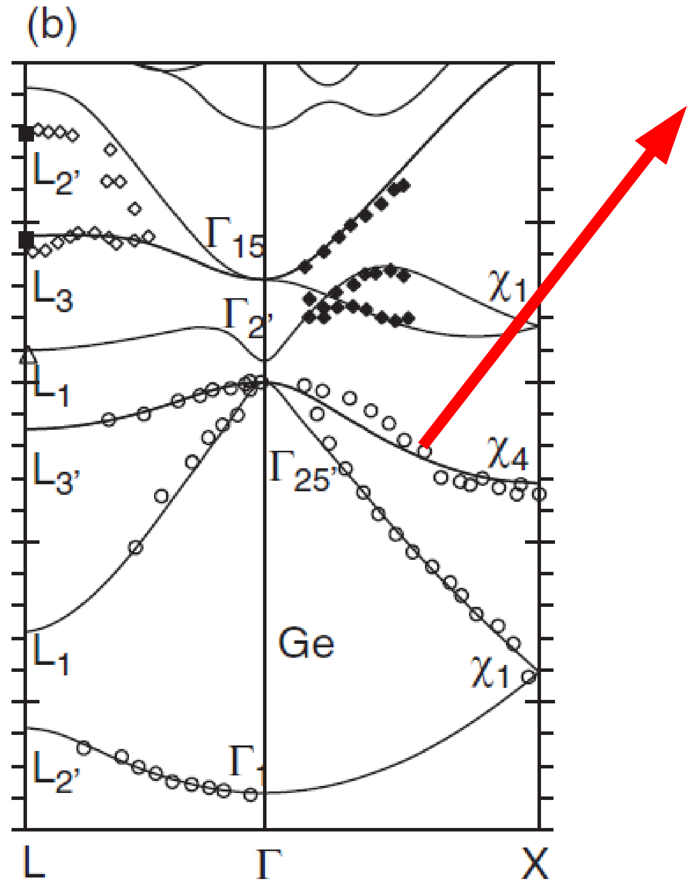
From Damascelli et al., RMP 75, 473 (2003)

+......

→ From functionals to applications: photoemission



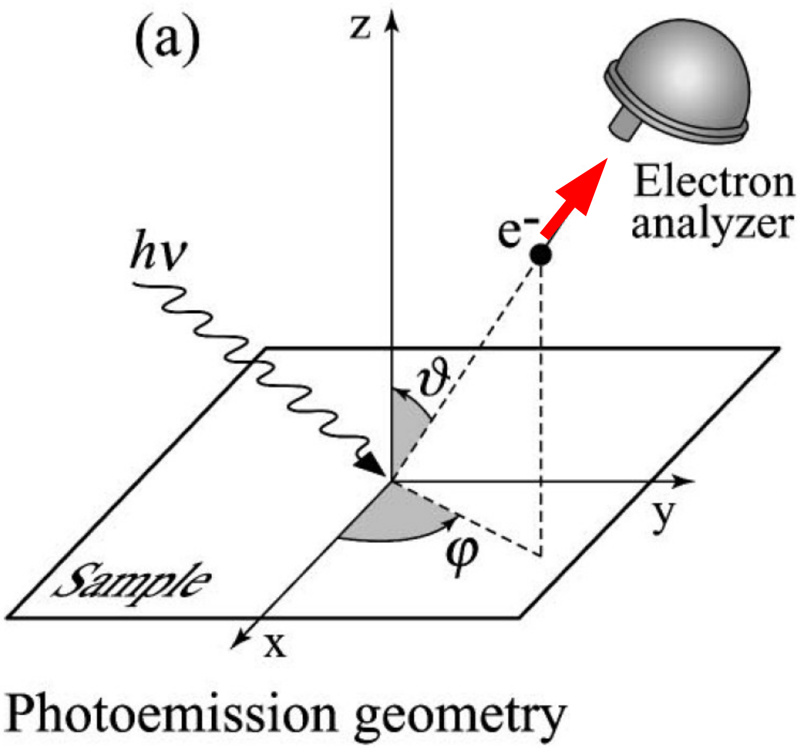
Photoemission geometry

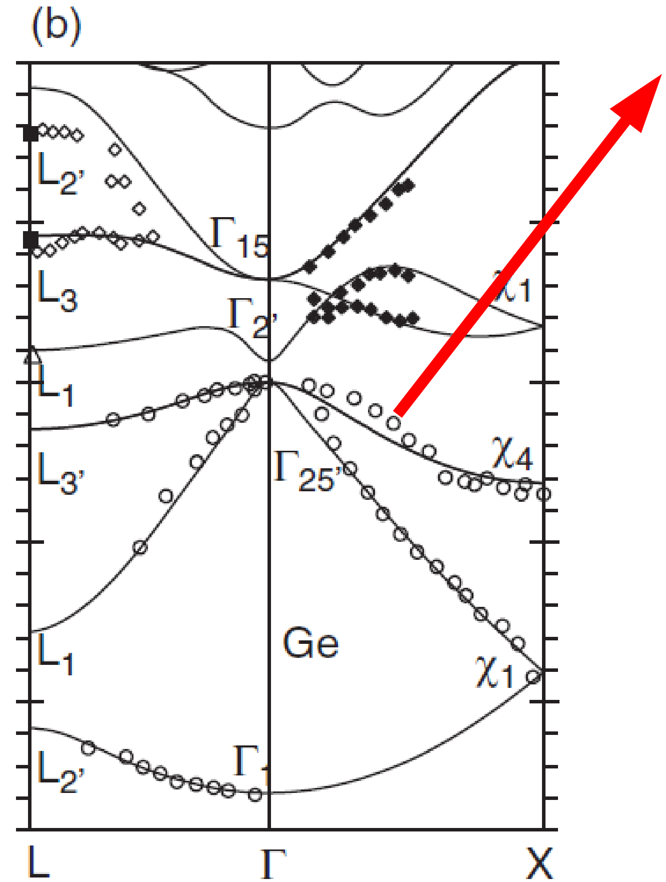


From Damascelli et al., RMP 75, 473 (2003)

+......

→ From functionals to applications: photoemission

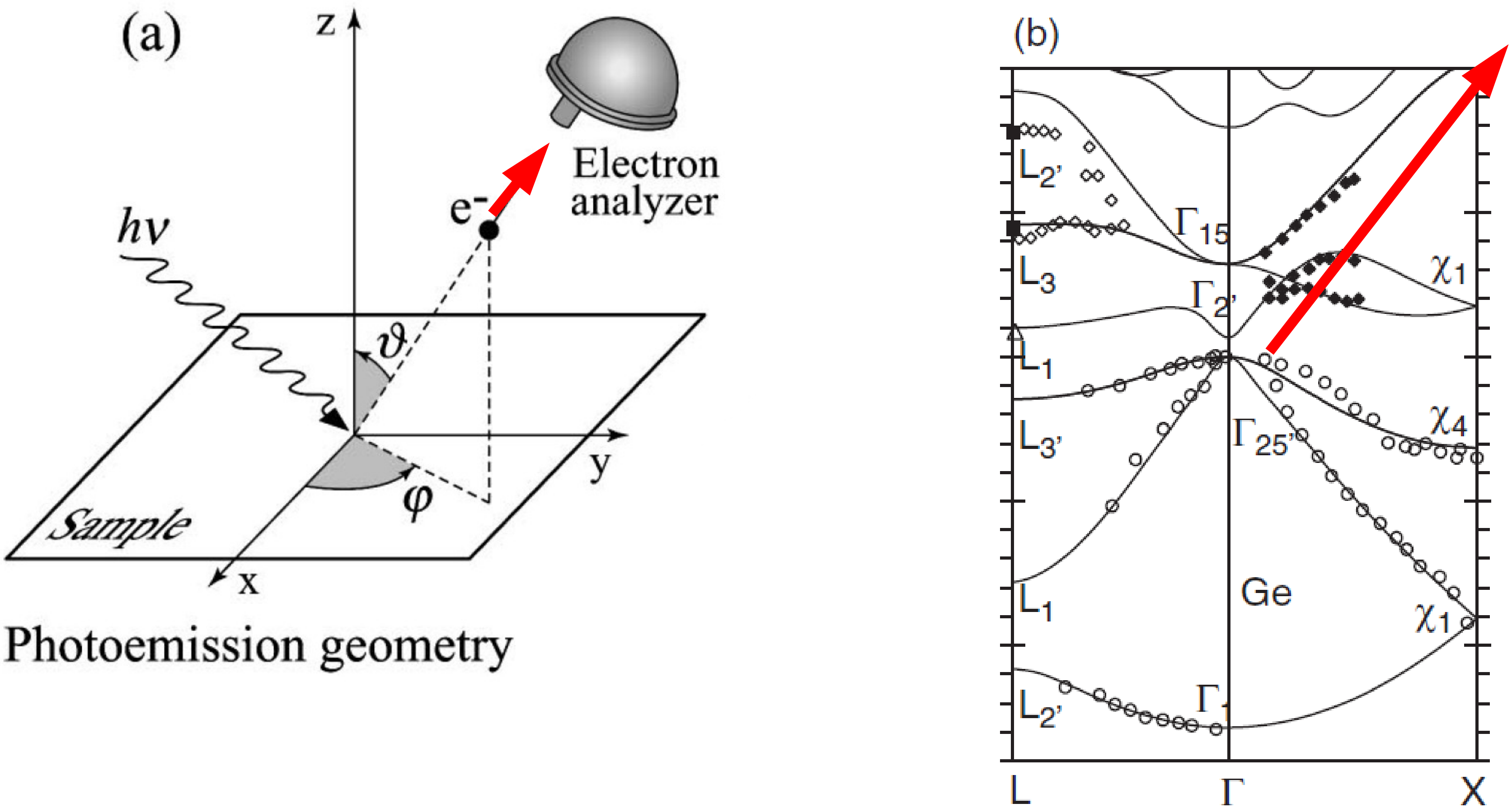




From Damascelli et al., RMP 75, 473 (2003)

+......

