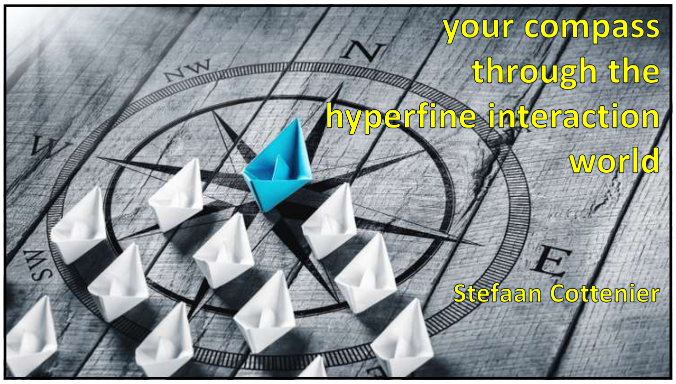


1

2

3

Second

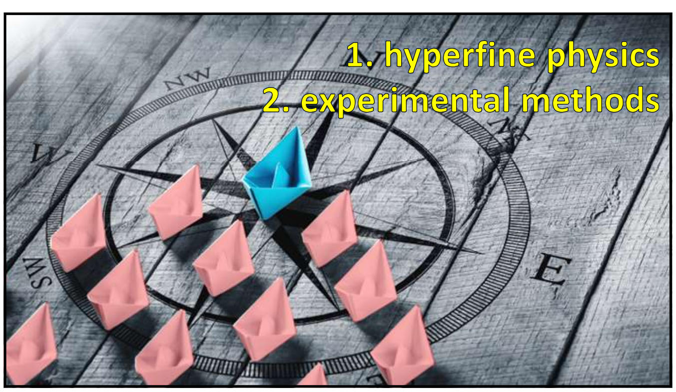
The **second** (symbol: **s**) is the unit of time in the International System of Units (SI), historically defined as $^1/_{86400}$ of a day – this factor derived from the division of the day first into 24 hours, then to 60 minutes and finally to 60 seconds each (24 × 60 × 60 = 86400). "Minute" comes from the Latin *pars minuta prima*, meaning "first small part", and "second" comes from the *pars minuta secunda*, "second small part".

The current and formal definition in the International System of Units (SI) is more precise:

> The second [...] is defined by taking the fixed numerical value of the caesium frequency, $\Delta\nu_{Cs}$, the unperturbed ground-state hyperfine transition frequency of the caesium 133 atom, to be 9 192 631 770 when expressed in the unit Hz, which is equal to s^{-1}.[1]

This current definition was adopted in 1967 when it became feasible to define the second based on fundamental properties of nature with caesium clocks.[2] Because the speed of Earth's rotation varies and is slowing ever so slightly, a leap second is added at irregular intervals to civil time[nb 1] to keep clocks in sync with Earth's rotation.

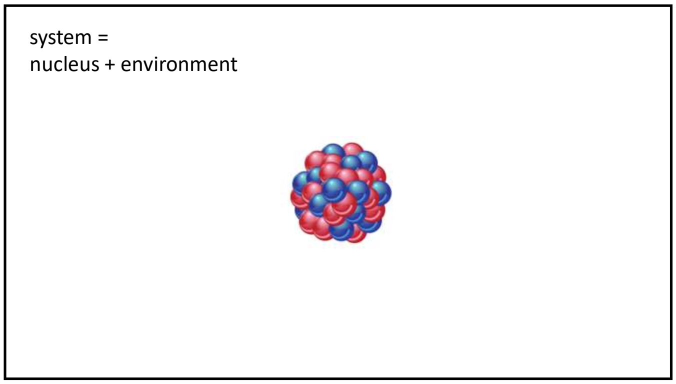
4



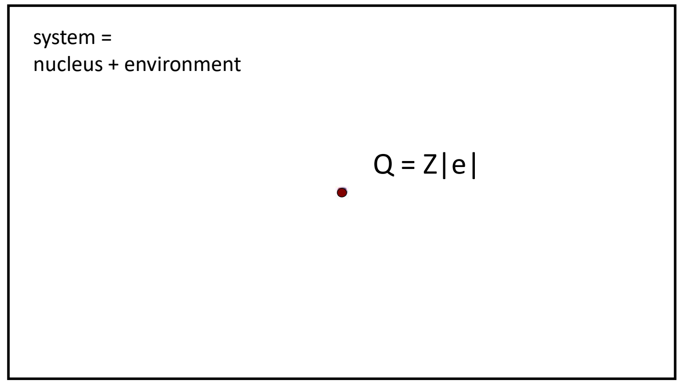
5

define
"system"

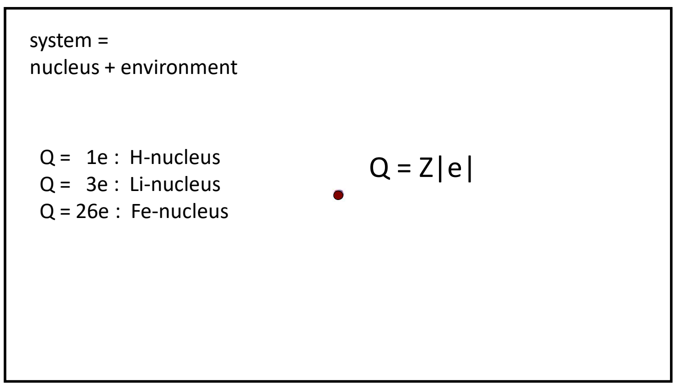
6


system =
nucleus + environment

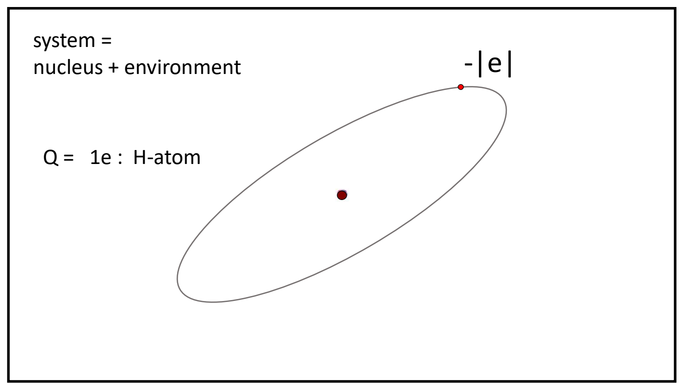
7


system =
nucleus + environment
Q = Z|e|

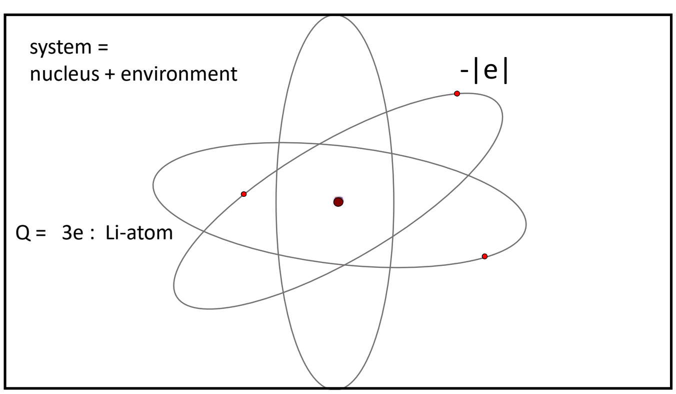
8


system =
nucleus + environment
Q = 1e : H-nucleus
Q = 3e : Li-nucleus
Q = 26e : Fe-nucleus
Q = Z|e|

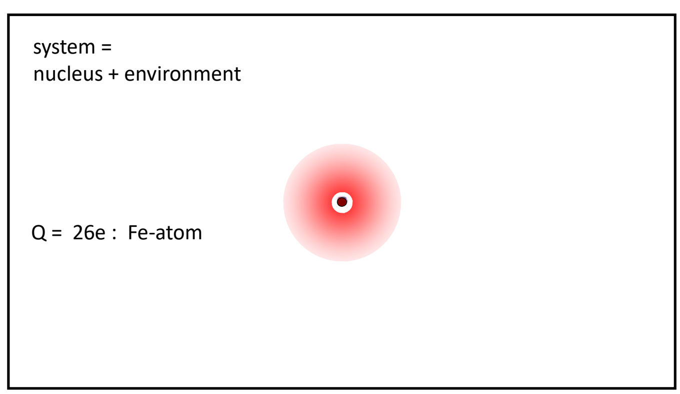
9


system =
nucleus + environment
-|e|
Q = 1e : H-atom

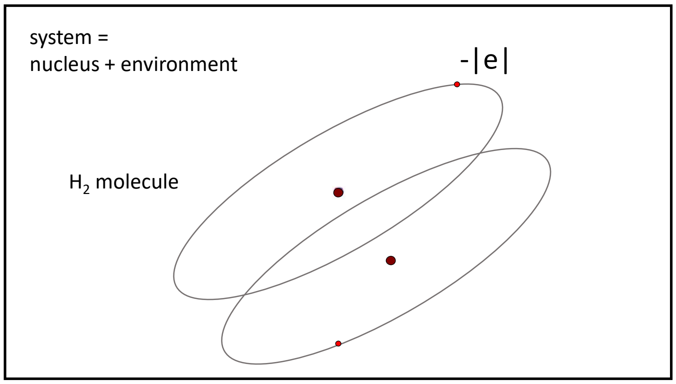
10


system =
nucleus + environment
-|e|
Q = 3e : Li-atom

11


system =
nucleus + environment
Q = 26e : Fe-atom

12



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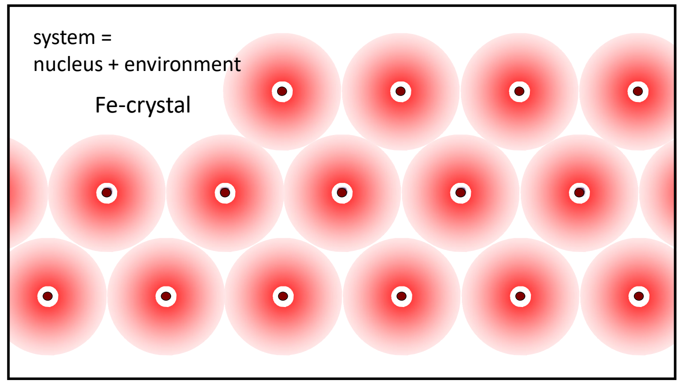

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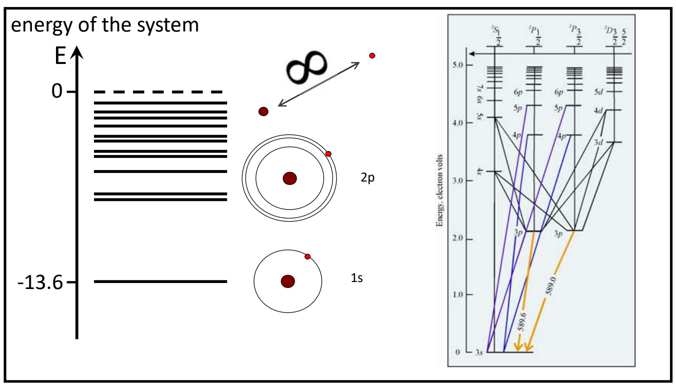

