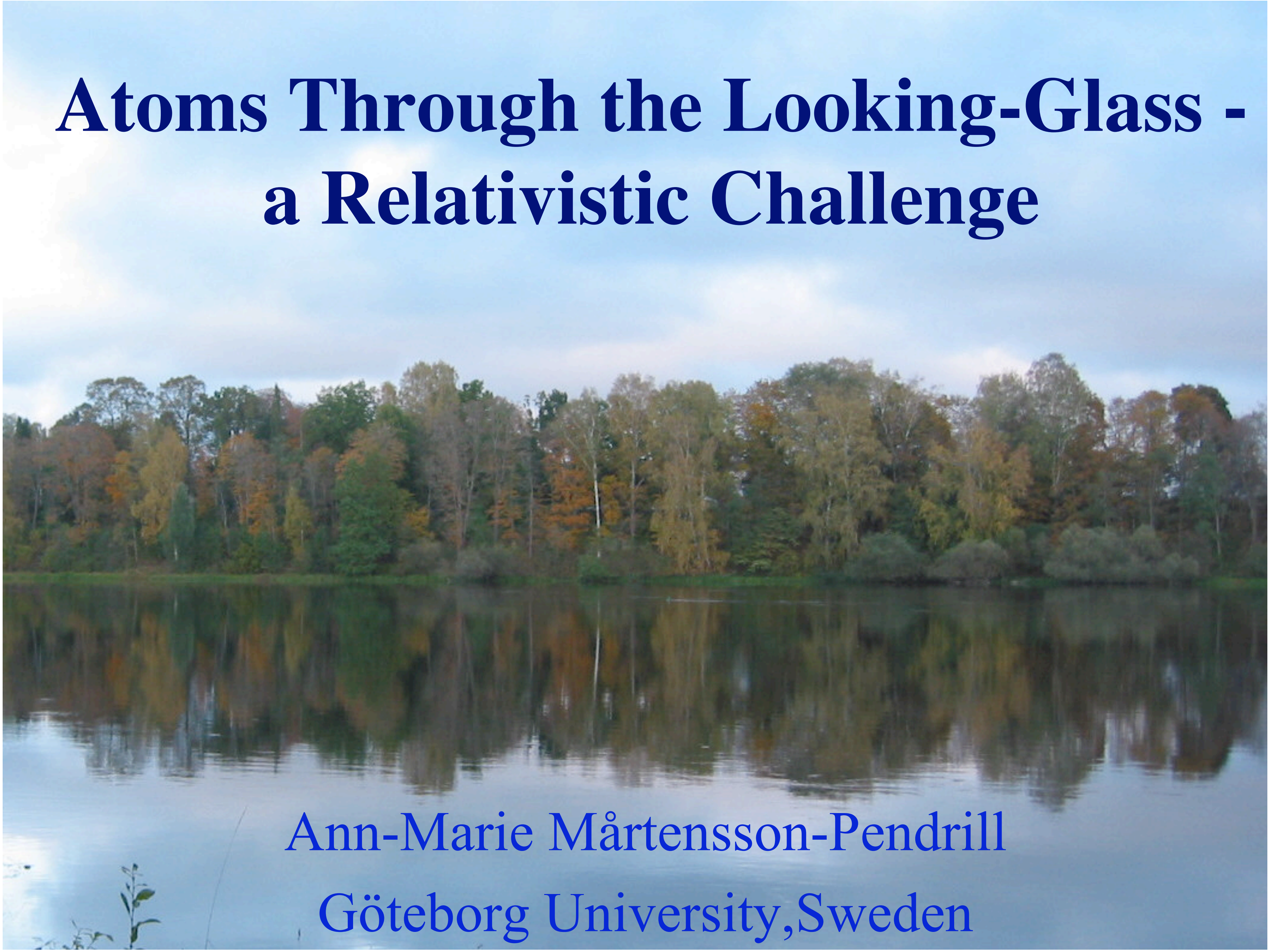


Atoms Through the Looking-Glass - a Relativistic Challenge

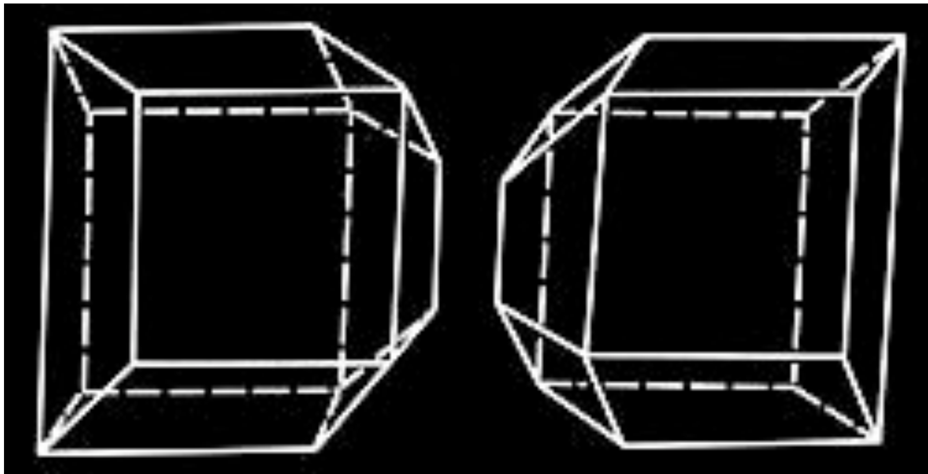
Ann-Marie Mårtensson-Pendrill

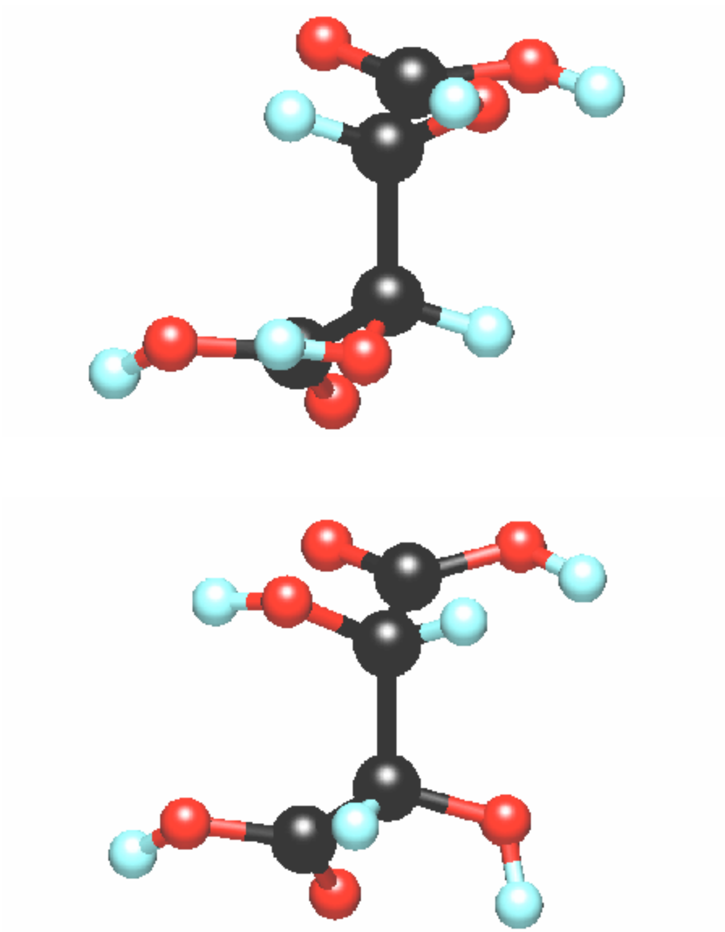
Göteborg University,Sweden

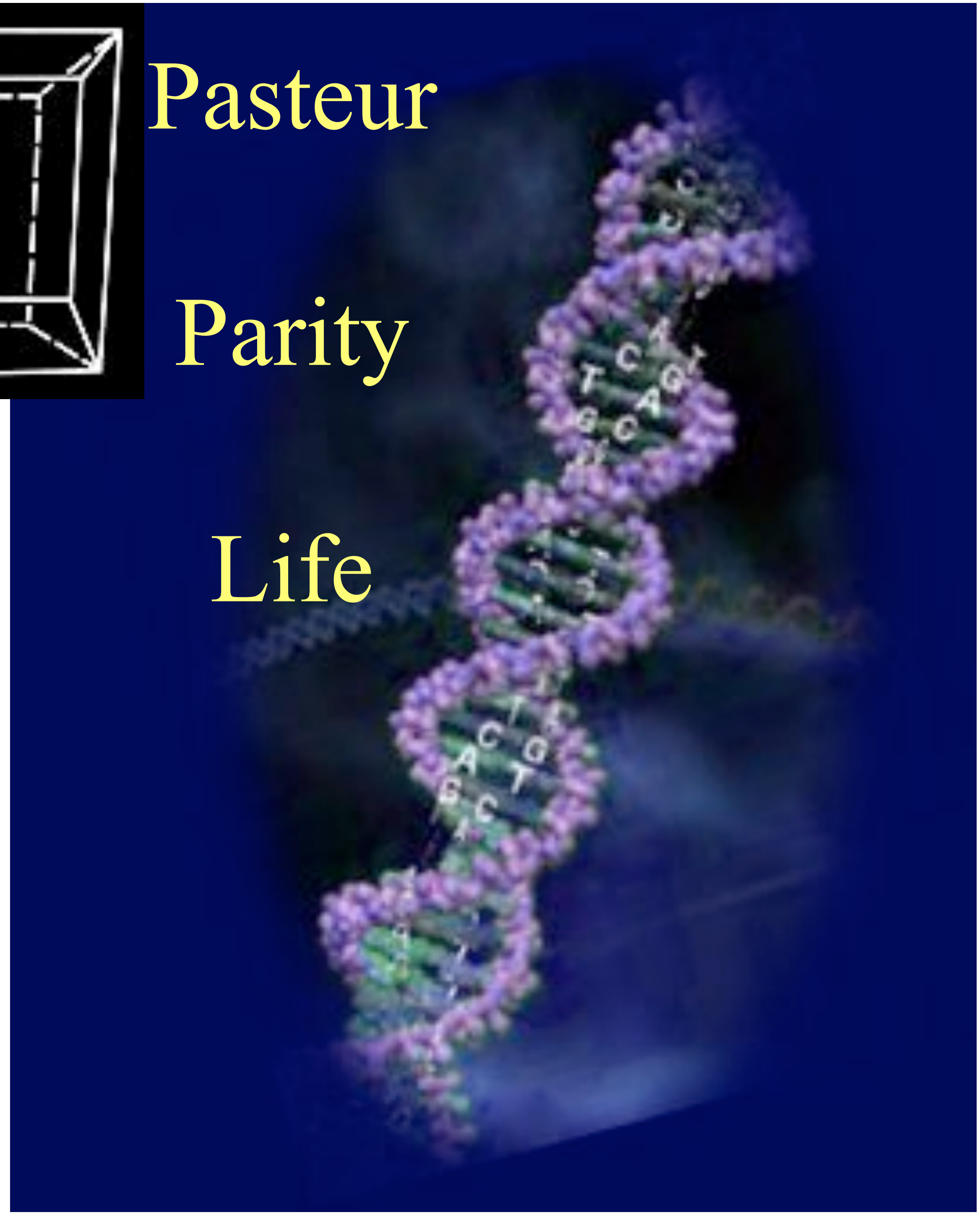
Two Decades of EBIT spectra Five Decades after Parity Revolution

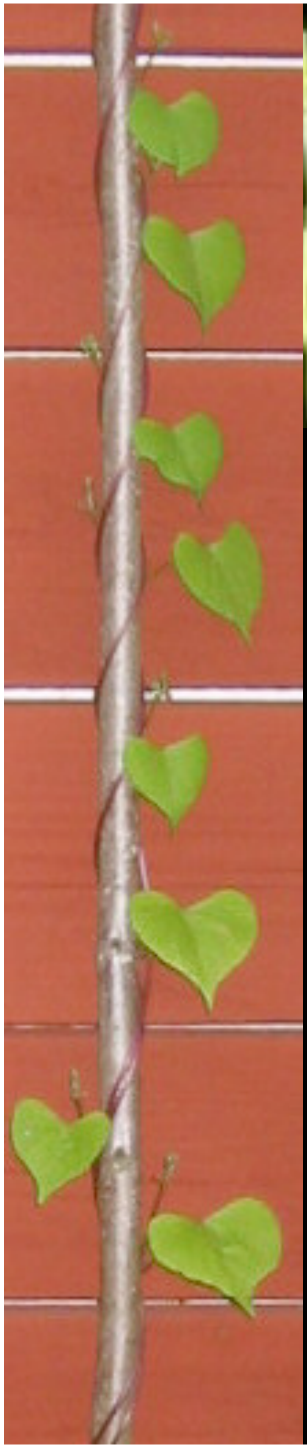
- Left-right - Parity
- Atomic Parity Non-Conservation
- Atomic calculations – ex: HFS, IS
- Relativistic calculations
- Nuclear distributions, EDM
- Bohr-Weisskopf effect - EBIT