→ From functionals to applications: photoemission



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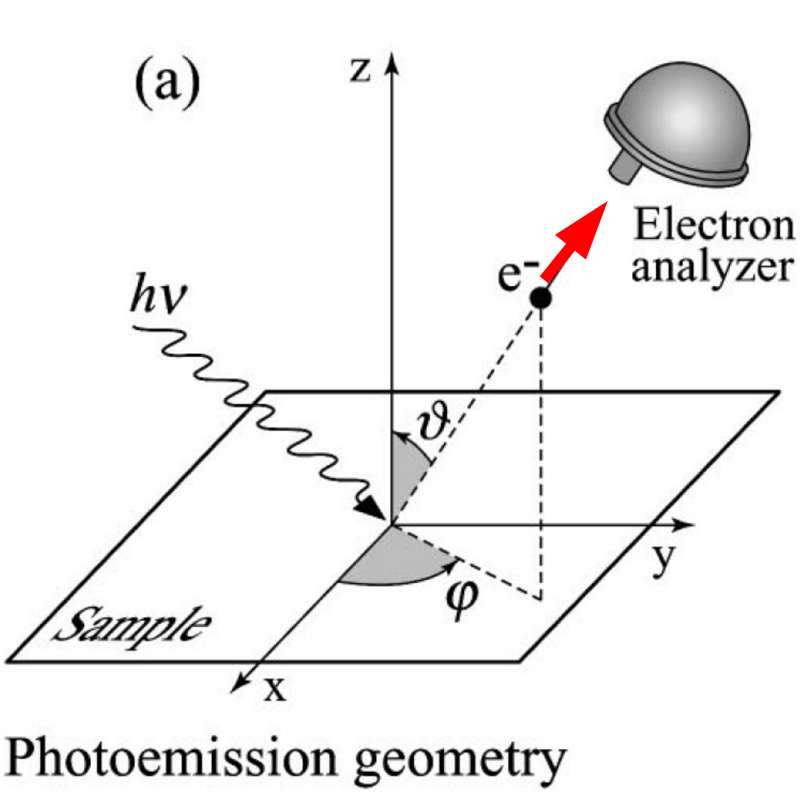
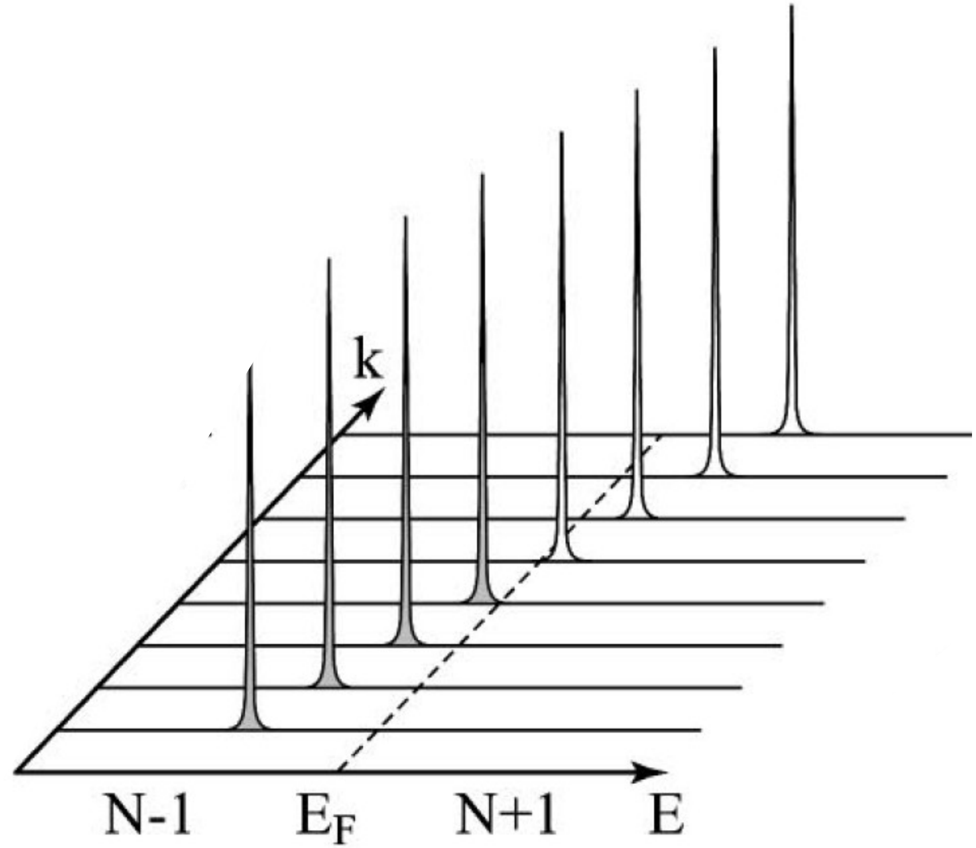
+......

→ From functionals to applications: photoemission





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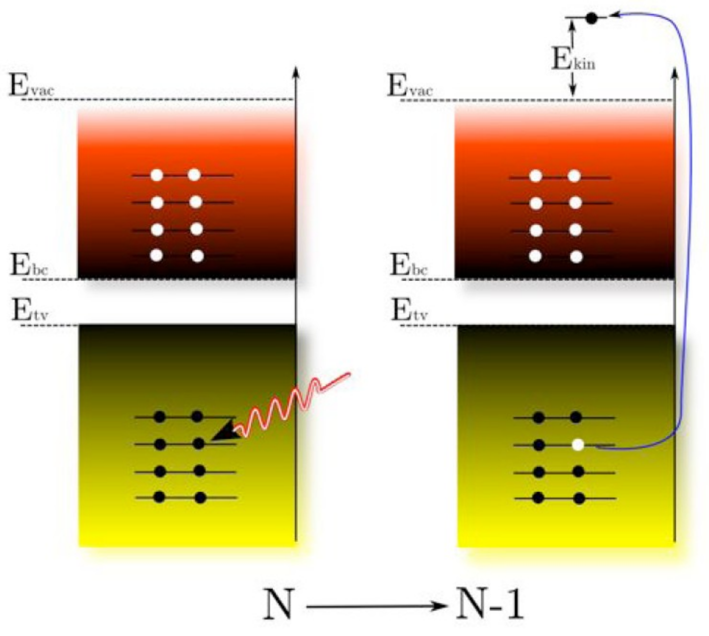
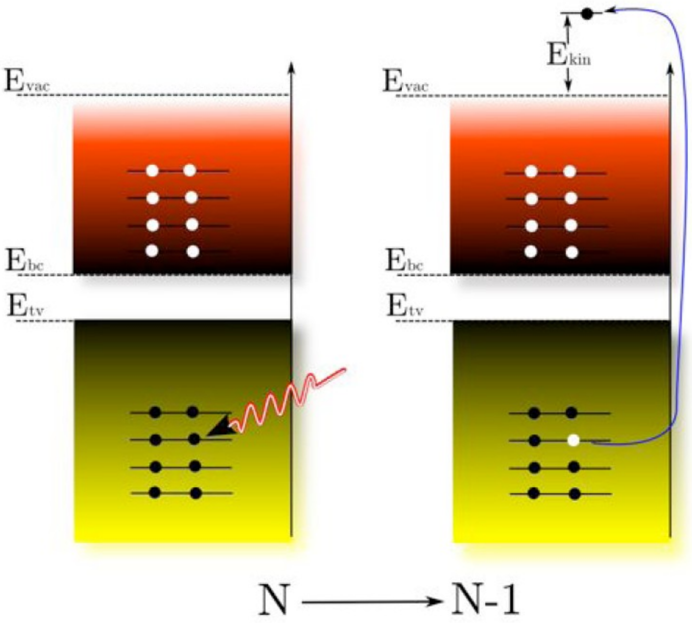
+......

Photoemission



$$E_i = E(N) - E(N-1, i)$$

Photoemission



Build another effective world!

$$E_i = E(N) - E(N-1, i)$$

Hartree-Fock

$$\left[-\frac{\nabla^2}{2} + V_{ext}(\mathbf{r}) + V_H(\mathbf{r})\right]\phi_i(\mathbf{r}) + \int d\mathbf{r}' V_x(\mathbf{r},\mathbf{r}')\phi_i(\mathbf{r}') = E_i\phi_i(\mathbf{r})$$

Non-local potential in an effective world!!!

What are the differences???

Kohn-Sham

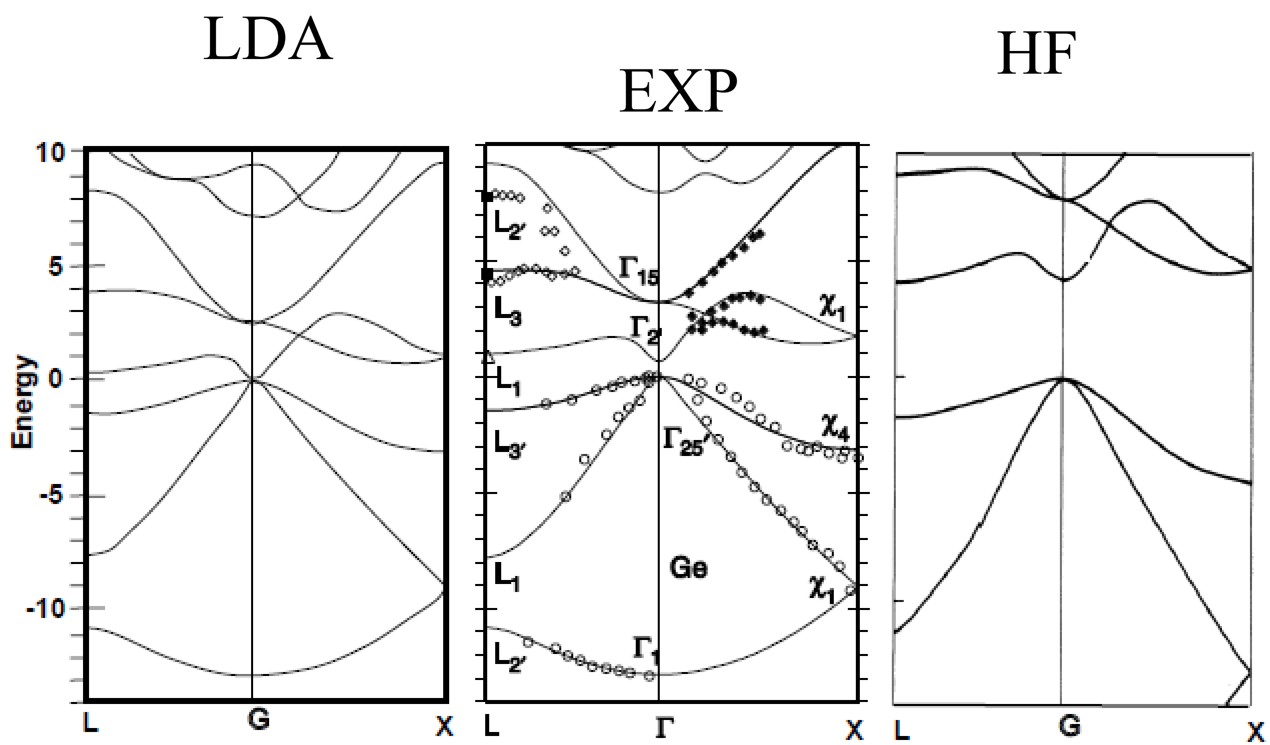
$$\left[-\frac{\nabla^2}{2} + V_{ext}(\mathbf{r}) + V_H(\mathbf{r})\right]\varphi_i(\mathbf{r}) + V_{xc}(\mathbf{r})\varphi_i(\mathbf{r}) = \epsilon_i\varphi_i(\mathbf{r})$$

Hartree-Fock

$$\left[-\frac{\nabla^2}{2} + V_{ext}(\mathbf{r}) + V_H(\mathbf{r})\right]\phi_i(\mathbf{r}) + \int d\mathbf{r}' V_x(\mathbf{r},\mathbf{r}')\phi_i(\mathbf{r}') = E_i\phi_i(\mathbf{r})$$

