Atomic and molecular calculations for studies of fundamental symmetries

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- Weak interactions and standard model

- Violation of inversion symmetry P and time-reversal symmetry T in atomic physics.

- Weak charge, anapole moment, and Schiff moment of the nucleus and electric dipole moment of the electron.

- High accuracy *ab initio* calculations for atoms. Correlations, relativistic and QED effects.

- Semiempirical and *ab initio* calculations of P-odd and P,T-odd effects in diatomic molecules.

  - *Ab initio* calculations of the energy difference between mirror molecules.

References

- J S M Ginges and V V Flambaum,
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  E-print: `physics/0309054` (2003)

- M Quack,
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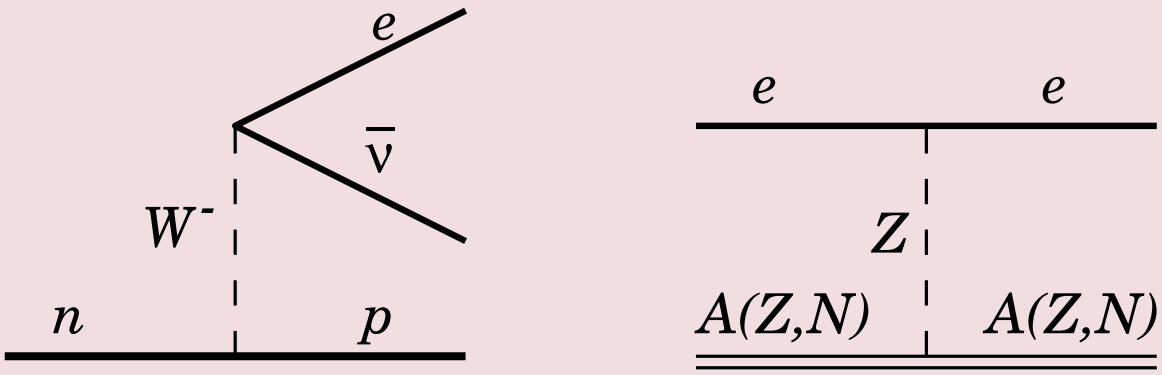
Charged and neutral weak currents



Charged currents can be seen in nuclear decays and other inelastic processes, while neutral currents can be also seen in elastic scattering. In atomic physics they lead to additional non-Coulomb interaction of the electrons with the nucleus and with each other.

Because of the very large mass of Z-boson, the weak interaction is contact on atomic scale. It includes P-even, P-odd (PNC), and P,T-odd parts. P-even part leads to small corrections to isotope shift and to hyperfine structure.

Effective P-odd electron-nucleus interaction

$$\begin{aligned} H_P &= H_P^{\mathrm{nsi}} + H_P^{\mathrm{nsd}} \\ &= \frac{G_{\mathrm{F}}}{\sqrt{2}}\left(-\frac{Q_{\mathrm{W}}}{2}\gamma_5 + \frac{\kappa}{I}\,\gamma_0\vec{\gamma}\vec{I}\right)\rho(\vec{r}), \end{aligned}$$

where $G_F \approx 1.2225 \cdot 10^{-14}$ a.u. is the Fermi constant, $\vec{I}$ is nuclear spin, $\vec{\gamma}_i$ are Dirac matrices, and $\rho(\vec{r})$ is nuclear density.

Dimensionless constants Q_{W} and κ characterize the strength of the NSI and NSD parts respectively. In the lowest order the standard model gives:

$$Q_{\mathrm{W}} = -N + Z(1 - 4\sin^2\theta_{\mathrm{W}}) \approx -N,$$

where N is the number of neutrons and θ_{W} is Weinberg angle. Radiative corrections to this expression change Q_{W} by few percent:

$$Q_{\mathrm{W}} = -0.9857\,N + 0.0675\,Z.$$

The coupling constant κ is given by:

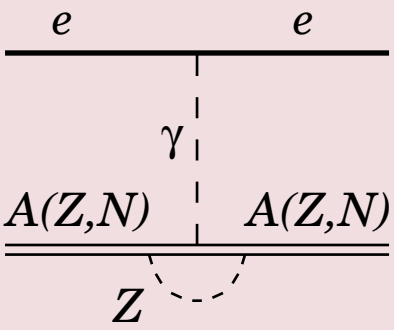
$$\kappa = (-1)^{I+1/2-l}\,\frac{I+1/2}{I+1}\kappa_A + \kappa_2 + \kappa_{Q_w},$$

where κ_A is the anapole moment constant, $\kappa_2 \approx -0.05$ corresponds to the weak neutral currents, and κ_{Q_w} appears as a radiative correction to the NSI part. For the shell model of the nucleus Flambaum and Khriplovich obtained:

$$\kappa_A \approx 1.15 \cdot 10^{-3} A^{2/3} \mu_n\, g_n,$$

where μ_n and g_n are magnetic moment and weak coupling constant of the unpaired nucleon ($g_p \approx 4.5$; $g_n \lesssim 1$).