- Right-handed seashells
- Left-handed honeysuckles
- Righthanded bindweed …

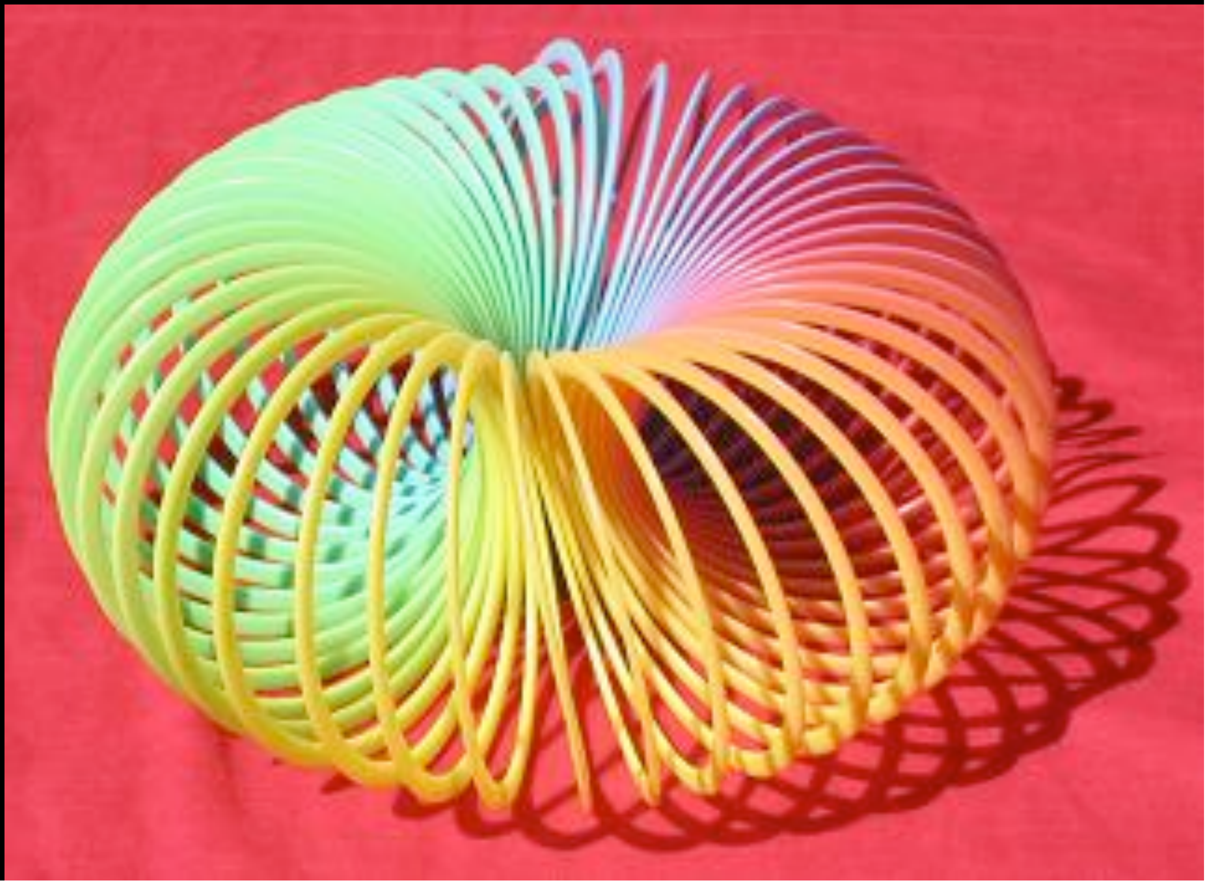


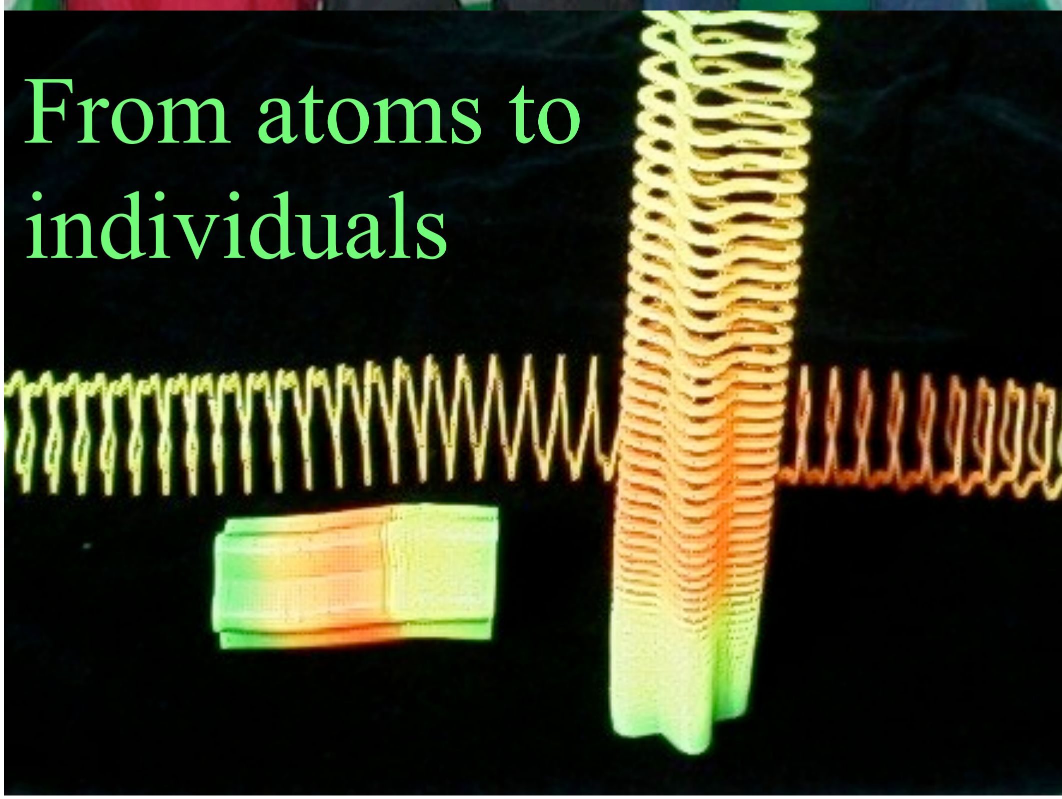



Pasteur
Parity
Life



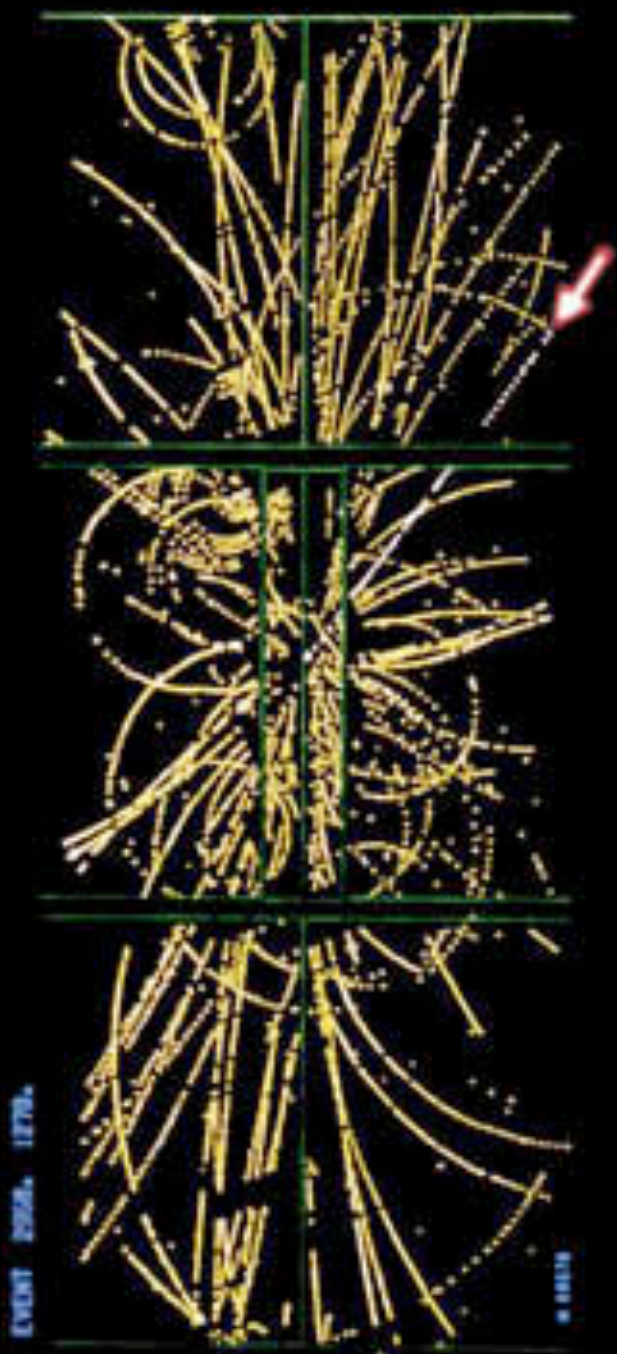
Left- or – right- handed ?




From atoms to individuals

Inversion
Rotation

Left-
handed
-
Right -
handed
?



Parity Revolution 1956-1967

Lee and Yang

Wu et al:

Beta Decay of Co

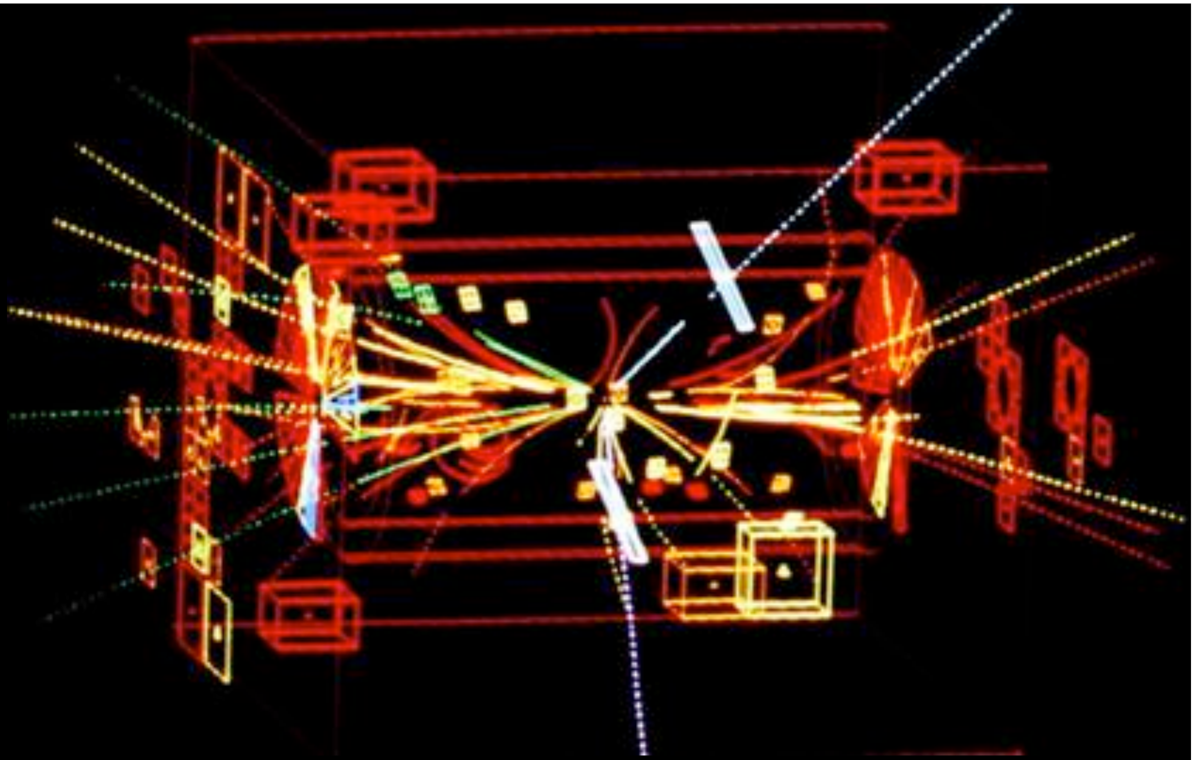
W-boson – discovered at CERN 1983

Atomic Parity Non-Conservation (PNC)?

Neutral Weak Currents

–

Z- Boson Discovered at CERN in 1983



Z-boson exchange modifies the electron-nucleus interaction

Z -boson :

As heavy as a Sr atom – *short* range interaction

Search for atomic PNC
Bouchiat and Bouchiat, 1974

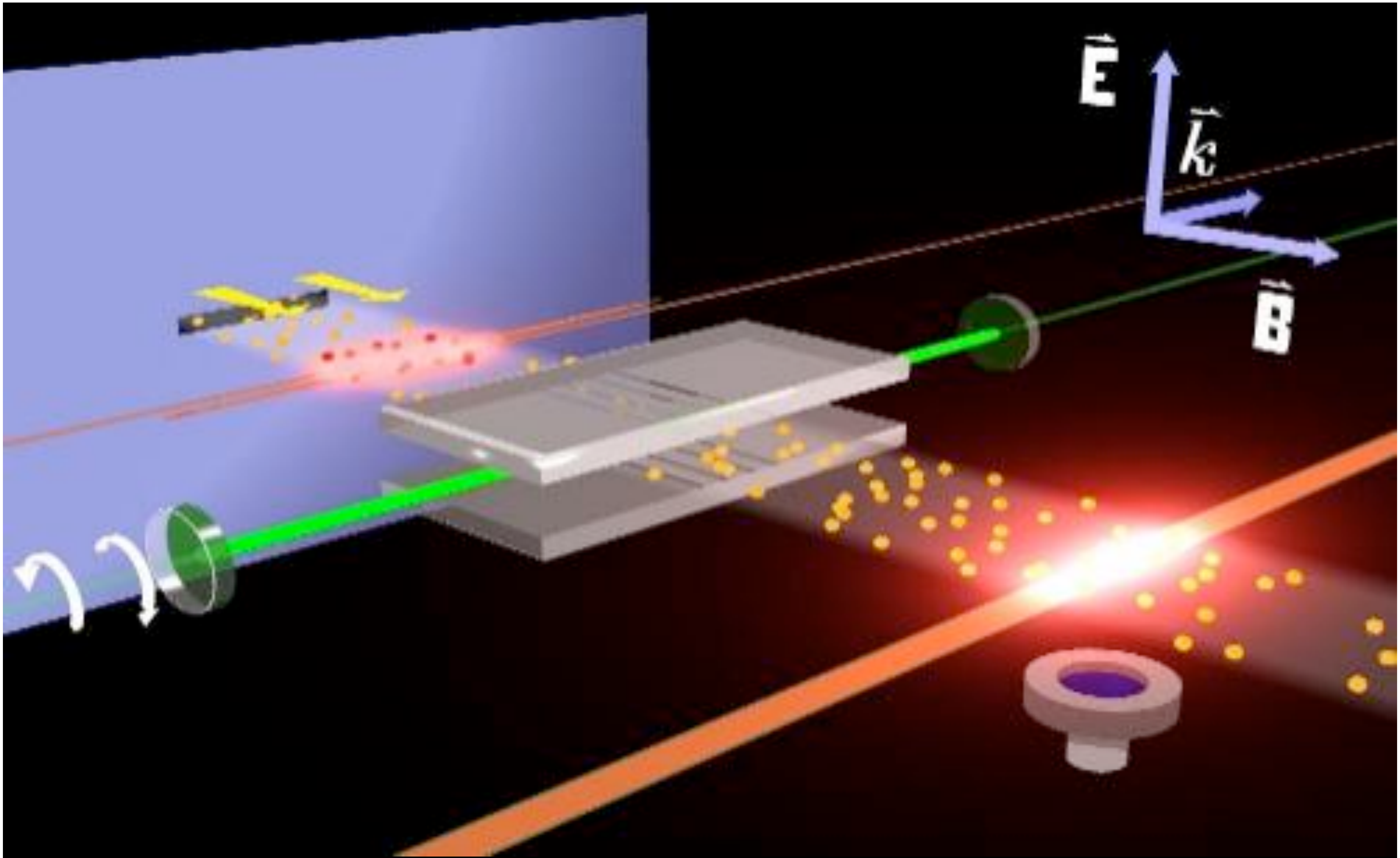
Z3 enhancement (short range)
Possible for heavy atoms

Z^3

Candidates:
Cs, Bi, Tl, Pb, Yb, Sm, Fr …

Paris, Oxford, Seattle, Novosibirsk,
Berkeley, Boulder …

Relativistic effects, nuclear size …



Colorado setup

Atomic theory in the 70s

Energies

Transition probabilities

MCHF / MCDF

CI

RPA

Hyperfine structure …

- Atomic many-body calculations
- Core polarization, all orders
- MBPT
- All- orders –
- Coupled-Cluster
- Non-relativistic