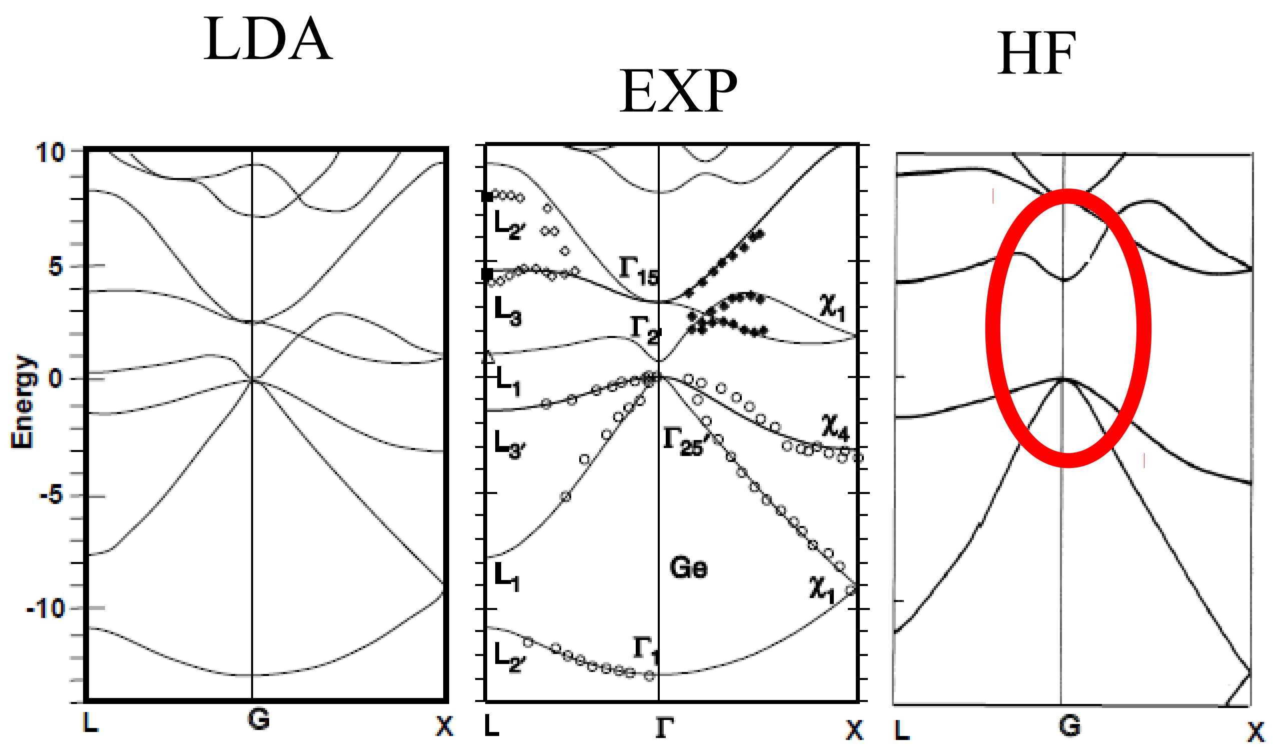
Non-local potential in an effective world!!!

→ More complicated effective worlds



Bandstructure of germanium, theory versus experiment

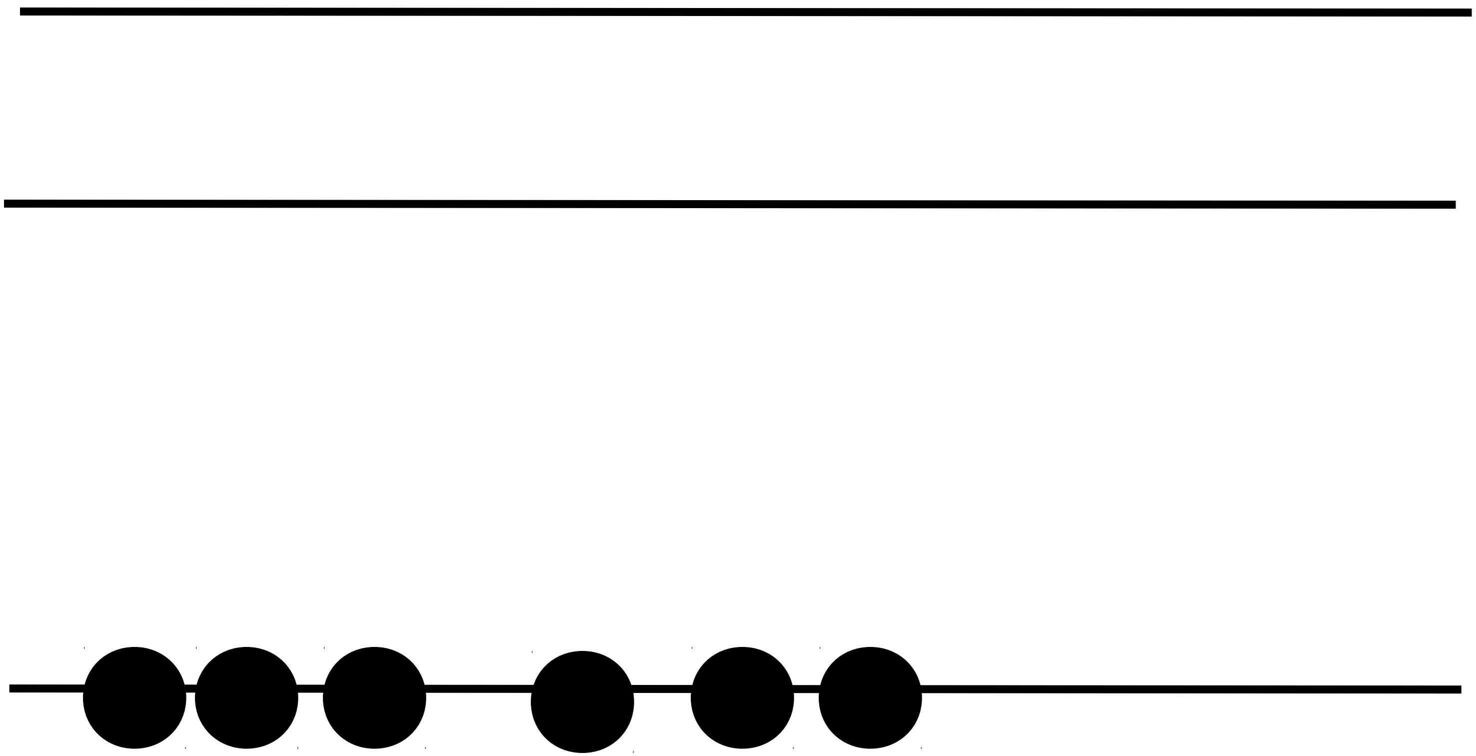
→ More complicated effective worlds

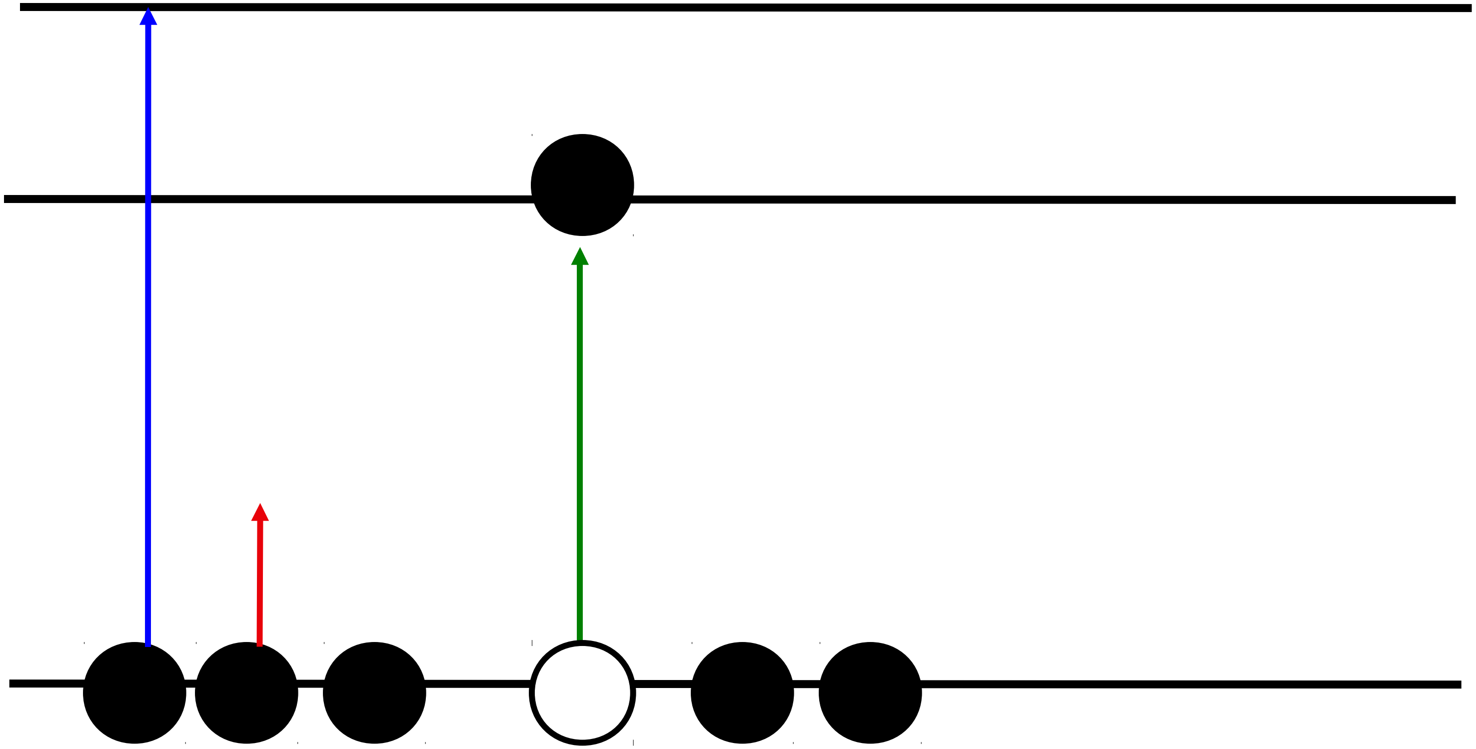


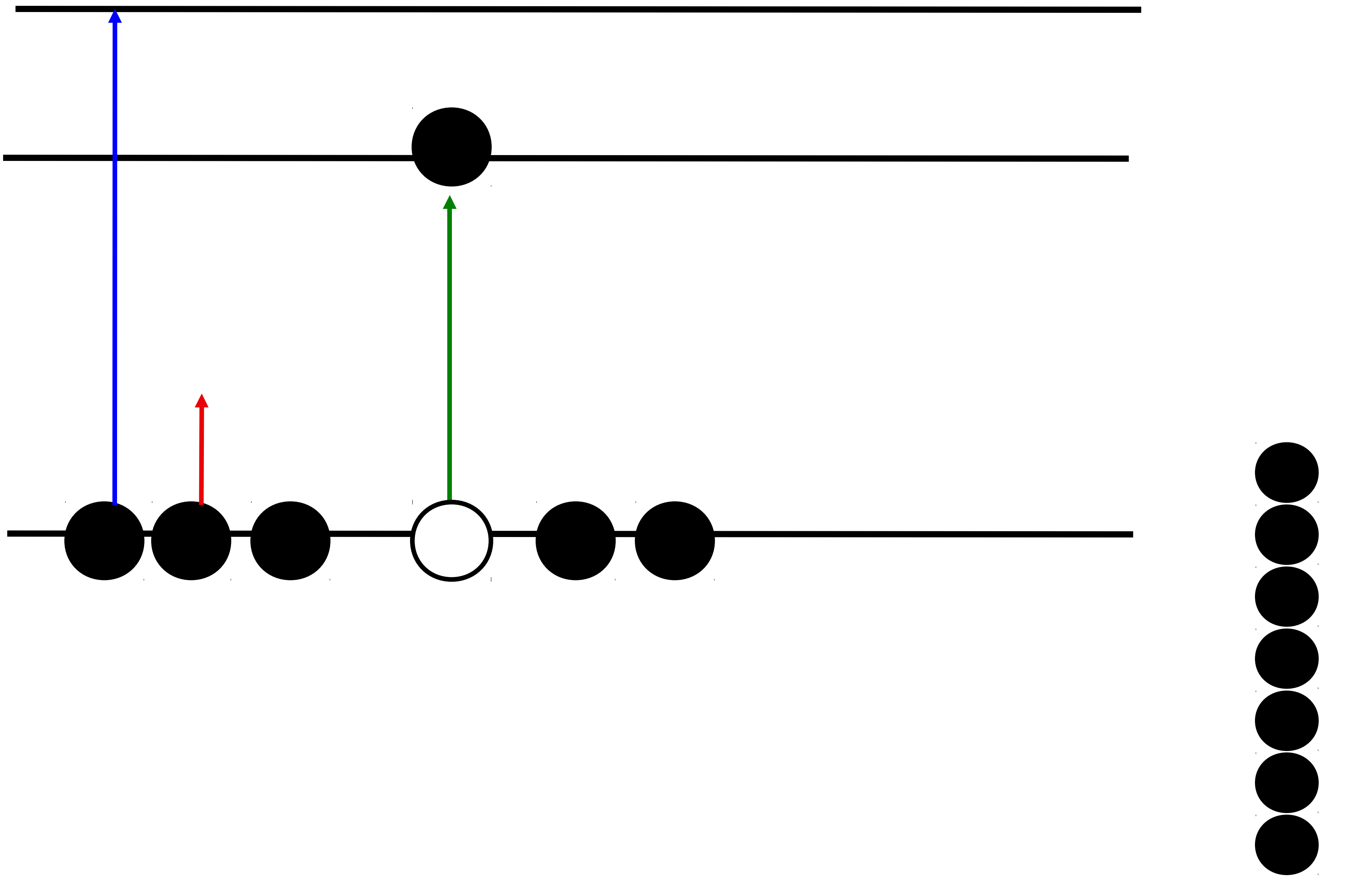
Bandstructure of germanium, theory versus experiment