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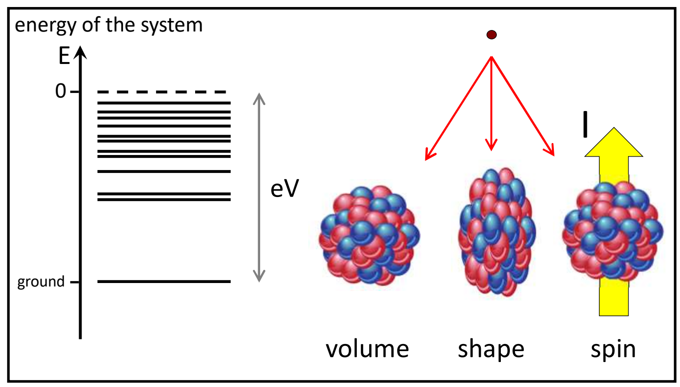

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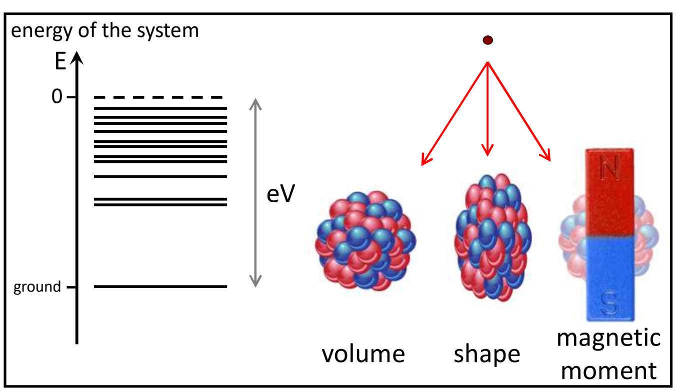

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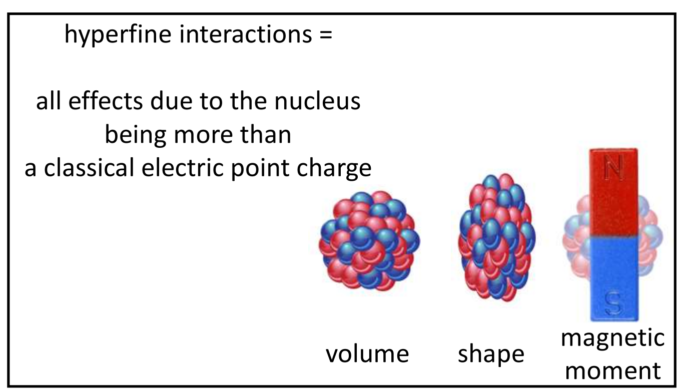

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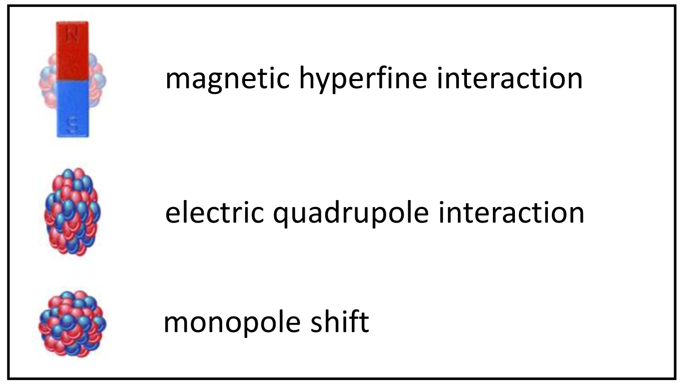

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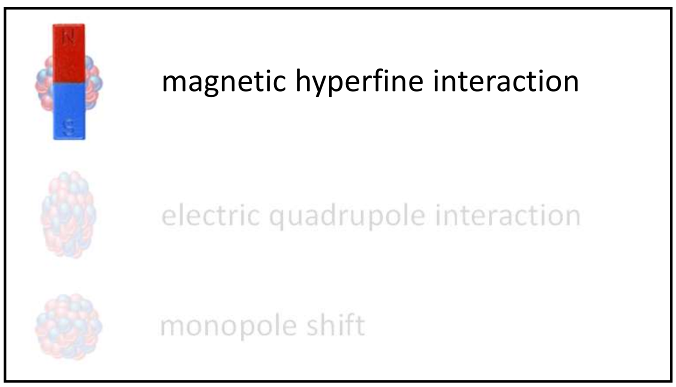

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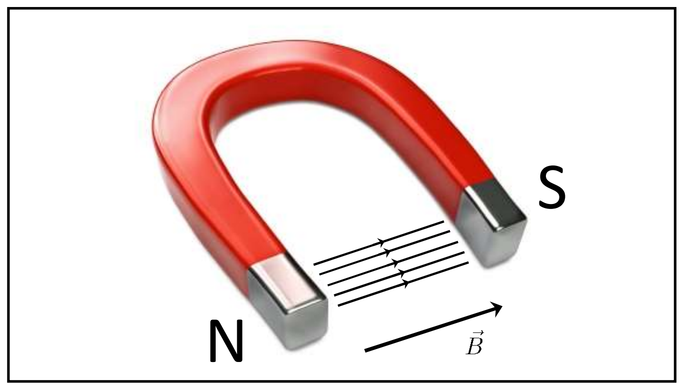

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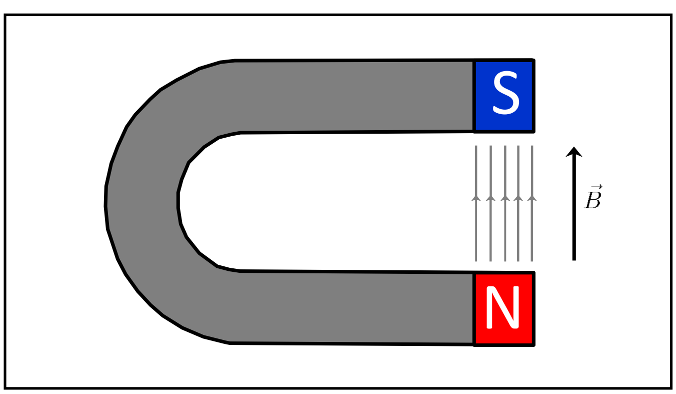

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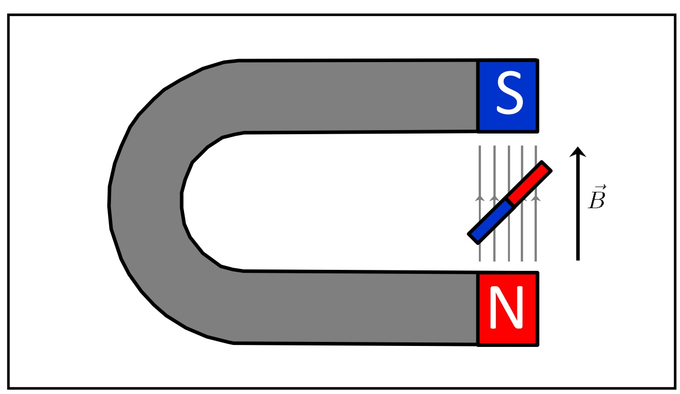

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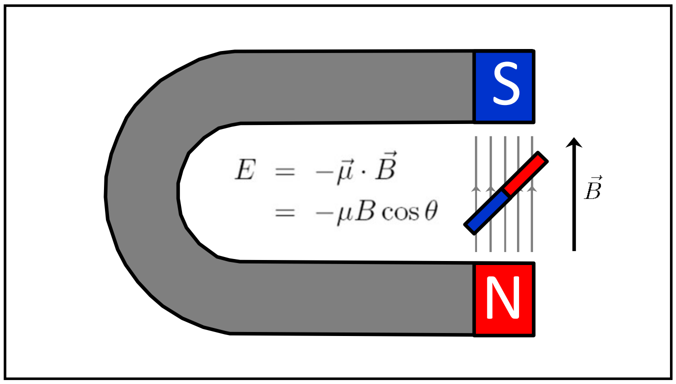

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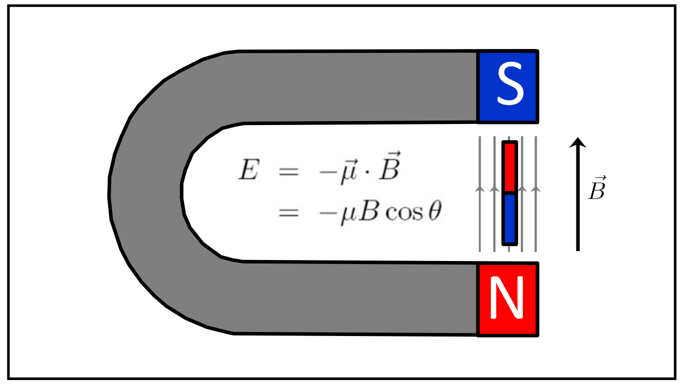

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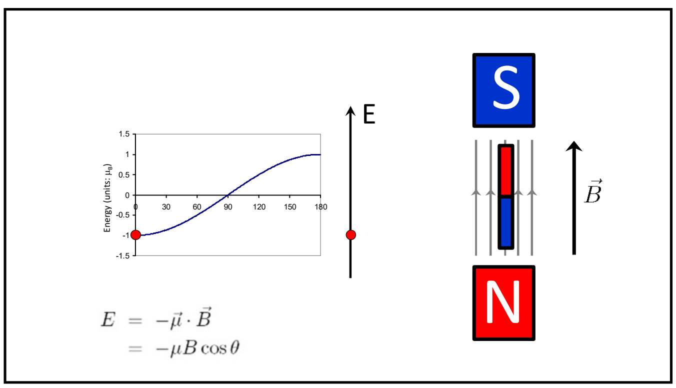

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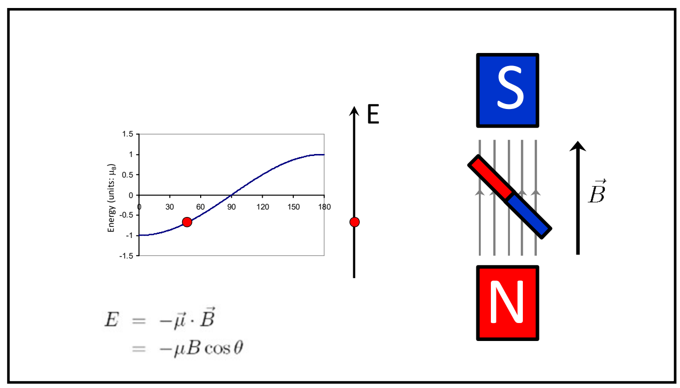

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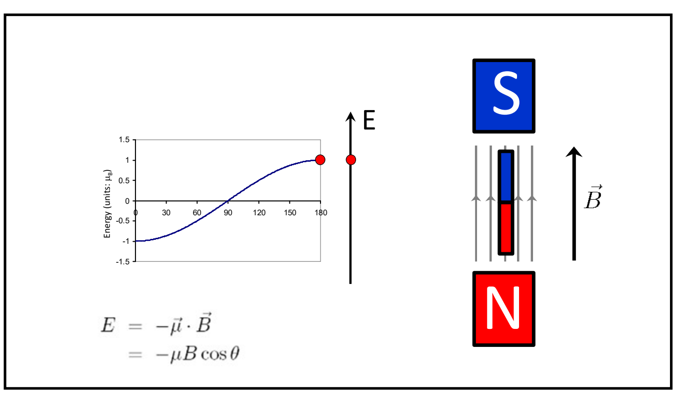

