Evaluation of the energy shift for the Pauli-forbidden X-ray transitions

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"Hunt for the "impossible atoms": the quest for a tiny violation of the Pauli Exclusion Principle. Implications for physics, cosmology and philosophy,"

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John Templeton Foundation

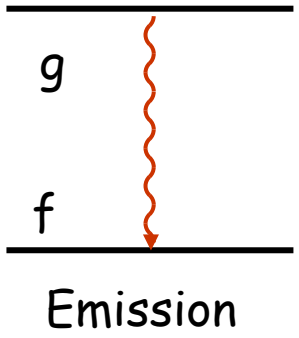
Overview of the seminar

- **From usual X-ray transitions to Pauli-forbidden ones**
  - **The Fermi golden rule: transition-matrix elements**
  - **The (non-relativistic) many-body wave-function: the effect of antisymmetrization**
  - **Full calculation of transition rate and energy-shift by the relativistic Multi-Configuration Dirac-Fock code**
  - **A relatively simple estimation of the energy-shift**
  - **Conclusions: and what about the 'new' electrons ?**
- **Is it possible to detect a transient violation of the Pauli principle at the subattosecond time scale ?**
  - **The Corinaldesi's paper**
  - **Retarded interactions of the E.M. field and Zitterbewegung: towards a non-orthodox view ?**

The Fermi golden rule: transition-matrix elements

Typical values of absorption edges (X-ray data booklet)

	Z	K	L_1	L_2	L_3	M_1	M_2	M_3	M_4	M_5
H	1	13.6								
C	6	284.2	37.3							
O	8	543.1	41.6							
V	23	5465	626.7	519.8	512.1					
Fe	26	7112	844.6	719.9	706.8	91.3	52.7	52.7		
Cu	29	8979	1096.7	952.3	932.7	122.5	77.3	75.1		
Ag	47	25514	3806	3524	3351	719.0	603.8	573.0	374.0	368.3
U	92	115606	21757	20948	17166	5548	5182	4303	3728	3552



A typical emission process from state ϕ_g to state ϕ_f: $\sigma_{fg} = \frac{2\pi h\alpha}{\omega m^2}\left|\langle\varphi_f|\hat{O}|\varphi_g\rangle\right|^2 \delta(E_f - E_g - \hbar\omega)$

where: $\hat{O} = (\vec{P}.\vec{\varepsilon} + i\vec{S}.\vec{k}\times\vec{\varepsilon})e^{i\vec{k}.\vec{r}}$ *so that:*

$$\langle f|\hat{O}_E|g\rangle = \left\langle f\left|\vec{P}.\vec{\varepsilon}\left(1 + i\vec{k}.\vec{r} - \frac{1}{2}(\vec{k}.\vec{r})^2 + \cdots\right)\right|g\right\rangle$$

$$\langle f|\hat{O}_B|g\rangle = \left\langle f\left|i\vec{S}.\vec{k}\times\vec{\varepsilon}\left(1 + i\vec{k}.\vec{r} - \frac{1}{2}(\vec{k}.\vec{r})^2 + \cdots\right)\right|g\right\rangle$$

Only pick up ◯ *and rewrite it:* $\langle f|\hat{O}_{Ed}|g\rangle = \langle f|\vec{P}.\vec{\varepsilon}|g\rangle = i\frac{m}{\hbar}(E_f - E_g)\langle f|\vec{\varepsilon}.\vec{r}|g\rangle$

with: $\vec{P}.\vec{\varepsilon} = \frac{m}{i\hbar}[\vec{\varepsilon}.\vec{r}, H_0]$ *and:* $\langle f|[\vec{\varepsilon}.\vec{r}, H_0]|g\rangle = (E_g - E_f)\langle f|\vec{\varepsilon}.\vec{r}|g\rangle$

By summing over all states: $\sigma = 4\pi^2\alpha\hbar\omega\sum_{fg}\left|\langle\varphi_f|o|\varphi_g\rangle\right|^2 \delta(E_f - E_g - \hbar\omega)$ **with o = ε . r**

We remind that: $\langle\varphi_n|\hat{O}|\varphi_g\rangle = \iiint_{espace}\varphi_n^*(r,\Omega)\hat{O}(r,\Omega)\varphi_g(r,\Omega)r^2 dr d\Omega$ **a space integral**

The many-body wave-function and the Schrödinger equation

The ultimate goal of most approaches in solid-state physics and quantum chemistry is to solve the time-independent problem (usually with Schrödinger Hamiltonian):

$$\hat{H}\Psi_i(\vec{x}_1,\vec{x}_2,...,\vec{x}_N,\vec{R}_1,\vec{R}_2,...,\vec{R}_M) = E_i\Psi_i(\vec{x}_1,\vec{x}_2,...,\vec{x}_N,\vec{R}_1,\vec{R}_2,...,\vec{R}_M)$$

where (M=number of nuclei, N=number of electrons):

$$\hat{H} = -\frac{1}{2}\sum_{i=1}^{N}\nabla_i^2 - \frac{1}{2}\sum_{A=1}^{M}\frac{1}{M_A}\nabla_A^2 - \sum_{i=1}^{N}\sum_{A=1}^{M}\frac{Z_A}{r_{iA}} + \sum_{i=1}^{N}\sum_{j>i}^{N}\frac{1}{r_{ij}} + \sum_{A=1}^{M}\sum_{B>A}^{M}\frac{Z_A Z_B}{R_{AB}}$$

In the Born-Oppenheimer approximation we need to solve the problem: $\hat{H}_{elec}\Psi_{elec} = E_{elec}\Psi_{elec}$

with $$\hat{H}_{elec} = -\frac{1}{2}\sum_{i=1}^{N}\nabla_i^2 - \sum_{i=1}^{N}\sum_{A=1}^{M}\frac{Z_A}{r_{iA}} + \sum_{i=1}^{N}\sum_{j>i}^{N}\frac{1}{r_{ij}} = \hat{T} + \hat{V}_{Ne} + \hat{V}_{ee}$$