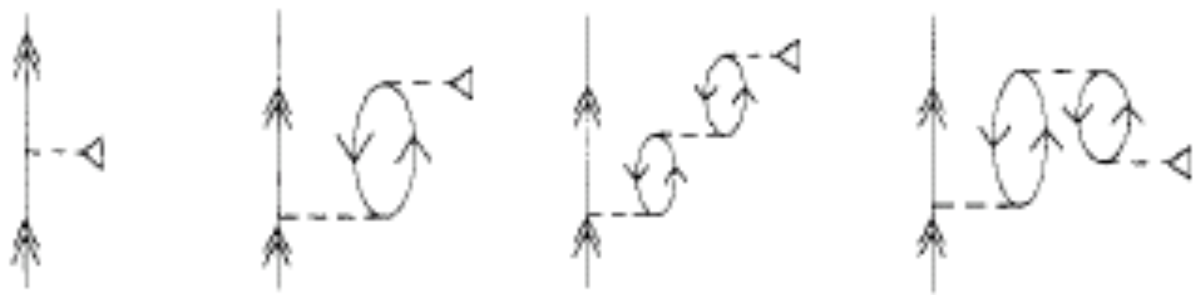
Helium-like systems

- Double CI – ”exact”
- All order pair equation – ”exact”
- Basis set questions / grid size + numerics

Essentially exact calculations possible

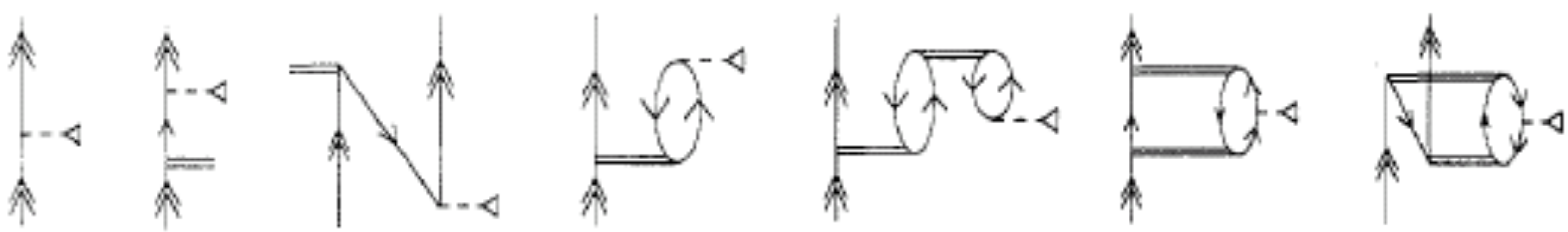
Hylleraas, Pekeris, Drake …

”RPA”, Core polarization, Single excitations to all orders:



(For HFS – only exchange)

+CORRELATION (double exc. all orders)



(a) (b) (c) (d) (e) (f) (g)

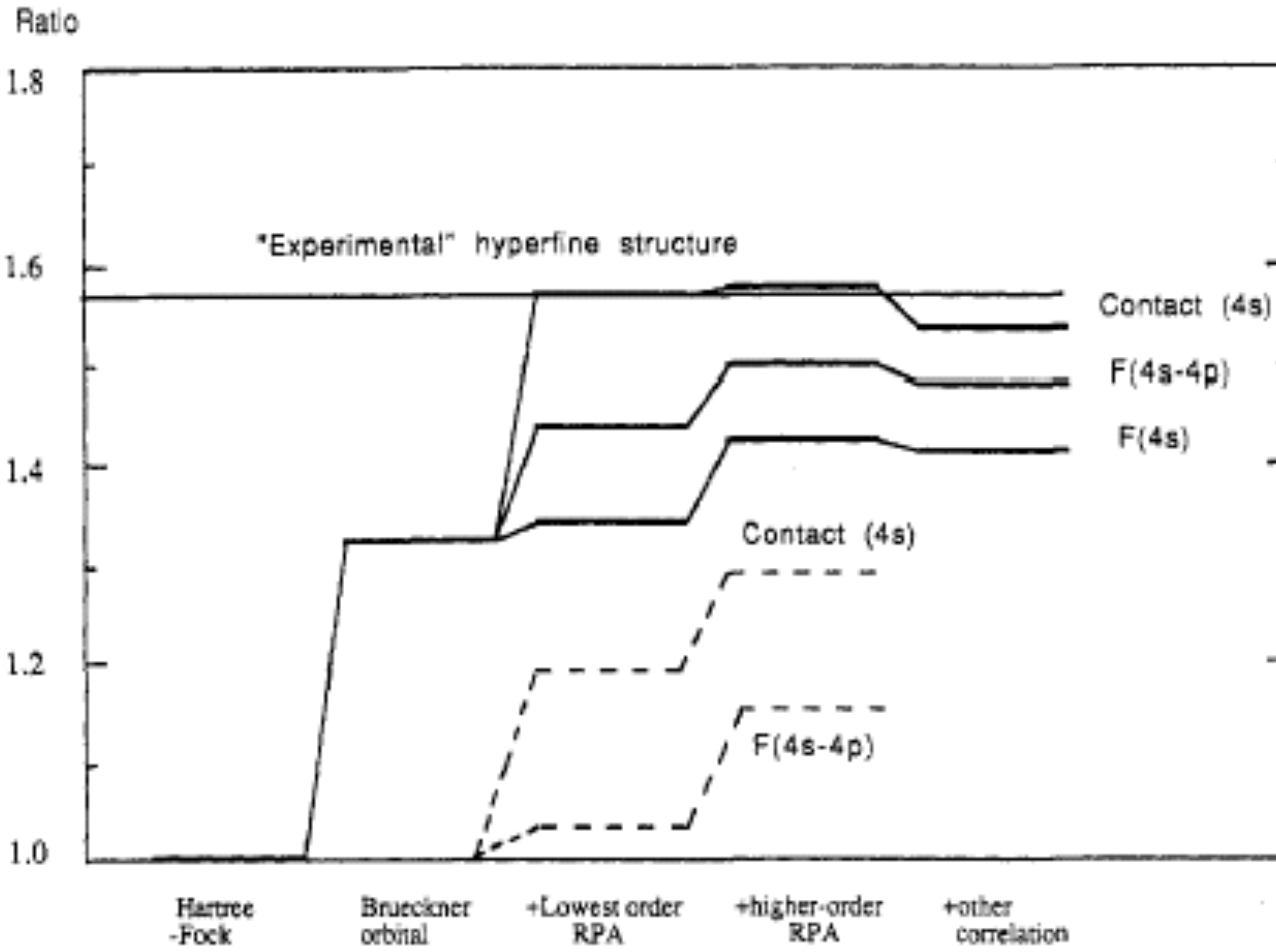
”BRUECKNER ORBITALS”

”RPA”

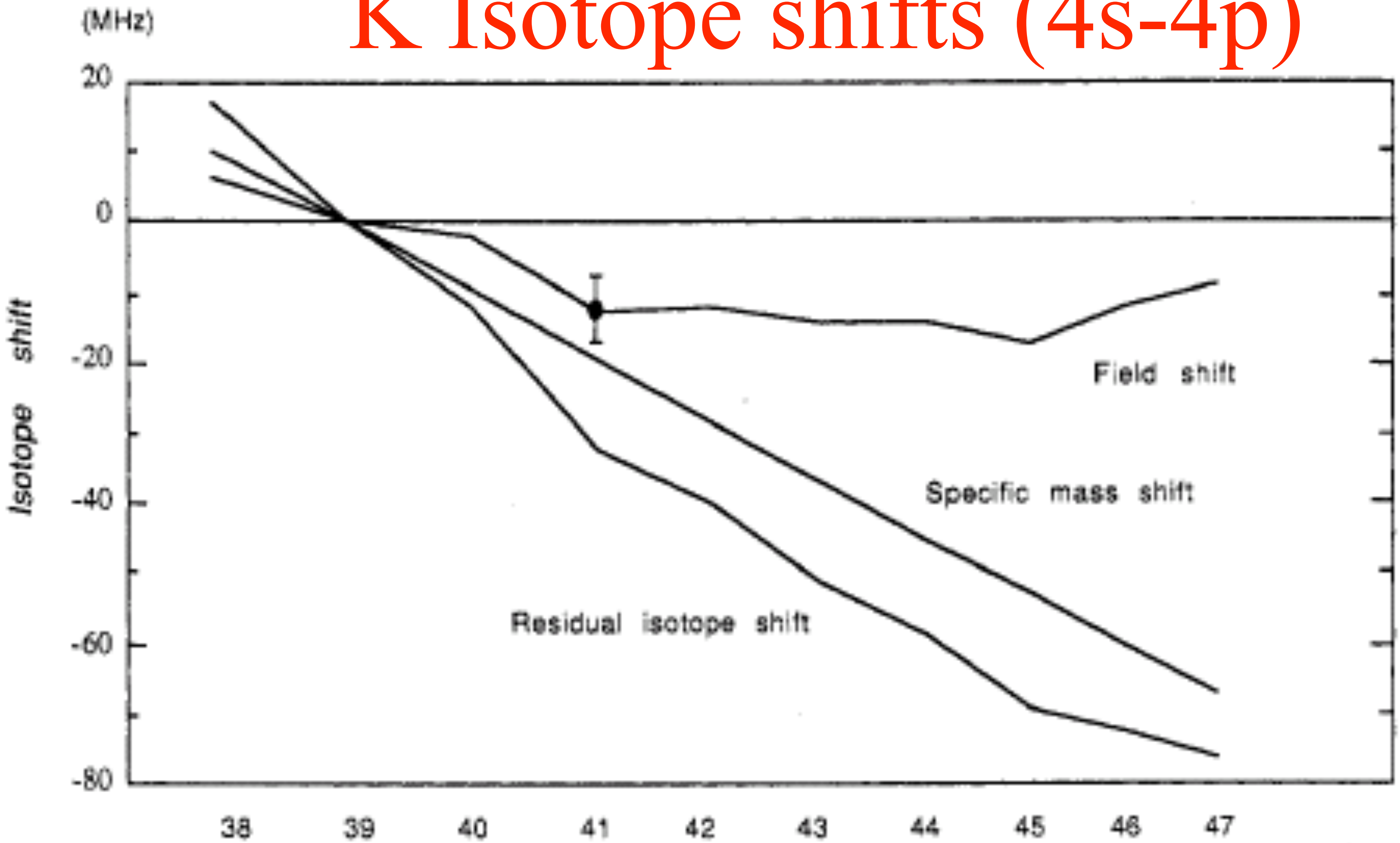
Other Correlation

Exempel: K – HFS + FS

(AMMP et al 1990)



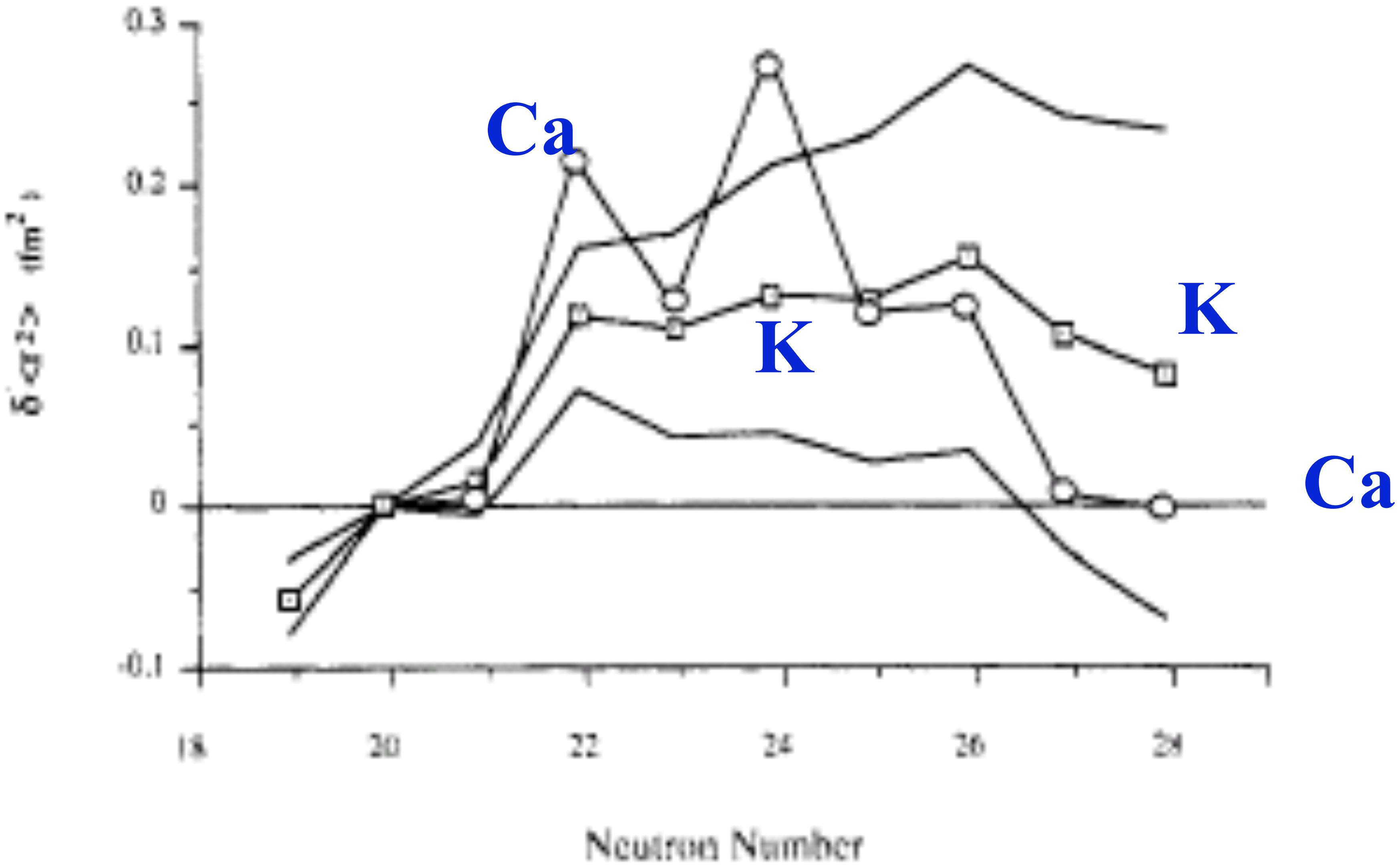
K Isotope shifts (4s-4p)



$$\delta\nu^{AA'} = \left(K^{\mathrm{NMS}} + K^{\mathrm{SMS}}\right)\left(\frac{1}{M_A} - \frac{1}{M'_A}\right) + F\kappa\delta\langle r^2\rangle^{AA'}$$

