Accurate calculations for polyvalent heavy atoms

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Atoms as probes for *new physics*

- Violation of discrete symmetries
- Violation of the local Lorentz invariance
- Time variation of the fundamental constants
- Exotic long-range interactions
- Interactions with Dark Matter & Dark Energy

Sometimes we study qualitative effects and sometimes we look for quantitative disagreements. In both cases we can not check atomic theory directly.

Symmetry violation & time-dependence of fundamental constants

- We calculate atomic sensitivity to some perturbation.
- Typically a few percent accuracy is sufficient.
- Usually highest sensitivity is found in complex atoms (i.e. heavy, polyvalent, with accidental degeneracies, etc.)

We need universal method and some tools to control the accuracy. Usually we calculate similar properties, which can be measured (spectra, transition rates, g-factors, HFS, polarizabilities).

Non-perturbative methods

- A typical example is configuration interaction (CI) method.
- It works very well for few electron systems.
- The size of CI space scales exponentially with the number of electrons.
- Becomes ineffective for number of electrons of the order of 10.

Many-body perturbation theory

Perturbation theory is effective when there is small parameter $\lambda \ll 1$

$$E_i^{\lambda} = E_i^{(0)} + a_i\lambda^2 + b_i\lambda^3 + c_i\lambda^4 + \ldots$$

In atomic theory if we start with some mean-field potential U_0 the residual interaction