And the total energy is given by: $E_{tot} = E_{elec} + E_{nuc}$

where $$E_{nuc} = \sum_{A=1}^{M}\sum_{B>A}^{M}\frac{Z_A Z_B}{R_{AB}}$$

The effect of antisymmetrization: the exchange interaction

In order to impose the antisymmetrization of the electrons, we need to write the total wave function as a Slater determinant (or as a linear combination of Slater determinants):

$$\Psi_0 \approx \Psi_{HF} = \frac{1}{\sqrt{N!}} \begin{vmatrix} \psi_1(\vec{x}_1) & \psi_2(\vec{x}_1) & \dots & \psi_N(\vec{x}_1) \\ \psi_1(\vec{x}_2) & \psi_2(\vec{x}_2) & \dots & \psi_N(\vec{x}_2) \\ \vdots & \vdots & & \vdots \\ \psi_1(\vec{x}_N) & \psi_2(\vec{x}_N) & \dots & \psi_N(\vec{x}_N) \end{vmatrix}$$

here each ψ_i represents a spin-orbital, single particle wave function

The Hartree-Fock approximation is a method to find the single-particle orthogonal orbitals ψ_i that minimize the total energy E_{HF} of the wave-function Ψ_{HF}. The expectation value is:

$$E_{HF} = \langle \Psi_{HF} | \hat{H} | \Psi_{HF} \rangle = \sum_{i=1}^{N} H_i + \frac{1}{2} \sum_{i,j=1}^{N} (J_{ij} - K_{ij})$$

where $H_i \equiv \int \psi_i^*(\vec{x}) \left[-\frac{1}{2}\nabla^2 - V_{ext}(\vec{x}) \right] \psi_i(\vec{x}) \, d\vec{x}$ **represents the kinetic + the electron-nucleus energy**

$J_{ij} = \int \int \psi_i(\vec{x}_1)\psi_i^*(\vec{x}_1) \frac{1}{r_{12}} \psi_j^*(\vec{x}_2)\psi_j(\vec{x}_2) d\vec{x}_1 d\vec{x}_2$ **is the Coulomb integral >0**

and $K_{ij} = \int \int \psi_i^*(\vec{x}_1)\psi_j(\vec{x}_1) \frac{1}{r_{12}} \psi_i(\vec{x}_2)\psi_j^*(\vec{x}_2) d\vec{x}_1 d\vec{x}_2$ **is the exchange integral**

The Hartree-Fock approximation

The minimization of the previous energy functional with the normalization conditions $\int \psi_i^*(\vec{x})\psi_j(\vec{x})d\vec{x} = \delta_{ij}$

leads to the Hartree-Fock equations: $\hat{f}\ \psi_i = \epsilon_i\ \psi_i\ , i = 1, 2, ..., N$ **with** $\hat{f} = -\frac{1}{2}\nabla_i^2 - \sum_A^M \frac{Z_A}{r_{iA}} + V_{HF}(i)$

In spite of their apparent Schrödinger-like form, the Hartree-Fock equations are non-linear, as:

$$V_{HF}(\vec{x}_1) = \sum_j^N \left(\hat{J}_j(\vec{x}_1) - \hat{K}_j(\vec{x}_1)\right) \quad \text{with} \quad \begin{cases} \hat{J}_j(\vec{x}_1) = \int |\psi_j(\vec{x}_2)|^2 \frac{1}{r_{12}}\, d\vec{x}_2 \\ \hat{K}_j(\vec{x}_1)\ \psi_i(\vec{x}_1) = \int \psi_j^*(\vec{x}_2) \frac{1}{r_{12}} \psi_i(\vec{x}_2)\, d\vec{x}_2\ \psi_j(\vec{x}_1) \end{cases}$$

The exchange interaction $K_j(x_i)$ has no classical analog and depends on the spin and orbital variables

The Hartree-Fock potential V_{HF} is non-local and non-linear (it depends on ψ):
the equations must be solved self-consistently

This is what is done by the MCDF code, except that it works with the Dirac hamiltonian
and it uses multiconfiguration (linear combinations of) Slater determinants

The relativistic Multi-Configuration Dirac-Fock code

*From J.P. Desclaux and collaborators, PRA **17**, 1804 (1978) & PRA **42**, 5139 (1990)*

Hamiltonian up to order α^2

$$\hat{H} = \sum_{i=1}^{n} \hat{h}_D(i) + \sum_{i>j}^{n} \frac{1}{r_{ij}}$$

$$= \sum_{i=1}^{n} \left[\phi(r_i) + c\vec{\alpha}(i) \cdot \vec{p}(i) + mc^2 \right] + \sum_{i>j}^{n} \frac{1}{r_{ij}}$$

with the addition of the Breit term:

$$\hat{g}^B(i,j) = -\frac{1}{r_{ij}} \left\{ \alpha_i \cdot \alpha_j + \frac{(\alpha_i \cdot r_{ij})(\alpha_j \cdot r_{ij})}{r_{ij}^2} \right\}$$

The other main difference with the non-relativistic case is due to the bi-spinor form of the single-particle wave-functions

$$\phi_i^{j,m_j}(+) = \frac{1}{r} \begin{Bmatrix} p_i(r)\chi_i^{(+)} \\ iq_i(r)\chi_i^{(-)} \end{Bmatrix}$$

$$\phi_i^{j,m_j}(-) = \frac{1}{r} \begin{Bmatrix} -p_i(r)\chi_i^{(-)} \\ iq_i(r)\chi_i^{(+)} \end{Bmatrix}$$

Relativistic corrections to the Hartree-Fock equations tend to be largest in the region immediately surrounding the nucleus (bigger kinetic energy). Therefore core orbitals are usually much more affected than valence orbitals

The relativistic MCDF code

http://www.lkb.upmc.fr/metrologysimplesystems/mdfgme-a-general-purpose-multiconfiguration-dirac-foc-program/

Transitions for Copper

Transition	Pauli obeying transitions	Pauli violating transitions		Energy difference
	Standard transition Energy [eV]	Energy [eV]	Transition probability velocity [1/s]	$E_{standard}$-E_{VIP} [eV]
$2p_{1/2}$ ==» $1s_{1/2}$ ($K_{\alpha 2}$)	8,047.78	7,728.92	2.6372675E+14	318.86
$2p_{3/2}$==» $1s_{1/2}$ ($K_{\alpha 1}$)	8,027.83	7,746.73	2.5690970E+14	279.84
$3p_{1/2}$ ==» $1s_{1/2}$ ($K_{\beta 2}$)	8,905.413	8,529.54	2.7657639E+13	375.873
$3p_{3/2}$==» $1s_{1/2}$ ($K_{\beta 1}$)	8,905.413	8,531.69	2.6737747E+13	373.723
$3d_{3/2}$==»$2p_{3/2}$ ($L_{\alpha 2}$)	929.7	822.84	5.9864102E+07	106.86
$3d_{5/2}$==»$2p_{3/2}$ ($L_{\alpha 1}$)	929.7	822.83	3.4922759E+08	106.87
$3d_{3/2}$==»$2p_{1/2}$ ($L_{\beta 1}$)	949.84	841.91	3.0154308E+08	107.93
$3s_{1/2}$ ==» $2p_{1/2}$	832.1	762.04	3.7036365E+11	70.06
$3s_{1/2}$ ==» $2p_{3/2}$	811.7	742.97	7.8424473E+11	68.73
$3d_{5/2}$ ==» 1s (**D**irect **R**adiative **R**ecombination)	8,977.14	8,570.82	1.2125697E+06	406.32

