Theory of the hyperfine structure in polyvalent atoms, including symmetry violating nuclear moments

M G Kozlov

PNPI

ECT* Trento 2015

Plan

1. CI+MBPT & CI+AO methods
2. Effective operators
3. Hyperfine structure
4. P-odd and P,T-odd nuclear moments
5. Molecules

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 approximation H_0 the residual interaction

$$V' = H - H_0$$

is not small. Thus, in general $\lambda \approx 1$ and MBPT does not work!

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:

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

Then we can write:

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

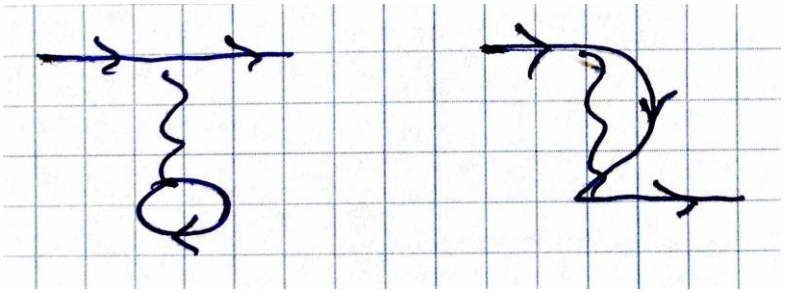
And now λ_{eff} can be small.

Effective Hamiltonian for valence electrons

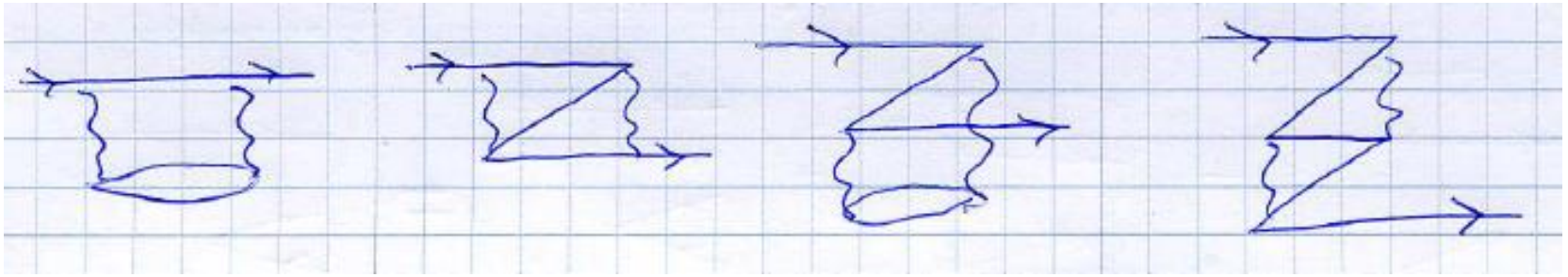
- We define valence space so that all core electrons are frozen.
- We use MBPT to form H_{eff} in the valence space.
- We diagonalize effective Hamiltonian using configuration interaction method.
- Zero order Hamiltonian is the valence Hamiltonian in the frozen core approximation.

Bruckner Goldstone diagrams for One-particle MEs of H_{eff}

Zero order:

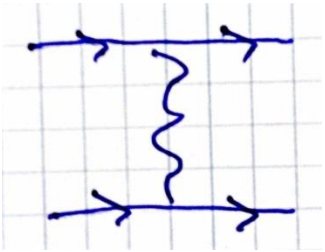


Second order:

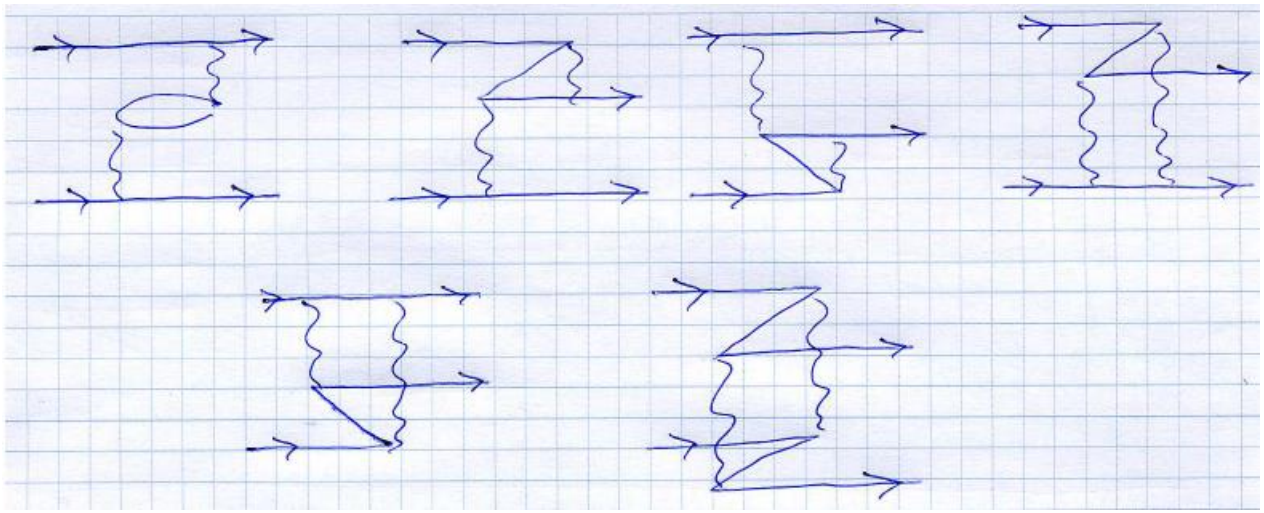


Two-particle ME of H_{eff}

Zero order:



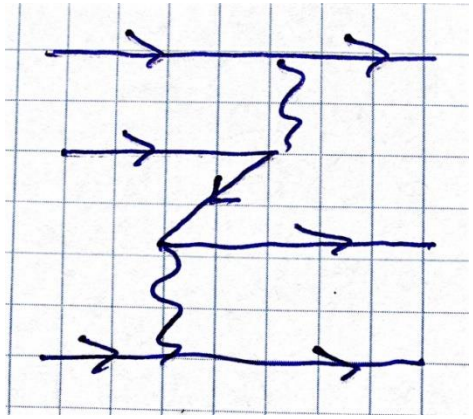
Second order:



Three-particle ME of H_{eff}

Zero order: None!

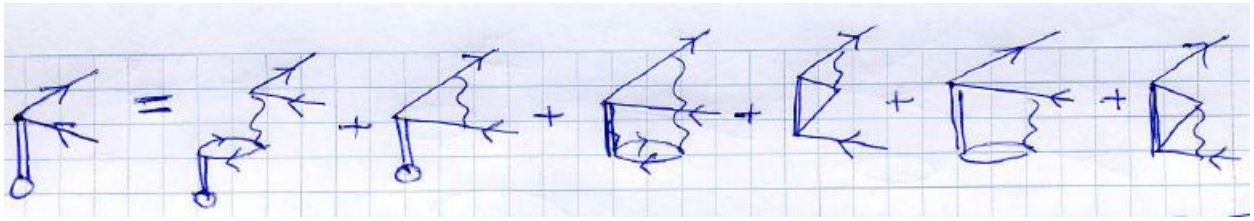
Second order:

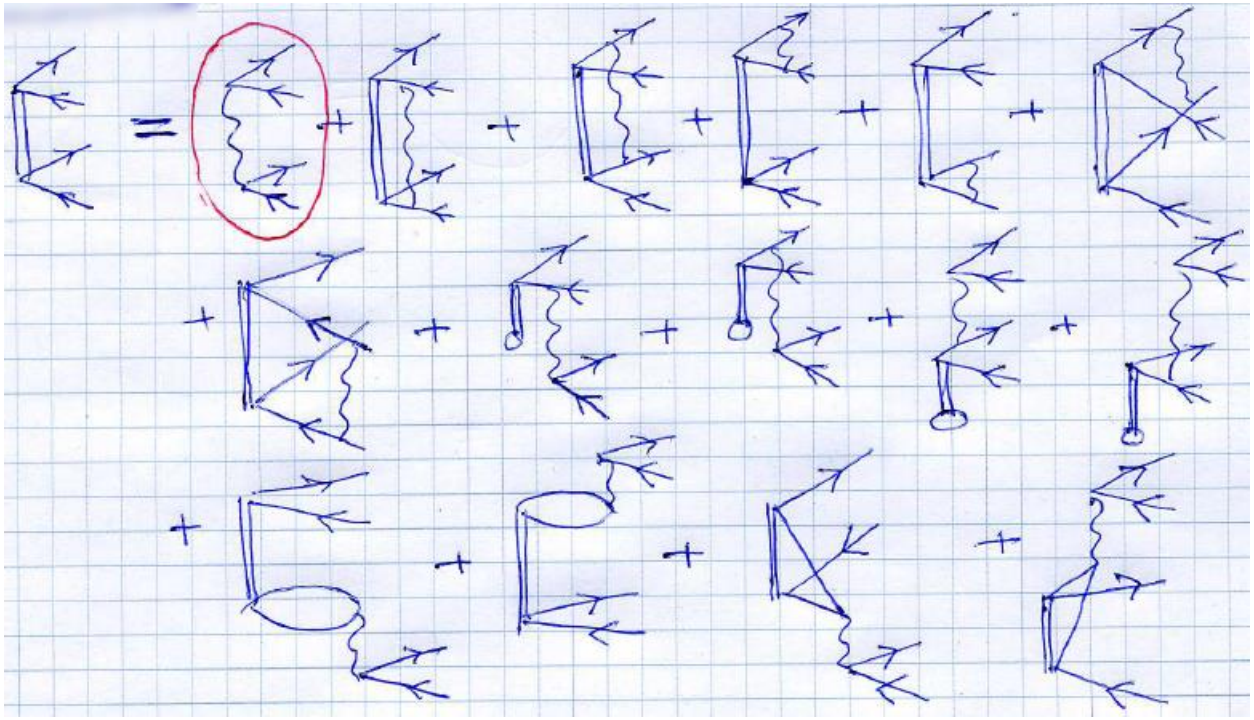


Coupled cluster equations for H_{eff}

1. Core cluster amplitudes:

1-e





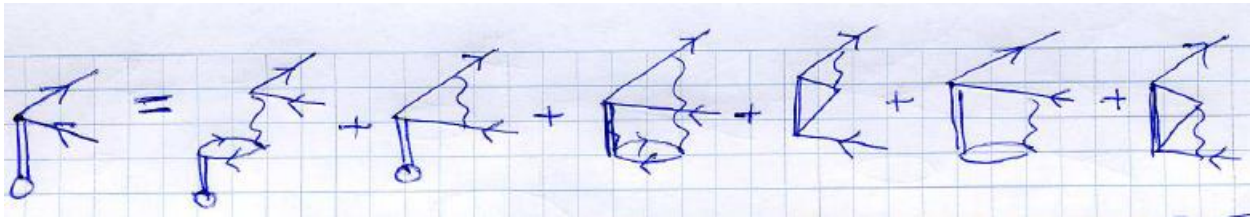
2-e

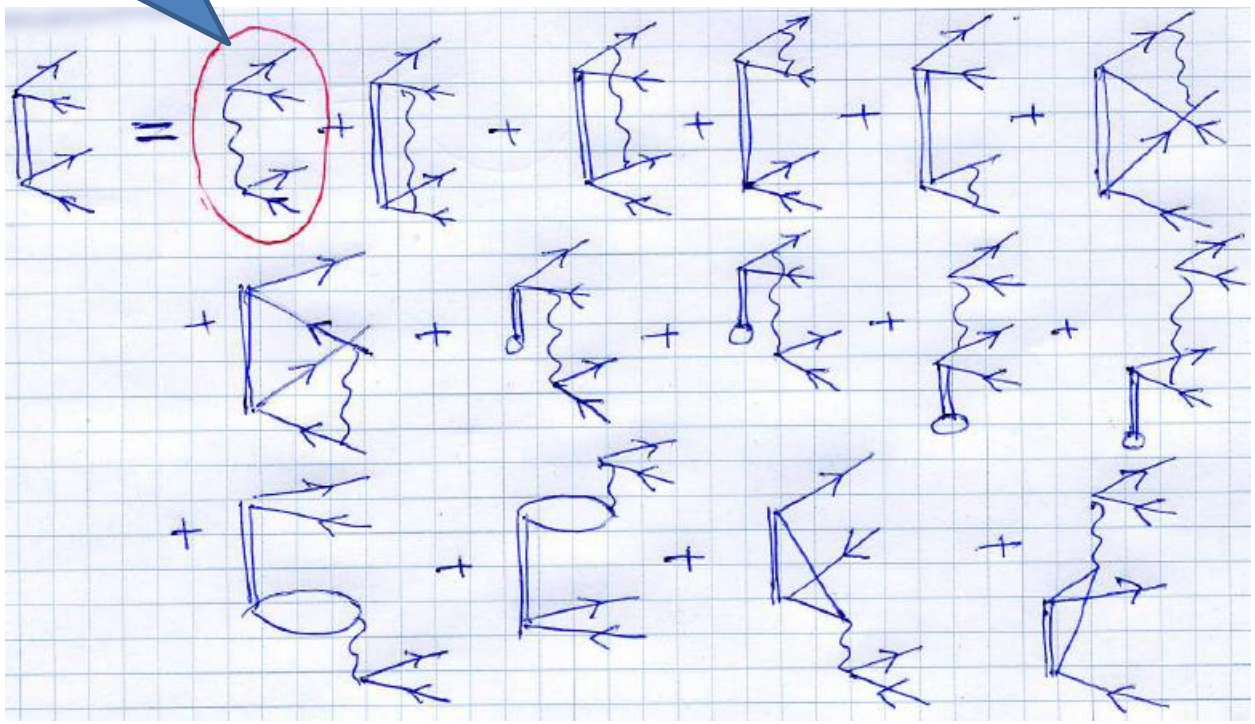
Coupled cluster equations for H_{eff}