Nuclear recoil

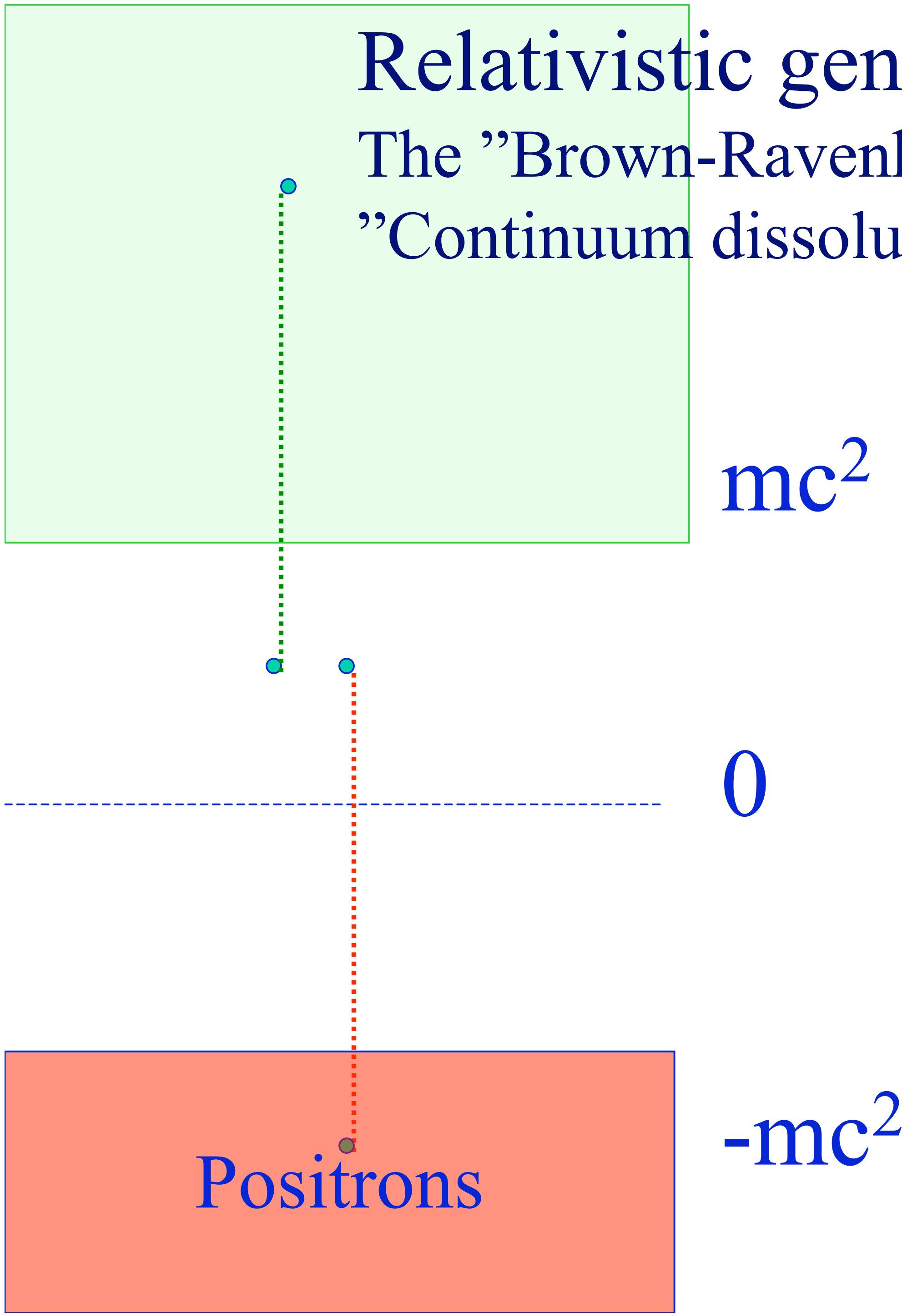
K – Ca isotopes charge radii



Relativistic generalizations

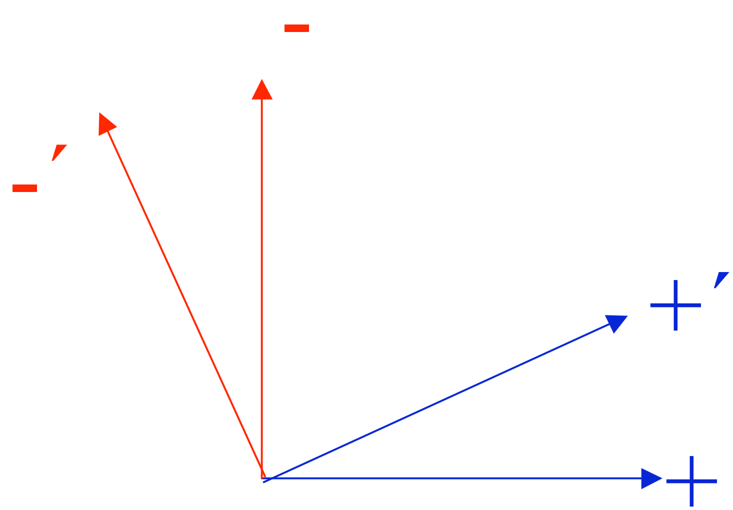
The "Brown-Ravenhall Disease"

"Continuum dissolution"



Warning! A complete orbital set includes both positive and negative energy states!

Projection operators



What is positive ?

”Free choice”

Free electrons – nuclear potential – Dirac–Fock?

”Furry picture”

Implementations of Projection operators

- Explicit insertion
- By construction of orbital set, keeping only positive energy part
- Implicit – through boundary conditions – relations upper/lower component (MCDF e.g.)

> 1986 (Trieste meeting)
> Methods under development
> Indiana, Göteborg, Novosibirsk, Oxford

…

L-extrapolation Helium

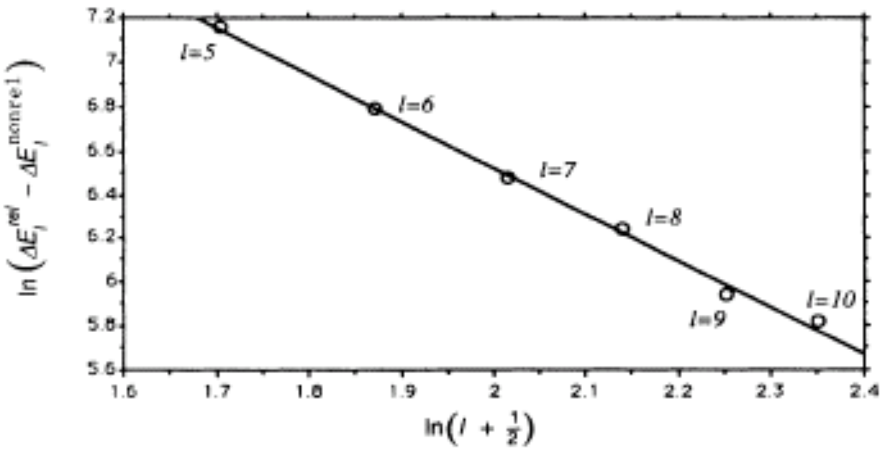


FIG. 2. Log-log plot of the relativistic corrections to the partial-wave increments of the Coulomb correlation energy of helium (from Table III).

ns and limits of the relativistic all-order Coulomb correlation valuated relative to $E_0 + E_1 = -2.750\,114\,97$ a.u. using hydro-, the differences to nonrelativistic (nonrel) results from Ref. 8 .u.).

		E_l^{rel}	$\Delta E_l^{rel} - \Delta E_l^{nonrel}$	$E_l^{rel} - E_l^{nonrel}$
		−129 049 58	−2080.9	−2080.9
		−150 535 37	168.4	−1912.4
2	−224 993	−152 785 30	68.5	−1844.0
3	−553 90	−153 339 20	33.2	−1810.8
4	−197 32	−153 536 52	19.3	−1791.4
5	−8698	−153 632 50	12.8	−1778.6
6	−4409	−153 667 59	8.9	−1769.7
7	−2466	−153 692 25	6.5	−1763.3
8	−1485	−153 707 10	5.1	−1758.1
9	−947	−153 716 56	3.8	−1754.4
10	−631	−153 722 88	3.4	−1751.0
$\sum_{l=11}^{\infty}$	−1866[a]		36[b]	
$\sum_{l=0}^{\infty}$		−153 741 54		−1715
Drake[c]		−153 741 52		−1714

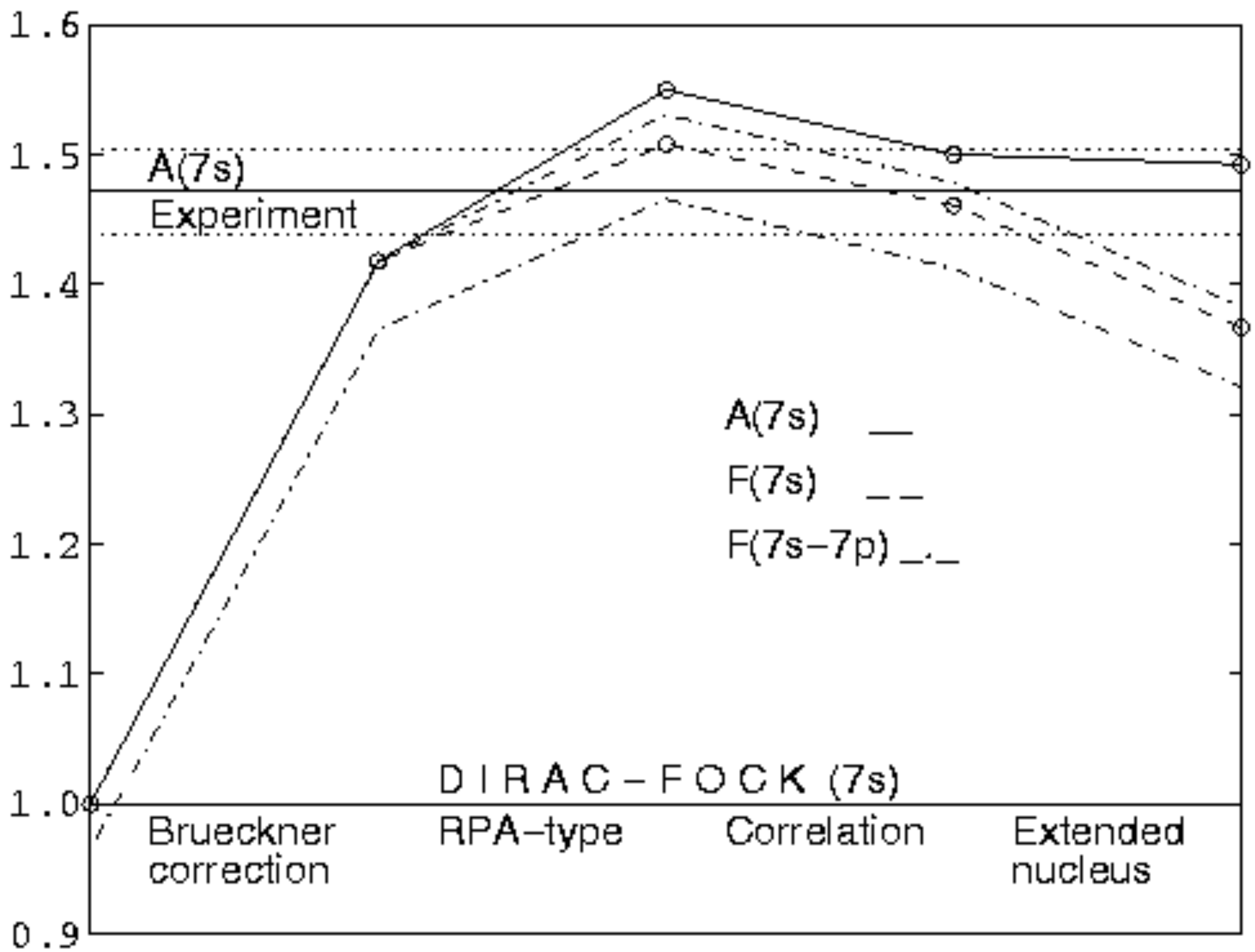
[a]Adding the relativistic corrections from Eq. (29) to the nonrelativistic tail from Ref. 8.
[b]From Eq. (29).
[c]Deduced from Drake, Ref. 13 (see Table I).

Non-relativistic Part L^{-4}

Relativistic Part L^{-2}

Salomonson Öster 1989

Many electrons: Example
Fr, HFS (A), IS (F)