The relativistic MCDF code

http://www.lkb.upmc.fr/metrologysimplesystems/mdfgme-a-general-purpose-multiconfiguration-dirac-foc-program/

Transitions for Gold

Transition	Pauli obeying transitions	Pauli violating transitions		Energy difference
	Standard transition Energy [eV]	Energy [eV]	Transition probability velocity [1/s]	$E_{standard}$-E_{VIP} [eV]
$2p_{1/2}$ ==» $1s_{1/2}$ ($K_{\alpha 2}$)	66,990.73	66,207.58	2.1042335E+16	783.15
$2p_{3/2}$==» $1s_{1/2}$ ($K_{\alpha 1}$)	68,804.50	68,002.09	1.7835326E+16	802.41
$3p_{1/2}$ ==» $1s_{1/2}$ ($K_{\beta 2}$)	77,575.01	76,547.92	3.8657822E+15	1,027.09
$3p_{3/2}$==» $1s_{1/2}$ ($K_{\beta 1}$)	77,979.80	76,937.91	3.6994027E+15	1,041.89
$3d_{3/2}$==»$2p_{3/2}$ ($L_{\alpha 2}$)	9,628.05	9,374.76	1.9441580E+14	253.29
$3d_{5/2}$==»$2p_{3/2}$ ($L_{\alpha 1}$)	9,713.44	9,457.85	1.1406776E+15	255.59
$3d_{3/2}$==»$2p_{1/2}$ ($L_{\beta 1}$)	11,442.45	11,169.27	1.1012516E+15	273.18
$3s_{1/2}$ ==» $2p_{1/2}$	10,308.41	10,081.34	6.1287637E+13	227.07
$3s_{1/2}$==» $2p_{3/2}$	8,494.03	8,286.83	1.9449551E+14	207.2
$5d_{5/2}$ ==» 1s (DRD)	80,391.1	79,465.62	1.7569882E+09	925.48

Transitions for Lead

Transition	Pauli obeying transitions	Pauli violating transitions		Energy difference
	Standard transition Energy [eV]	Energy [eV]	Transition probability velocity [1/s]	$E_{standard}$-E_{VIP} [eV]
$2p_{1/2}$ ==» $1s_{1/2}$ ($K_{\alpha 2}$)	72,805.42	71,992.03	2.4680208E+16	813.39
$2p_{3/2}$==» $1s_{1/2}$ ($K_{\alpha 1}$)	74,970.11	74,133.89	2.0639102E+16	836.22
$3p_{1/2}$ ==» $1s_{1/2}$ ($K_{\beta 2}$)	84,450.45	83,385.36	4.5414771E+15	1,065.09
$3p_{3/2}$==» $1s_{1/2}$ ($K_{\beta 1}$)	84,939.08	83,856.44	4.3479248E+15	1,082.64
$3d_{3/2}$==»$2p_{3/2}$ ($L_{\alpha 2}$)	10,449.59	10,188.23	2.3146352E+14	261.36
$3d_{5/2}$==»$2p_{3/2}$ ($L_{\alpha 1}$)	10,551.60	10,287.71	1.3570636E+15	263.89
$3d_{3/2}$==»$2p_{1/2}$ ($L_{\beta 1}$)	12,613.80	12,330.02	1.3246599E+15	283.78
$3s_{1/2}$ ==» $2p_{1/2}$	11,349.4	11,116.39	7.4132768E+13	233.01
$3s_{1/2}$==» $2p_{3/2}$	9,184.56	8,974.38	2.4205005E+14	210.18
$5d_{5/2}$ ==» 1s(DRD)	87,589	86,686.79	5.8880291E+11	902.21

The relativistic MCDF code

http://www.lkb.upmc.fr/metrologysimplesystems/mdfgme-a-general-purpose-multiconfiguration-dirac-foc-program/

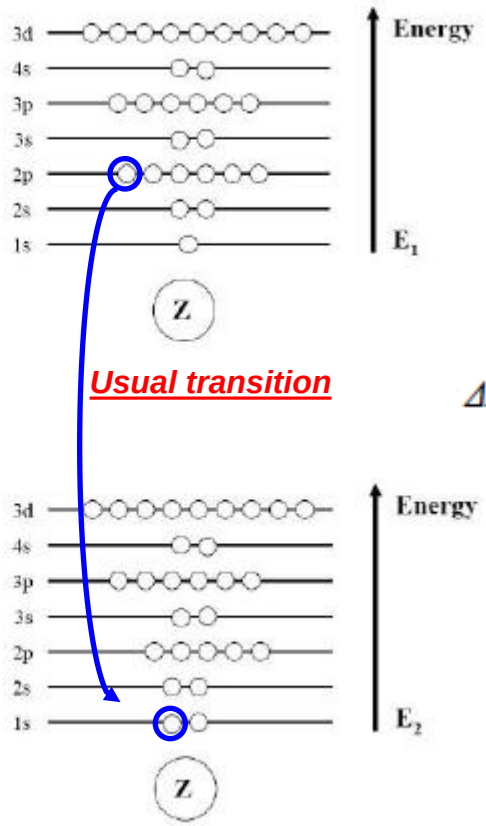
An example of input file…

Sample input file $k_{\alpha 2}$ transition

```
*501  Cu Trial
   scfmdf max
   hdimdf max
   maelam max
   pncgme maX
   podmdf max
   poemdf max
   :
   mod_lightspeed=n
   nz=29
   mdf  do_ener=y  keep_ener=n  binary_ener=y  do_scf=y
   Breit=full    mag_scf=n    diag_afterSCF=n
   vacpol_scf=y
   Electric  mulpol=1
   use_mcdfener=y
   sub_offset=n
   opt_relax=y
   ret_lorentz=n
   opt_qedel=y :
   mod_mesh=n
   exotic=y   tstf
   mod_nuc=n
   nbeli=29  nbelf=29
   def_config=given
   1s2 2s2 2p6 (2p@])1 3s2 3p6 3d10 :
end
   1s2 (1s@])1 2s2 2p6 3s2 3p6 3d10 :
end
   jjti=1   mjti=1
   jjtf=1   mjtf=1
   iflagp=y
   neigv=1
#initial state parameters
   icmul=0  iprt_energ=1
   NORBSC=0 :
   NSTEP=0
   lregul=n modtest=n
   modsolv_orb=n
   mod_odlm=n
    :
#final state parameters
   neigv=1
   icmul=0  iprt_energ=1
   NORBSC=0 :
   NSTEP=0
   lregul=n modtest=n
   modsolv_orb=n
   mod_odlm=n
```