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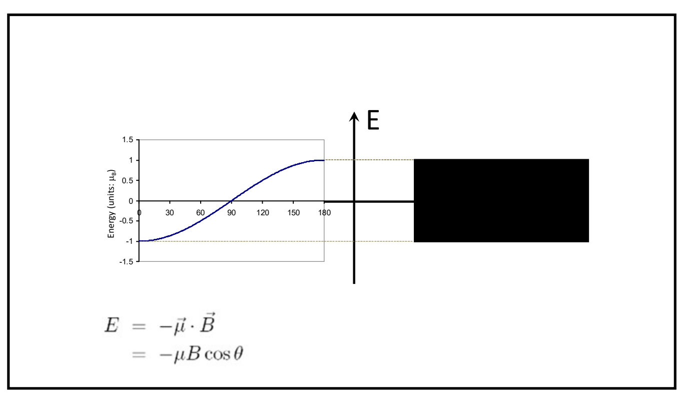

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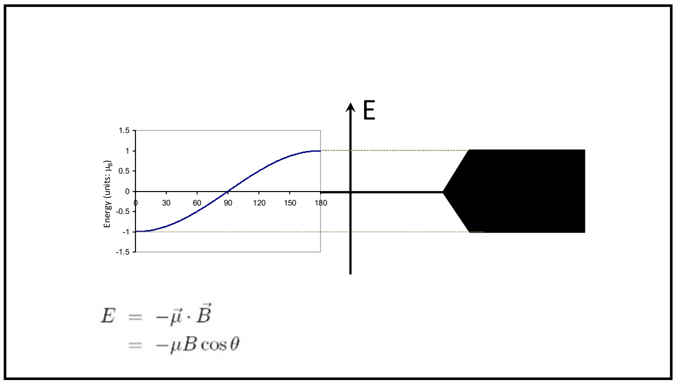

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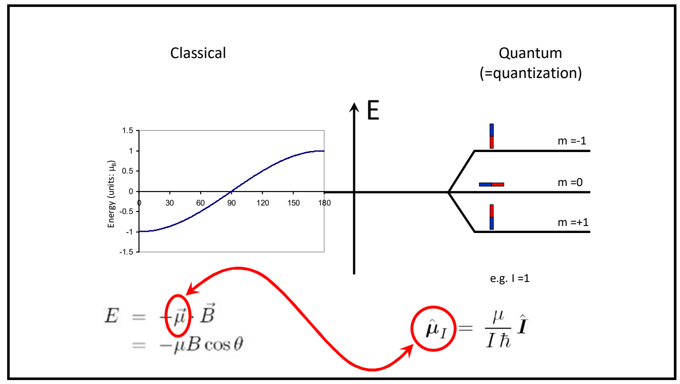

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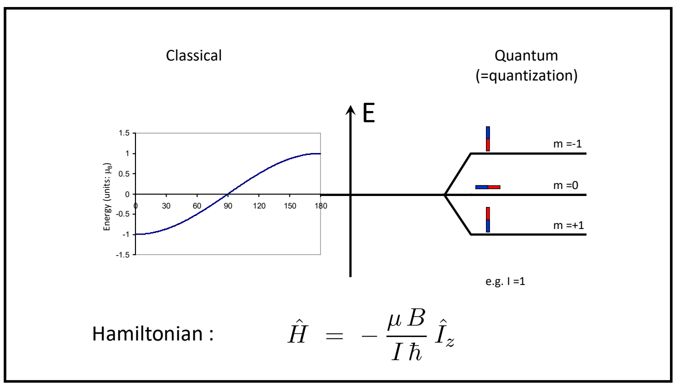

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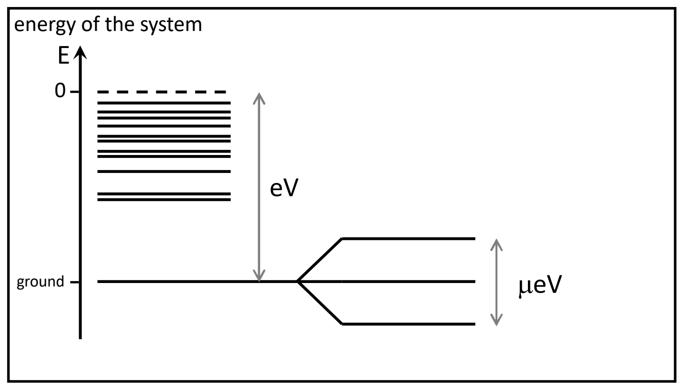

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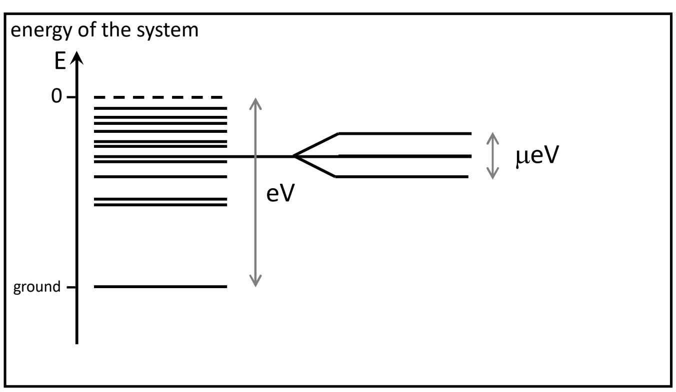

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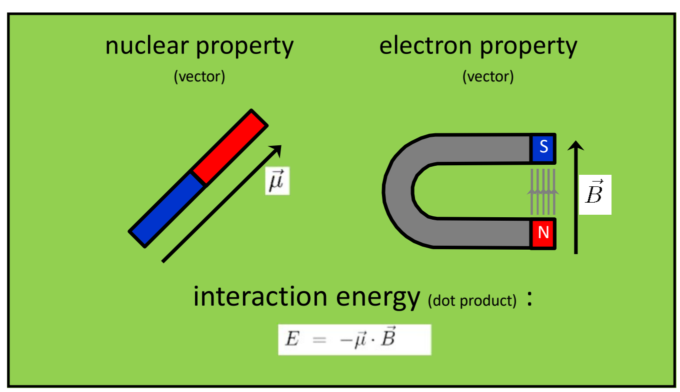
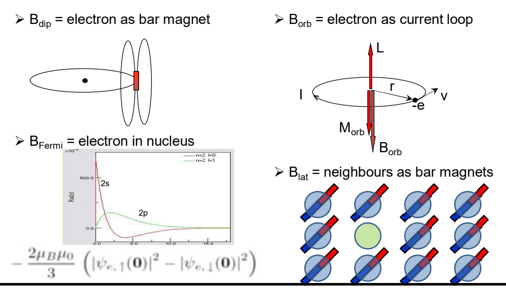


36

Source of magnetic fields at the nuclear site in an atom/solid

$B_{tot} = B_{dip} + B_{orb} + B_{fermi} + B_{lat}$



37

How to do it in WIEN2k ?

Magnetic hyperfine field

In regular scf file:
`:HFFxxx` (Fermi contact contribution)

After post-processing with LAPWDM :
- orbital hyperfine field ("3 3" in case.indmc)
- dipolar hyperfine field ("3 5" in case.indmc)

in case.scfdmup

```
------------------- top of file: case.indm -------------------
-9.                  Emin cutoff energy
 1                   number of atoms for which density matrix is calculated
 1  1  2     index of 1st atom, number of L's, L1
 0 0         r-index, (l,s)-index
------------------- bottom of file ----------------------
```

After post-processing with DIPAN :
- lattice contribution

in case.outputdipan

more info:
UG 7.8 (lapwdm)
UG 8.3 (dipan)

38

How to do it in WIEN2k ?

Magnetic hyperfine field

step-by-step tutorial video : https://youtu.be/L4t5ZAJAsoY

In regular scf file:
`:HFFxxx` (Fermi conta

After post-processing with LAPWDM :
- orbital hyperfine field ("3 3" in case.indmc)
- dipolar hyperfine field ("3 5" in case.indmc)

in case.scfdmup

```
------------------- top of file: case.indm -------------------
-9.                  Emin cutoff energy
 1                   number of atoms for which density matrix is calculated
 1  1  2     index of 1st atom, number of L's, L1
 0 0         r-index, (l,s)-index
------------------- bottom of file ----------------------
```

After post-processing with DIPAN :
- lattice contribution

in case.outputdipan

more info:
UG 7.8 (lapwdm)
UG 8.3 (dipan)

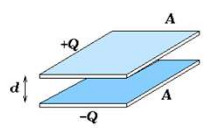
39

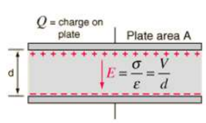
magnetic hyperfine interaction

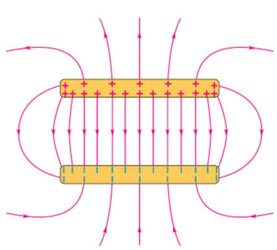
electric quadrupole interaction

monopole shift

40







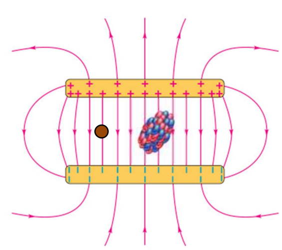
41

- Force on a point charge:

$$\vec{F} = Q\vec{E}$$

- Force on a general charge:

$$\vec{F} = \int \vec{E}\, dQ = Q\vec{E}$$



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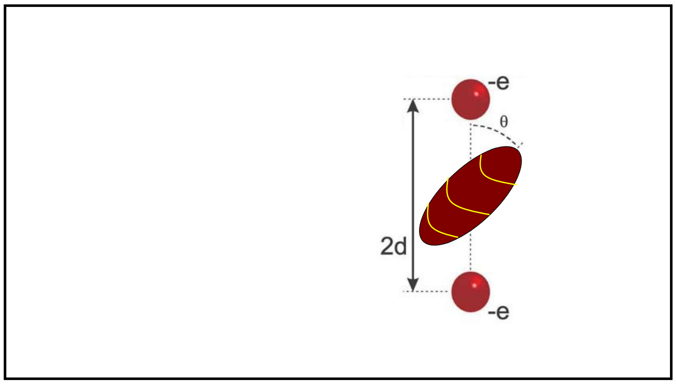

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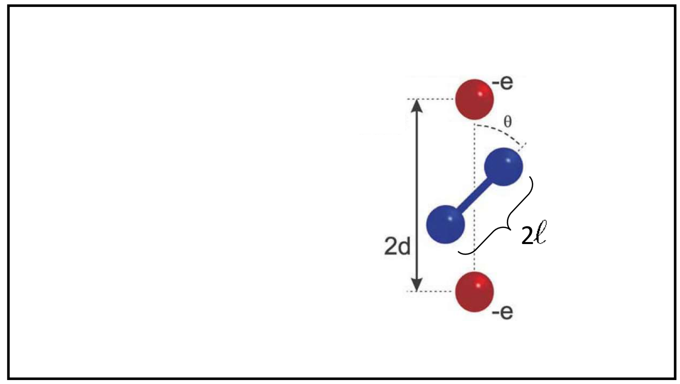