For heavy nuclei with unpaired proton $\kappa_A \gg \kappa_2, \kappa_{Q_w}$. Nuclear anapole moment is given by the diagram:



Effective P,T-odd electron-nucleus interaction

$$H_{P,T} = \mathrm{i}\frac{G_\mathrm{F}}{\sqrt{2}}\left(Zk_1\gamma_0\gamma_5 + \frac{k_2}{I}\vec{\gamma}\vec{I}\right)\rho(\vec{r}),$$

where k_1 and k_2 are dimensionless constants.

P,T-odd interactions also induce P,T-odd electromagnetic moments of the particles: the so called Schiff moment S and magnetic quadrupole moment M of the nucleus and the electric dipole moment (EDM) of the electron d_e. The latter leads to the following P,T-odd effective electron Hamiltonian:

$$H_\mathrm{EDM} = -2d_e\begin{pmatrix} 0 & 0 \\ 0 & \vec{\sigma} \end{pmatrix}\vec{\nabla}\phi,$$

where ϕ is the electrostatic potential on the electron.

All P- and P,T-odd interactions in atom are described by rather singular effective operators and their matrix elements rapidly grow with Z.

Z-scaling of the PNC interaction

The estimate for the valence matrix element of the operator H_P is (in a.u.)

$$\begin{aligned} H_P^{\rm nsi} &\sim 10^{-16} Z\,|\psi_{\rm val}(0)|^2\,Q_w, \\ H_P^{\rm nsd} &\sim 10^{-16} Z\,|\psi_{\rm val}(0)|^2\,\kappa. \end{aligned}$$

For heavy atoms the wave function at the origin is large:

$$\psi_{\rm val}(0) \sim \sqrt{ZR(Z)},$$

where $R(Z)$ is relativistic enhancement factor

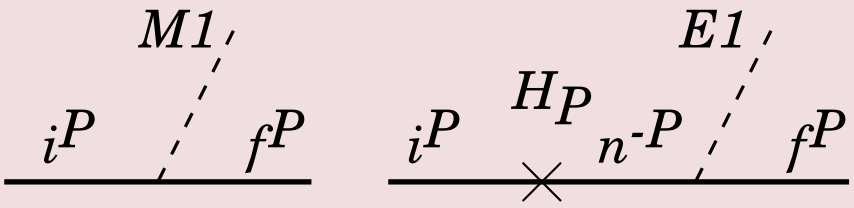
$$R(1) = 1; \qquad R(80) \approx 10.$$

As a result, valence amplitudes for the operator H_P are of the order of (Bouchiat and Bouchiat, 1974):

$$\begin{aligned} \langle p_{1/2}|H_P^{\rm nsi}|s_{1/2}\rangle &\sim 10^{-16} Z^3 R(Z), \\ \langle p_{1/2}|H_P^{\rm nsd}|s_{1/2}\rangle &\sim 10^{-16} Z^2 R(Z)\,\kappa \frac{\langle \vec{I}\cdot\vec{j}\rangle}{I}. \end{aligned}$$

Typical PNC effects in atomic spectra

Parity selection rules forbid $E1$ and $M1$ transitions to take place simultaneously. P-odd interaction leads to the interference of these amplitudes. This interference manifests itself in a form of pseudo-scalar correlations, such as optical activity of the atomic vapor.



Calculation of the PNC effects requires knowledge of atomic valence states and Green's function for both short and long distances.

What limits the accuracy of atomic theory?

- Relativistic effects and finite nuclear size effects are extremely important for all P- and P,T-odd interactions.

- Correlation corrections to the transition frequencies and allowed $E1$-transition amplitudes are typically $\sim$10%; for the PNC interactions they can reach $\sim$30%.

- QED corrections to the frequencies in heavy atoms are typically $\sim$0.1%. For the PNC amplitudes they can reach $\sim$1%.