A simple estimation of the energy shift

The case of K_α emission for copper



$$\Delta E' = E_1 - E_2 \approx 8042 \text{ eV}$$

$$E_3 = E_1 + V_{1s\_Z} + V_{2p\_Z} + V_{1s\_e^-} + V_{2p\_e^-} + V_{1s\_1s} + V_{2p\_2p} + 3V_{1s\_2p}$$

$$E_4 = E_2 + V_{1s\_Z} + V_{2p\_Z} + V_{1s\_e^-} + V_{2p\_e^-} + 2V_{1s\_1s} + 3V_{1s\_2p}$$

with:

$$V_{1s\_1s} \approx 483 \text{ eV}$$

$$V_{2p\_2p} \approx 110 \text{ eV}$$

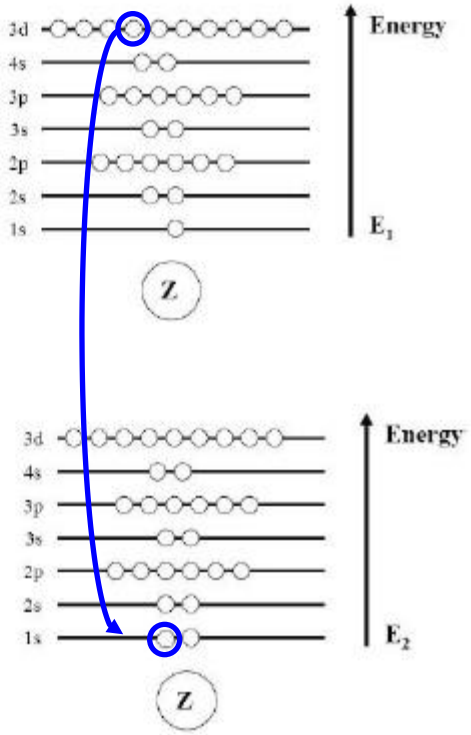
$$\Delta E = \Delta E' - (V_{1s\_1s} - V_{2p\_2p}) \approx 7669 \text{ eV}$$

A simple estimation of the energy shift

The case of K_β emission for copper: as before, but $\Delta E'$=8905 eV and $V_{3p\text{-}3p}$ = 20 eV. So:

$$\Delta E = \Delta E' - (V_{1s\_1s} - V_{3p\_3p}) \approx 8442 \text{ eV}.$$

The case of K-edge emission for copper



$$\tilde{E}_3 = \tilde{E}_1 + V_{1s\_Z} + V_{1s\_e^-} + V_{1s\_1s} + V_{1s\_3d}$$

$$\tilde{E}_4 = \tilde{E}_2 + V_{1s\_Z} + V_{1s\_e^-} + 2V_{1s\_1s}$$

here $\Delta E'$=8979 eV,

$V_{1s\text{-}1s}$ = 483 eV and

$V_{1s\text{-}1s}$ = 38 eV

So, we get:

$$\Delta E = \Delta E' - (V_{1s\_1s} - V_{1s\_3d}) \approx 8534 \text{ eV}.$$

What about the 'new' ('fresh') electrons ?

Overview of the seminar

- From usual X-ray transitions to Pauli-forbidden ones
  - A relatively simple estimation of the energy-shift
  - The Fermi golden rule: transition-matrix elements
  - The interaction hamiltonian: non-relativistic state
  - The many-body wave-function: the effect of antisymmetrization
  - Full calculation of the energy-shift by the relativistic Dirac-Fock MCDF code
  - Conclusions: and what about the ‘new’ electrons ?

- **Is it possible to detect a transient violation of the Pauli principle at the subattosecond time scale ?**
  - **The Corinaldesi’s paper**
  - **Retarded interactions of the E.M. field and Zitterbewegung: towards a non-orthodox view ?**

Premise

Corinaldesi's idea that Pauli principle can be violated in short time transients

SUPPLEMENTO AL NUOVO CIMENTO N. 3, 1967
VOLUME V

Model of a Dynamical Theory of the Pauli Principle.

E. CORINALDESI
Department of Physics, Boston University - Boston, Mass.

(ricevuto il 4 Marzo 1967)

This note does not question the fact that nature seems to order systems of « identical » bosons and fermions in a special way which we describe by means of symmetric and antisymmetric wave functions. Our only aim is to show that this ordering may be conceived as a dynamical process of which only the final stage is normally observed.

Premise

Corinaldesi's idea that Pauli principle can be violated in short time transients

Consider the 2-particle Lagrangian of the conventional non-relativistic theory:

$$\mathscr{L} = -\frac{\hbar^2}{2m}\left(\nabla_1\psi^\dagger\cdot\nabla_1\psi + \nabla_2\psi^\dagger\cdot\nabla_2\psi\right) - V\psi^\dagger\psi + \ldots + \frac{\hbar}{2i}\left(\frac{\partial\psi^\dagger}{\partial t}\psi - \psi^\dagger\frac{\partial\psi}{\partial t}\right)$$

And add to it the following non-linear term (written here for fermions):

$$\mathcal{L}_{non-lin} = \tfrac{1}{2}\left(\Psi^+(1,2)+\Psi^+(2,1)\right)\left(\Psi(1,2)+\Psi(2,1)\right)\left(i\ln\xi\right)^3$$

where: $$\xi = \frac{\left(\Psi^+(1,2)+\Psi^+(2,1)\right)\left(\Psi(1,2)-\Psi(2,1)\right)}{\left(\Psi^+(1,2)-\Psi^+(2,1)\right)\left(\Psi(1,2)+\Psi(2,1)\right)}$$ is a phase !

Notice that the non-linear term is zero for both non-overlapping fermions (ξ=1, so lnξ =0), and for symmetrized wave-functions, because $\Psi(1,2) = -\Psi(2,1)$ (!!!)

Premise

Corinaldesi's idea that Pauli principle can be violated in short time transients

Define: $$N^{(sym)} = \tfrac{1}{2}\int \left(\Psi^{+}(1,2) - \Psi^{+}(2,1)\right)\left(\Psi(1,2) - \Psi(2,1)\right) d^3x_1 d^3x_2$$

$$N^{(no-sym)} = \tfrac{1}{2}\int \left(\Psi^{+}(1,2) + \Psi^{+}(2,1)\right)\left(\Psi(1,2) + \Psi(2,1)\right) d^3x_1 d^3x_2$$

In this framework, the equation of motion leads to the interesting properties:

1) When the two wave-packets do not overlap, then: $N^{(sym)} = N^{(no-sym)} = 1$

2) When the two wave-packets start overlapping, then: $\begin{cases} \dfrac{dN^{(sym)}}{dt} \geq 0 \\ \dfrac{dN^{(no-sym)}}{dt} \leq 0 \end{cases}$ **up to:** $\begin{cases} N^{(sym)} = 2 \\ N^{(no-sym)} = 0 \end{cases}$

with the property (conservation of probability) : $$\frac{dN^{(sym)}}{dt} + \frac{dN^{(no-sym)}}{dt} = 0$$

Corinaldesi's conclusions

Corinaldesi's idea is that Pauli principle can be violated in short time transients

Conclusions of Corinaldesi's paper:

The new Schrödinger equation can be expected to yield physical predictions differing from those derived from the conventional theory, when times are involved which are shorter than a characteristic « symmetrization time ».