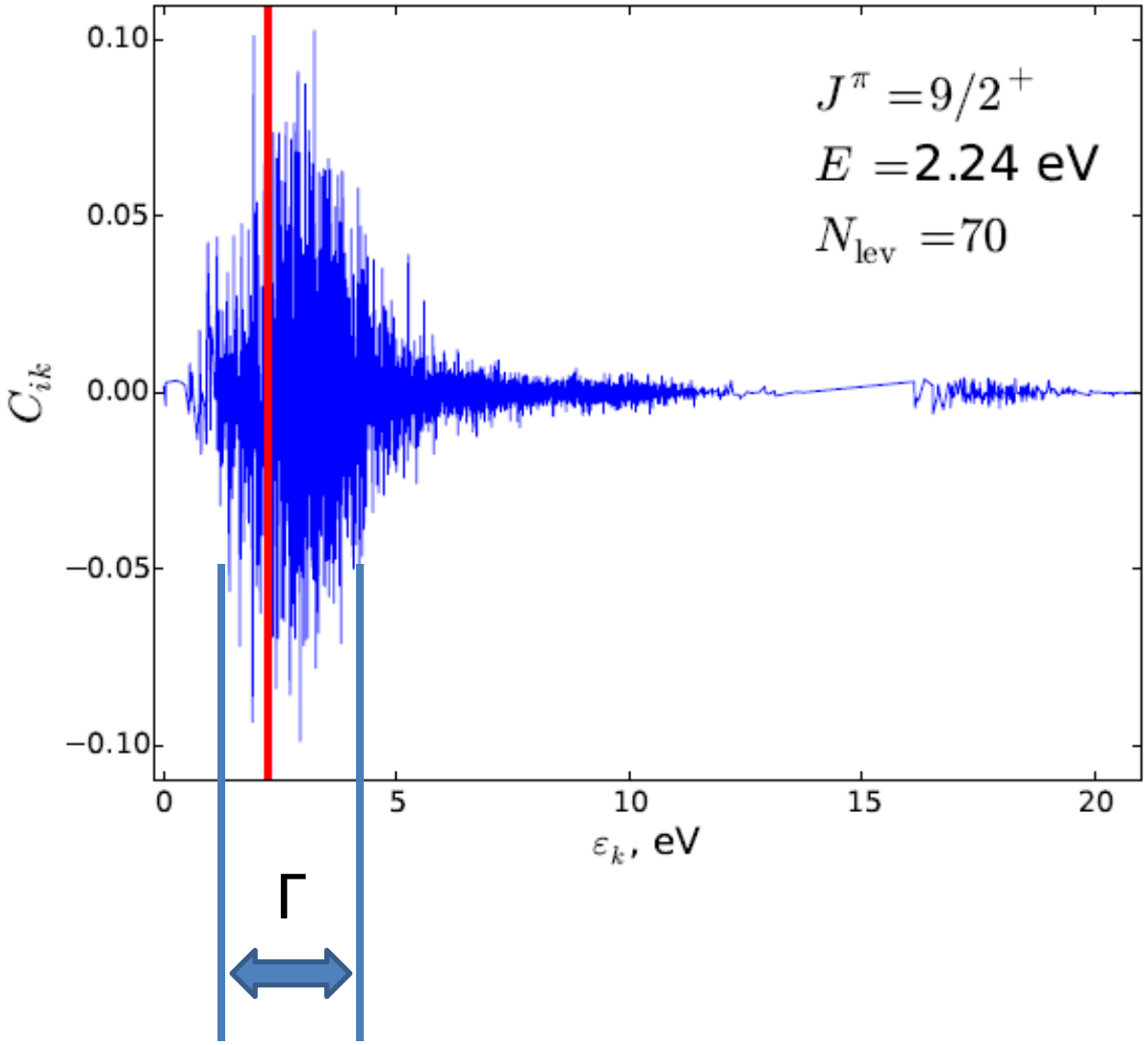
$$V' = V - U_0$$

is not small. Thus, in general, $\lambda \approx V'/\Delta \sim 1$ and MBPT does not work!

Residual interaction

If $V' \gg D$, where D is distance between levels, then V' mixes basis states within spreading width

$$\Gamma = 2\pi\langle V'\rangle^2/D$$



Structure of the eigenstate of Protactinium atom. $\Gamma \approx 2$ eV.

[A.Viatkina, MK, V Flambaum, PRA **95**, 022503 (2017)]

Effective small parameter for core-valence correlation corrections

Let us single out the core with excitation energy Δ_{cv} >>1. Then for the core-valence correlations we can introduce

$$\lambda_{\text{eff}} = \frac{\langle V' \rangle}{\Delta_{cv}}$$

Comparing this to the correlation correction:

$$\delta E_{cv} = \frac{\langle V' \rangle^2}{\Delta_{cv}}$$

we can write:

$$\lambda_{\text{eff}} = \sqrt{\frac{\delta E_{cv}}{\Delta_{cv}}}$$

And now λ_{eff} can be small.

CI+MBPT method

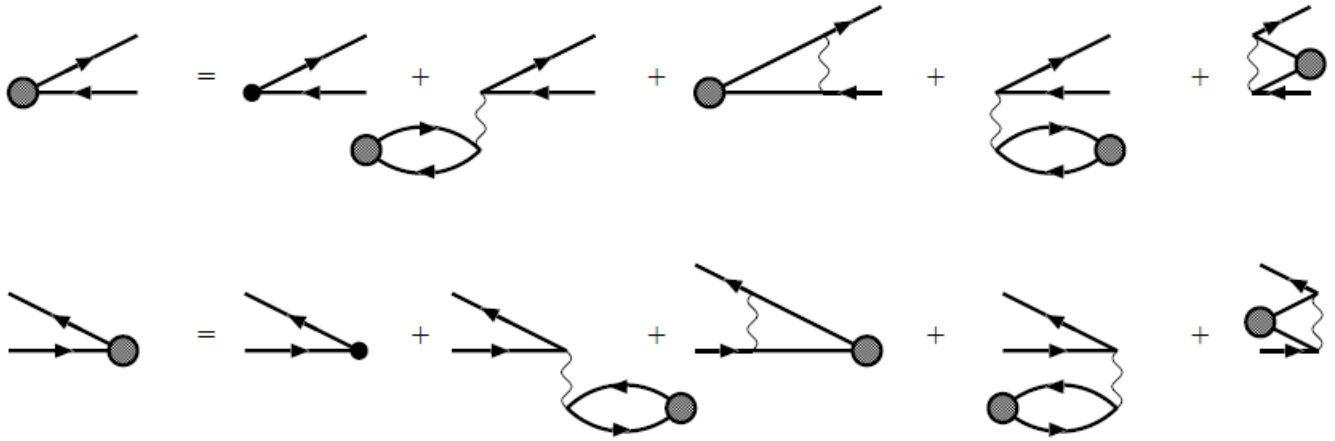
- Valence correlations are treated within configuration interaction (CI) method.
- Core-valence & core-core are accounted for by many-body perturbation theory (MBPT).
- Second order MBPT is used to form effective Hamiltonian in the valence CI space.
- Effective operators are formed for all valence observables.