$\Rightarrow$ We need to account for all these effects if we want to test standard model on the level of radiative corrections (1%).

What do we know about weak charges and anapole moments of the nuclei?

The most accurate experiments were made for Cs, Tl, and Bi. The theory for Cs is much simpler than for Tl, and Bi appears to be too complicated to make accurate calculations.

Combining experimental results for PNC amplitudes with atomic calculations one can get "experimental" values for the weak charges of the nuclei:

$$\begin{aligned} Q_w(^{133}\mathrm{Cs}) &= -72.5(3)_{\mathrm{expt}}(5)_{\mathrm{theor}}\,, \\ Q_w(^{205}\mathrm{Tl}) &= -114\,(1)_{\mathrm{expt}}(3)_{\mathrm{theor}}\,, \end{aligned}$$

and standard model predictions are:

$$\begin{aligned} Q_w^{\mathrm{SM}}(^{133}\mathrm{Cs}) &= -73.09(3)\,, \\ Q_w^{\mathrm{SM}}(^{205}\mathrm{Tl}) &= -116.7(1)\,. \end{aligned}$$

Experimental values for anapole moments are:

$$\begin{aligned} \kappa_A(^{133}\mathrm{Cs}) &= 0.36(6), \\ \kappa_A(^{205}\mathrm{Tl}) &= -0.26(27). \end{aligned}$$

$E1_{\rm PNC}$ amplitude for $6p_{1/2} \to 6p_{3/2}$ transition in ^{205}Tl ($i \cdot 10^{-10}(-Q_w/N)$ a.u.).

CI	-6.408
$H_{\rm eff}$ & RPA	-0.725
A_σ	$+0.241$
$A_{\rm sbt}$	$+0.180$
$A_{\rm tp}$	-0.082
SR	-0.006
Subtotal	-6.81
Normalization	$+0.14$
Rad. Corr.	$+0.05$
Total	-6.61

$M1$ amplitude (10^{-3} a.u.)	
CI+MBPT-II	4.145
MBPT-III(1e)	4.149

$$\mathcal{R} = 10^8 \times {\rm Im}\frac{E1_{\rm PNC}{}^1}{M1_1}$$

$$\left(Q_w = Q_w^{\rm SM} = -116.7\right)$$

$$-15.0(4)$$

Experimental and theoretical values of $\mathcal{R} = 10^8 \times \frac{\mathrm{Im}E1_{\mathrm{PNC}}}{M1}$ for $6p_{1/2} \rightarrow 6p_{3/2}$ transition in ^{205}Tl

Experiment

Oxford	Edwards *et al* (1995)	−15.68 (45)
	Majumder & Tsai (1999)[1]	−15.36 (45)
Seattle	Vetter *et al* (1995)	−14.68 (17)

Theory[2]

(Standard model value $Q_W = -116.8$ assumed)

Novosibirsk	Dzuba *et al.* (1987)	−15.0 (5)
Notre Dame	Liu *et al.* (1996)	−16.0 (10)
Gatchina-ND	Kozlov *et al.* (2001)	−15.0 (4)

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[1] reanalysis of the Oxford experiment

[2] includes QED radiative correction (-0.7)% (Kuchiev & Flambaum (02); Milstein, Sushkov, & Terekhov (02))

Molecular enhancement of the nuclear anapole moment

In atoms $H_P^{\rm nsd}$ mixes levels of opposite parity, which are typically separated by $\Delta E_{\rm at} \sim 0.1\,$a.u. Therefore, the mixing is of the order of

$$\delta\psi_{\rm pnc} \sim \frac{\langle H_P^{\rm nsd}\rangle_{\rm at}}{\Delta E_{\rm at}} \sim 10^{-15} Z^2 R(Z)\,\kappa.$$

In molecules the levels of the opposite parity are separated by the rotational interval, which is typically $\Delta E_{\rm rot} \sim 10^{-5}$ a.u. Thus, the mixing is now

$$\delta\psi_{\rm pnc} \sim \frac{\langle H_P^{\rm nsd}\rangle_{\rm mol}}{\Delta E_{\rm rot}} \sim 10^{-12} Z^2 R(Z)\,\kappa,$$

where we assumed that molecular matrix element is 10 times smaller, than atomic one.