For charged fermions this would amount to a reformulation of electromagnetic interactions in which the electromagnetic field would play the role of a symmetrizing agent (!)

This, of course, leaves three questions open:

1) How could the electromagnetic field act this way ?
2) What would be a typical value for the «symmetrization time» ?
3) How could it be possible to measure it ?

A note for future purposes…

Wave-like behaviour should not be identified with Ψ !

1 **Newton eq.**

(in Hamilton-Jacobi form for a statistical set)

$$i\hbar\frac{\partial\Psi(\vec{r},t)}{\partial t}=-\frac{\hbar^2\nabla^2}{2m}\Psi(\vec{r},t)+V(\vec{r},t)\Psi(\vec{r},t)+\frac{\hbar^2\nabla^2\left|\Psi(\vec{r},t)\right|}{2m\left|\Psi(\vec{r},t)\right|}\Psi(\vec{r},t)$$

2 **Schrödinger eq.** with

$$i\hbar\frac{\partial\Psi(\vec{r},t)}{\partial t}=-\frac{\hbar^2\nabla^2}{2m}\Psi(\vec{r},t)+V(\vec{r},t)\Psi(\vec{r},t)$$

$$\left|\Psi(\vec{r},t)\right|^2=1,\quad\forall\ (\vec{r},t)$$

A note for future purposes…

Schrödinger's equation can be written non-linearly:

See Holland, "The Quantum Theory of Motion", Cambridge 1993

$$i\hbar\frac{\partial\Psi(r,t)}{\partial t}=-\frac{\hbar^2\nabla^2}{2m}\Psi(r,t)+V(r,t)\Psi(r,t)$$

If we put: $\Psi(\vec{x},t)=R(\vec{x},t)e^{iS(\vec{x},t)/\hbar}$ and separate Re and Im:

$$\Rightarrow\begin{cases}-\dfrac{\partial S}{\partial t}=\dfrac{(\nabla S)^2}{2m}+V(r)+Q\equiv E & \text{(Hamilton-Jacobi equation)}\\ \vec{\nabla}\cdot\vec{J}-\dfrac{\partial\rho}{\partial t}=0 & \text{(continuity equation)}\end{cases}$$

$$\begin{cases}\rho=\Psi^*\Psi=R(\vec{x},t)^2\\ \vec{j}=\frac{i\hbar}{2m}(\Psi\vec{\nabla}\Psi^*-\Psi^*\vec{\nabla}\Psi)\end{cases}$$

where: $Q=-\dfrac{\hbar^2}{2m}\dfrac{\nabla^2R}{R}$ is called quantum potential

Corinaldesi's conclusions

Corinaldesi's idea is that Pauli principle can be violated in short time transients

Conclusions of Corinaldesi's paper:

The new Schrödinger equation can be expected to yield physical predictions differing from those derived from the conventional theory, when times are involved which are shorter than a characteristic « symmetrization time ».

For charged fermions this would amount to a reformulation of electromagnetic interactions in which the electromagnetic field would play the role of a symmetrizing agent (!)

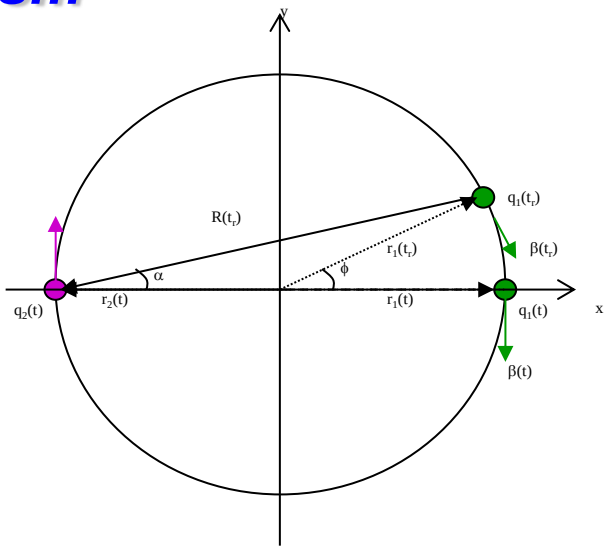
This, of course, leaves three questions open:

1) How could the electromagnetic field act this way ?
2) What would be a typical value for the «symmetrization time» ?
3) How could it be possible to measure it ?

Reminder of classical electromagnetism

Expression of the Lienard-Wieckert retarded electric field at q_2:

$$\vec{E}(R,t)=\frac{q_1(1-\beta^2)(\hat{R}-\vec{\beta}(t_r))}{R^2(1-\hat{R}\cdot\vec{\beta}(t_r))^3}+\frac{q_1\hat{R}\times[(\hat{R}-\vec{\beta}(t_r))\times\dot{\vec{\beta}}(t_r)]}{cR(1-\hat{R}\cdot\vec{\beta}(t_r))^3}$$



The rate of work done by q_1 on q_2 to order β^4 is: $W_2=\dfrac{\mu_0 q_1 q_2 a^2}{6\pi c}$

Oscillating dipoles: Lienard/Wiechert emitting power $p_{emit}=\dfrac{\mu_0 q_1^2}{6\pi c}\dfrac{a^2-\frac{(\vec{v}\times\vec{a})^2}{c^2}}{1-\frac{v^2}{c^2}}$

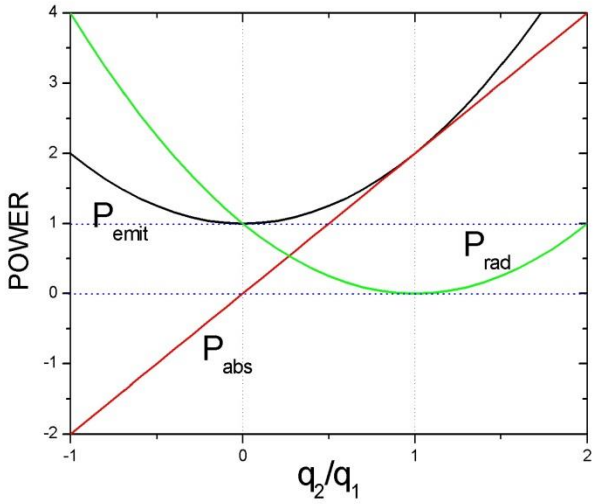
$$\Rightarrow p_{abs}=W_1+W_2\cong 2\frac{\mu_0 q_1 q_2}{6\pi c}a^2$$

$$\Rightarrow p_{rad}=p_{emit}-p_{abs}$$

$$\Rightarrow \textit{If } \vec{v}\perp\vec{a} \Rightarrow p_{emit}=\frac{\mu_0 q_1^2}{6\pi c}a^2$$