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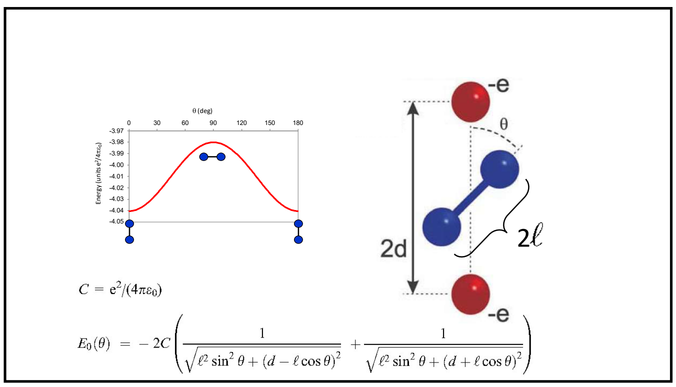

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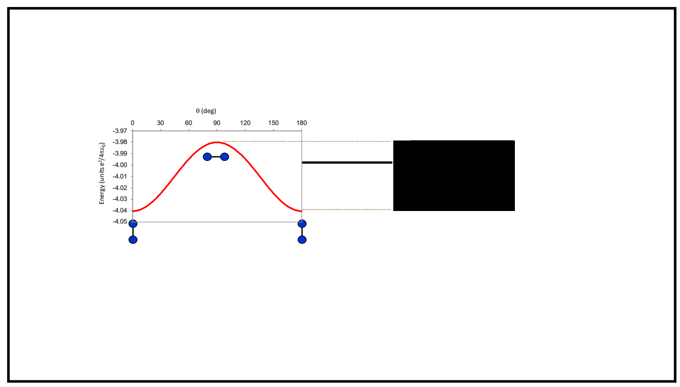

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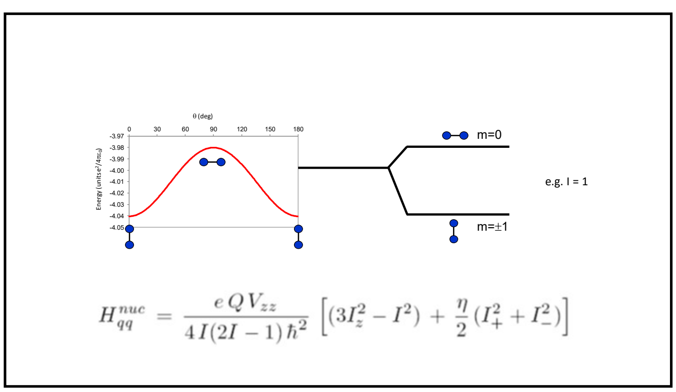

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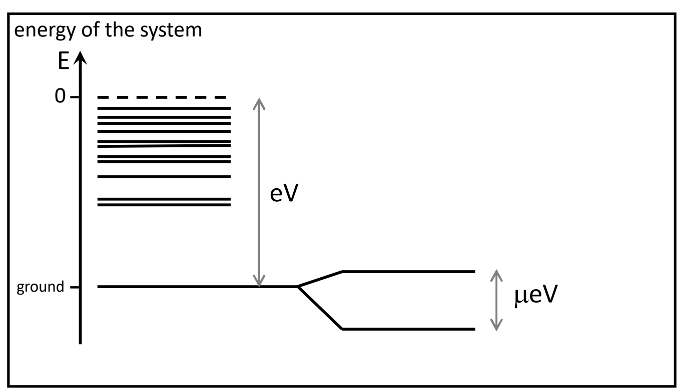

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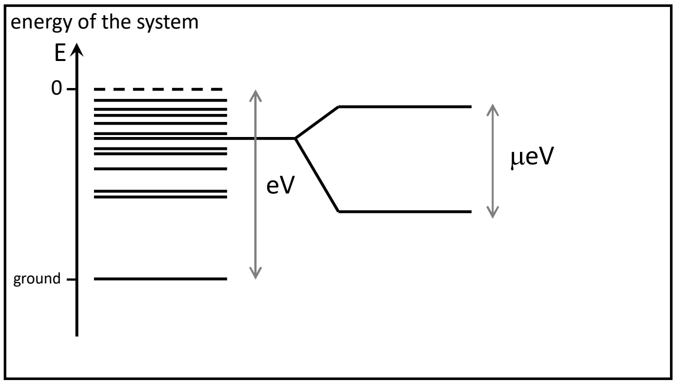

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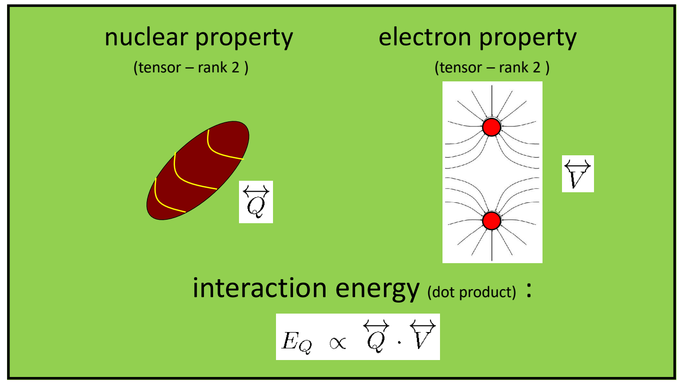


50

How to do it in WIEN2k ?

Electric-field gradient

In regular scf file:

```
:EFGxxx
:ETAxxx
Main directions of the EFG
```

} 5 degrees of freedom

Full analysis printed in case.output2
if EFG keyword in case.in2 is put (UG 7.6)
(split into many different contributions)

more info:
- Blaha, Schwarz, Dederichs, PRB 37 (1988) 2792
- EFG document in wien2k FAQ (Katrin Koch, SC)

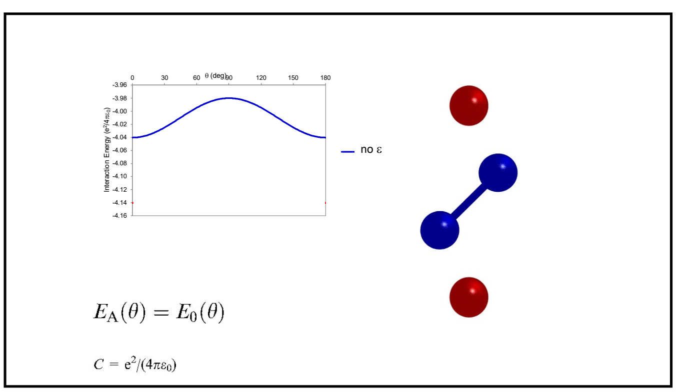
51

magnetic hyperfine interaction

electric quadrupole interaction

monopole shift

52



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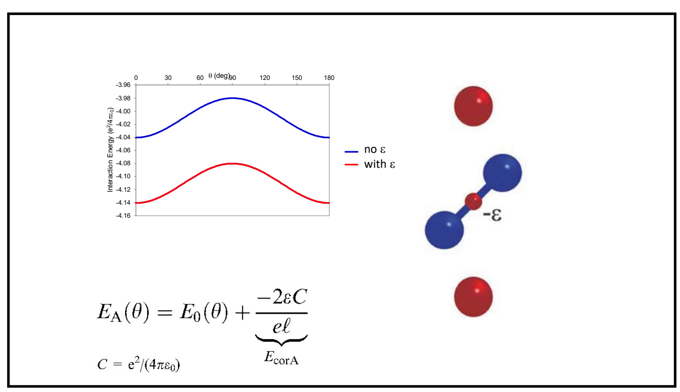

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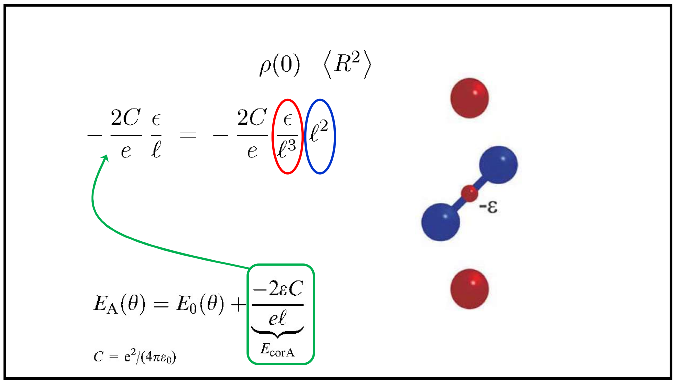

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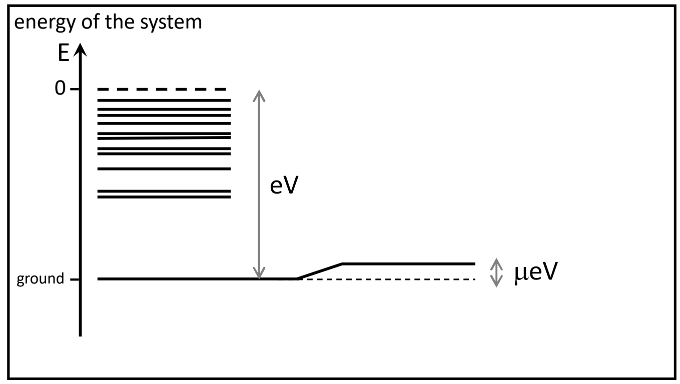

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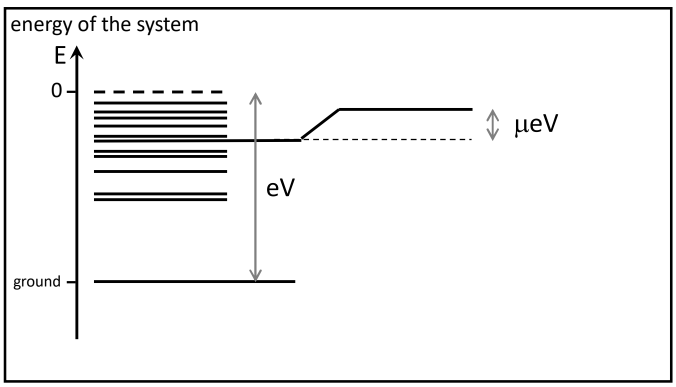

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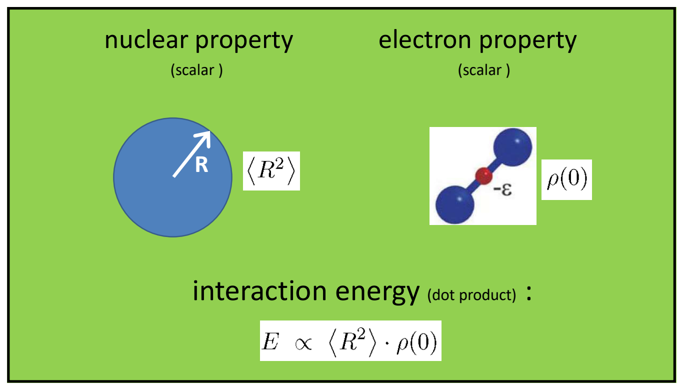

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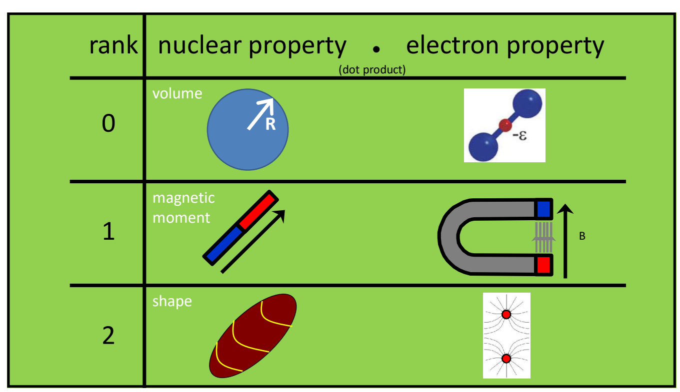
How to do it in WIEN2k ?