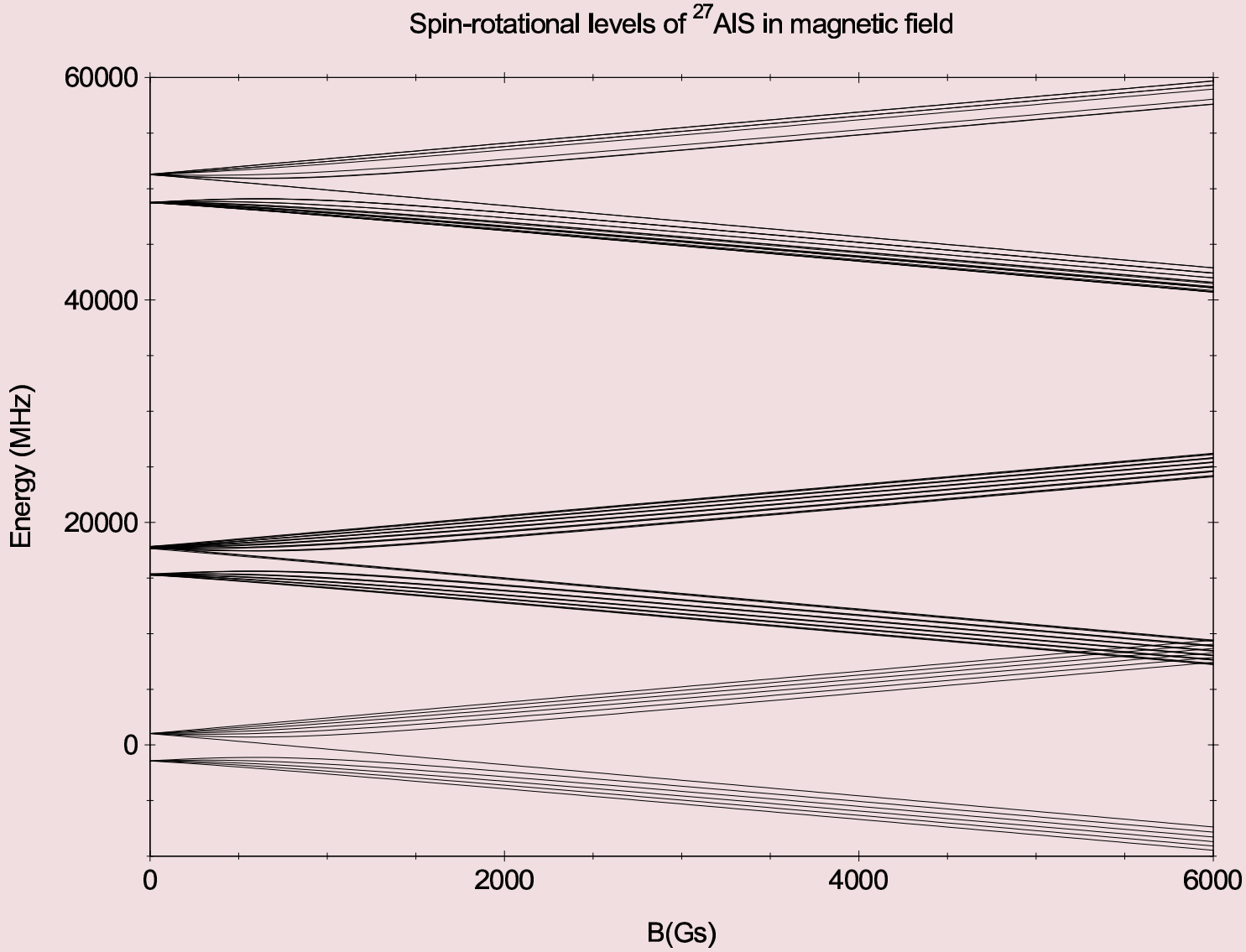
In molecules we can further enhance PNC mixing by crossing the levels of opposite parity in the magnetic field.