Effective Hamiltonian for valence electrons

- We define valence space so that all core electrons are frozen.
- We use MBPT to form H_{eff} in the valence space.
- We diagonalize effective Hamiltonian using configuration interaction method.
- Zero order Hamiltonian is the valence Hamiltonian in the frozen core approximation.

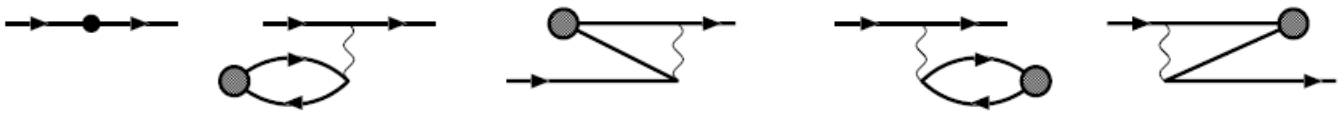
Effective operators for observables

RPA for core

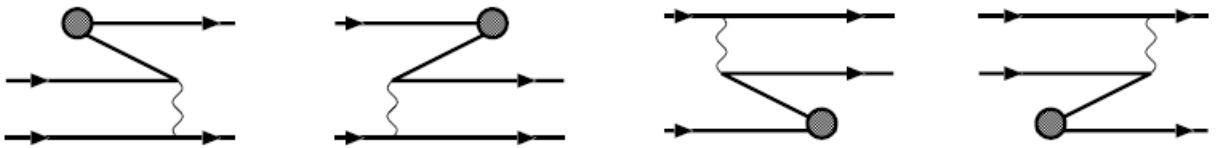


Valence amplitudes

1-e



2-e



Advantages

- Applicable to atoms and ions with arbitrary number of closed shells including superheavy elements.
- Applicable to polyvalent atoms.
- Computationally inexpensive.
- Allows to calculate large variety of properties, which depends mainly on valence electrons.
- Some high-order MBPT corrections can be included within CI+all-order (CI+AO).