Isomer shift calculations

In regular scf file:

`:RTOxxx` = electron density near the nucleus of atom xxx (i.e. at the first radial mesh point, typically 0.0005 au)

59



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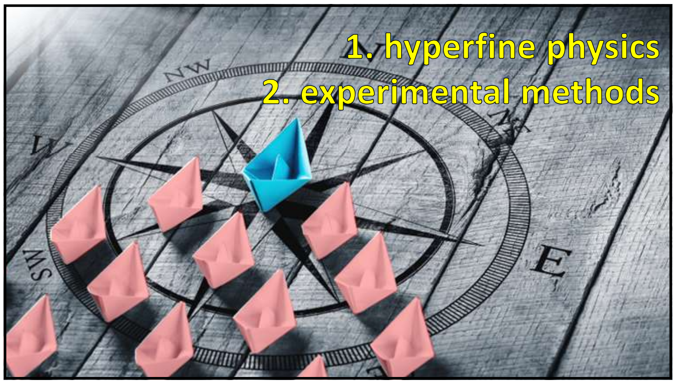


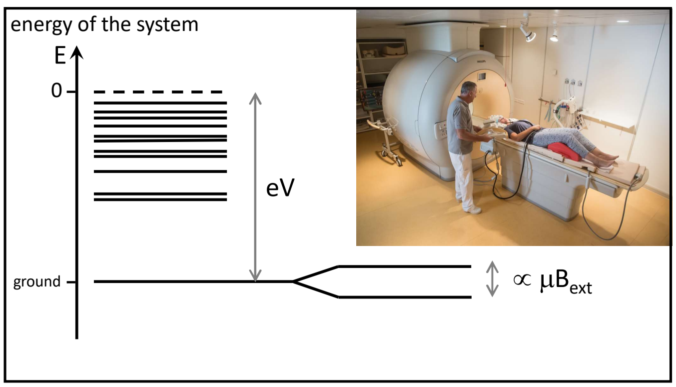
61

experimental hyperfine methods =

all methods of which
the experimental signal is affected
by a nucleus that is more than
a classical electric point charge

All methods that are based on transitions
between levels that are shifted or split
by hyperfine interactions

62



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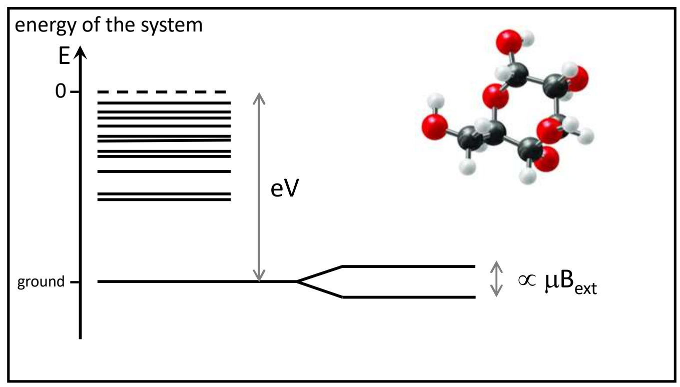

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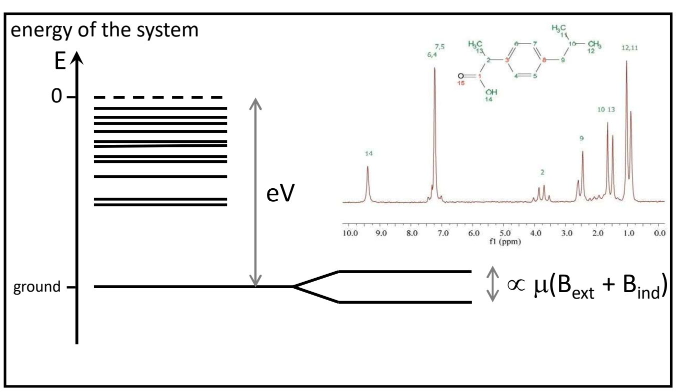

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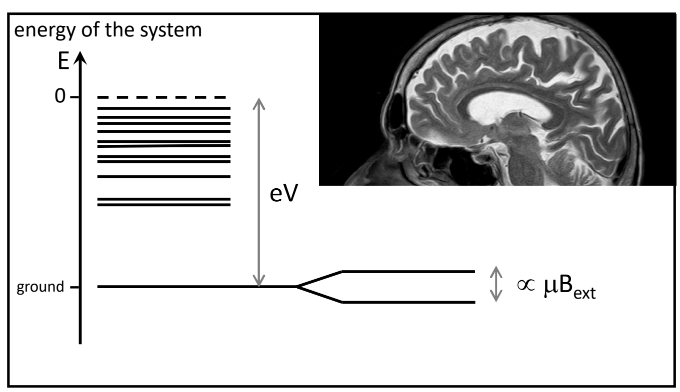

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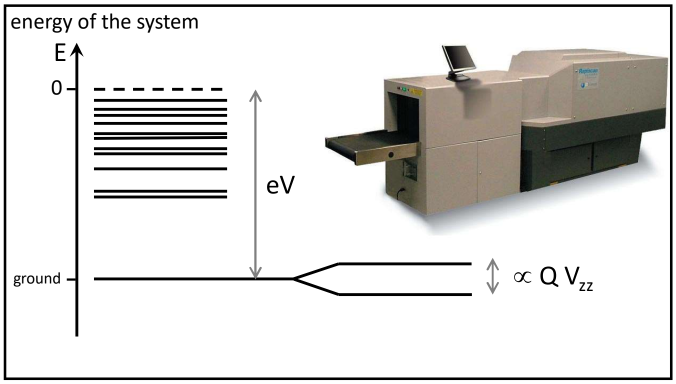

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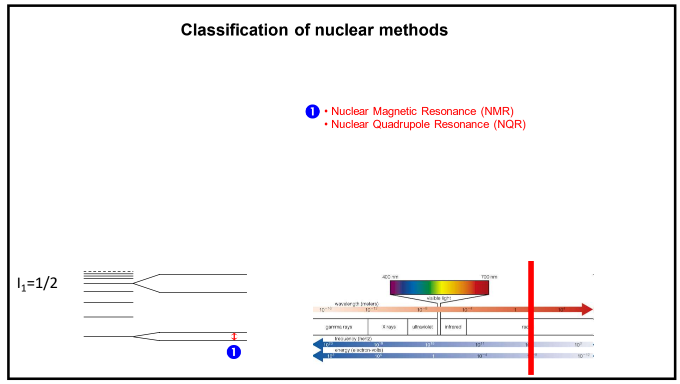

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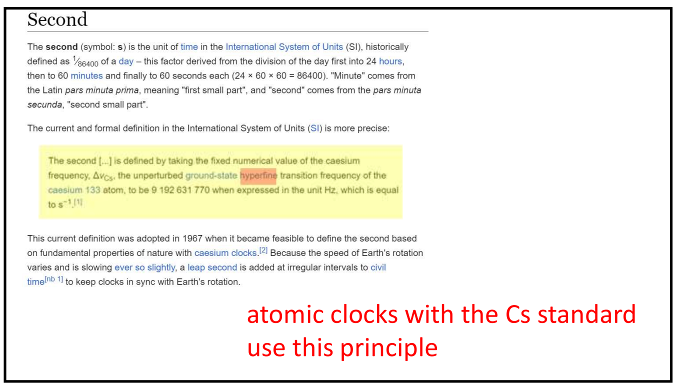


Second

The **second** (symbol: **s**) is the unit of time in the International System of Units (SI), historically defined as $^1/_{86400}$ of a day – this factor derived from the division of the day first into 24 hours, then to 60 minutes and finally to 60 seconds each (24 × 60 × 60 = 86400). "Minute" comes from the Latin *pars minuta prima*, meaning "first small part", and "second" comes from the *pars minuta secunda*, "second small part".

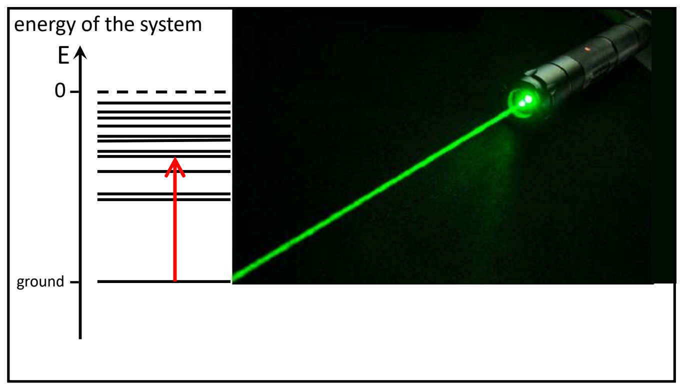
The current and formal definition in the International System of Units (SI) is more precise:

> The second [...] is defined by taking the fixed numerical value of the caesium frequency, $\Delta\nu_{Cs}$, the unperturbed ground-state hyperfine transition frequency of the caesium 133 atom, to be 9 192 631 770 when expressed in the unit Hz, which is equal to s^{-1}.[1]

This current definition was adopted in 1967 when it became feasible to define the second based on fundamental properties of nature with caesium clocks.[2] Because the speed of Earth's rotation varies and is slowing ever so slightly, a leap second is added at irregular intervals to civil time[nb 1] to keep clocks in sync with Earth's rotation.

atomic clocks with the Cs standard use this principle

69



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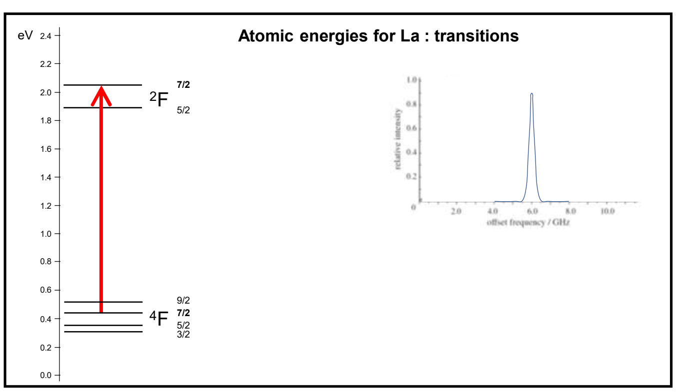