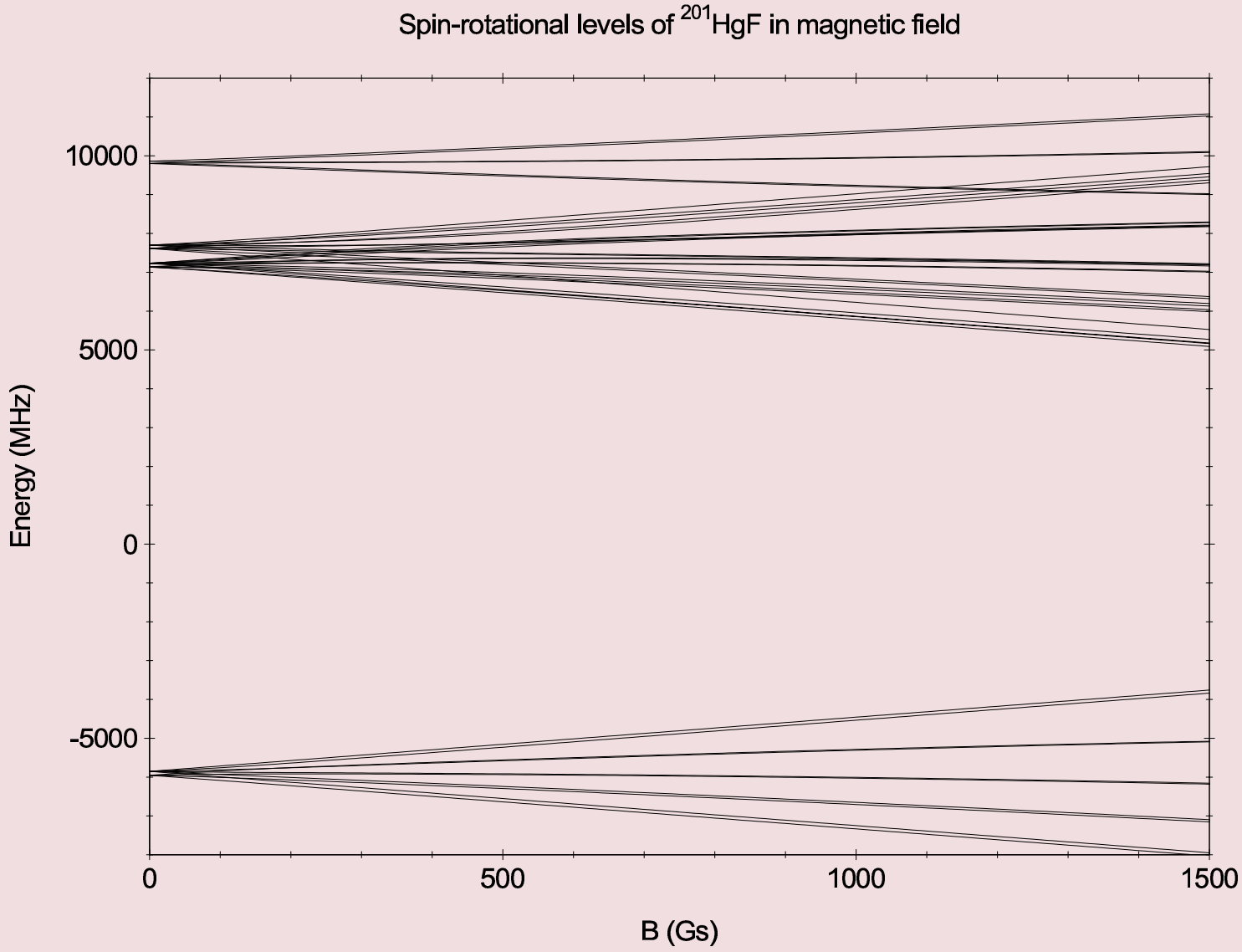
Spin-rotational degrees of freadom

of the diatomic molecule with unpaired electron (diatomic radical) can be described by the spin-rotational Hamiltonian:

$$\begin{aligned} H_{\rm sr} &= B\vec{N}^2 + \gamma\,\vec{s}\cdot\vec{N} + \vec{s}\hat{\boldsymbol{A}}\vec{I} \\ &+ \mu_0\;\vec{s}\hat{\boldsymbol{G}}\vec{B} - D\,\vec{n}\cdot\vec{E} \\ &+ W_P\,\kappa\left(\vec{n}\times\vec{s}\cdot\vec{I}\right) + W_d\,d_e\,\vec{s}\cdot\vec{n}\,. \end{aligned}$$

In this expression $\vec{I}$ is the nuclear spin (we assume the second spin to be zero); $\vec{s}$ is the (effective) spin of the unpaired electron;$\vec{N}$ is the rotational angular momentum; B and γ are the rotational and the spin-doubling constants.
Tensors $\hat{\boldsymbol{A}}$ and $\hat{\boldsymbol{G}}$ describe the hyperfine structure on the nucleus and interaction with the magnetic field $\vec{B}$; μ_0 is the Bohr magneton;$\vec{n}$ is the molecular axis unit vector and $\vec{E}$ is external electric fields.
W_P and W_d are the PNC electronic matrix elements.