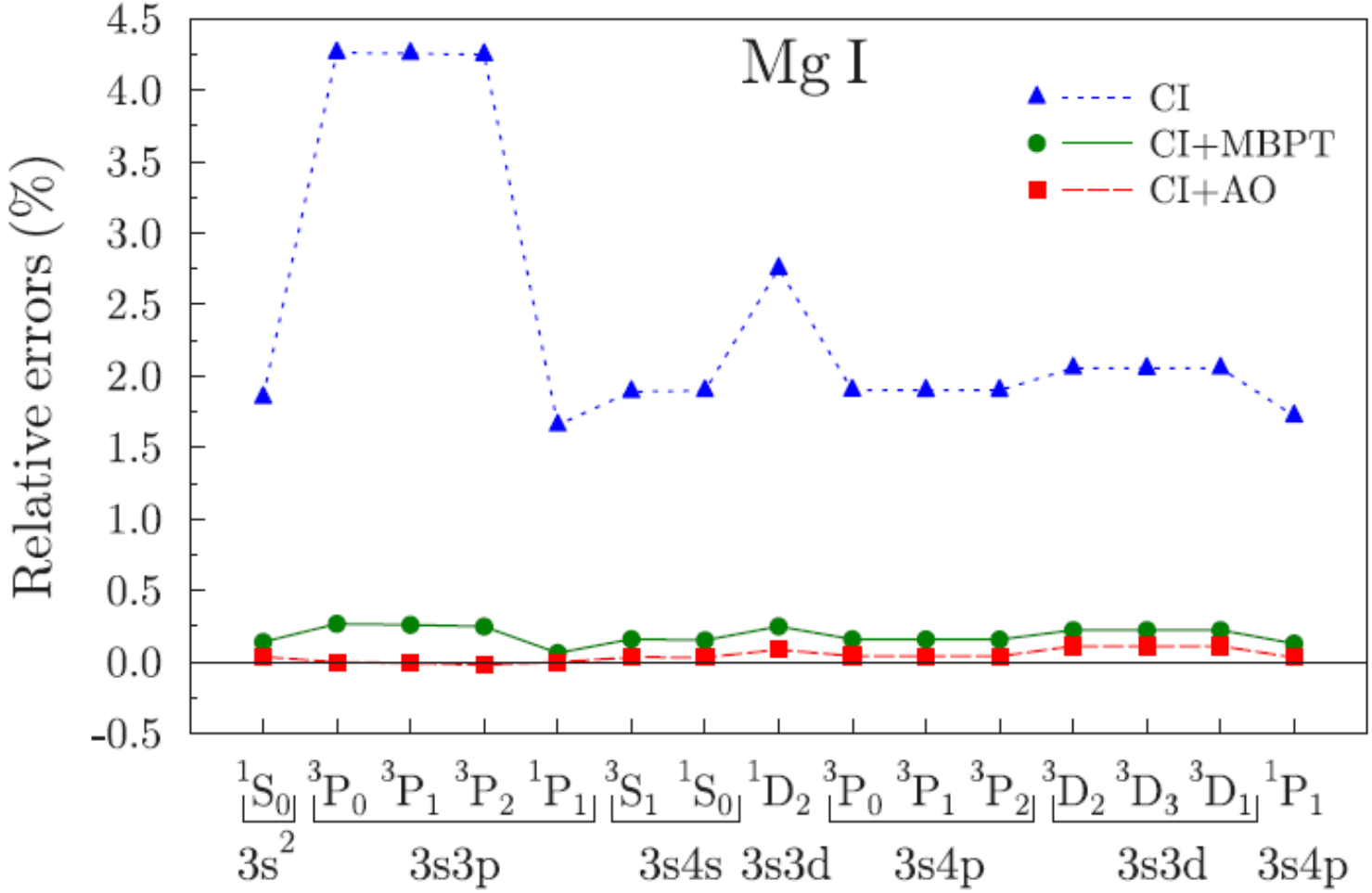
Limitations

- Difficult to include high-order MBPT corrections consistently:
  - energy-dependence of the effective Hamiltonian;
  - effective many particle interactions.
- Difficult to use for atoms with too many electrons in the open shells:
  - CI space grows too fast;
  - choice of the mean field.
- Generally, the method can not be used for quantitative tests of fundamental physics.

Status of the method

- CI+MBPT & CI+AO is used by several groups in Australia, USA, & Russia. Recently: China & Germany(?).
- About a hundred papers published.
- Effects: PNC, EDMs, LLI, α-variation, etc.
- Computer package is available from CPC. Additional programs and scripts are on ResearchGate (https://www.researchgate.net/project/Atomic-calculations-using-CI-MBPT-and-CI-AO-all-order-methods)

Accuracy of CI, CI+MBPT, & CI+AO for Mg I



[E Konovalova & MK, PRA, **92**, 042508 (2015)]

HFS of ^{205}Tl (MHz)

	$A_{6p_{1/2}}$	$A_{6p_{3/2}}$	$A_{7s_{1/2}}$	$A_{7p_{1/2}}$	$A_{7p_{3/2}}$	$A_{6d_{3/2}}$	$A_{6d_{5/2}}$
DF	17339	1291	7579	1940	187	21	9
CI	924	−1369	3799	−102	112	−185	391
$H_{\rm eff}$	3428	−45	765	331	−56	114	−226
$A_{\rm RPA}$	959	359	1031	103	73	5	15
A_{σ}	−1071	−31	−269	−92	−9	3	−5
$A_{\rm sbt}$	−1389	−161	−75	−113	−19	−19	−8
$A_{\rm tp}$	1731	120	−22	133	4	21	7
$A_{\rm SR}$	209	88	−29	14	6	−1	0
Norm.	−467	−4	−113	−20	−3	0	0
Total	21663	248	12666	2193	295	−41	183
Theor. [a]	21760	−1919	12470	2070	195		
Theor. [b]	21300	339	12760				
Theor. [c]	21623	264	12307	2157	315	−35	184
Expt.	21311	265	12297	2155	309	−43	229