$\Rightarrow$ Total radiated power of the system proportional to the square of the dipole moment:

$$p_{rad}=\frac{\mu_0(q_1-q_2)^2}{6\pi c}a^2$$



Retarded differential equations

General characteristics of RDE:

1) Solutions are quantized due to retardation (no scale invariance)

Instead of an algebraic associated equation, you end up with a transcendental (trigonometric) associated equation → quantized solutions

2) Need for a whole set of past data in the interval $[0,t_r]$

For example: $\dot{x}(t) = x(t - \frac{\pi}{2})$

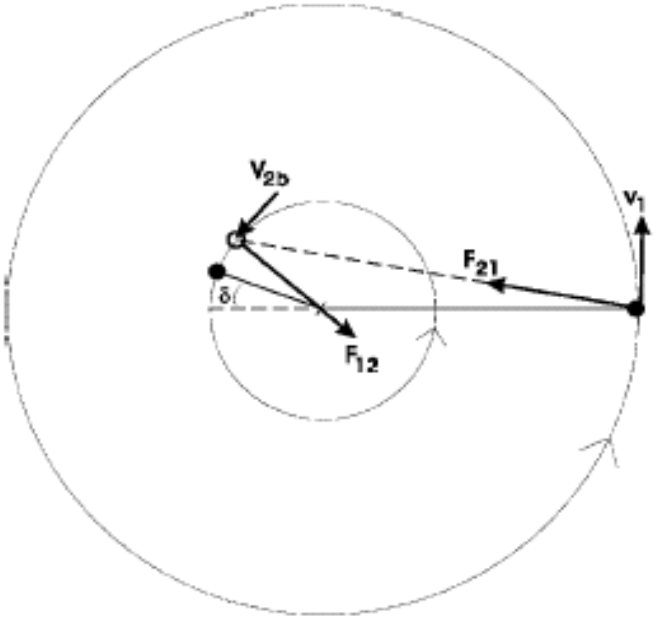
$\Rightarrow \quad x(t) = a\cos t + b\sin t$ …for any a and b !

Ping-pong motion in hydrogen atom

*L. Page and N. Adams, American Journal of Physics **13**, 141 (1945)*

The infinite proton-mass limit is a singular condition that cannot be treated perturbatively (it does not allow retardation effects)

Angular momentum is not conserved !
(purely under the action of internal forces)



Results of Lyapunov stability analysis:

Jayme De Luca, Phys. Rev. E 73, 026221 (2006)

1) ***Resonant orbits are quantized naturally because of delay***
2) ***Angular momenta are ~ integer multiples of a constant***

⇒ Ping-pong phenomenon is a non-trivial feature absent in ODE

Ping-pong motion in hydrogen atom

Jayme De Luca, Phys. Rev. E 73, 026221 (2006)

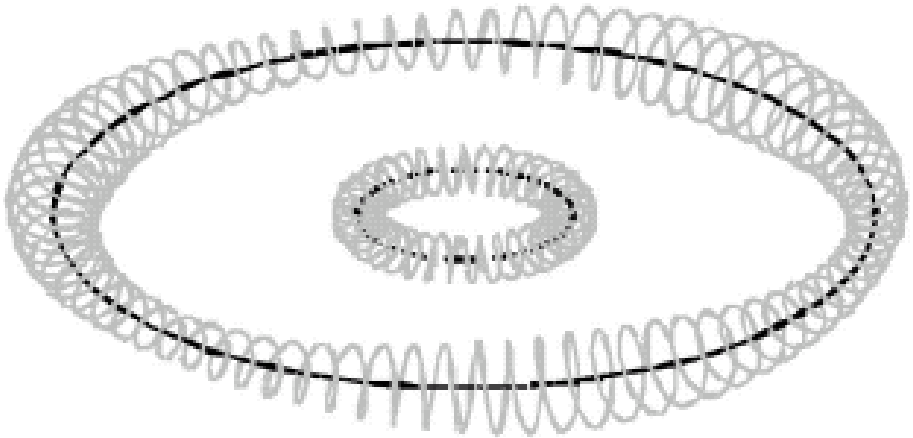
The infinite proton-mass limit is a singular condition that cannot be treated perturbatively (it does not allow retardation effects)

Action for the electron: $$\int \frac{1-\vec{v}_1\cdot\vec{v}_{2r}}{r_{12r}(1-\vec{n}_{12r}\cdot\vec{v}_{2r})}dt_1$$

$\vec{v}_1$ **= electron velocity**

$\vec{v}_{2r}$ **= retarded proton velocity ;** $\vec{n}_{12r}=\dfrac{\vec{r}_{12r}}{r_{12r}}$

r_{12r} **= electron-proton distance at the retarded time**



Beatings of modes leads to a no-radiation Poynting condition !

Dirac equation & ZBW (Hestenes' interpretation)

*D. Hestenes, J. Math. Phys. **8**, 798-808 (1967), **14**, 893-905 (1973), **16**, 556-572 (1975), **16**, 573-583 (1975), Am. J. Phys., **47**, 399-415 (1979), Foundations of Physics, Vol. **40**, 1-54 (2010)*

Dirac equation: $$\left(\alpha_0 mc^2 + \sum_{j=1}^{3} \alpha_j p_j c \right) \psi(\mathbf{x},t) = i\hbar \frac{\partial \psi}{\partial t}(\mathbf{x},t)$$

with $\alpha_\mu\alpha_\nu+\alpha_\nu\alpha_\mu=2\delta_{\mu\nu}$

Zitterbewegung: $$\vec{\mathrm{v}} \equiv \frac{\mathrm{d}\vec{\mathrm{x}}}{\mathrm{dt}} = \frac{i}{\hbar}[H,\vec{\mathrm{x}}] = c\vec{\alpha}$$

$$i\hbar \frac{\mathrm{d}\vec{\alpha}}{\mathrm{dt}} = -2c\vec{p} + 2H\vec{\alpha} \Rightarrow \textbf{free particle (p \& H constant):} \quad \frac{\mathrm{d}\vec{\mathrm{x}}}{\mathrm{dt}} = c^2 H^{-1}\vec{p} + c\vec{\alpha}_0 e^{-2iHt/\hbar}$$