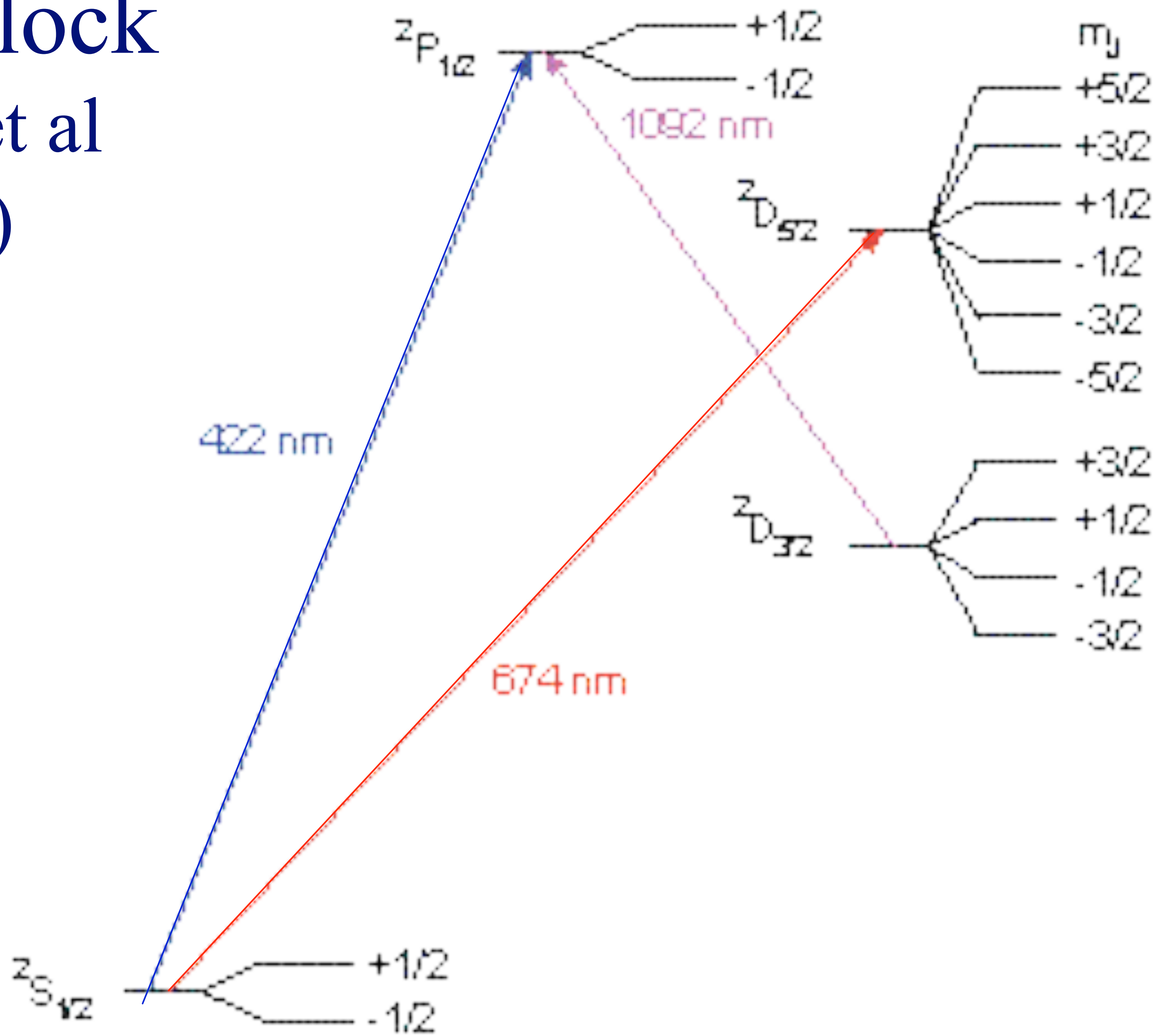


RMBPT – Coupled Cluster

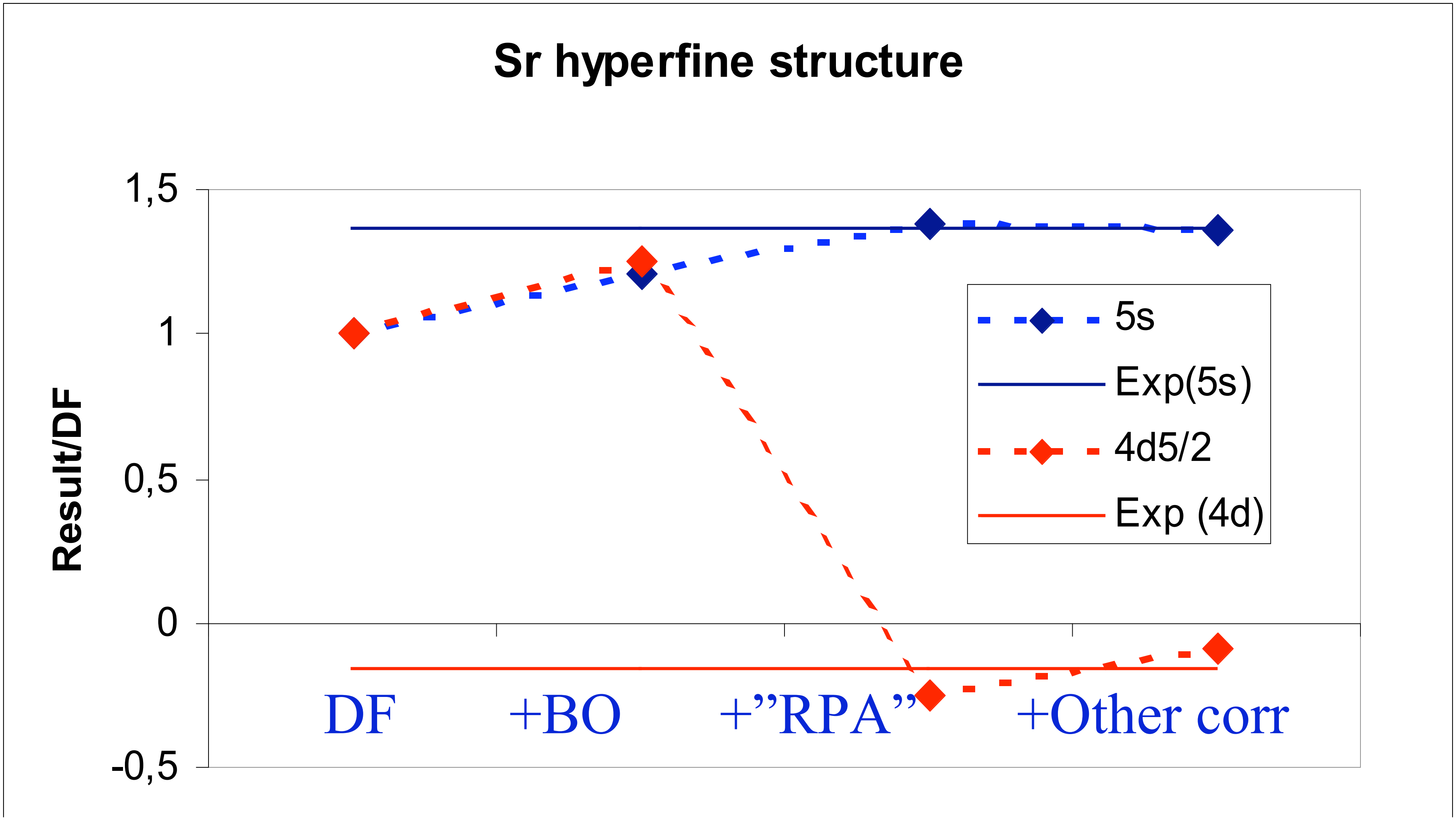
Single and double excitations (CCSD)

(AMMP 1999)

Sr ion clock
(Klein et al NPL)



Hfs of $4d_{5/2}$?



Theory:

1 MHz (AMMP,2002)

2.507 MHz (Yu et al, 2004)

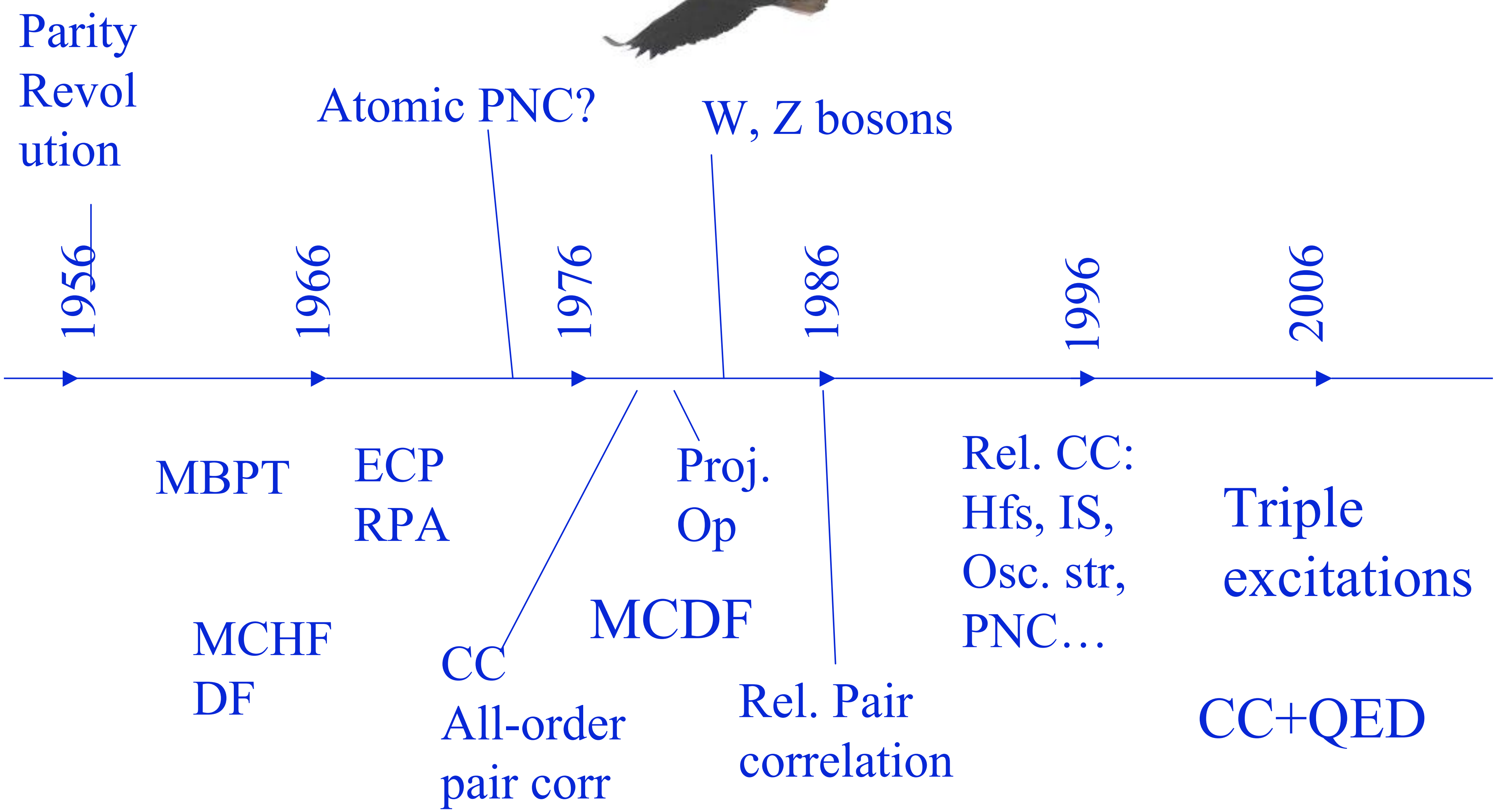
-2.77 MHz (Itano, 2006)

$A(4d_{5/2})$

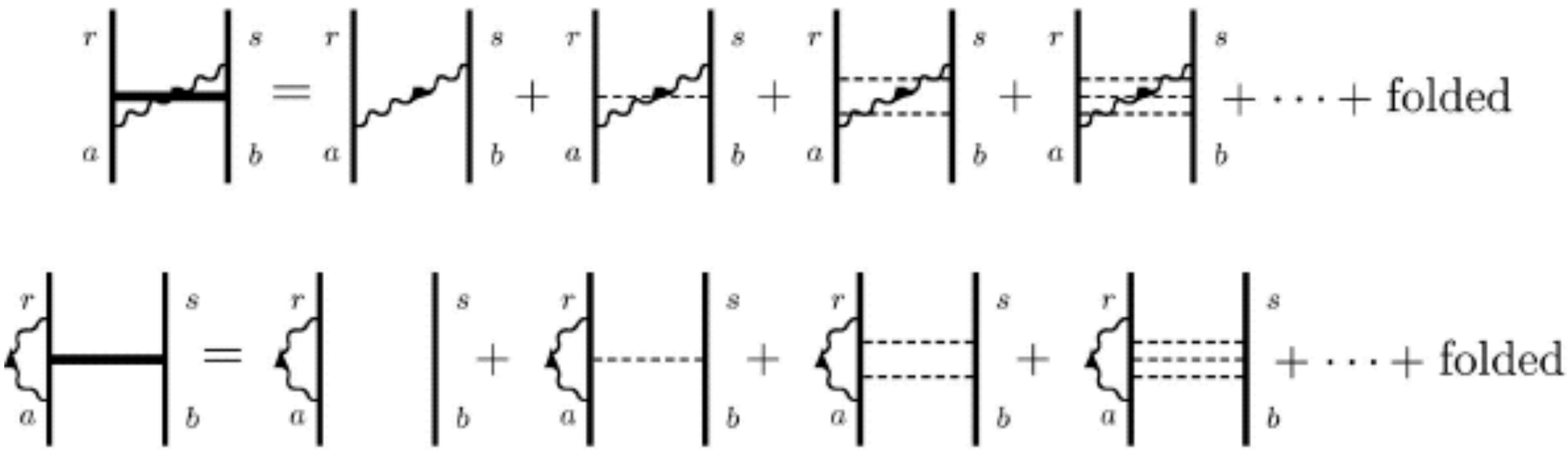
Exp: 2.1743(14)MHz

(Barwood et al 2003)

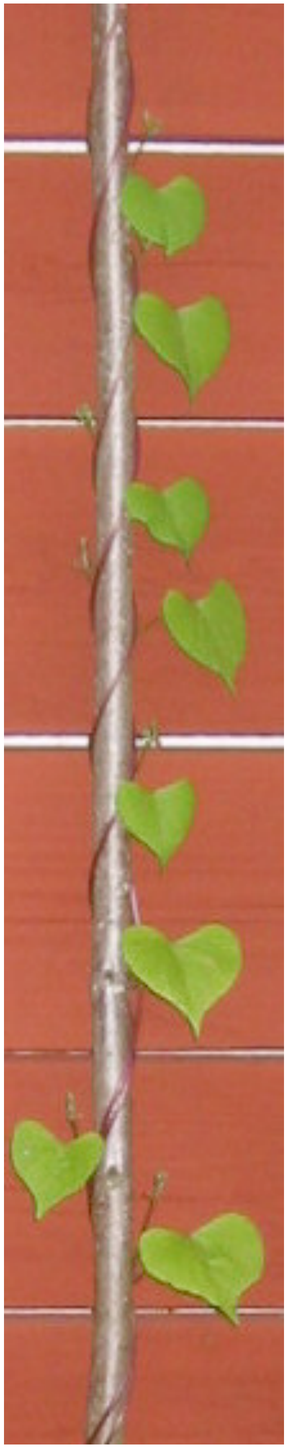
Timeline


Parity Revol ution
Atomic PNC?
W, Z bosons
1956
1966
1976
1986
1996
2006
MBPT
MCHF DF
ECP RPA
CC All-order pair corr
Proj. Op
MCDF
Rel. Pair correlation
Rel. CC: Hfs, IS, Osc. str, PNC…
Triple excitations
CC+QED

Combination of CC and QED



Lindgren, Salomonson, Hedendahl 2006



PNC-interaction

$$H^{PNC} = G\, Q_W\, \gamma_5\, \rho_n(r) / \sqrt{8} + \ldots$$

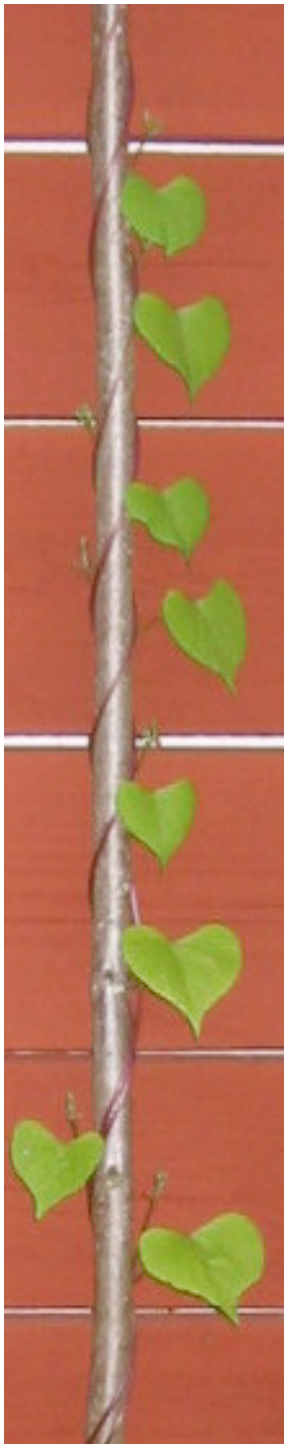
Proportional to weak charge:

$$Q_W \cong (1\text{-}4 \sin^2 \theta_W) Z - N$$

$$\sin^2 \theta_W \cong 0.23$$

Study PNC in isotope chain (e.g. Fr)–
eliminates need for atomic theory?
But $\rho_n(r)$ may vary

Neutron distribution ?