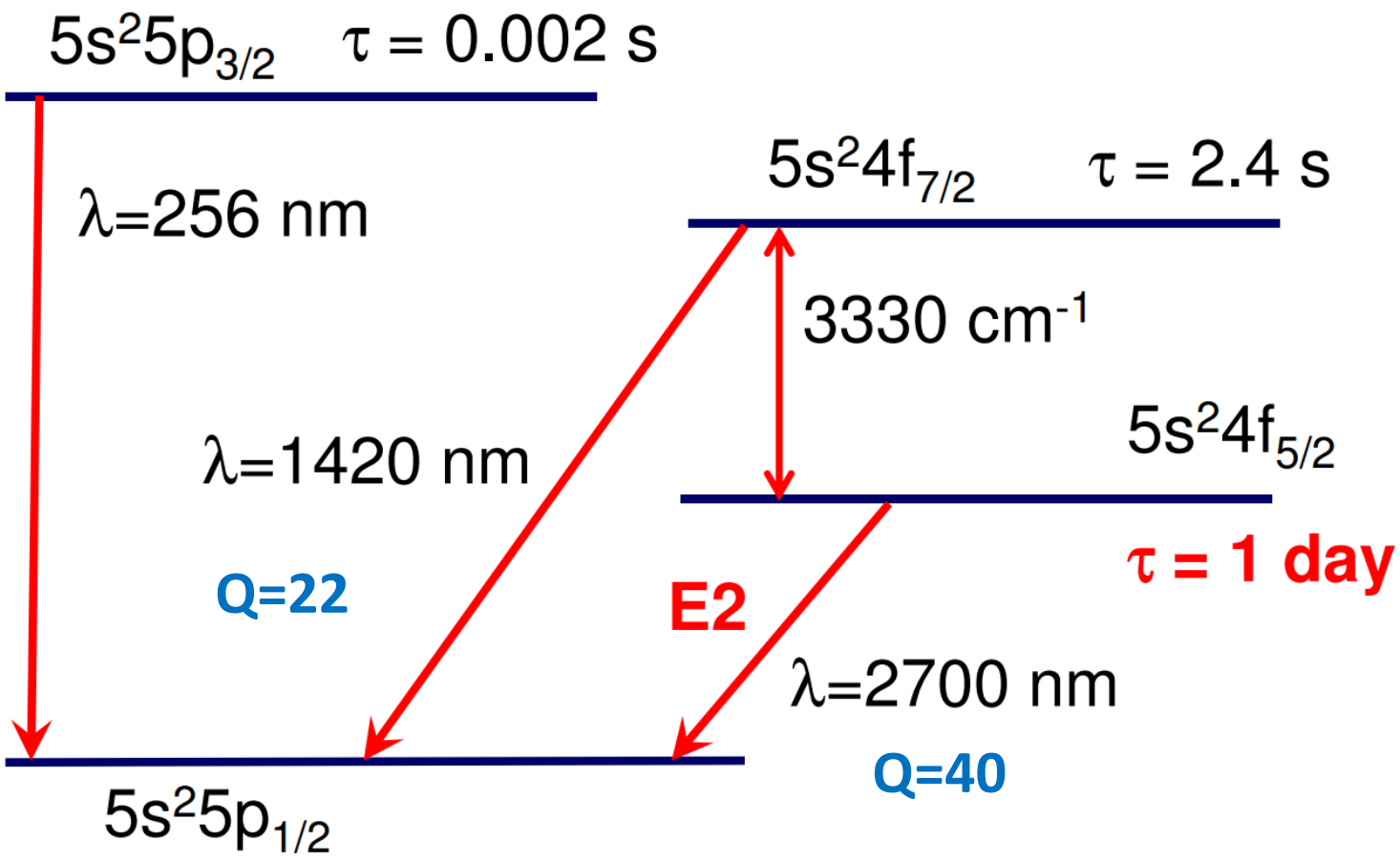
[MK, S G Porsev, & W R Johnson, 2001]

Polarizabilities of $^1S_0$ & $^3P_0$ clock states in B^+, Al^+, & In^+ ions

Ion		CI	CI + MBPT	CI + all
B^+	$\alpha_0(2s^2\,{}^1S_0)$	9.575	9.613	9.624
	$\alpha_0(2s2p\,{}^3P_0^o)$	7.779	7.769	7.772
	$\Delta\alpha_0$	−1.796	−1.844	−1.851
Al^+	$\alpha_0(3s^2\,{}^1S_0)$	24.405	24.030	24.048
	$\alpha_0(3s3p\,{}^3P_0^o)$	24.874	24.523	24.543
	$\Delta\alpha_0$	0.469	0.493	0.495
In^+	$\alpha_0(5s^2\,{}^1S_0)$	26.27	23.83	24.01
	$\alpha_0(5s5p\,{}^3P_0^o)$	28.60	25.87	26.02
	$\Delta\alpha_0$	2.33	2.04	2.01