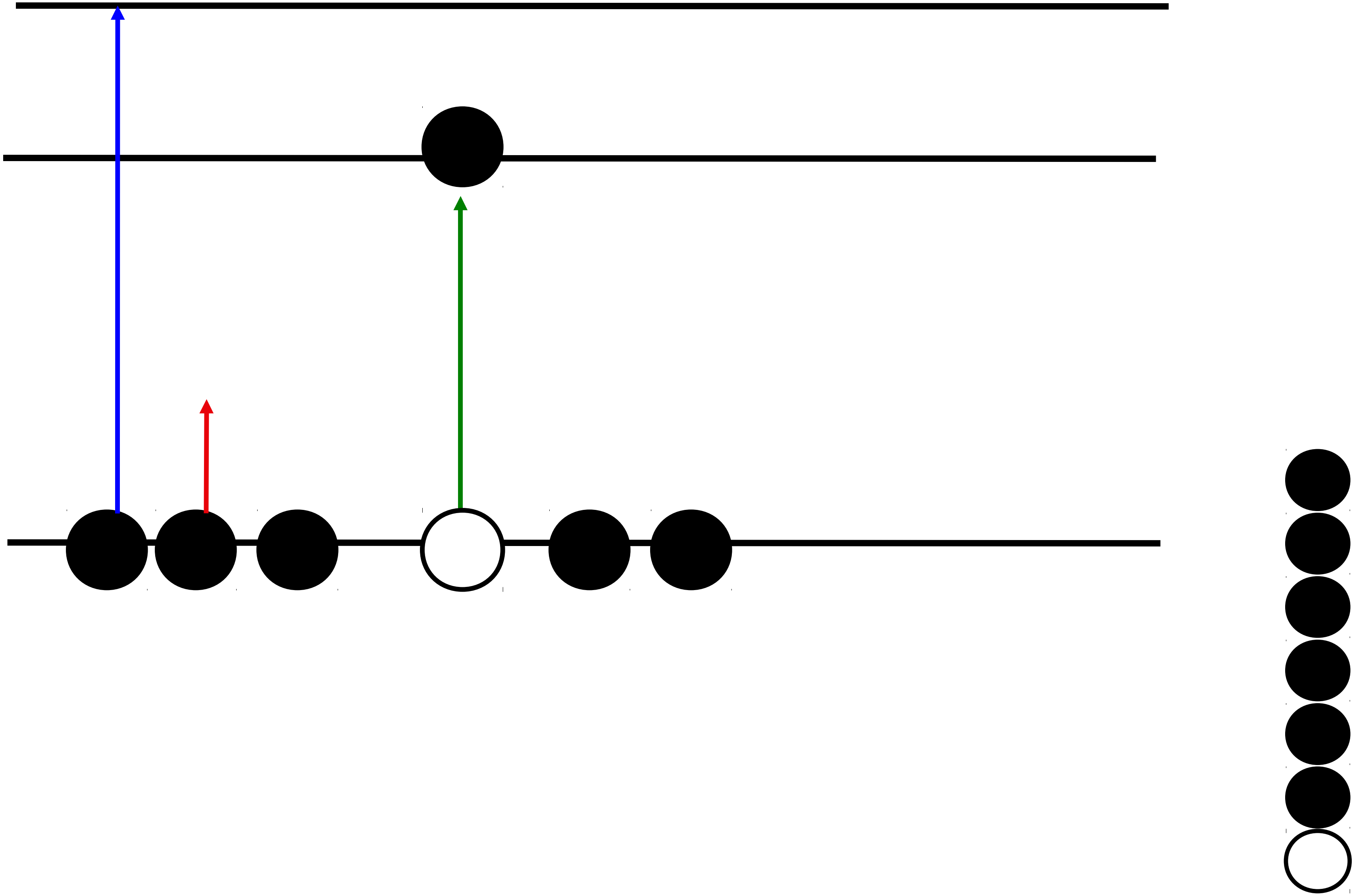
What is wrong with Hartree-Fock?