Parity Non-Conservation in Cs

$Q_W(^{133}Cs) = -72.61(28)_{exp}(73)_{exp}$

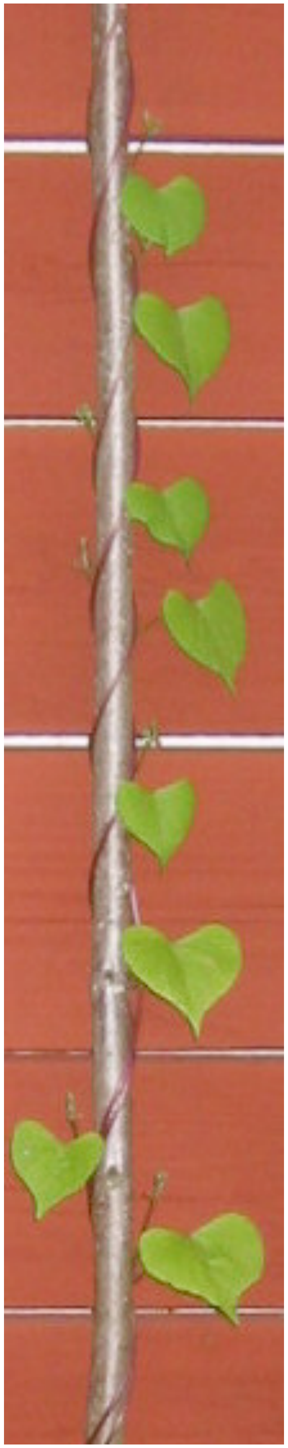
Exp: Wieman et al (1999) + …

Derevianko (2000, 2001) +
Blundell et al (1988, 1990, 1992),
Flambaum et al (1989, …2000)

Including Breit interaction (0.9%) +
Estimate of correction for difference
neutron- proton distribution (-0.2%)

Standard Model

$Q_W(^{133}Cs) = -73.20(13)$



Neutron EDM ?

The argument against an electric dipole moment of a nucleus or elementary particle raises directly the question of parity.

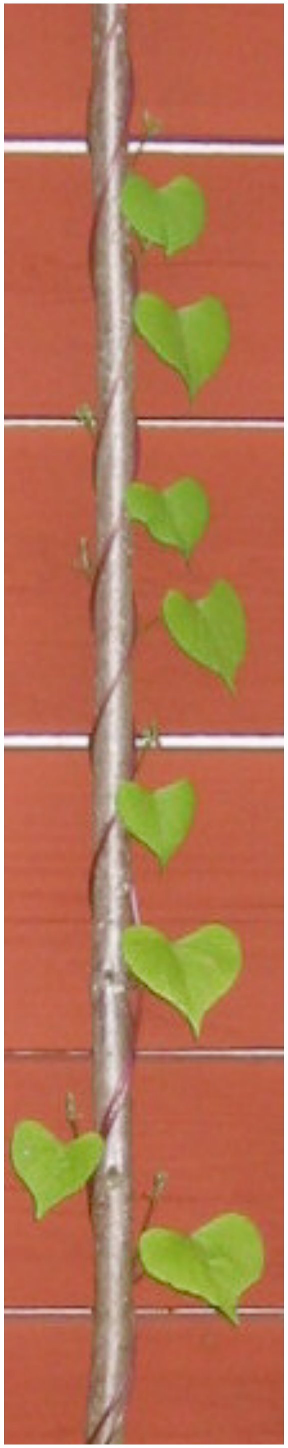
But there is no compelling reason for excluding this possibility.

The validity of the parity assumption must rest on experimental evidence. …

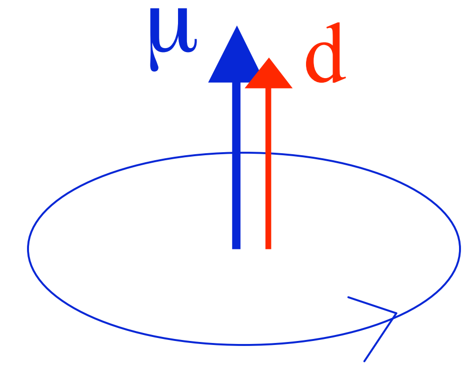
The experimental evidence is not as conclusive as generally supposed.

(Purcell and Ramsey 1950)

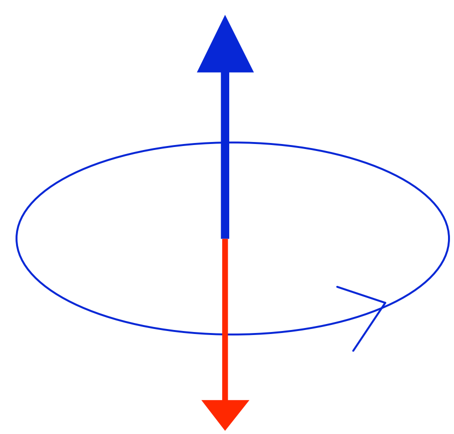
EDM ?



A nucleon with an electric dipole moment would show an asymmetry between left- and right-handed systems; in one system, the electric dipole would be parallel to the angular momentum, in the other, anti-parallel.

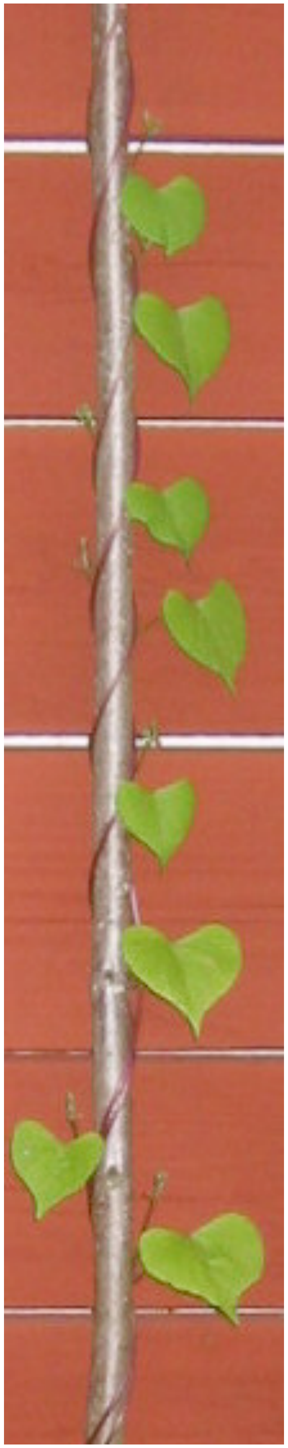


(P)



Purcell and Ramsey (1950)

$|D| < 3 \times 10^{-18}$ cm



Neutron EDM
Baker et al, PRL 97, 131801 (2006)

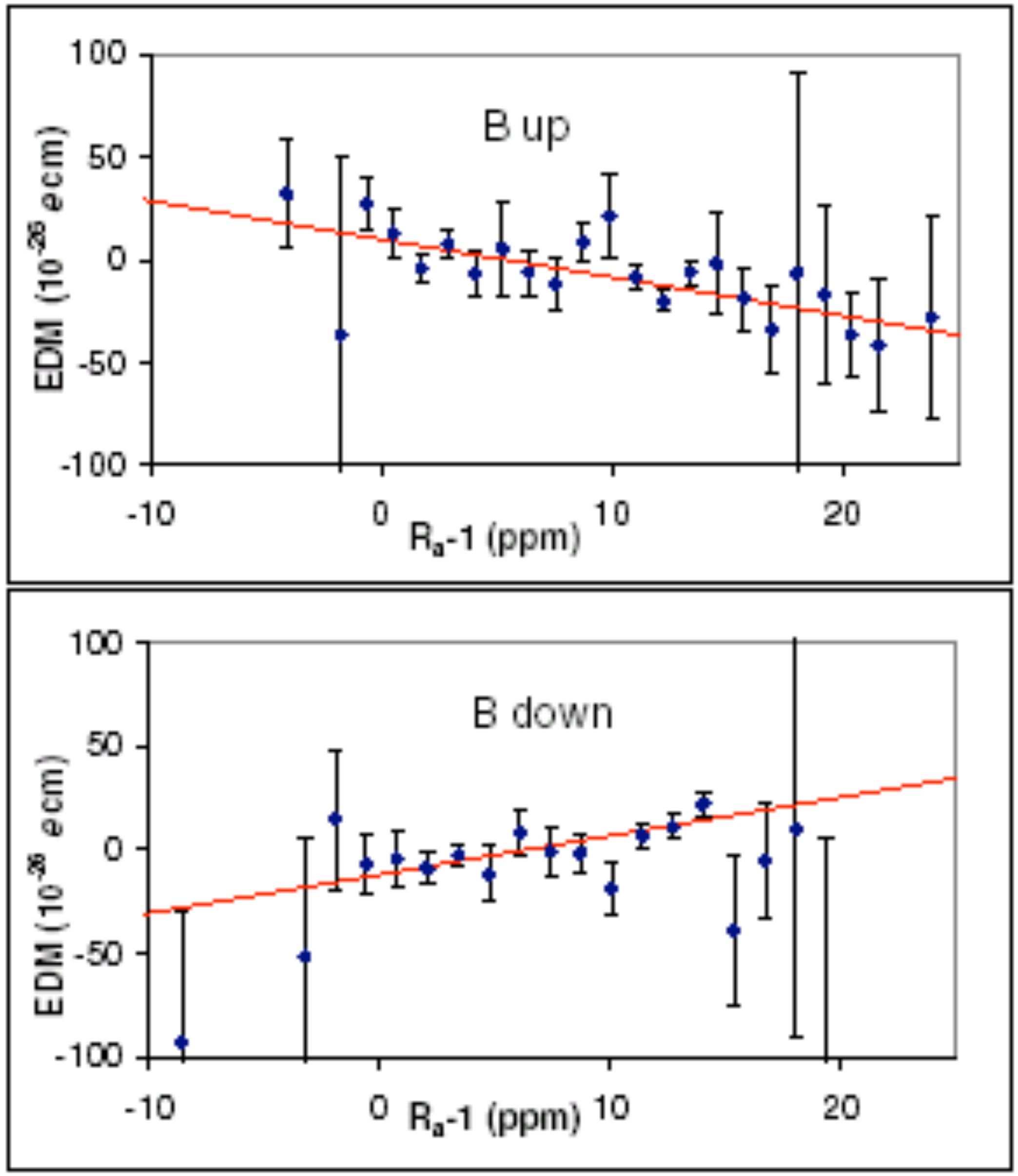
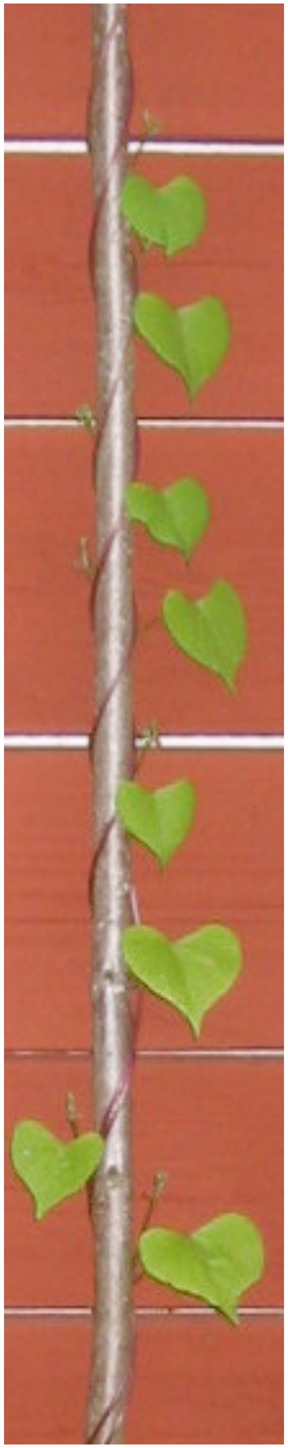


FIG. 2 (color online). Measured EDM (binned data) as function of the relative frequency shift of neutrons and Hg.



Neutron EDM limits

$|D| < 3 \times 10^{-18}$ cm (1950)

Purcell and Ramsey

$|D| < 5 \times 10^{-20}$ cm (1957)

$|D| < 3 \times 10^{-24}$ cm (1977)

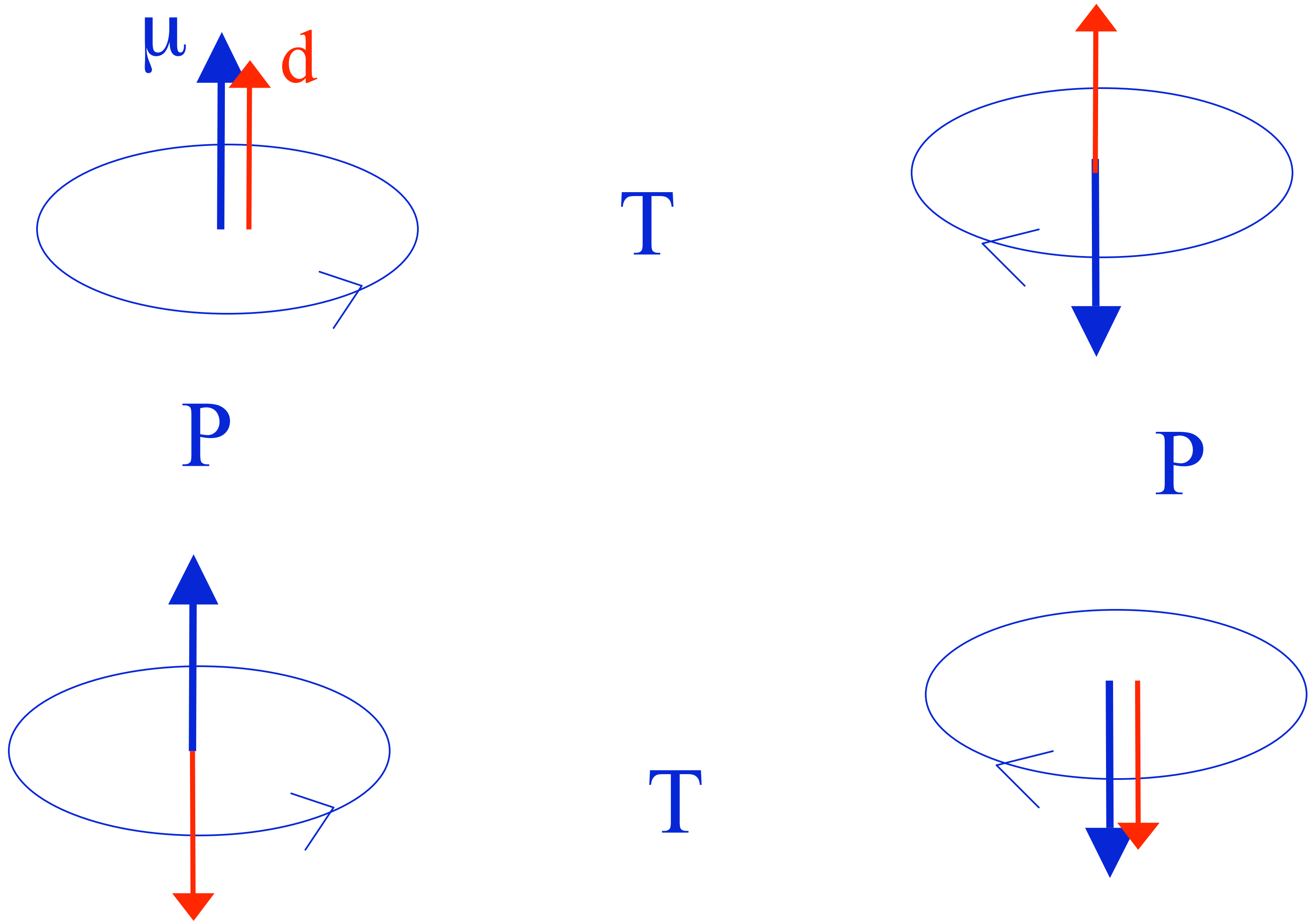
$|D| < 6 \times 10^{-25}$ cm (1982)

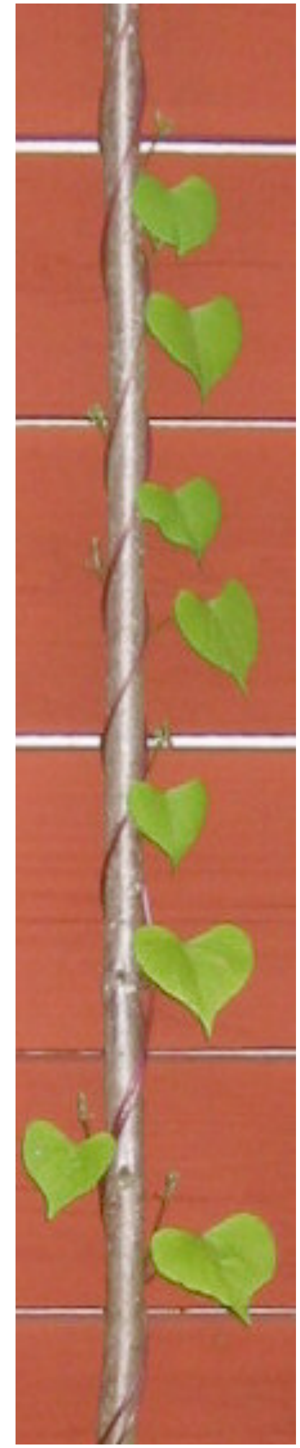
…

$|D| < 2.9 \times 10^{-26}$ cm (2006)

Why no EDM?