1. Core cluster amplitudes:

1-e

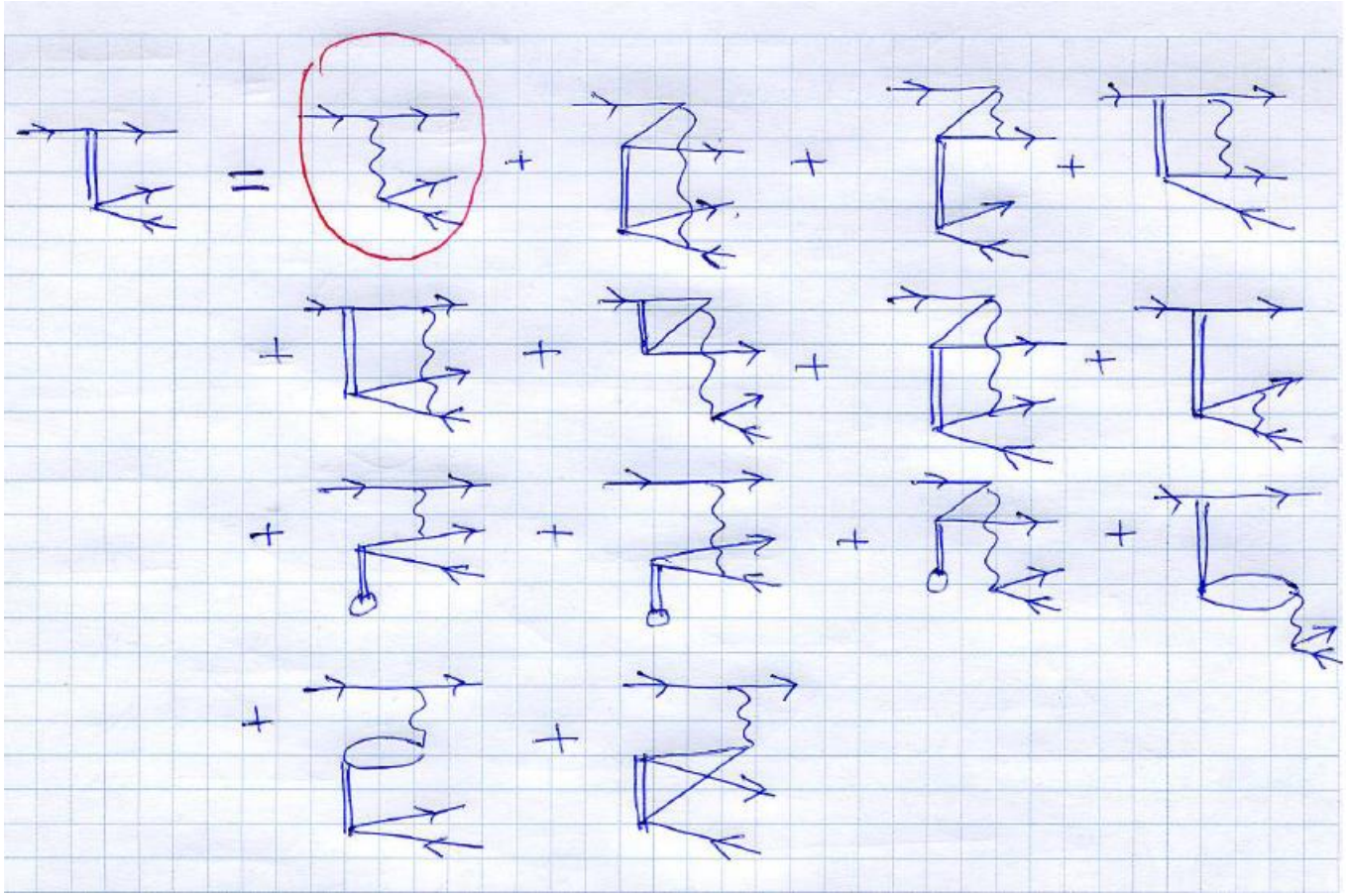
The only zero order term



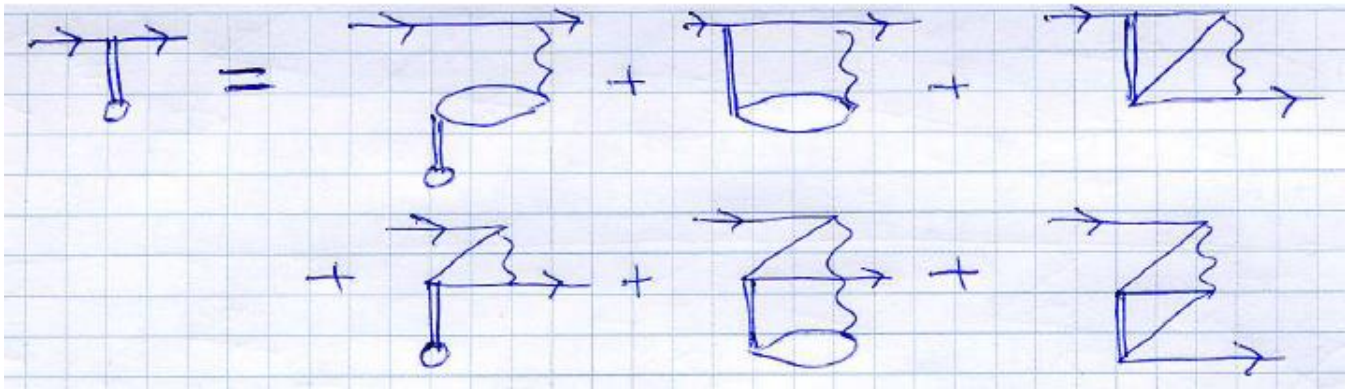


2-e

2. Core-valence cluster amplitudes:

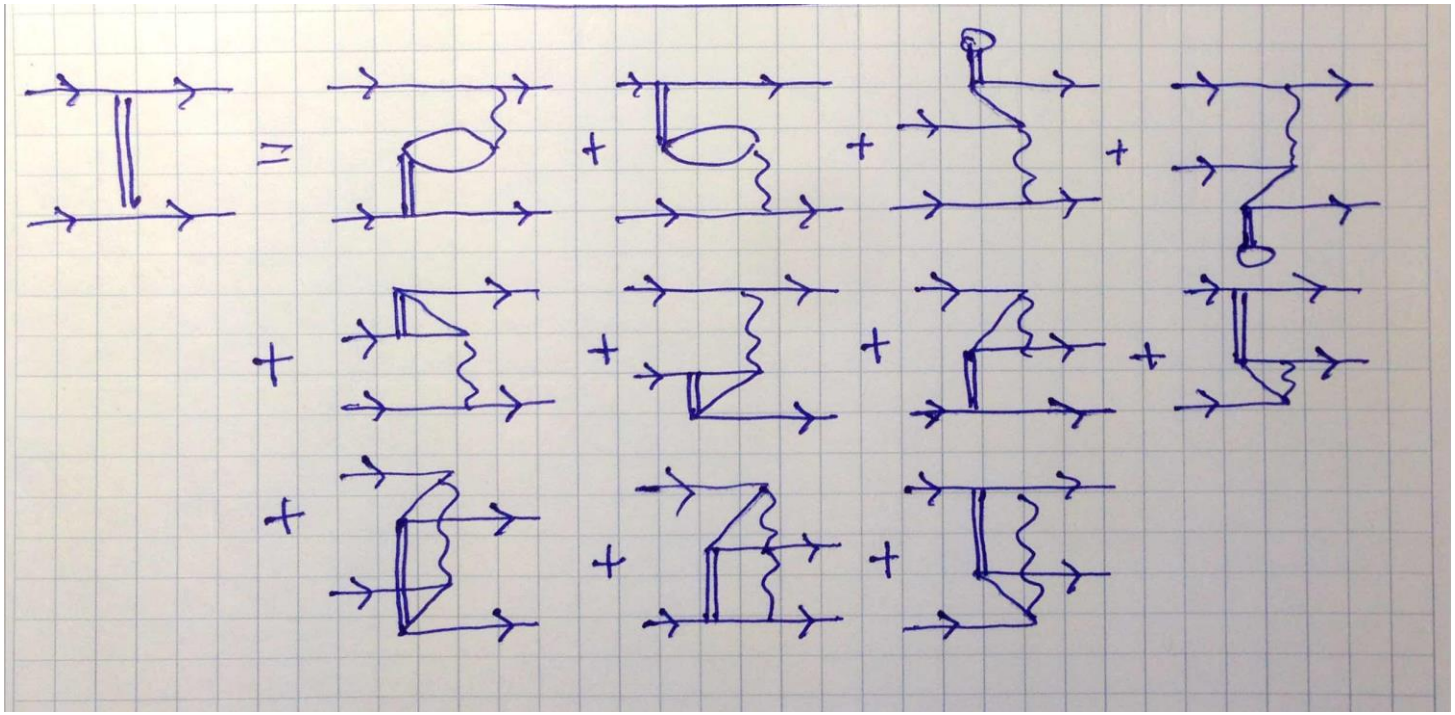


3. Valence cluster amplitudes:



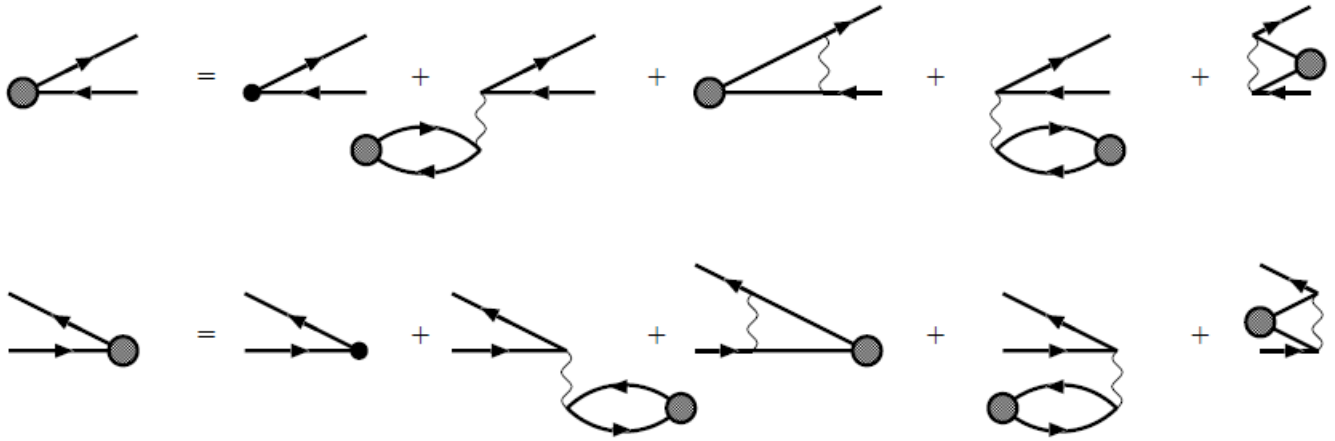
1-e

2-e



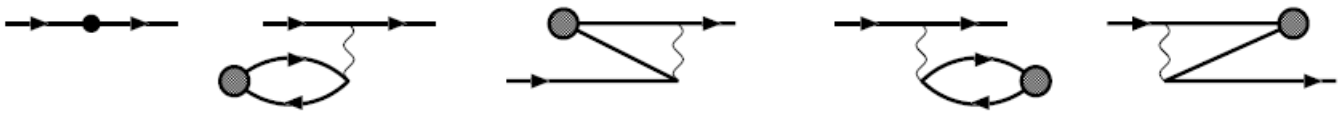
Effective operators for observables

RPA for core

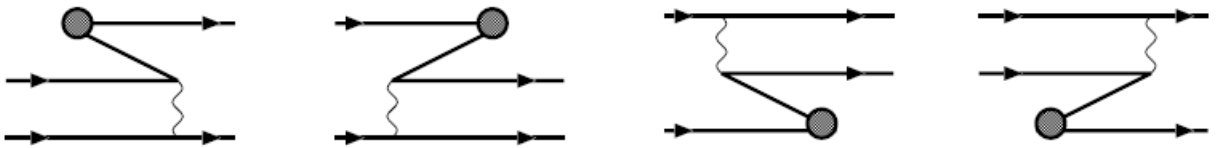


Valence amplitudes

1-e

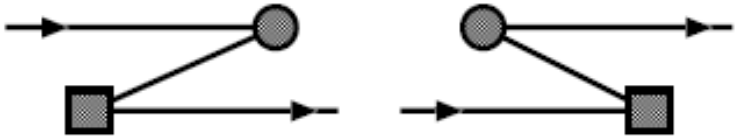


2-e

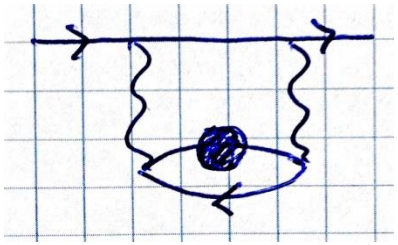


Some high order corrections to effective operators

Self-energy



Structural radiation



Normalization correction $\langle \Phi_i | 1 - \partial_E \Sigma(E) | \Phi_k \rangle_{E=E_{\mathrm{av}}} = \delta_{ik}$