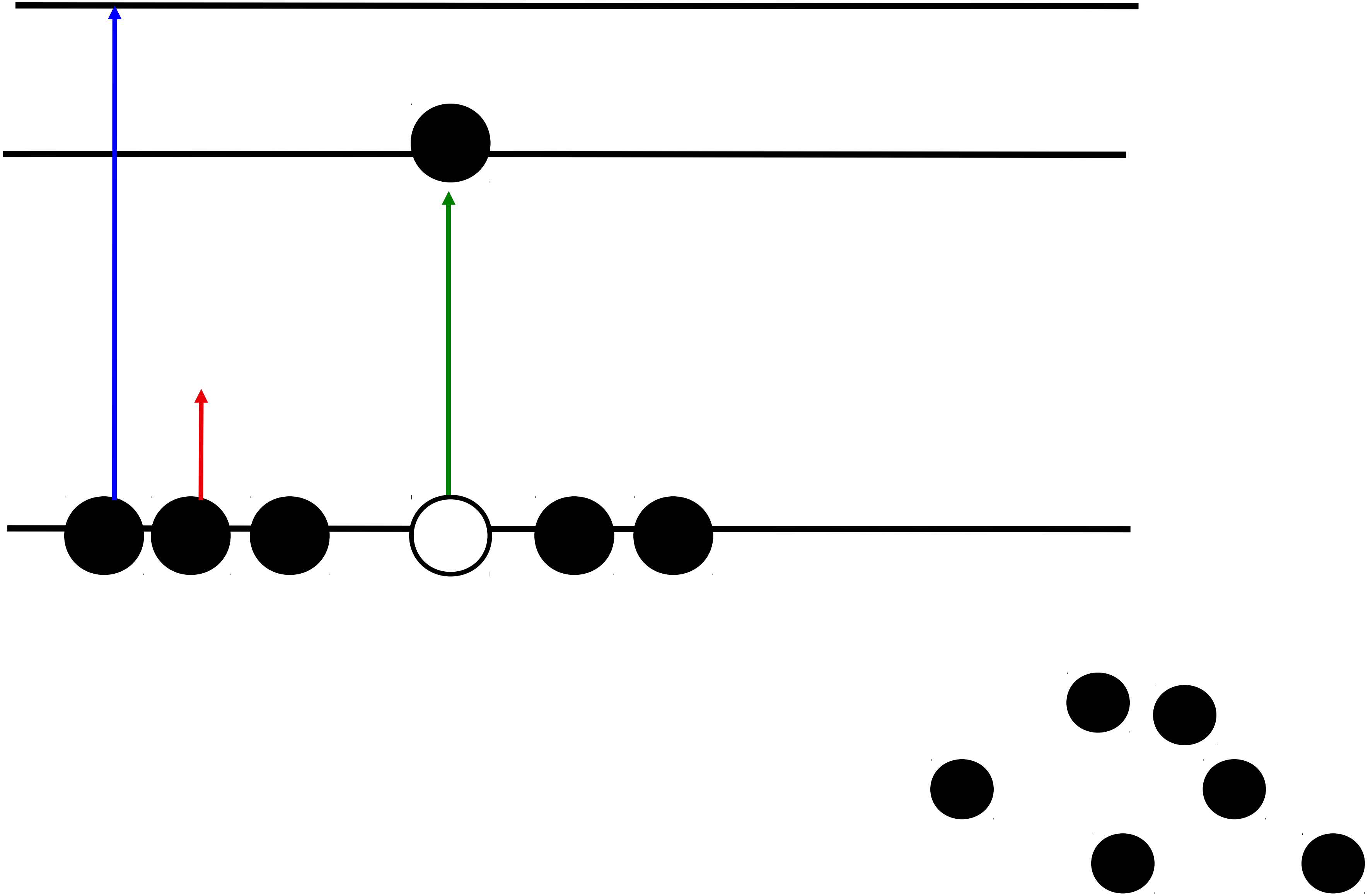
→ The many-body problem

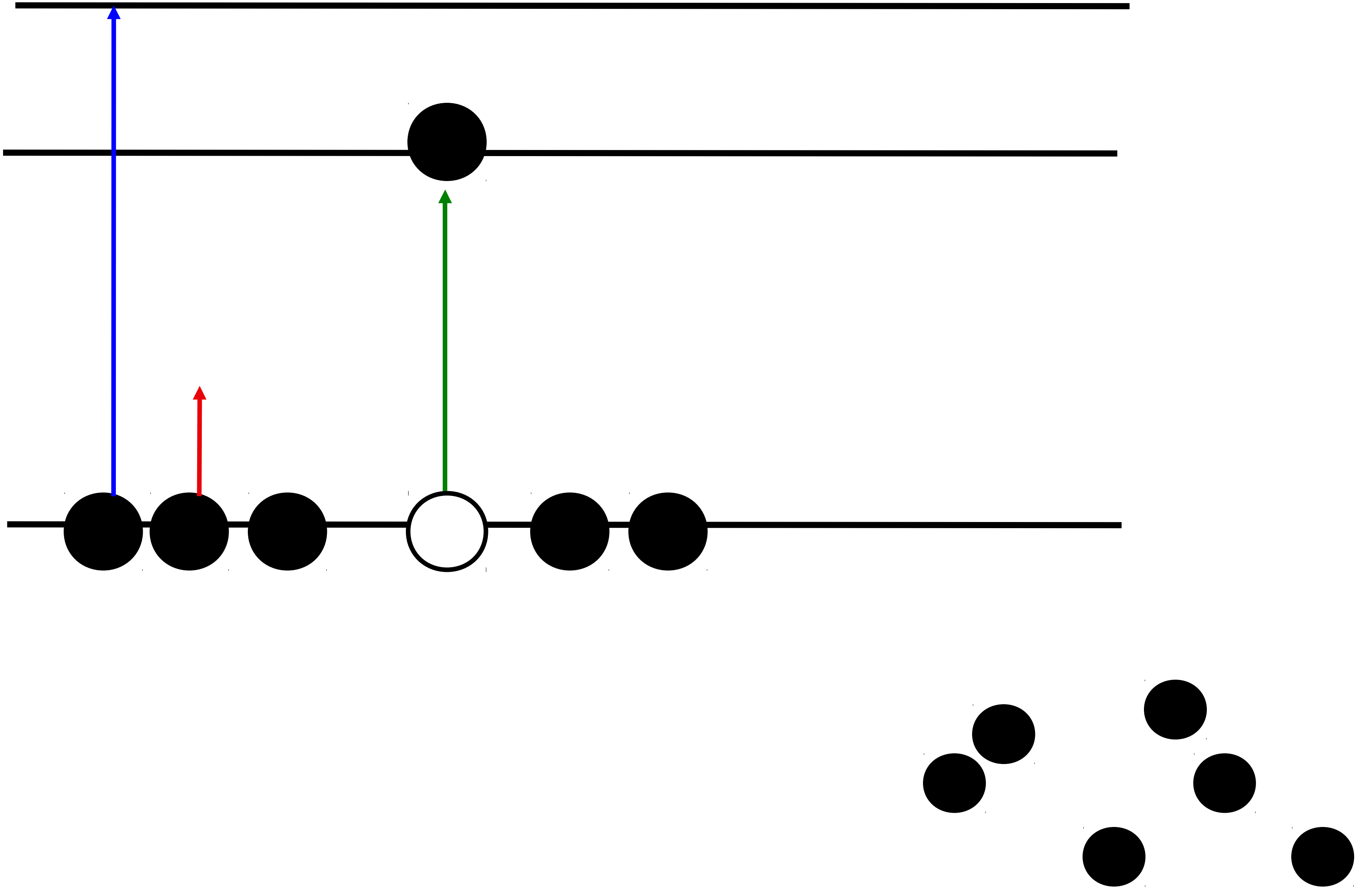


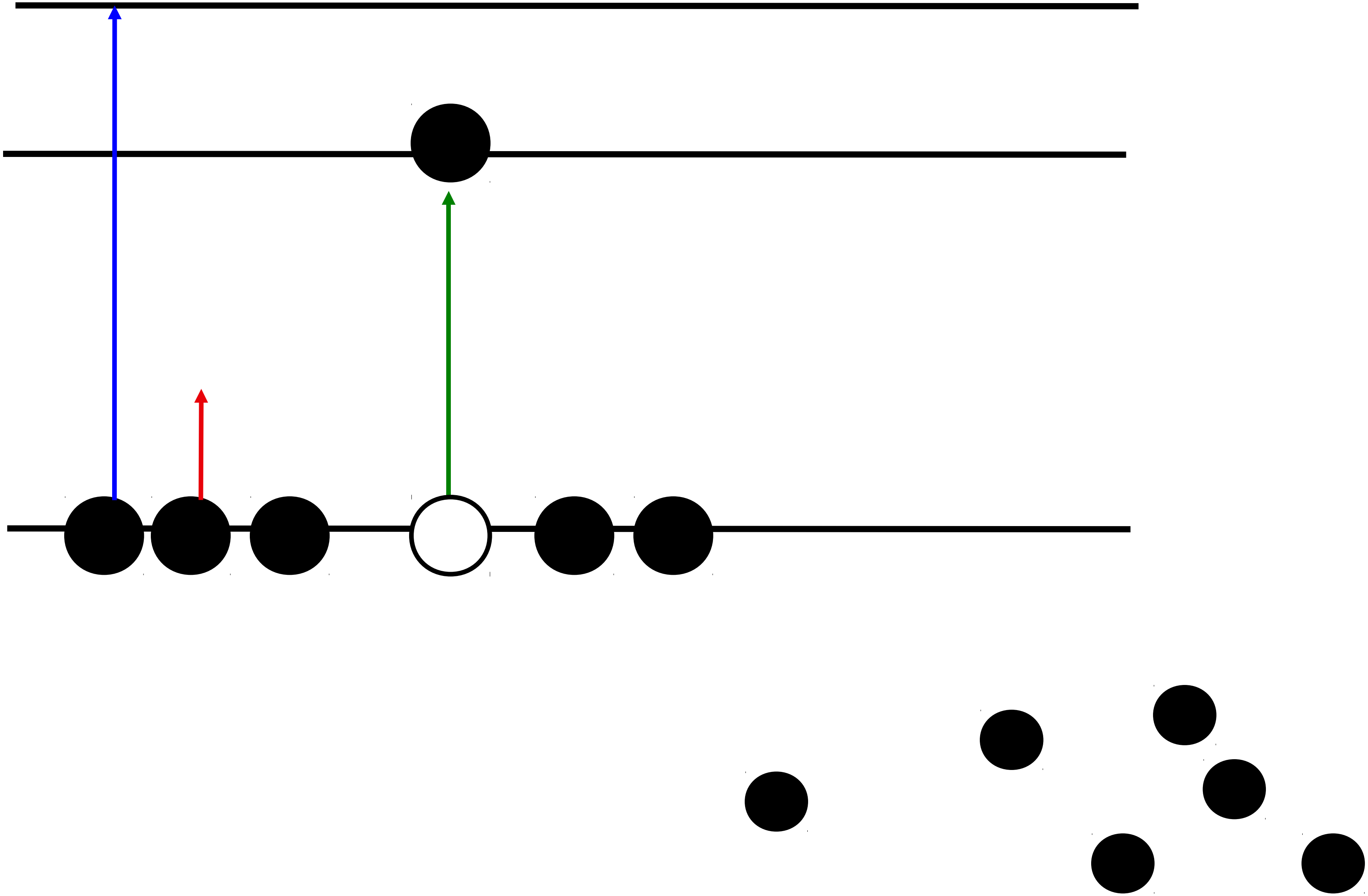


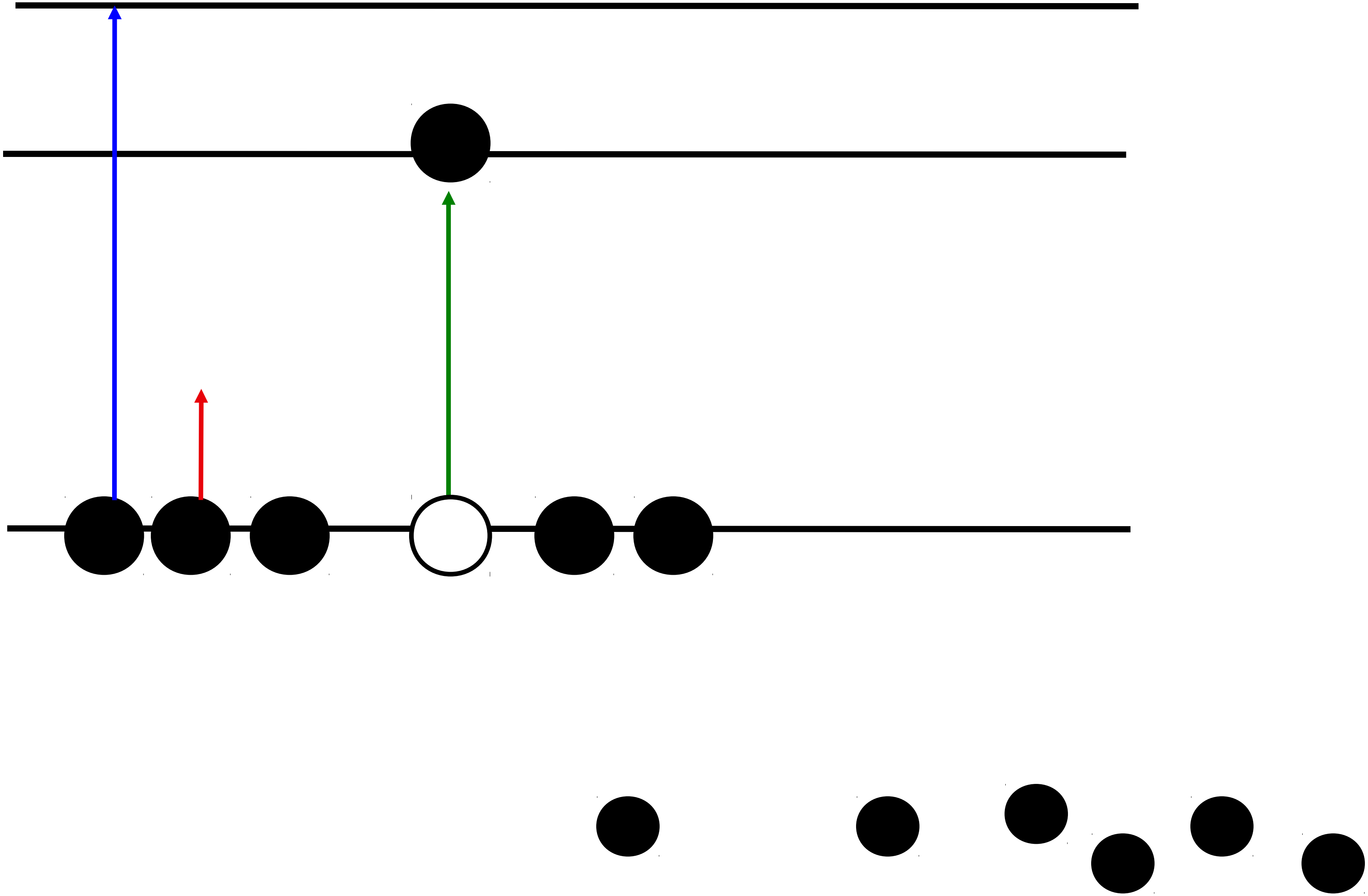