⇒ from which we get:

$$\vec{\mathrm{x}}(\mathrm{t}) = \vec{\mathrm{x}}_0 + c^2 H^{-1}\vec{p}t + \tfrac{1}{2} i\hbar c\vec{\alpha}_0 H^{-1} e^{-2iHt/\hbar}$$

$$= \vec{\mathrm{x}}_{\mathrm{A}}(\mathrm{t}) + \vec{\xi}(t)$$

with $\omega_{ZBW} = \frac{H}{\hbar} = \frac{2mc^2}{\hbar}$

Moreover: $\vec{p} \to \vec{p} - e\vec{\mathrm{A}}(\vec{\mathrm{x}},t)$

From Dirac to Schrodinger equation

Non-relativistic limit of Gordon decomposition:

$$m\rho\,\vec{\mathrm{v}} = m\rho\,\vec{u} + \vec{\nabla}\times(\rho\,\vec{S}) \quad \Rightarrow \quad \vec{\mathrm{v}} = \vec{u} + \vec{w}$$

usual definition of momentum: $\vec{p} = i\hbar[\Psi^*(\vec{\nabla}\Psi) - (\vec{\nabla}\Psi^*)\Psi]$

However:

$$\begin{cases} \vec{\nabla}\cdot m\rho\,\vec{\mathrm{v}} = \vec{\nabla}\cdot m\rho\,\vec{\mathrm{u}} \quad \text{and} \\ \left\langle \vec{r}\times m\rho\,\vec{\mathrm{v}} \right\rangle = \left\langle \vec{r}\times m\rho\,\vec{u} \right\rangle + 2\left\langle \vec{S} \right\rangle \equiv \left\langle \vec{L} \right\rangle + 2\left\langle \vec{S} \right\rangle \end{cases}$$

$\Rightarrow$ v = charge velocity ; u = velocity of the center of mass

From Dirac to Schrodinger equation

Kinetic energy of u, v and w: $\frac{m\mathrm{v}^2}{2} = \frac{m\mathrm{u}^2}{2} + \frac{m\mathrm{w}^2}{2}$

$\Rightarrow$ if the spin is independent of position: $\vec{S}(\vec{r}) = \vec{S}$

the contribution of the α–ZBW motion $\vec{w} = \frac{\vec{\nabla}\rho \times \vec{S}}{m\rho}$

in the Hamiltonian is: $\frac{1}{2}mw^2 = \frac{S^2(\nabla\rho)^2}{2m\rho^2} = \frac{\hbar^2(\nabla\rho)^2}{8m\rho^2} \equiv Q$

See Holland, "The Quantum Theory of Motion", Cambridge 1993 and Recami and Salesi, PRA 57, 98 (1998)

This shows that, in the Schrödinger equation, $\hbar$ stands for twice the spin

Non-relativistic hydrogen atom

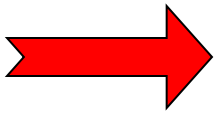
Given the Hamilton-Jacobi equation: $$-\frac{\partial S}{\partial t}=\frac{(\nabla S)^2}{2m}+V(r)+Q\equiv E$$

where: $$Q=-\frac{\hbar^2}{2m}\frac{\nabla^2 R}{R}$$ and: $$\Psi(\vec{x},t)=R(\vec{x},t)e^{iS(\vec{x},t)/\hbar}$$

the spin kinetic energy term Q is responsible for H-atom eigenvalues:

$$Q(100)=E_{1s}-V(r)$$ $$Q(200)=E_{2s}-V(r)$$ $$Q(210)=E_{2s}-V(r)$$

$$Q(21\pm 1)=E_{2s}-V(r)-\frac{\hbar^2}{2mr^2\sin^2\vartheta}=E_{2s}-V(r)-\frac{(\nabla S)^2}{2m}$$



the spin velocity field **w**(**r**) stabilizes only “true” orbitals

Dirac-relativistic hydrogen atom (I)

$$\Psi_{1s}(\vec{r},t)=\begin{pmatrix} g_{1s}(\vec{r}) \\ f_{1s}(\vec{r}) \end{pmatrix} e^{-iWt/\hbar} \qquad \text{with: } W = mc^2\sqrt{1-(Z\alpha)^2} \cong mc^2(1-\tfrac{1}{2}(Z\alpha)^2)$$

$$g_{1s}=\sqrt{\frac{8Z^3}{a_0^3}}\sqrt{\frac{W+mc^2}{2mc^2\Gamma(3)}}e^{-Zr/a_0} \quad \text{and} \quad f_{1s}=\sqrt{\frac{8Z^3}{a_0^3}}\sqrt{\frac{W-mc^2}{2mc^2\Gamma(3)}}e^{-Zr/a_0}$$

$$\Rightarrow \left\langle \vec{p}_{cl} \right\rangle_{1s} = \left\langle p_{cl}^2 \right\rangle_{1s} = 0 \quad \text{and} \quad \vec{p}_{nc} = \frac{\hbar}{2\rho(\vec{r})}\left(\vec{\nabla}\times(\overline{\Psi}\vec{\sigma}\Psi) - \tfrac{1}{c}\partial_t(\overline{\Psi}i\vec{\alpha}\Psi)\right)$$

with: $\overline{\Psi}\sigma_z\Psi = g_{1s}^2 + f_{1s}^2$ and $\overline{\Psi}i\alpha_y\Psi = 2g_{1s}f_{1s}$

$\Rightarrow$ We average over ZBW and get the same result as for Schrodinger equation… what if we did not average ?

Dirac-relativistic hydrogen atom (II)

Two oscillatory motions determined by W: $\Psi_{1s}(\vec{r},t)=\begin{pmatrix} g_{1s}(\vec{r}) \\ f_{1s}(\vec{r}) \end{pmatrix} e^{-iWt/\hbar}$

Composition of two frequencies:

$$\begin{cases} \hbar\omega_{free} = 2mc^2 \\ \hbar\omega_{1s} = Z^2\alpha^2 mc^2 \end{cases}$$

$\left(W \cong 2mc^2\left(1-\frac{1}{2}(Z\alpha)^2\right)\right)$

The 2 energies sum up as if the two motions were orthogonal

A possible composition:

Toroidal pattern

Dirac equation and the zitterbewegung (summary)