EDM – Violates P and T





1987,
Stockholm

Will a neutron EDM be discovered?

K-mesons …

Unless nature is malevolent against Norman Ramsey

… not necessarily in my life time

Ljungskile, Sweden, June 2006

TABLE I. Summary of limits (95% C.L.) set by the ^{199}Hg EDM and other experiments on model-independent and "naturalness" parameters.

Parameter	Limit from ^{199}Hg	Best other limit		Ref.
$\bar{\theta}_{QCD}$	1.5×10^{-10}	6×10^{-10}	n [3]	[6,11]
$\tilde{d}_d$ (cm)	7×10^{-27}	1.1×10^{-25}	n [3]	[6,12]
C_T	1×10^{-8}	5×10^{-7}	TlF [13]	[14]
C_S	3×10^{-7}	4×10^{-7}	Tl [4]	[14]
ε_q^{SUSY}	2×10^{-3}	1×10^{-2}	n [3]	[1]
ε^{Higgs}	$0.4/\tan\beta$	$0.7/\tan\beta$	Tl [4]	[1]
x^{LR}	1×10^{-3}	1×10^{-2}	n [3]	[1]

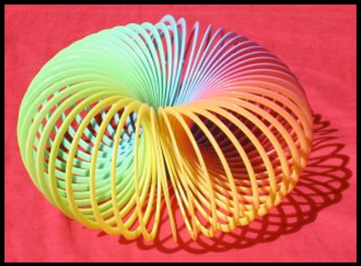
Romalis et al 2001

Parity Non-Conservation and Nuclear Structure ?

- EDM: $(< r_d^2 > - < r_c^2 >)$
  (Schiff moments) + ….

- Isotope Chains PNC– neutron distribution

- Anapole moments …



What is known about nuclear distributions?

Nuclear Charge Distributions

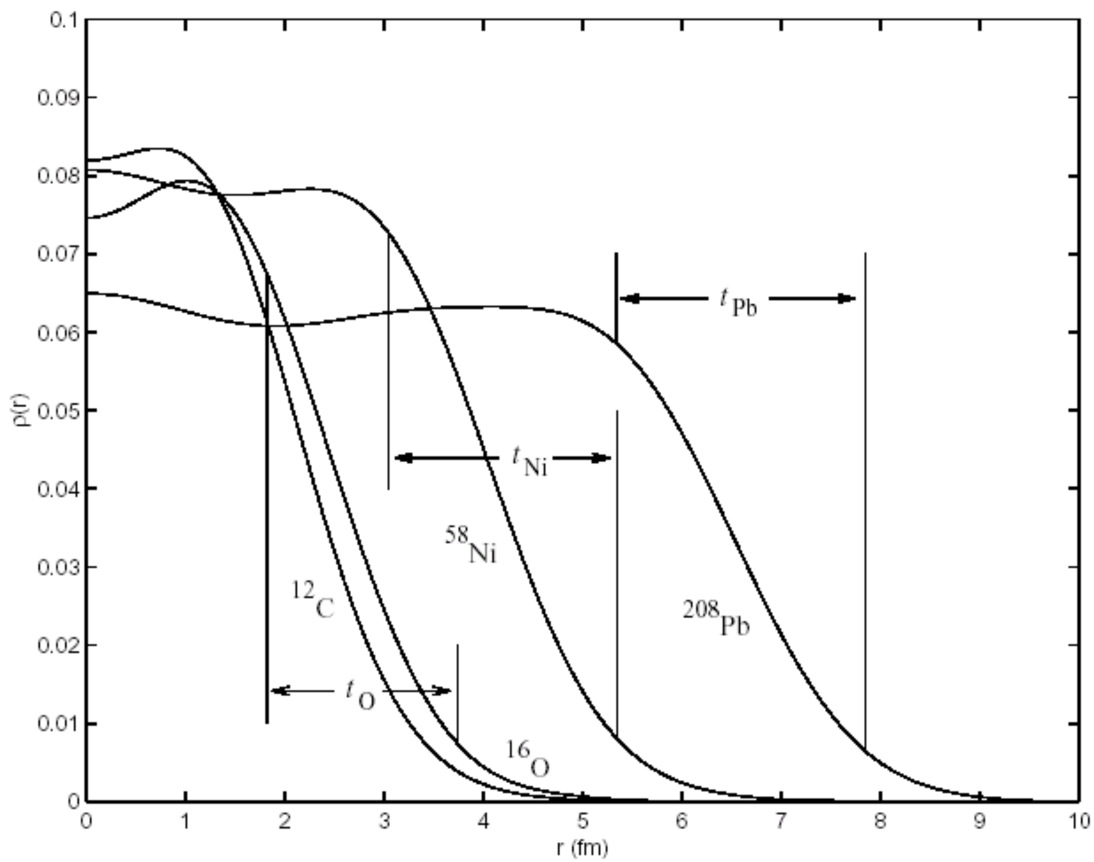
First approximation:

Homogeneous distribution:

$R = R_0 A^{1/3}$

$R_0 = 1.2$ fm

$\langle r^2 \rangle = 3 R^2/5$



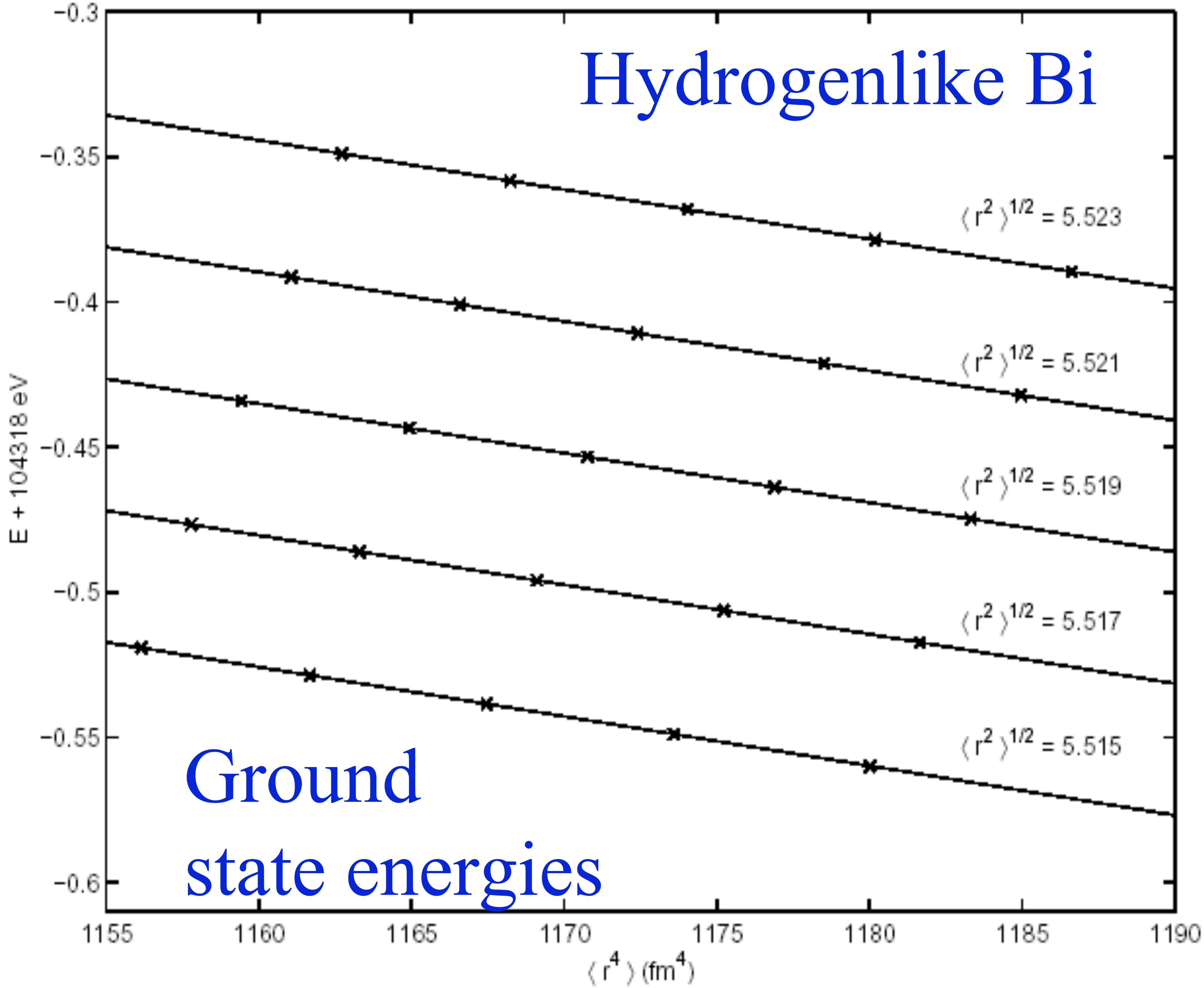
Fermi Distribution

$$\rho(r) = \frac{\rho_0}{1 + e^{(r-c)/a}}$$

$$\begin{aligned}
\langle r^2 \rangle &\approx \frac{3}{5}c^2 + \frac{7}{5}\pi^2 a^2 , \\
\langle r^4 \rangle &\approx \frac{3}{7}c^4 + \frac{18}{7}\pi^2 a^2 c^2 + \frac{31}{7}\pi^4 a^4 , \\
\langle r^6 \rangle &\approx \frac{3}{9}c^6 + \frac{11}{3}\pi^2 a^2 c^4 + \frac{239}{15}\pi^4 a^4 c^2 + \frac{127}{5}\pi^6 a^6
\end{aligned}$$

Homogeneous nuclear distribution, radius c

”Thickness parameter”, a


Hydrogenlike Bi
Ground
state energies
E + 104318 eV
⟨r⁴⟩ (fm⁴)
⟨r²⟩^1/2 = 5.523
⟨r²⟩^1/2 = 5.521
⟨r²⟩^1/2 = 5.519
⟨r²⟩^1/2 = 5.517
⟨r²⟩^1/2 = 5.515
−0.3
−0.35
−0.4
−0.45
−0.5
−0.55
−0.6
1155
1160
1165
1170
1175
1180
1185
1190

Francium Hyperfine anomalies

(Grossmann et al 1999
Sprouse 2006)

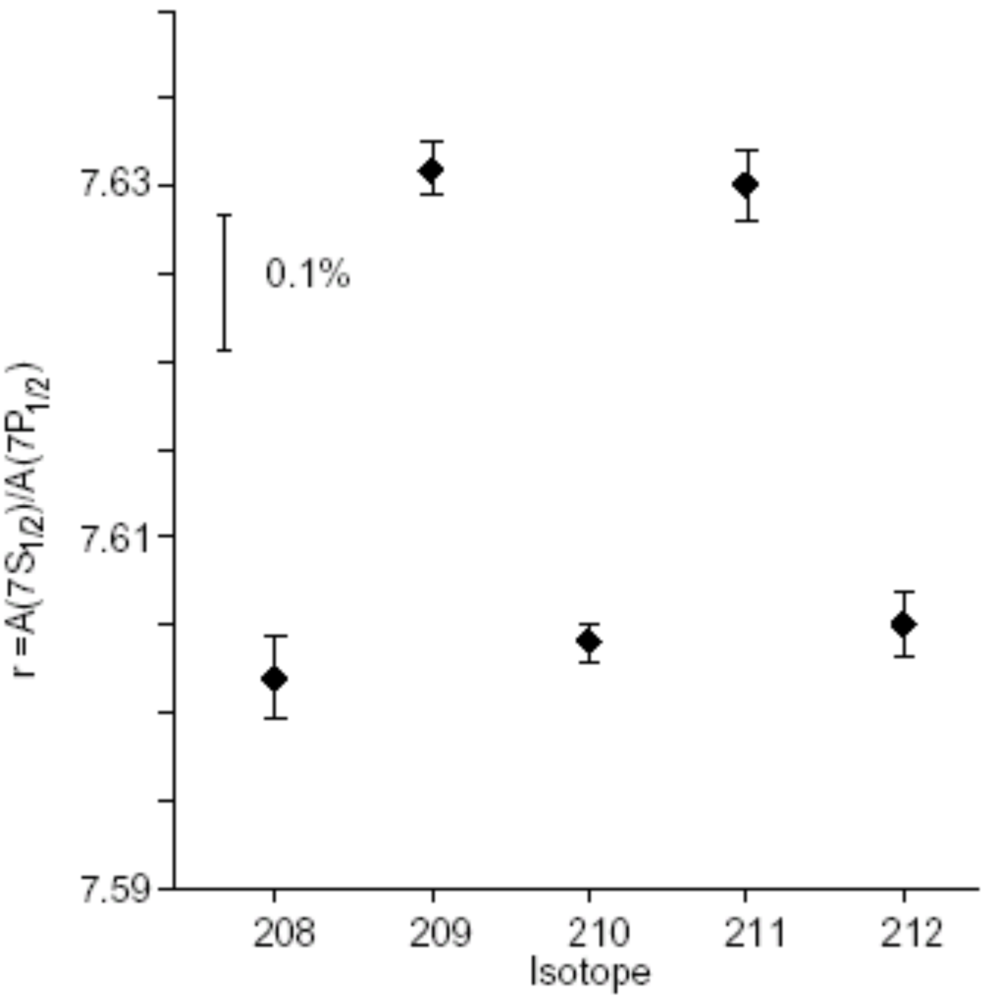


Figure 13. Ratio of hyperfine *A* magnetic dipole constants of $7S_{1/2}$ and $7P_{1/2}$ states observed for five different Fr isotopes. The s states come from the work of Coc *et al* [39] and the p states come from [28].