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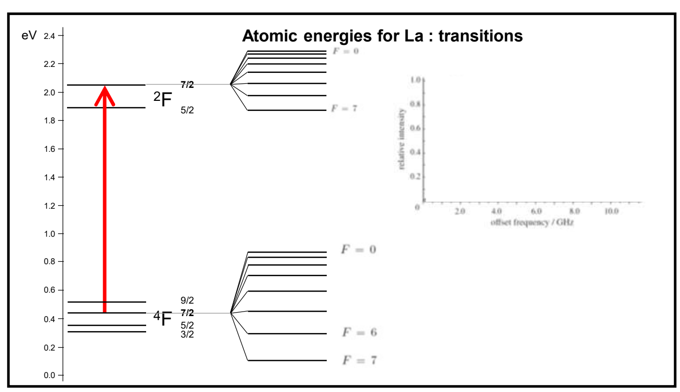

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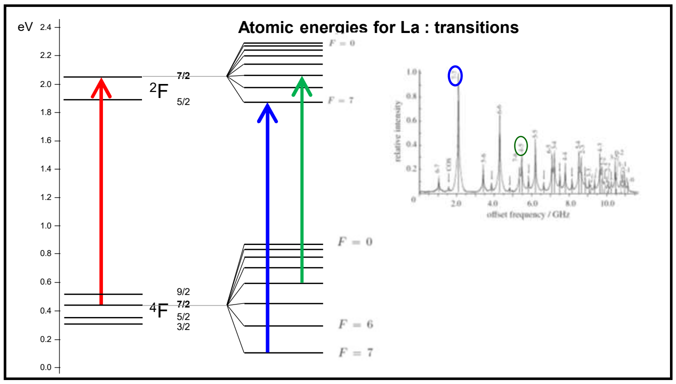

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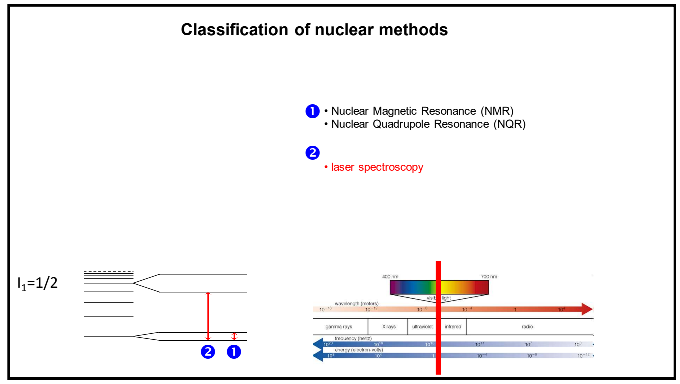

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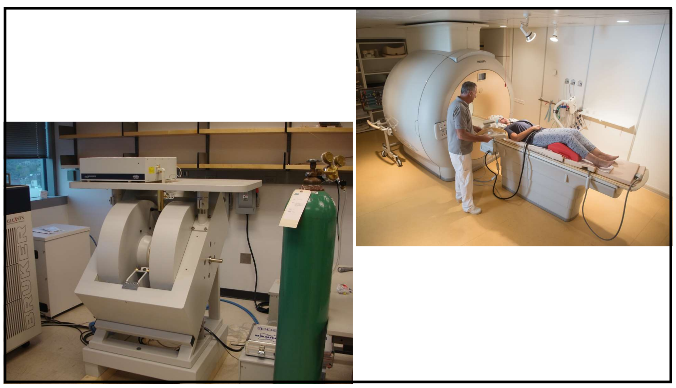

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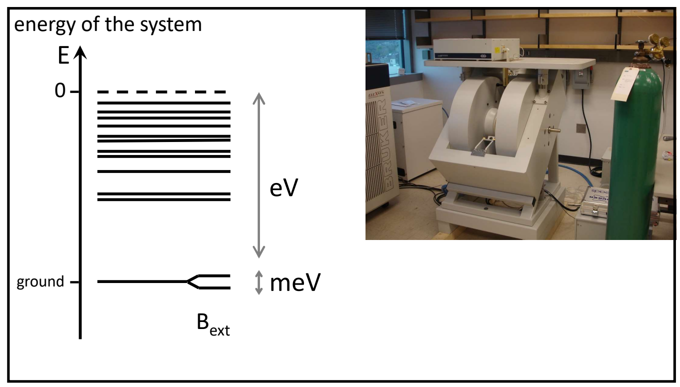

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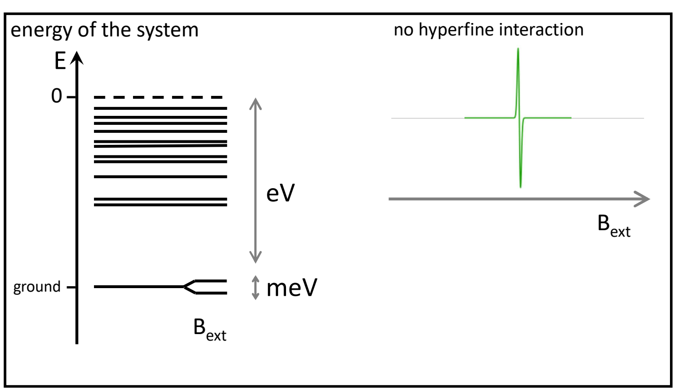

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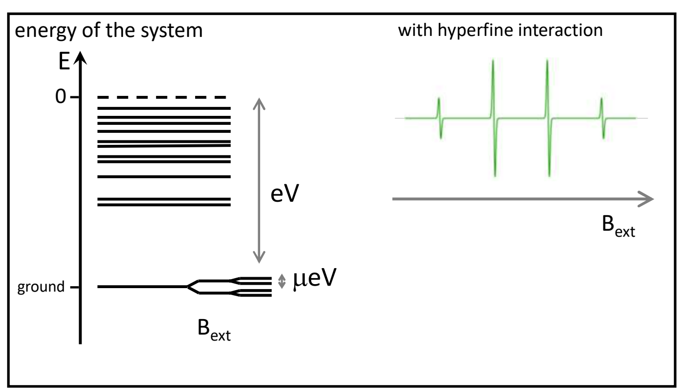

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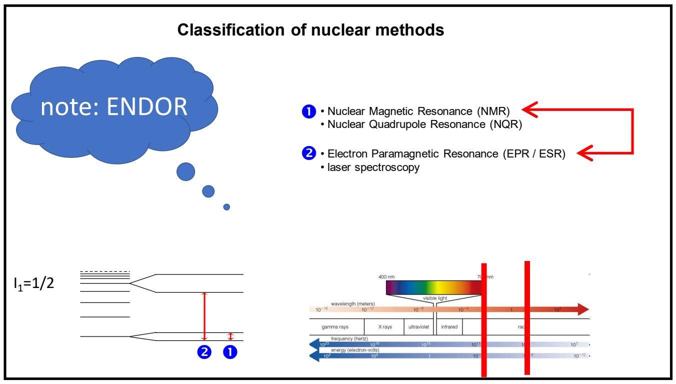

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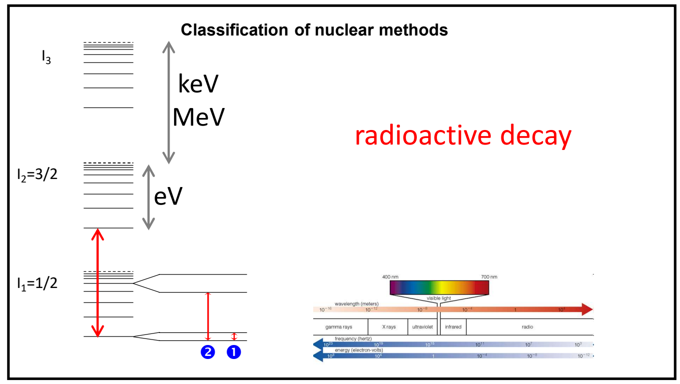

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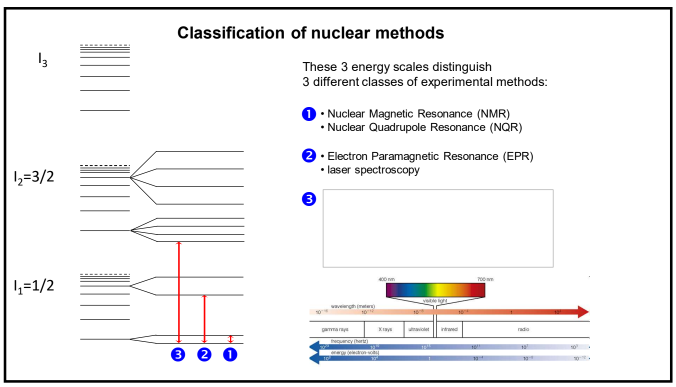

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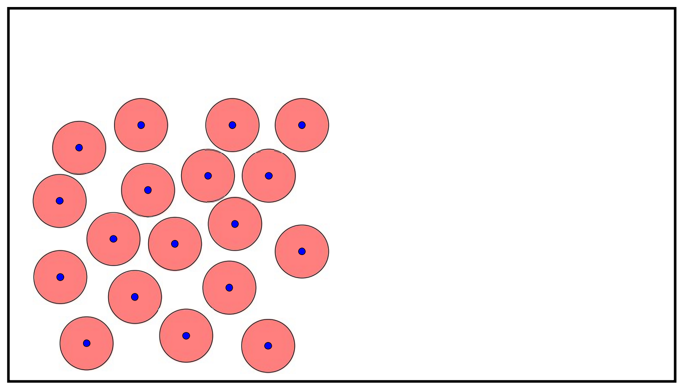

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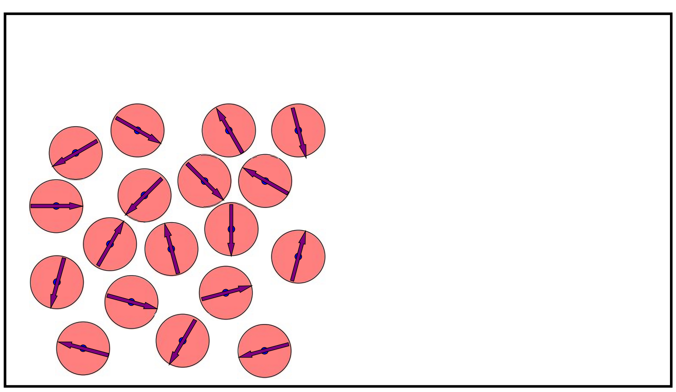

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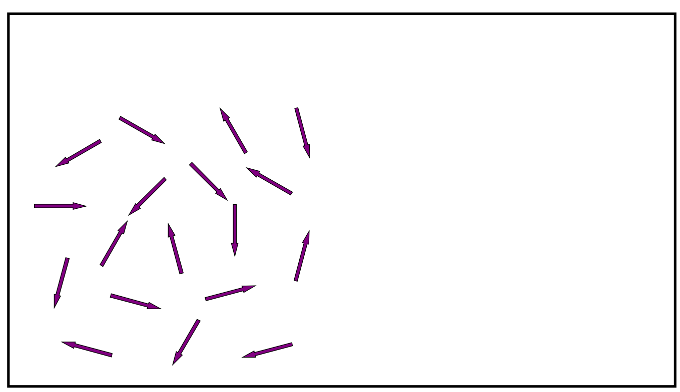