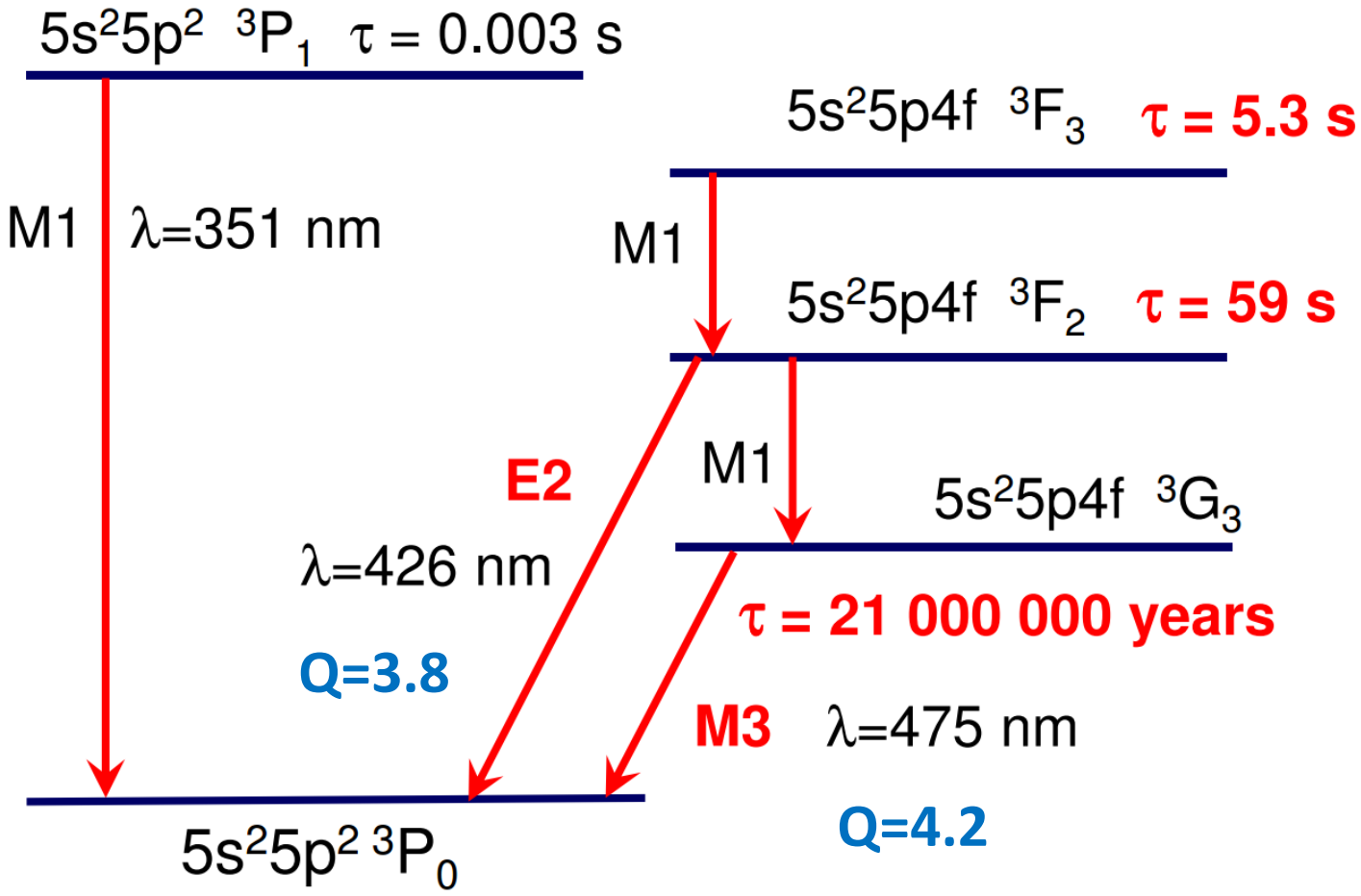
[M Safronova , MK, C Clark, PRL, **107**, 143006 (2011)]

In-like Pr^{10+}



[Safronova et al, PRL, **113**, 030801 (2014)]

Sn-like Pr^{9+}



[Safronova et al, PRL, **113**, 030801 (2014)]

Conclusions

- CI+MBPT is useful tool
- Computer package is available from CPC: http://cpc.cs.qub.ac.uk/summaries/AEWV_v1_0.html
- More details on RG: https://www.researchgate.net/project/Atomic-calculations-using-CI-MBPT-and-CI-AO-all-order-methods

Thanks!