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]

Final field method

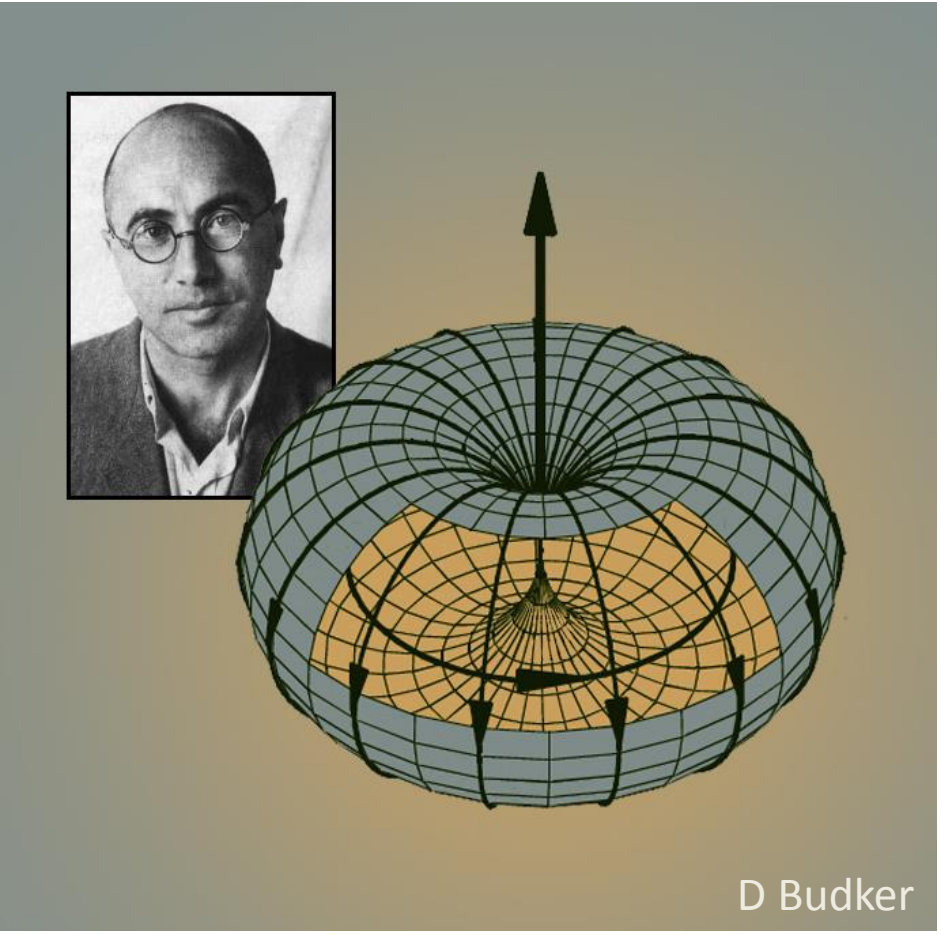
We can add perturbation directly to the effective Hamiltonian:

$$\widetilde{H}_{\text{eff}} = H_{\text{eff}} + \lambda V$$

Then we can find required correction as:

$$\delta E = \left.\frac{\partial \tilde{E}_{\text{eff}}}{\partial \lambda}\right|_{\lambda=1}$$

This is particular convenient for perturbations with the same symmetry as the Hamiltonian, e.g. for the isotope shifts. But we can sacrifice the symmetry to avoid using effective operators.