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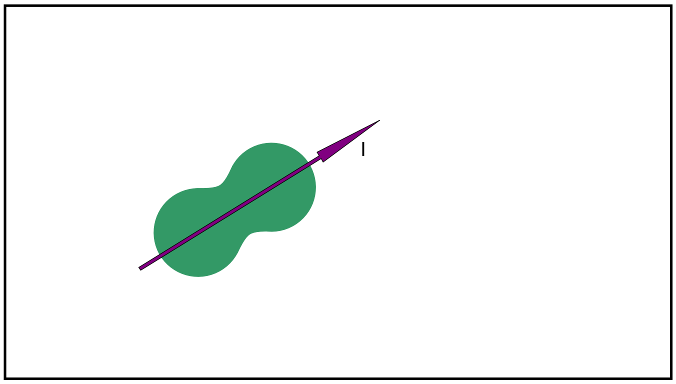

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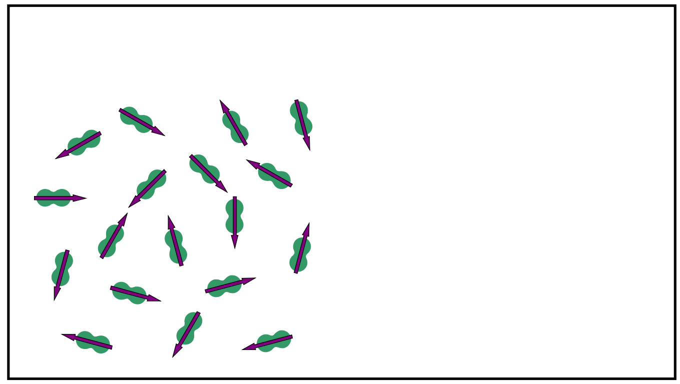

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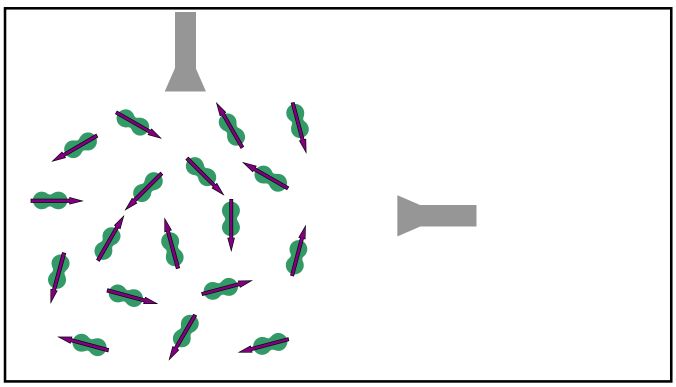

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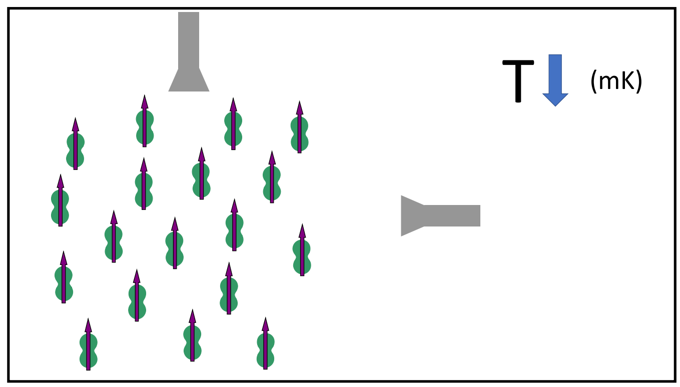

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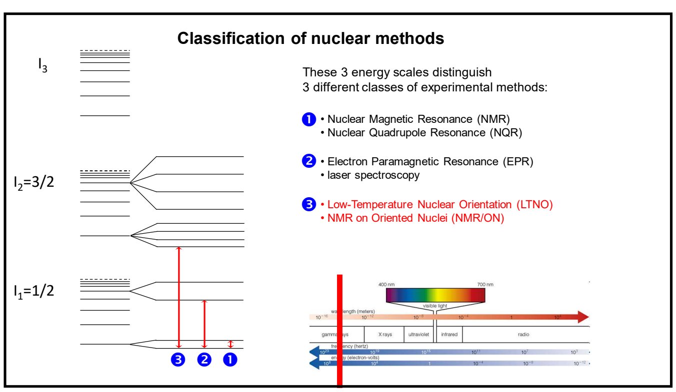

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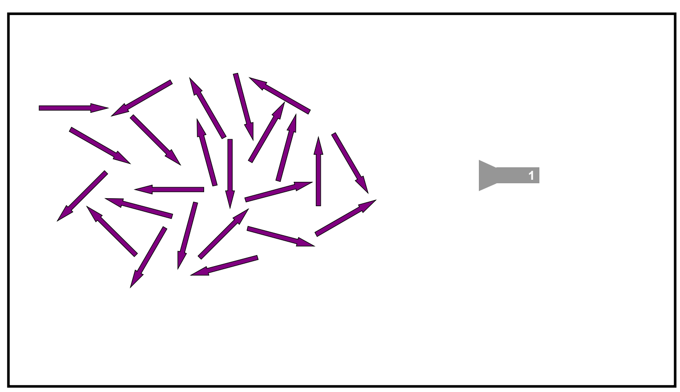

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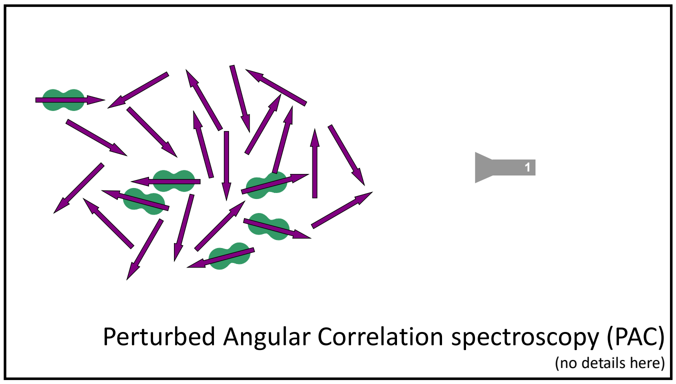

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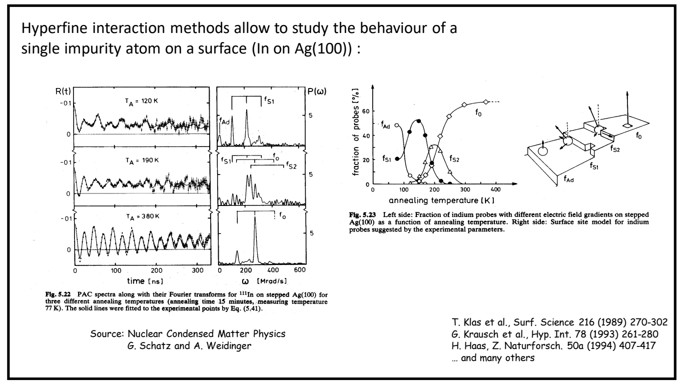

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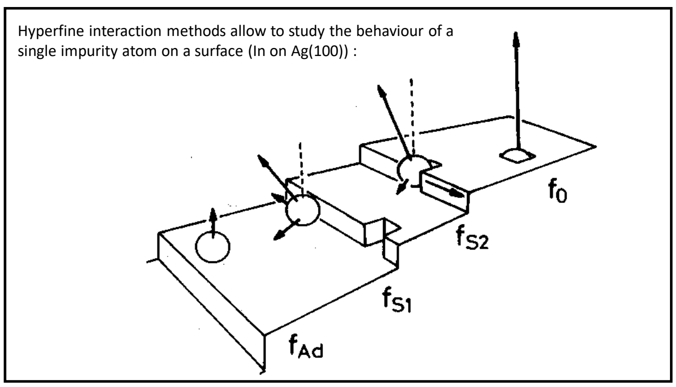

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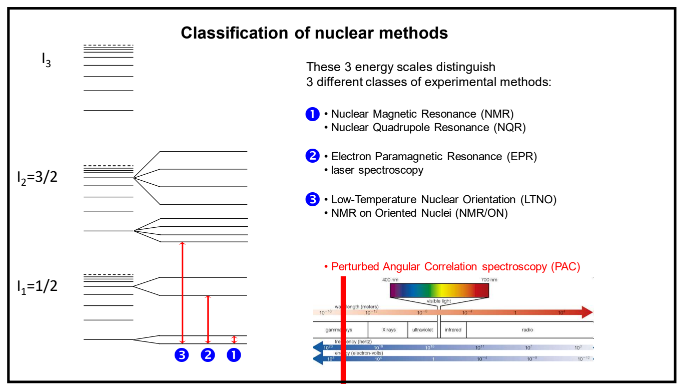

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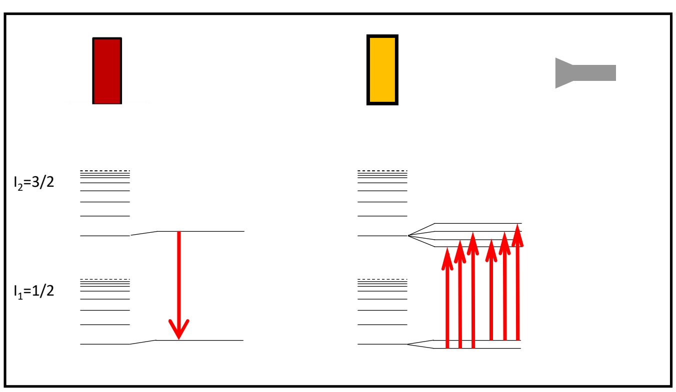

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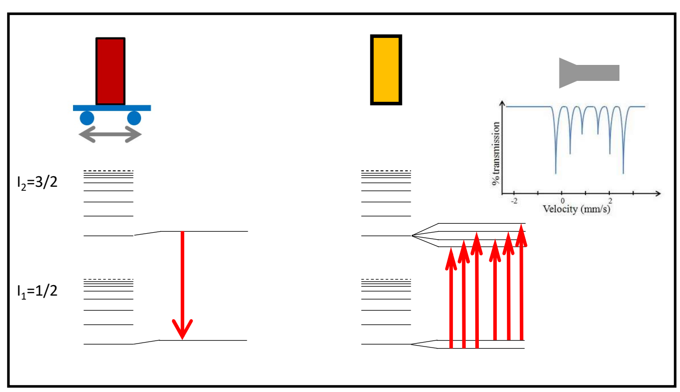

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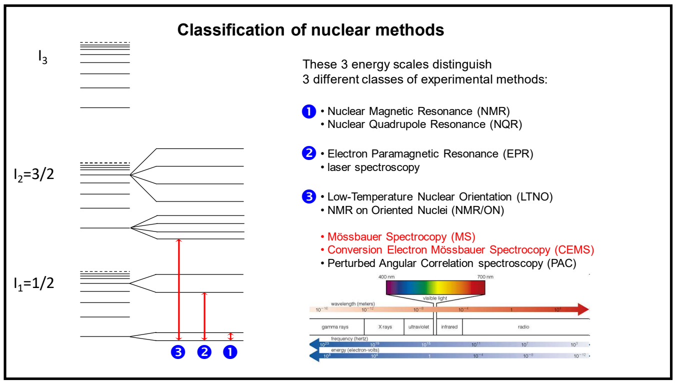