Ratio
$A(7s)/A(7p_{1/2})$

Odd-even staggering

Tl hyperfine anomalies

(A-M M-P 1995)

$\Delta\ (6p_{1/2}) = -1.04 \cdot 10^{-4}$ (Lurio Prodell 1956)

$\Delta\ (6p_{3/2}) = 16.26 \cdot 10^{-4}$ (Gould 1956)

$\Delta\ (7s_{1/2}) = -3.4(18) \cdot 10^{-4}$ (Hermann et al 1993)

Single particle:

$\Delta(ns_{1/2}) \,/\, \Delta\ (np_{1/2}) = 3.5$

$\Delta(np_{3/2}) = 0$

Many-body effects.
CCSD:

consistent with experimental data

"Breit Rosenthal" effect on HFS - Nuclear Charge Distribution

Correction $(1- \varepsilon_{BR})$ due to charge distribution:

$$\varepsilon_{BR} = b_2 < r_c^2 > + b_4 < r_c^4 > + b_6 < r_c^6 >$$

Parameters depend on l and j, but very weakly on n

But Breit-Rosenthal effect is insufficient …

Bohr-Weisskopf effect: Extract $\delta < r_m^2 >$

Bohr-Weisskopf effect:
Correction to hfs interaction for distributed nuclear magnetic moment

$$h_{\mathrm{BW}}^{\mathrm{hfs}} = \int \Big\{ \eta(R - r) \Big[g_s \Big(\frac{\mathbf{S}_n}{r^2} - \sqrt{10} (\mathbf{S}_n \mathbf{C}_n^2)^1 \frac{r}{R^3} \Big) + g_L \mathbf{L}_n \Big(\frac{1}{r^2} - \frac{r}{R^3} \Big) \Big] \times \boldsymbol{\alpha} \Big\} \rho_m(R) R^2 \, dR$$

$$\varepsilon_{\mathrm{BW}} = a_2 < r_m{}^2 > + a_4 < r_m{}^4 > + a_6 < r_m{}^6 >$$

Tl result (1995)

$$^{203:205}\delta < r_c{}^2 > = 0.115(3)\ \mathrm{fm}^2$$

(From muonic data, Engfer et al At Data Nucl. Data Tables1974)

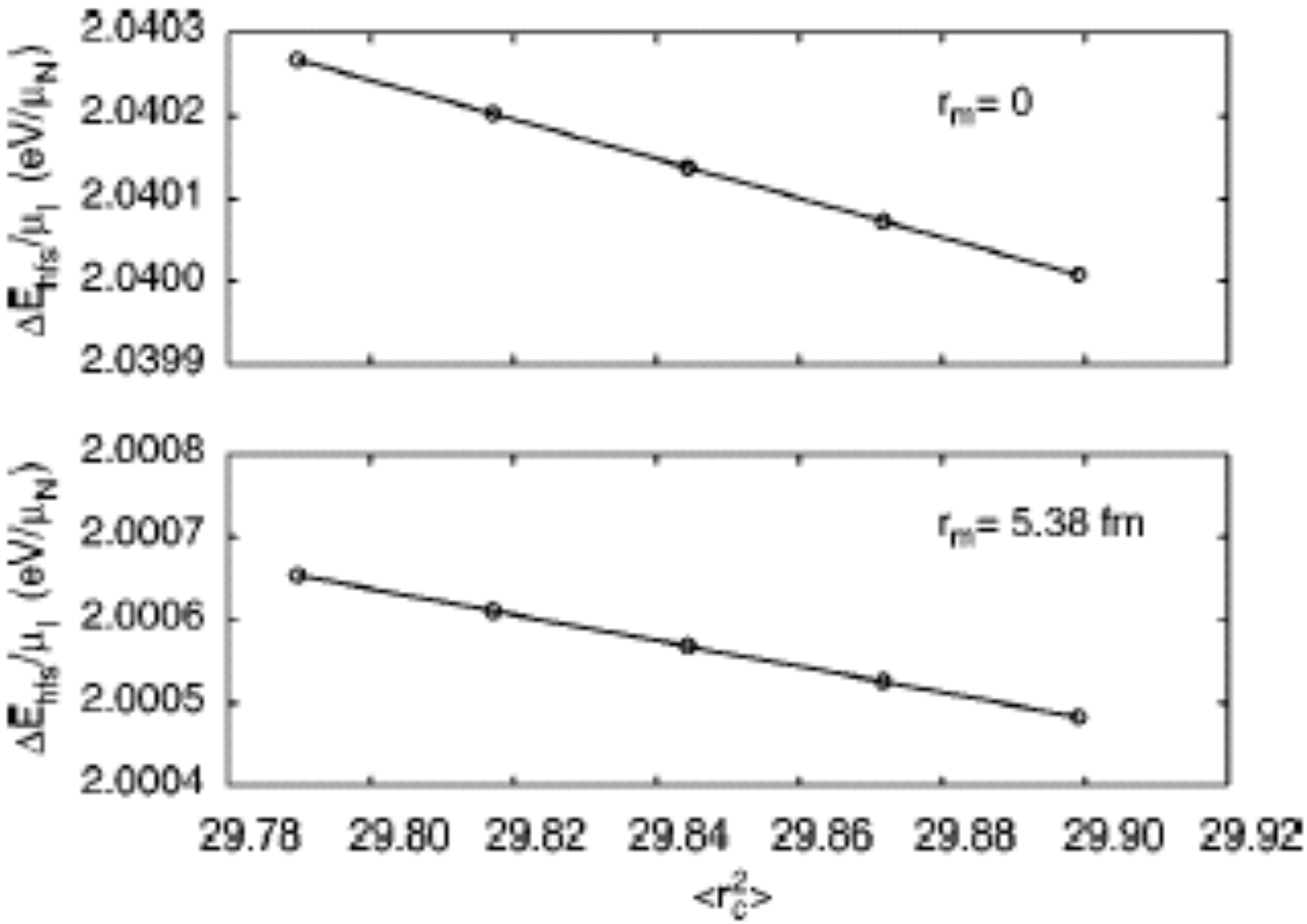
gives

$$^{203:205}\delta < r_m{}^2 > = 0.26(2)\ \mathrm{fm}^2$$

About equal contributions to
the hyperfine anomaly in Tl

Evidence for different distributions

Breit-Rosenthal and Bohr-Weisskopf effects are not independent



Tl

Hydrogen-like Tl
(Beiersdorfer et al 2001)

^{203}Tl:

$\varepsilon_{BW} = 2.212\%$ $\quad \langle r_m^{1/2} \rangle = 5.83(14)$fm

^{205}Tl:

$\varepsilon_{BW} = 2.248\%$ $\quad \langle r_m^{1/2} \rangle = 5.89(14)$fm

Larger than charge radii –
Challenging nuclear theory to reproduce

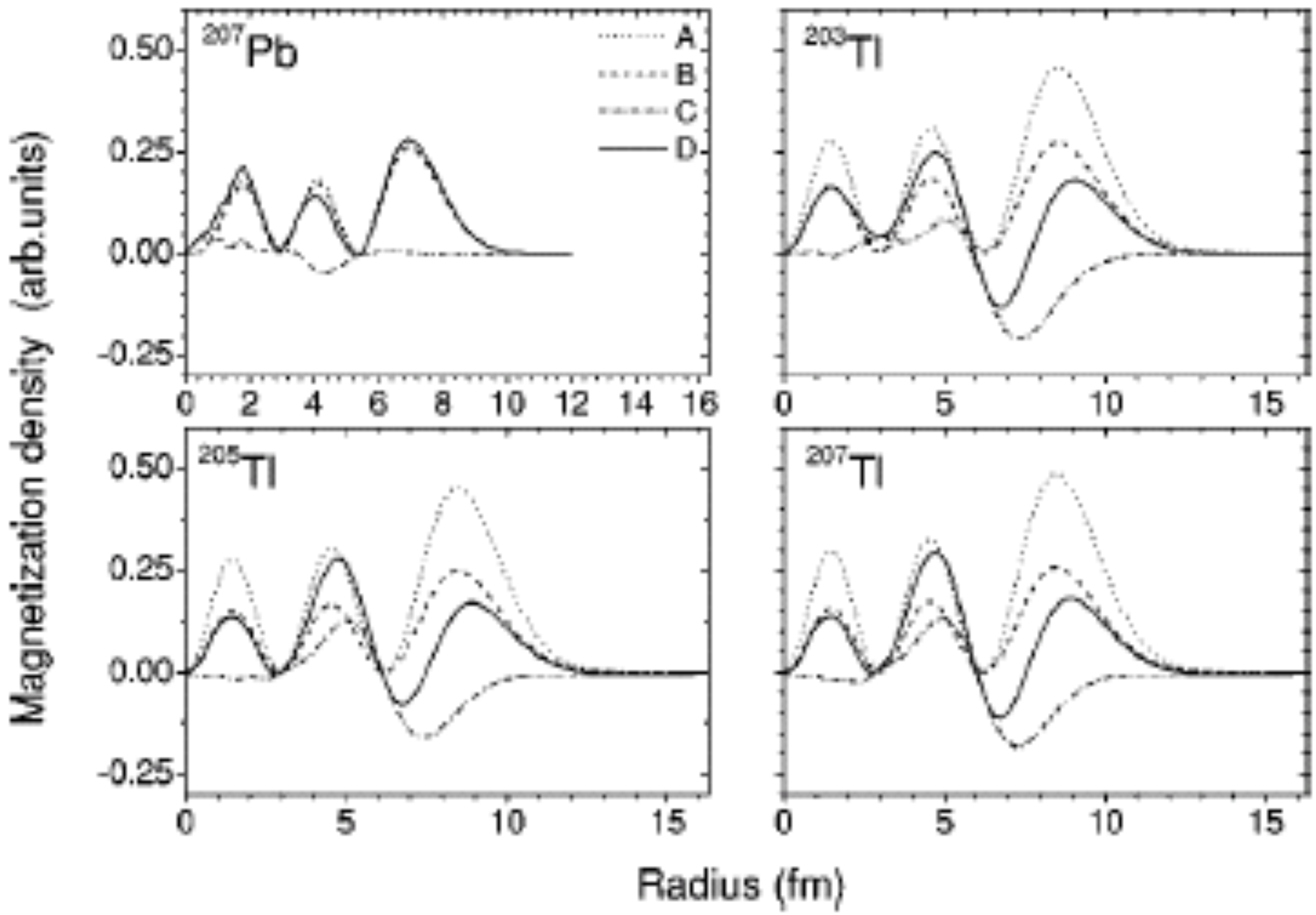


FIG. 3. Calculated magnetization distribution for ^{207}Pb and ^{203,205,207}Tl. Line *A* shows the single-particle result, line *B* has been normalized with the spectroscopic factor of the single particle, line *C* shows the contributions of diagonal and off-diagonal elements in DCM, and line *D* is the total magnetization.

Tomaselli et al, 2002

Experiment =

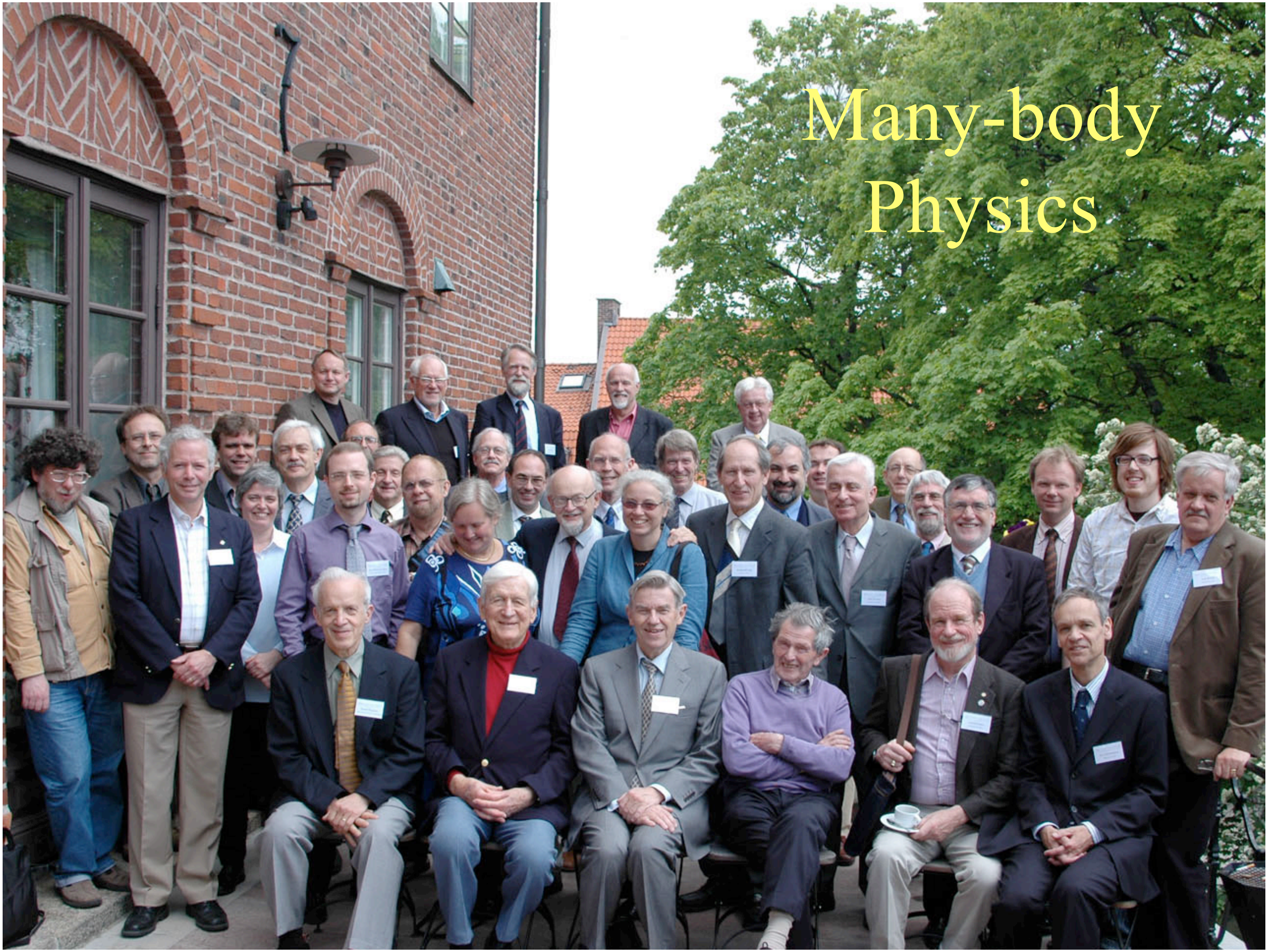
$$\text{QED} + \frac{\text{atom}}{\text{nucleus}} * \text{nucleus} + \text{new physics?}$$

Nuclear Challenge!

Atomic Physics at the Interface to Nuclear and Particle Physics

(INT, 1999)

Many-body methods also connect condensed matter theorists and quantum chemists (+TlF, YbF, PbO …)


Many-body
Physics