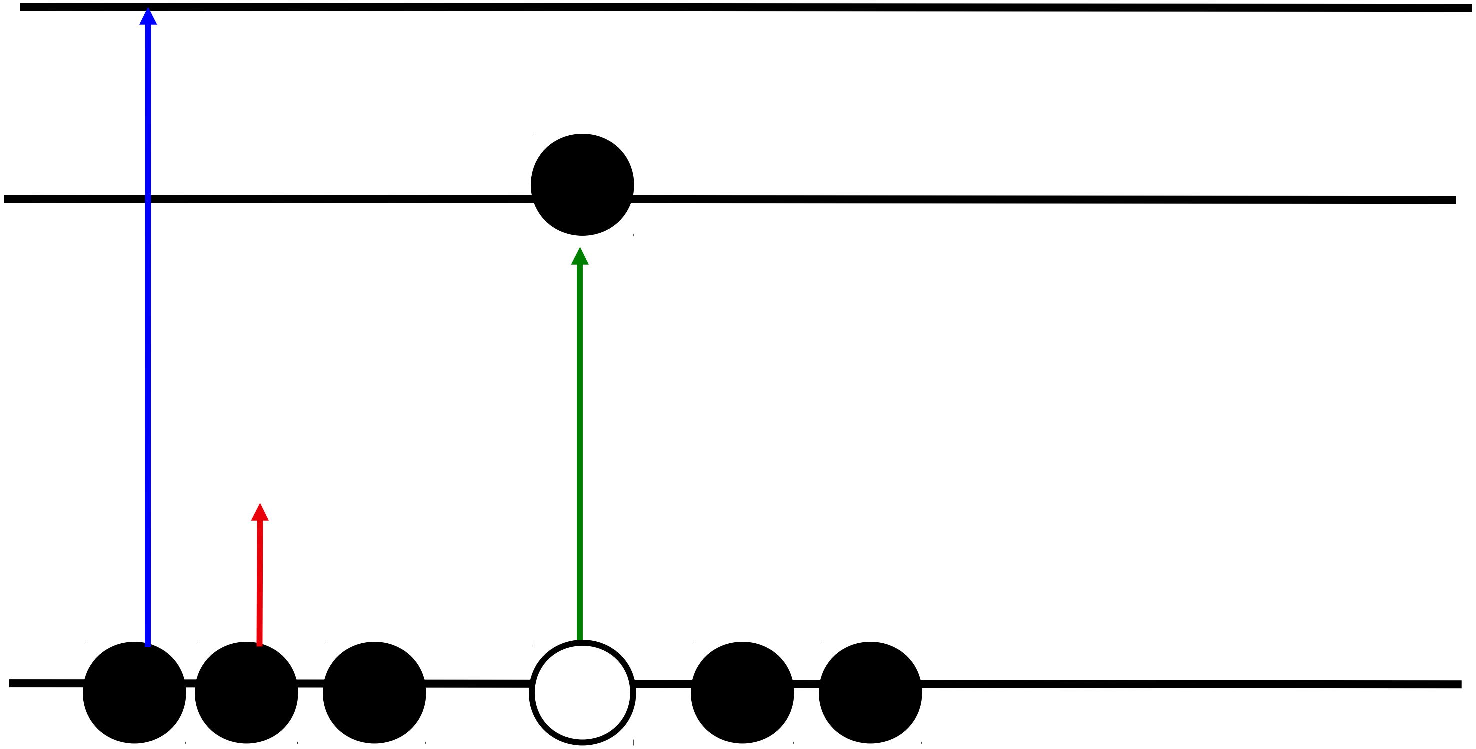




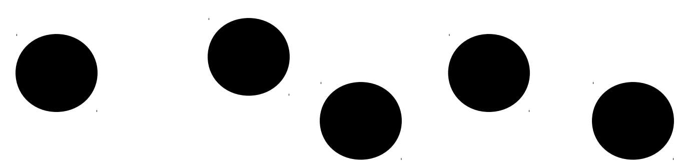


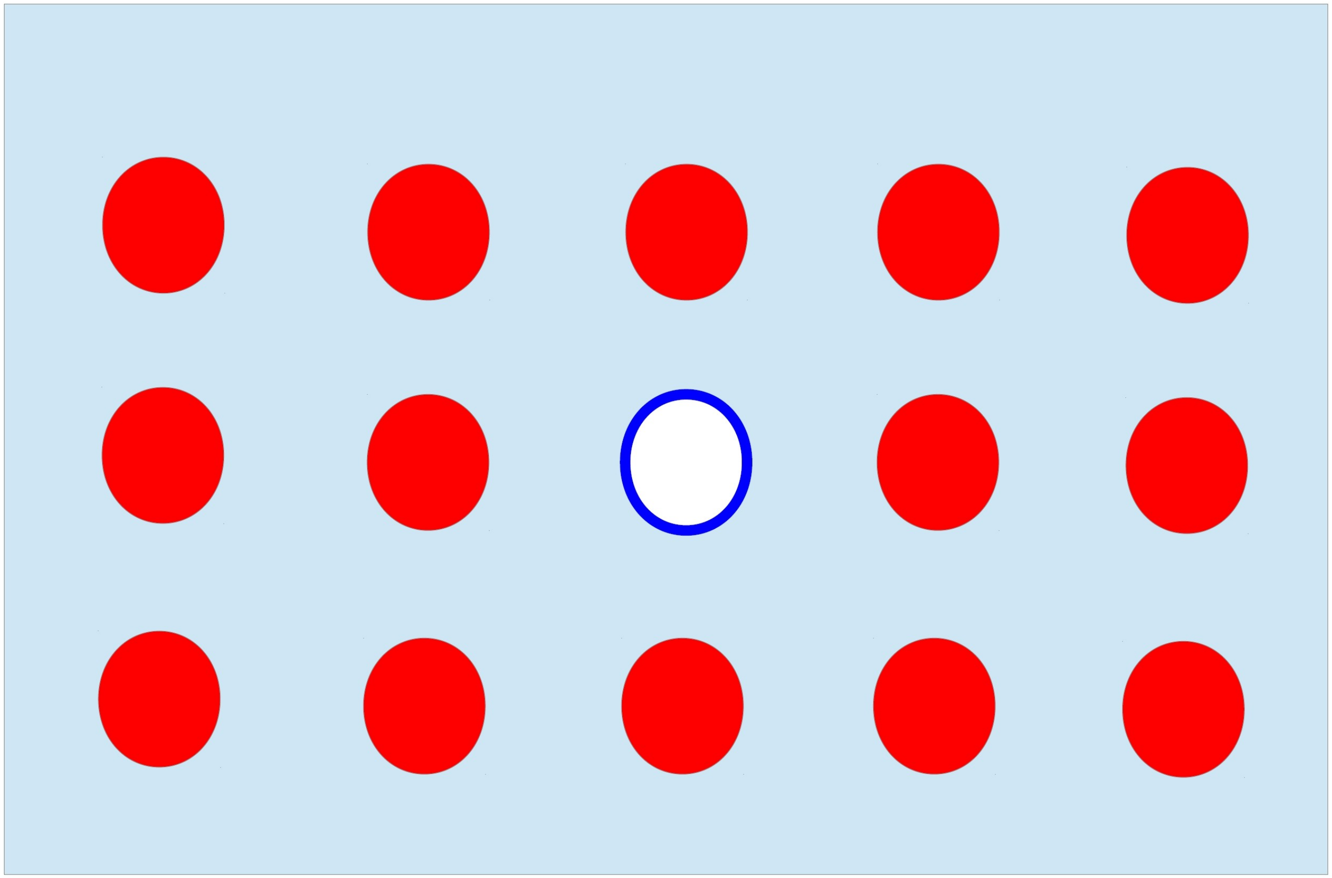




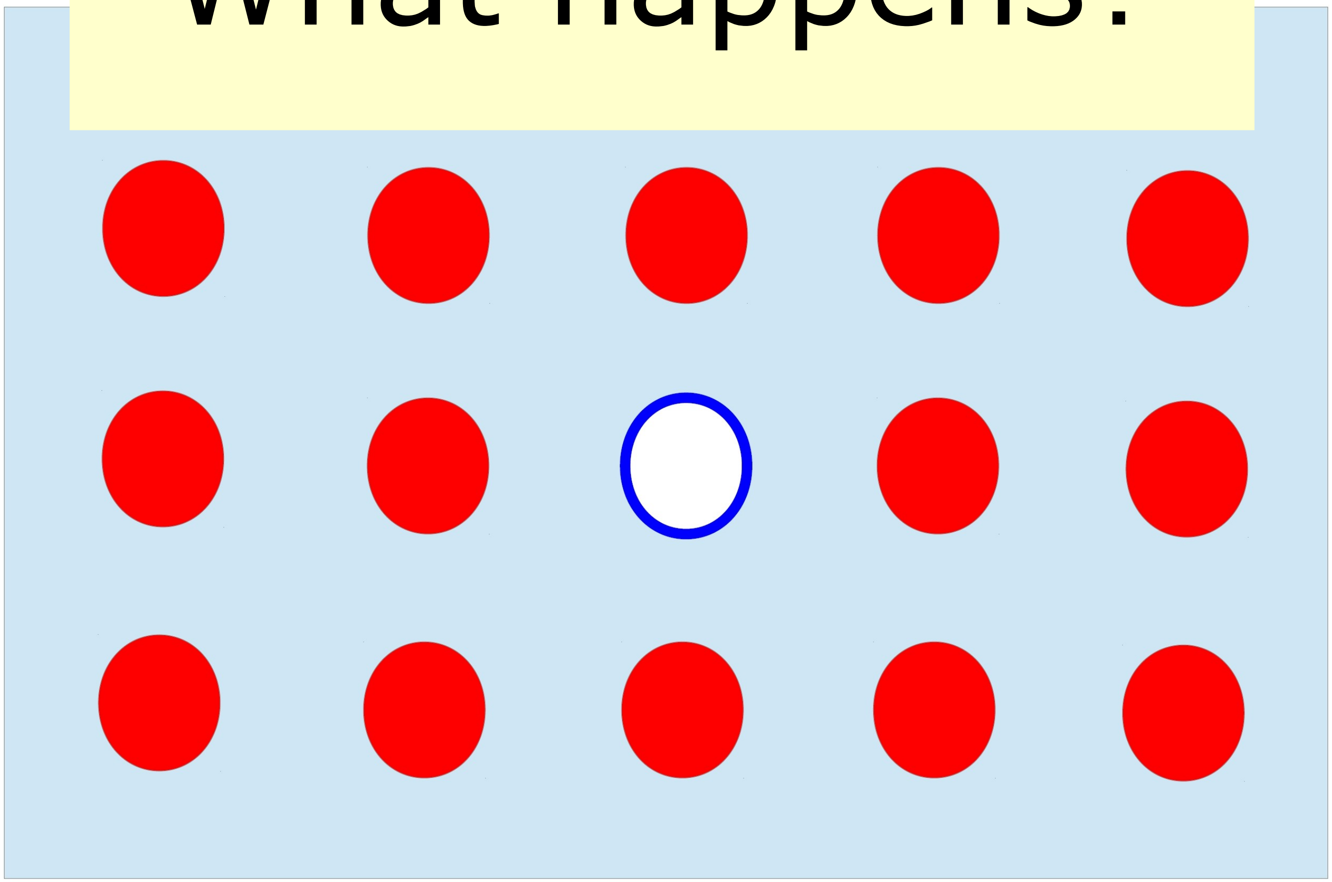


Electrons are interacting !!!