Nuclear anapole moment

$$\mathbf{a} = -\pi \int \mathbf{j}(r) r^2 d\mathbf{r}$$

Vector potential:

$$\mathbf{A} = \mathbf{a}\,\delta(\mathbf{r})$$

For relativistic case we need regularization:

$$\delta(\mathbf{r}) \to \rho_{\mathrm{nuc}}(\mathbf{r})$$

$$H_{\mathrm{AM}} = e\boldsymbol{\alpha}\mathbf{a}\rho_{\mathrm{nuc}}(\mathbf{r})$$

with $\mathbf{a} = \kappa_a \frac{\mathbf{I}}{I}$

Nuclear magnetic quadrupole moment

$$M_{mn} = \int (r_m \varepsilon_{nkl} + r_n \varepsilon_{mkl}) r_k J_l \, d\mathbf{r}$$

Atomic (P,T-odd) Hamiltonian has the form

$$H_{\mathrm{MQM}} = -\frac{1}{6} e \alpha_m \varepsilon_{mnk} M_{nl} \nabla_l \nabla_k \frac{1}{r}$$

Search for AM

- AM is indistinguishable from the NSD-PNC weak interaction and from the NSD radiative corrections to the PNC interaction with the weak charge of the nucleus.
- We can look for the PNC effects in the RF hyperfine transitions.
- AM is enhanced when we have close levels of opposite parity with $\Delta J = \pm 1$.
- AM is enhanced in diatomic radicals.

Search for MQM

- MQM is suppressed in diamagnetic systems.
- MQM effects are enhanced in paramagnetic radicals used to search for eEDM.
- Nuclear MQMs are enhanced in deformed nuclei.
- Molecular matrix elements for MQM and eEDM are related.
- MQM effects in paramagnetic molecules can dominate effects from the Schiff moment.

P,T-odd effective molecular Hamiltonian

$$H = W_d d_e \boldsymbol{S}\cdot\boldsymbol{n} + W_Q \frac{Q}{I}\boldsymbol{I}\cdot\boldsymbol{n} - \frac{W_M M}{2I(2I-1)}\boldsymbol{S}\hat{\boldsymbol{T}}\boldsymbol{n}.$$

$$M_{i,k} = 3M/[2I(2I-1)]T_{i,k},$$

$$T_{i,k} = I_i I_k + I_k I_i - \tfrac{2}{3}\delta_{i,k} I(I+1).$$

$$W_M = \frac{9R_M(Z)}{20r_0\alpha Z R_d(Z)} W_d$$

MQM in heavy diatomics

[V V Flambaum, D DeMille, and MK, 2014]

Molecule	I_t	State	$\lvert W_M \rvert$ 10^{33} Hz/ $e \cdot \mathrm{cm}^2$	$10^{25} d_p$/ $e \cdot \mathrm{cm}$	$\lvert W_M MS \rvert$ (μHz) $10^{10}\tilde{\theta}$	$10^{27}(\tilde{d}_u - \tilde{d}_d)$/ cm
^{135,137}BaF	$\frac{3}{2}$	$^2\Sigma_{1/2}$	0.83[a]	~0.1	1	0.6
^{173}YbF	$\frac{5}{2}$	$^2\Sigma_{1/2}$	2.1[b]	22	42	25
^{201}HgF	$\frac{3}{2}$	$^2\Sigma_{1/2}$	4.8[a]	~1	10	6
^{177}HfF$^+$	$\frac{7}{2}$	$^3\Delta_1$	0.5	20	33	20
^{179}HfF$^+$	$\frac{9}{2}$	$^3\Delta_1$	0.5	14	26	16
^{181}TaN	$\frac{7}{2}$	$^3\Delta_1$	~1	30	50	30
^{229}ThO	$\frac{5}{2}$	$^3\Delta_1$	1.9	~10	72	44
^{229}ThF$^+$	$\frac{5}{2}$	$^3\Delta_1$	1.7	~10	65	39

Conclusions

- We have effective technique to calculate hyperfine structure in atoms.
- The same method can be used for P-odd and P,T-odd effects in atoms.
- In diatomic molecules P-odd and P,T-odd effects are much stronger than in atoms.
- New generation of eEDM experiments with molecules can give information on P,T-odd nuclear forces.

Package for CI+MBPT calculations

[MK, S G Porsev, M S Safronova, and I I Typitsyn *Computer Physics Communications,* **195**, 197 (2015)]

- Dirac-Coulomb Hamiltonian in no-pair approximation
- $H_{\rm eff}$ is formed within second order MBPT
- 13 effective operators for observables in RPA approximation include:
  (a) hyperfine constants A & B
  (b) P-odd & P,T-odd interactions (PNC, AM, eEDM, MQM)
  (c) transition amplitudes *E1-E3* & *M1-M3*

Collaborators

- Vladimir Dzuba
- Victor Flambaum
- Sergey Porsev
- Marianna Safronova
- Ilya Tupitsyn

Thank you!