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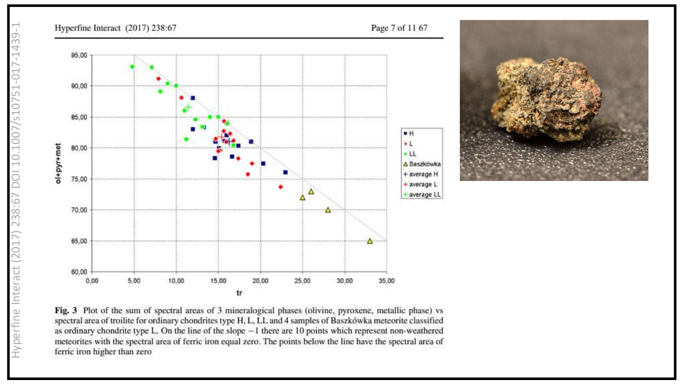

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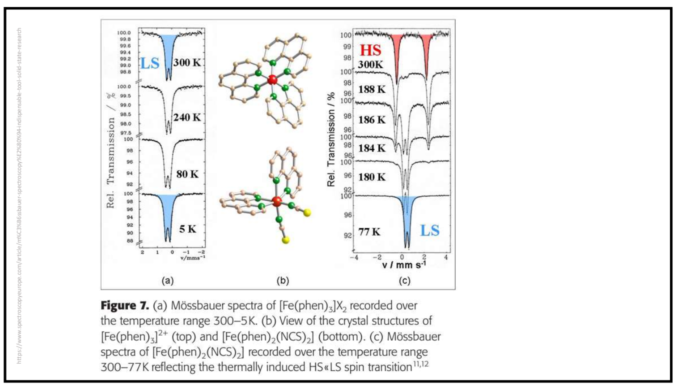

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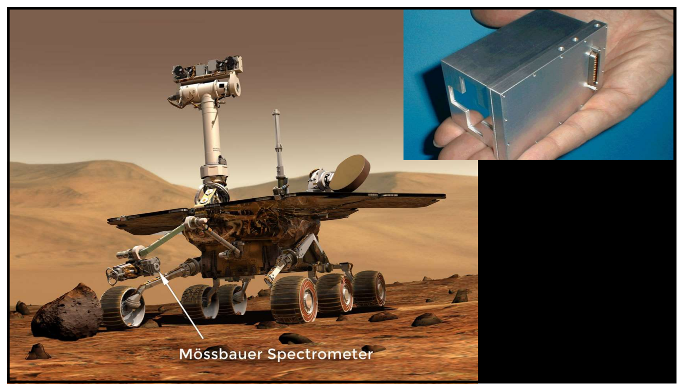

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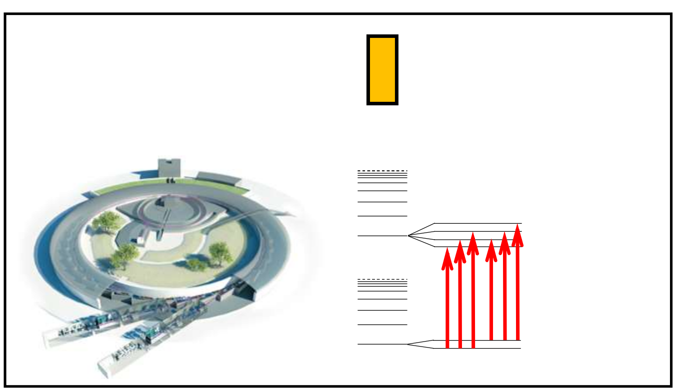

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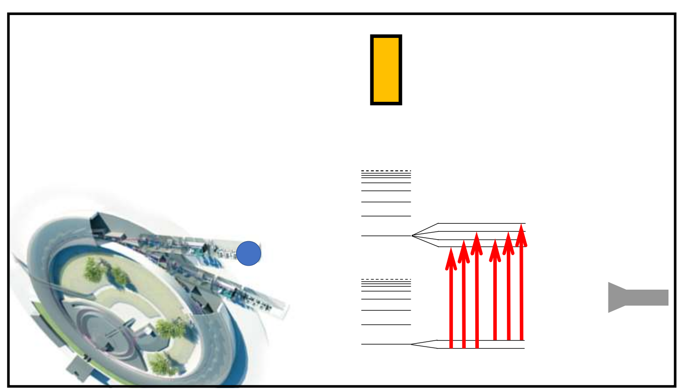

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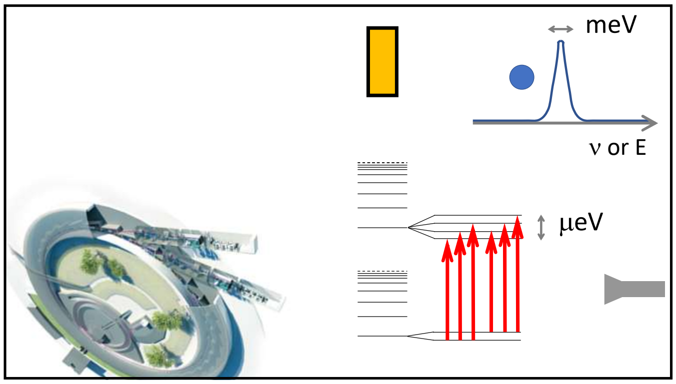

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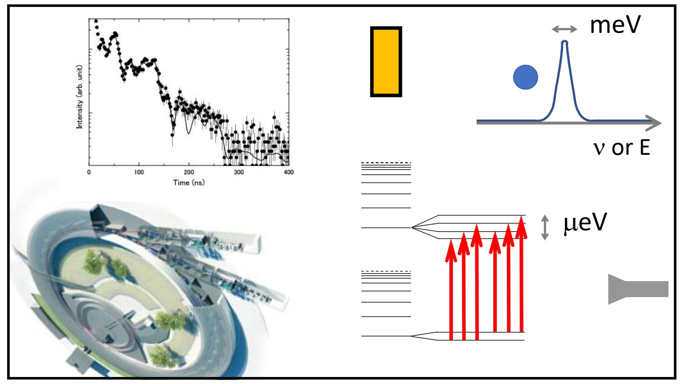

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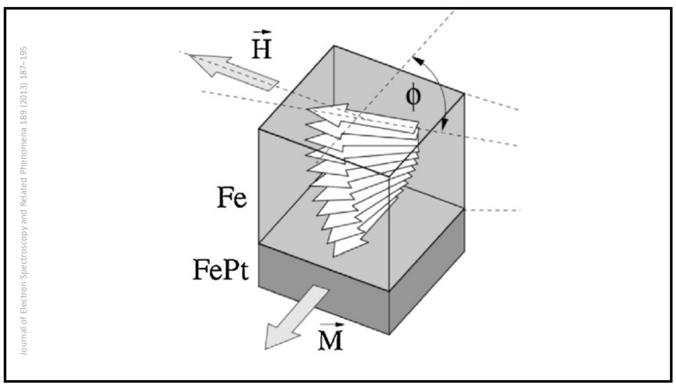

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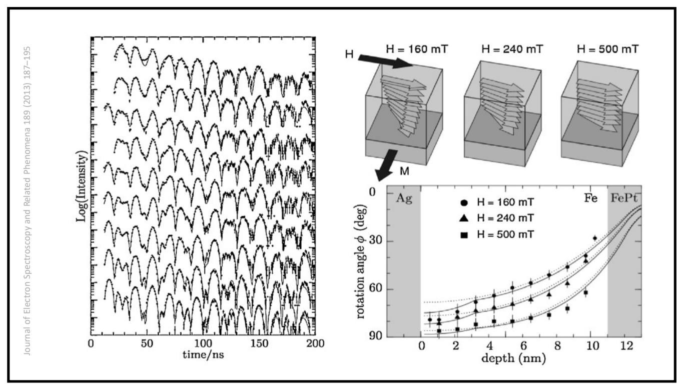

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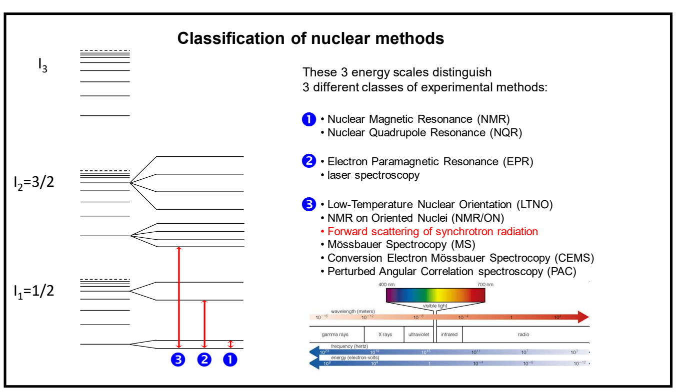

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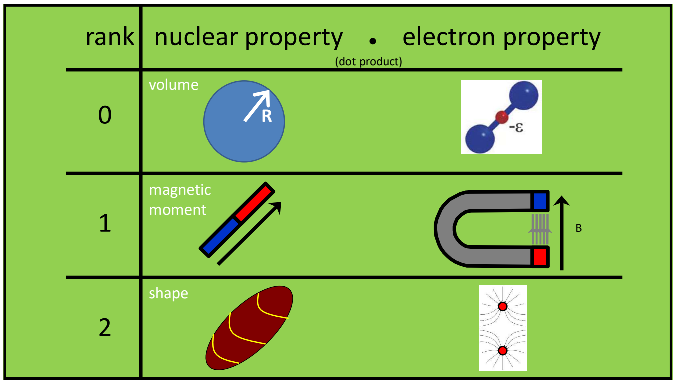

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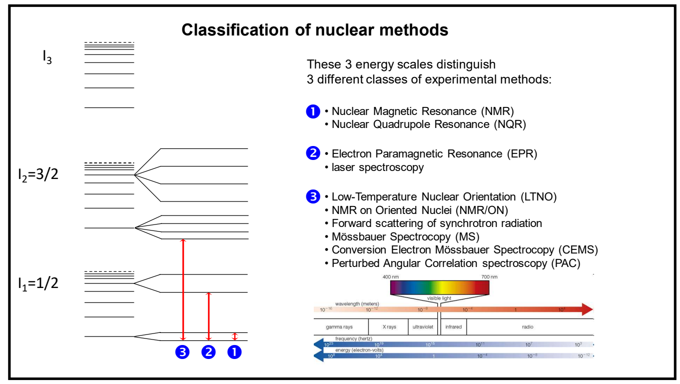

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45-minute version (as today) but without WIEN2k instructions :
https://youtu.be/_cMNuOQB3fI

step-by-step demo video for hyperfine fields with WIEN2k :
https://youtu.be/L4t5ZAJAsoY

course: www.hyperfinecourse.org
didactical approach : https://youtu.be/YsUk4P1f5DM

my Youtube channel : https://bit.ly/cottenier
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