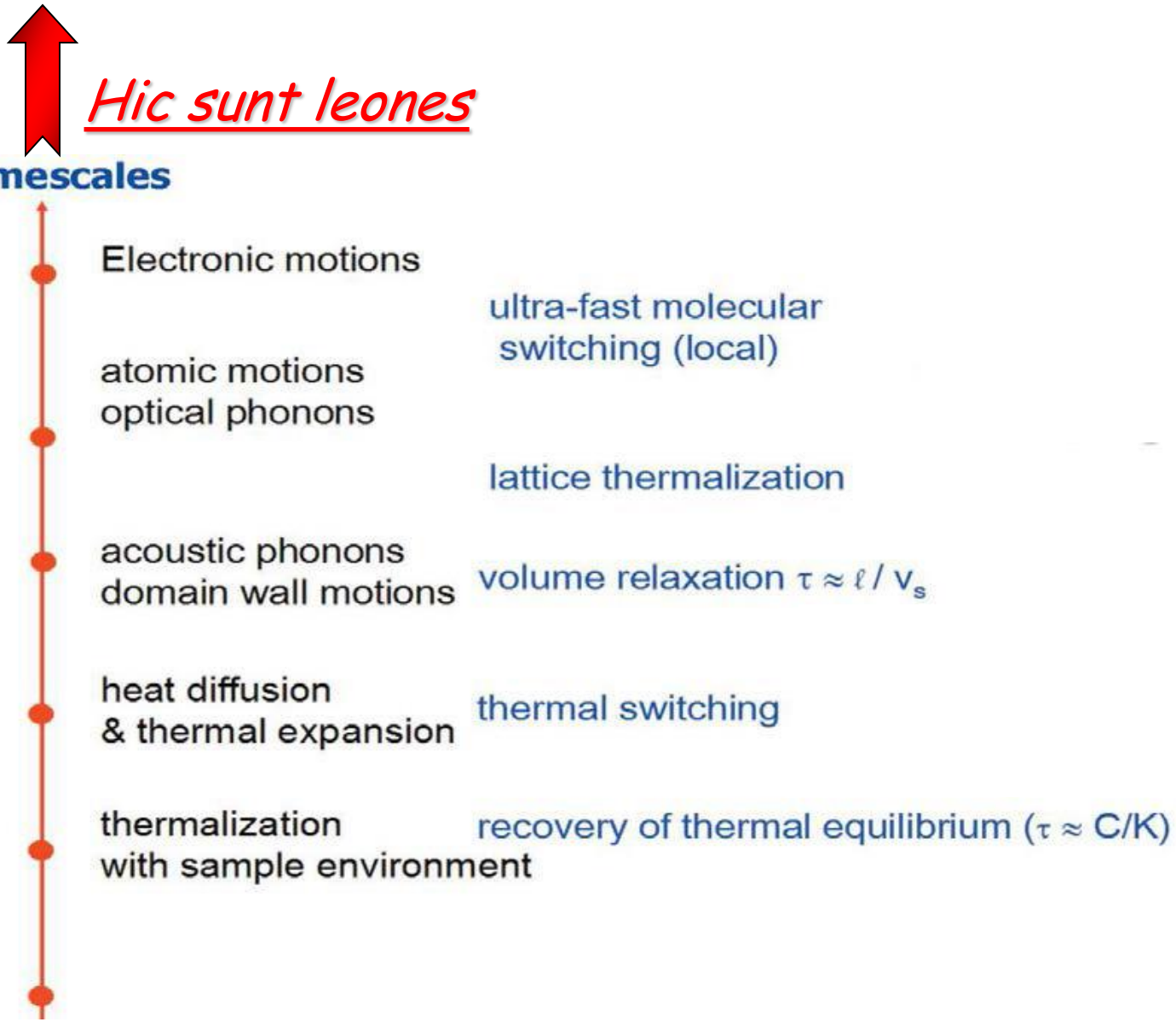
1) The motion of the electron is determined by the composition of two momenta: $\vec{p} = \vec{p}_{cl} + \vec{p}_{nc}$

2) p_{cl} is the motion of the center of mass and p_{nc} is the motion of a massless charge (moving at speed c)

3) both Schrodinger and Dirac equations (if properly interpreted) agree with this description: their expectation values correspond to averages on the ZBW frequency

4) Interestingly, the relativistic time-dilation and length-contraction are determined by the c.o.m. velocity, u.

5) The toroidal motion is responsible of the spin (and might be related to high-frequency parity-violation effects)


Hic sunt leones
timescales
10-15 s
Electronic motions
ultra-fast molecular switching (local)
atomic motions
optical phonons
10-12 s
lattice thermalization
10-9 s
acoustic phonons
domain wall motions
volume relaxation τ ≈ ℓ / vs
10-6 s
heat diffusion
& thermal expansion
thermal switching
10-3 s
thermalization
with sample environment
recovery of thermal equilibrium (τ ≈ C/K)
1 s

Back to PEP: two-electron atoms

How to extend this ZBW picture to the case of 2 electrons ?

$$\Rightarrow \begin{cases} P_{nc}^{(1)} = P^{(1)} - \hbar \nabla_{x_1} S(x_1, x_2) \\ P_{nc}^{(2)} = P^{(2)} - \hbar \nabla_{x_2} S(x_1, x_2) \end{cases}$$

$\Rightarrow$ ***Non-classical momentum of particle 1 depends on the position of particle 2 and vice-versa***

AJP, 1945 ➡

Action and Reaction Between Moving Charges

LEIGH PAGE AND NORMAN I. ADAMS, JR.
Yale University, New Haven, Connecticut

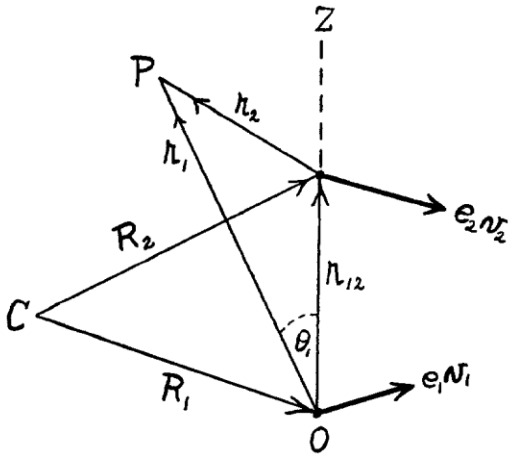


FIG. 1. Two moving charges.

$$\mathbf{G}_a = \frac{e_1 e_2}{2c^2}\left\{\mathbf{R}_2 \times \left(\frac{\mathbf{v}_1}{r} + \frac{\mathbf{v}_1 \cdot \mathbf{r}_{12}\mathbf{r}_{12}}{r^3}\right) + \mathbf{R}_1 \times \left(\frac{\mathbf{v}_2}{r} + \frac{\mathbf{v}_2 \cdot \mathbf{r}_{12}\mathbf{r}_{12}}{r^3}\right)\right\}$$

Comparing with Eq. (8) we see that the portion of the linear momentum involving the velocity $\mathbf{v}_1$ of the first particle is to be considered as located at the second particle, and *vice versa*.

Is it possible to detect a transient violation of the Pauli principle at the subattosecond scale ?

S. Di Matteo – IPR, University of Rennes 1 (France)

LNF Training School organized within the project:

"Hunt for the "impossible atoms": the quest for a tiny violation of the Pauli Exclusion Principle. Implications for physics, cosmology and philosophy,"

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John Templeton Foundation