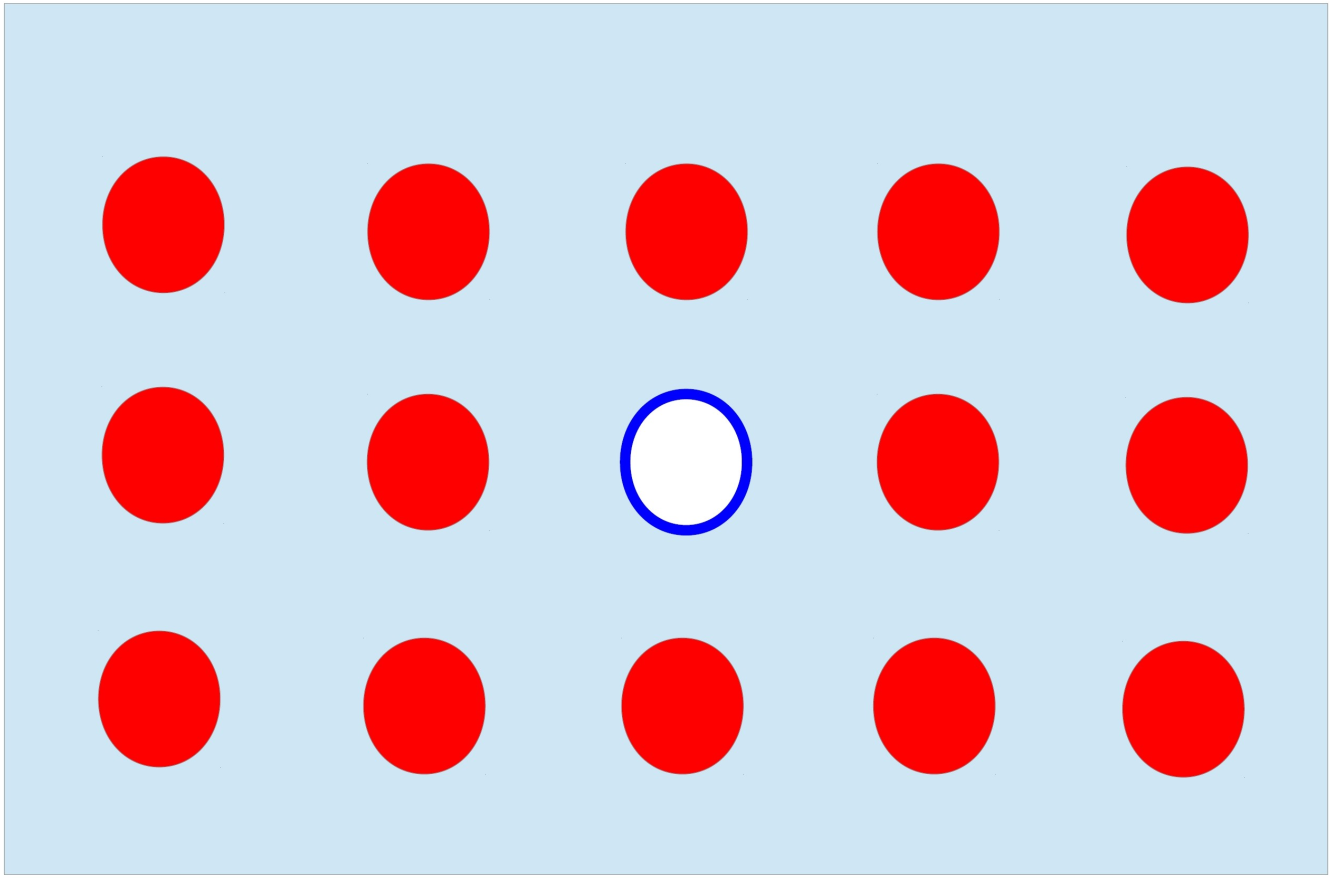




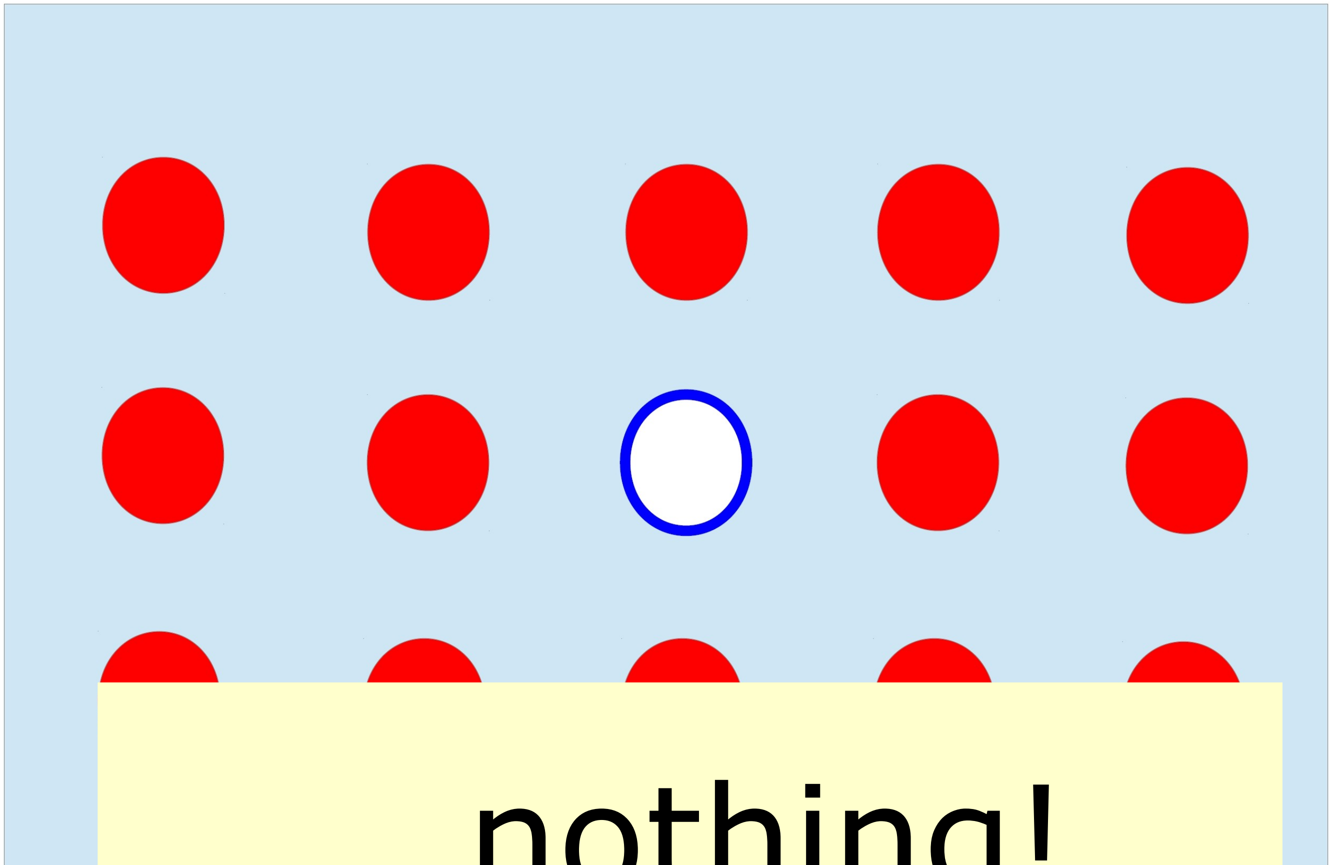
What happens?



Non-interacting particles

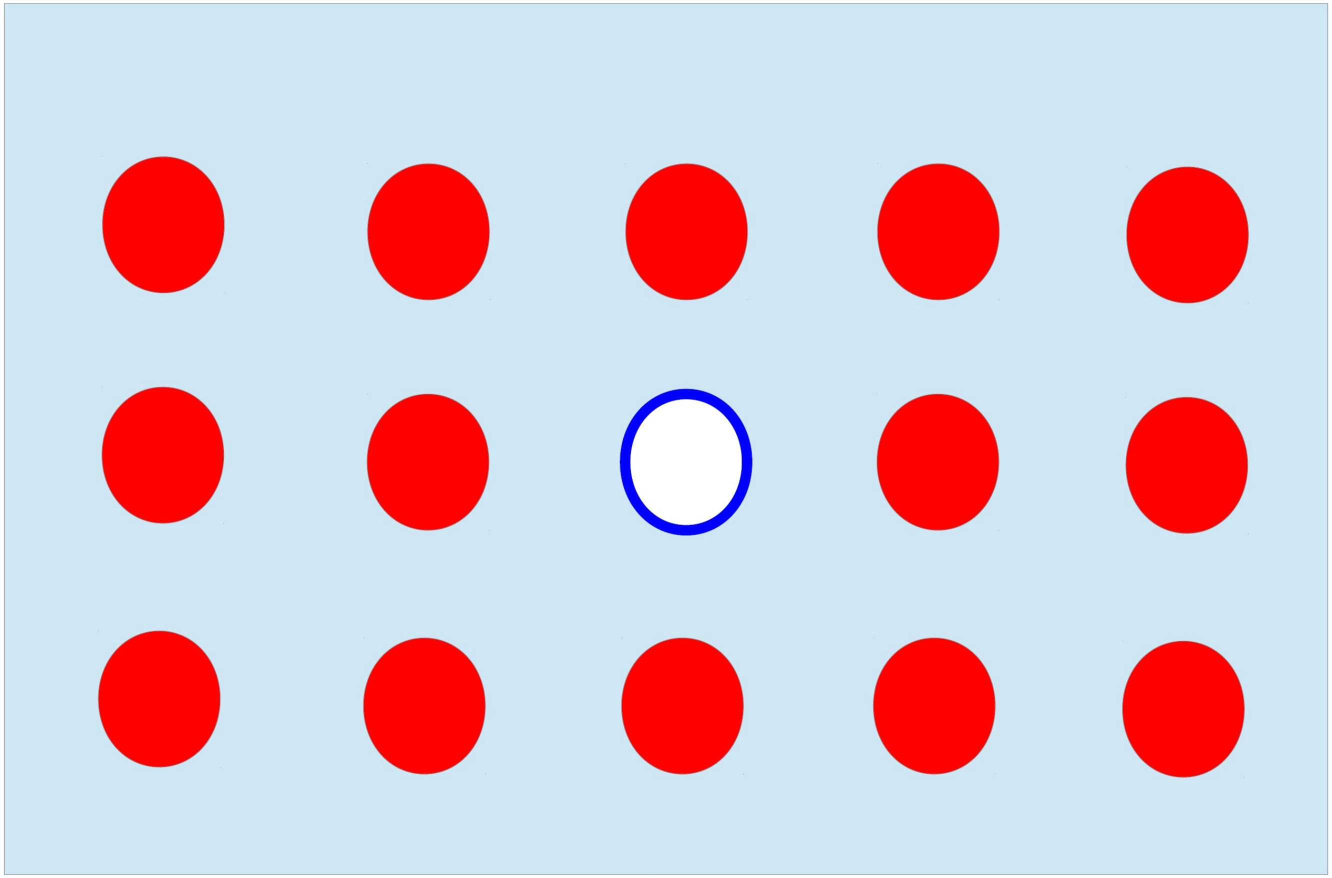


Non-interacting particles

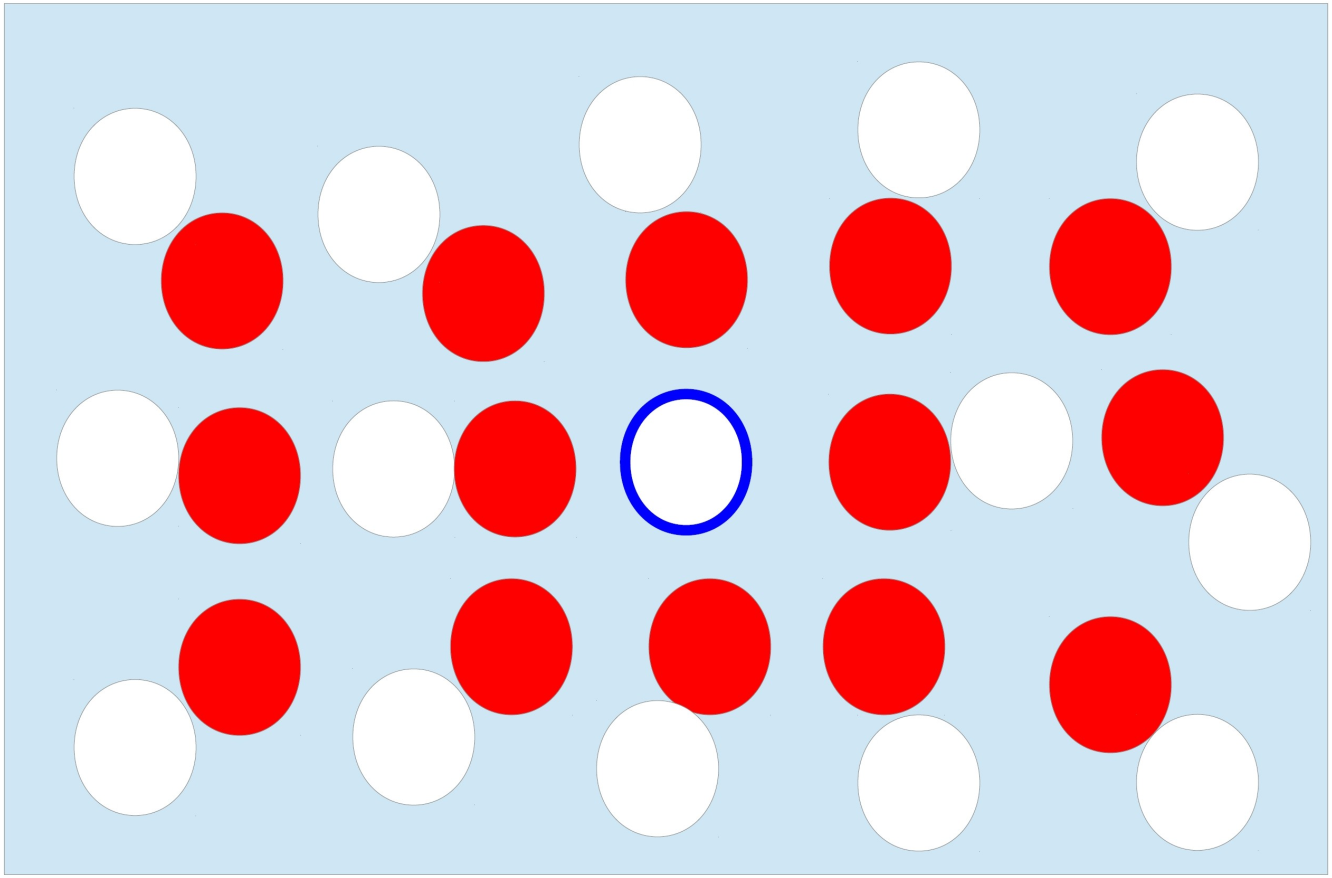


...nothing!

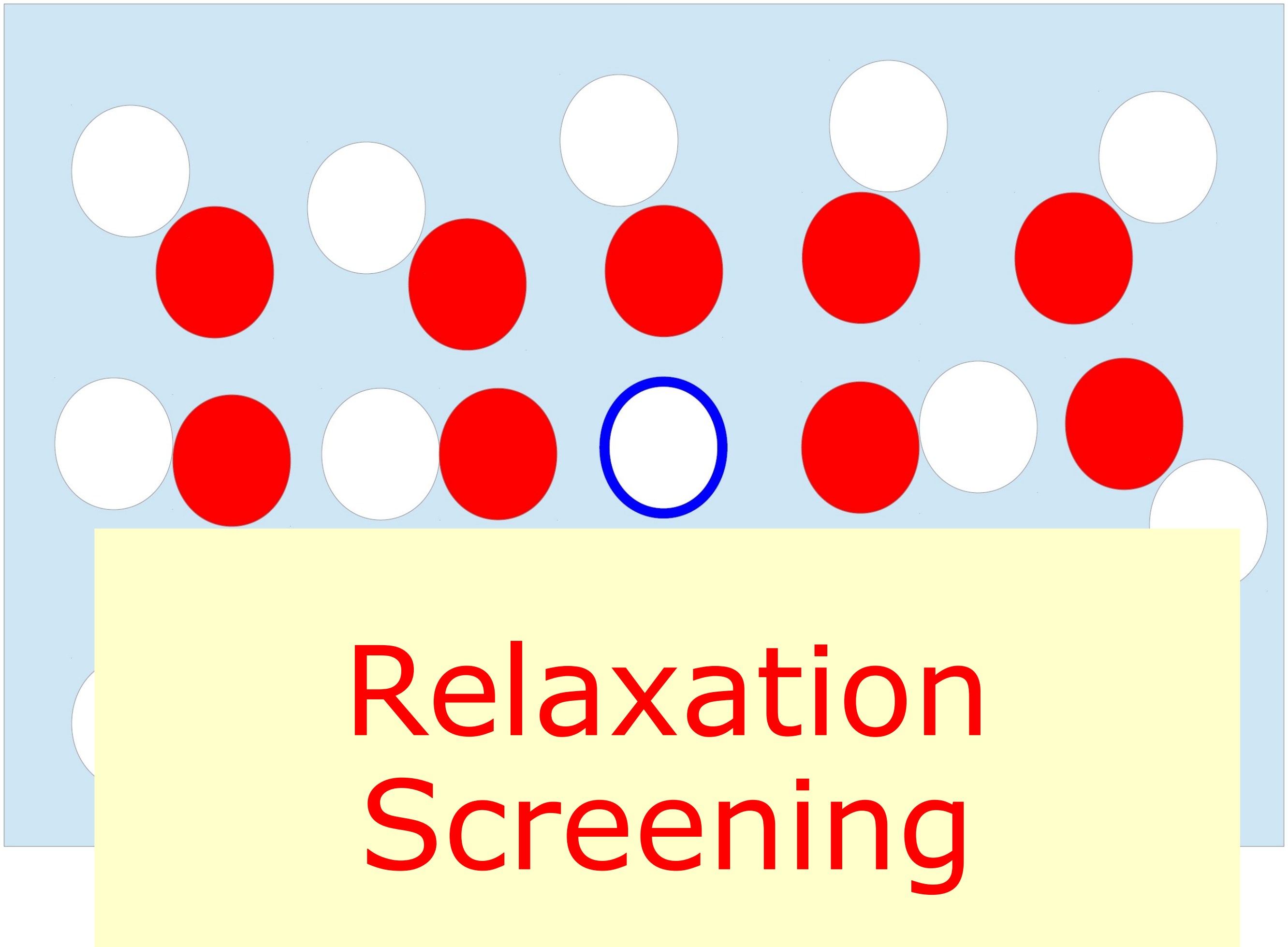
Interacting particles



Interacting particles



Interacting particles



Hartree-Fock

$$\left[-\frac{\nabla^2}{2} + V_{ext}(\mathbf{r}) + V_H(\mathbf{r})\right]\phi_i(\mathbf{r}) + \int d\mathbf{r}' V_x^F(\mathbf{r},\mathbf{r}')\phi_i(\mathbf{r}') = E_i\phi_i(\mathbf{r})$$

Hybrids = effective screening α

$$\left[-\frac{\nabla^2}{2} + V_{ext}(\mathbf{r}) + V_H(\mathbf{r}) + V_{xc}(\mathbf{r})\right]\phi_i(\mathbf{r}) + \alpha\int d\mathbf{r}'\left[V_x^F(\mathbf{r},\mathbf{r}') - V_x(\mathbf{r}')\delta(\mathbf{r}-\mathbf{r}')\right]\phi_i(\mathbf{r}') = E_i\phi_i(\mathbf{r})$$

LDA+U....

With screening

Hartree-Fock

With **dynamical screening:** GW

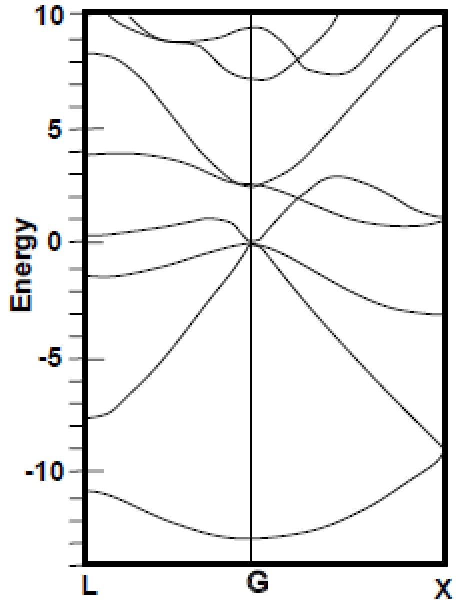
Hartree-Fock

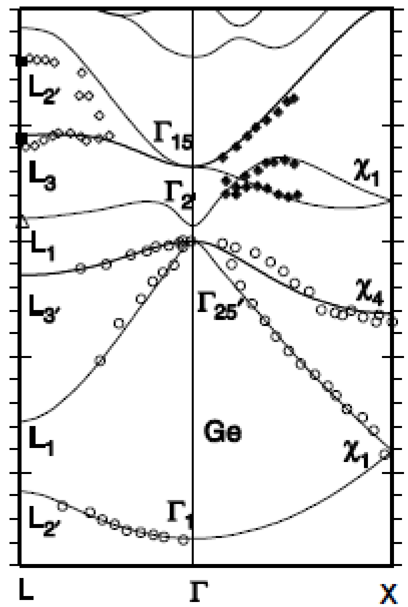
GW today: standard for bandstructures

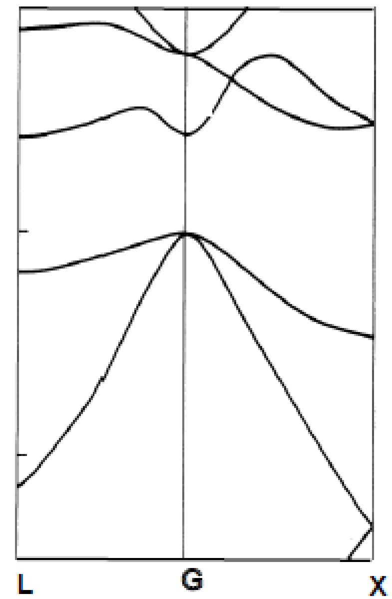
LDA

GW

HF







GW calculations, Rohlfing et al., PRB 48, 17791 (1993)

Bandstructure of germanium, theory versus experiment

A step back : finding our way in the many-body labyrinth

→ The many-body marvel

→ The many-body problem

→ Observables

→ Descriptors and density functional theory

→ Effective worlds and the Kohn-Sham auxiliary system

→ The two fundamental difficulties with KS

→ More complicated effective worlds: from KS to many-body (meeting on the way: Hartree-Fock, DFT+U, hybrids, GW,...)

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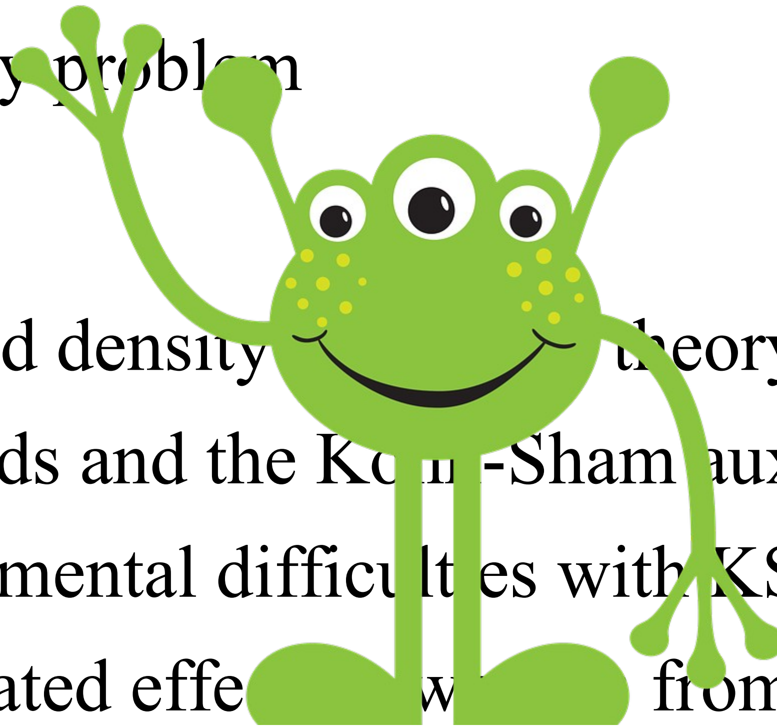

Project : participate in finding better auxiliary potentials

….with pencil and paper!!!!