Spin-rotational levels of ^{27}AlS in magnetic field
60000
40000
20000
0
Energy (MHz)
0
2000
4000
6000
B(Gs)


Spin-rotational levels of 201HgF in magnetic field
10000
5000
0
-5000
Energy (MHz)
0
500
1000
1500
B (Gs)

Is it possible to calculate W_P and W_d?

For many diatomic molecules parameters of the spin-rotational Hamiltonian are known from the experiments with free molecules, or with the molecules frosen in a noble gas matrix. That allows to calculate W_P and W_d semiempirically.

In the molecular frame the hyperfine tensor $\hat{\boldsymbol{A}}$ has the form:

$$\hat{\boldsymbol{A}} = \begin{pmatrix} A_\perp & 0 & 0 \\ 0 & A_\perp & 0 \\ 0 & 0 & A_\parallel \end{pmatrix},$$

where two parameters $A_\perp$ and $A_\parallel$ depend on the wave function of the unpaired electron in the visinity of the nucleus.

Parameters of the tensor $\hat{\boldsymbol{G}}$ give the relativistic corrections: in the nonrelativistic limit for the ${}^2\Sigma_{1/2}$, $\quad G_\perp = G_\parallel = 2$.

Semi-empirical wave function

The main assumption of the method is that the wave function of the molecule can be written as follows

$$|\Lambda,\Omega\rangle = |\lambda=\Lambda,\omega=\Omega\rangle_{\text{unpaired}}|\Lambda_c=0,\Omega_c=0\rangle_{\text{coupled}}.$$

In the vicinity of the heavy nucleus the wave function of the unpaired electron can be expanded in spherical waves

$$\begin{aligned} |\lambda,\omega\rangle &= \sum_k C_k|l,j,\omega\rangle, \\ k &= (l-j)(2j+1). \end{aligned}$$

Here $|l,j,\omega\rangle$ are four-component spherical waves:

$$|l,j,\omega\rangle = \begin{pmatrix} f_{l,j}Y^l_{j,\omega} \\ ig_{l,j}Y^{l'}_{j,\omega} \end{pmatrix},$$

where f and g are radial functions, $Y^l_{j,\omega}$ is the spherical spinor, $l' = 2j - l$.

At the small distances solutions of the Dirac equation are:

$$\begin{pmatrix} f_{l,j} \\ g_{l,j} \end{pmatrix} = \frac{k}{|k| Z^{1/2} r} \begin{pmatrix} (\gamma + k) J_{2\gamma}(x) - \frac{x}{2} J_{2\gamma-1}(x) \\ \alpha Z J_{2\gamma}(x) \end{pmatrix}$$
$$x = \sqrt{8Zr}$$
$$\gamma = \sqrt{(j+1/2)^2 - \alpha^2 Z^2}$$

For each $l \neq 0$ a pair of functions with $j = l - 1/2$ and $j = l + 1/2$ on the large distances have to form nonrelativistic function $|l, m_l = \lambda, \omega\rangle$. It reduces the number of independent parameters by imposing following restrictions (case of $\lambda = 0$):

$$p\text{-wave} \ : \ C_{-2} = -\sqrt{2} C_1,$$
$$d\text{-wave} \ : \ C_{-3} = -\sqrt{3/2} C_2, \ \ldots$$

The hyperfine axial tensor $\hat{\boldsymbol{A}}$:

$$\begin{aligned} A &\equiv \frac{A_{\parallel} + 2A_{\perp}}{3} \\ &= \frac{4}{3}C^2_{-1}h_{-1,-1} + \frac{4}{9}C^2_1 h_{1,1} + \frac{8}{9}C^2_{-2}h_{-2,-2} \\ &+ \; |!\frac{8}{15}C^2_2 h_{2,2} + \ldots \end{aligned}$$

$$\begin{aligned} A_d &\equiv \frac{A_{\parallel} - A_{\perp}}{3} \\ &= -\frac{8}{9}C^2_1 h_{1,1} - \frac{8}{45}C^2_{-2}h_{-2,-2} - \frac{8}{15}C^2_2 h_{2,2} + \ldots \end{aligned}$$

$$h_{k,k'} = -\frac{g_n \alpha}{2m_p}\int_0^{\infty}(f_k g_{k'} + g_k f_{k'})dr,$$

where g_n is the nuclear g-factor and m_p is the proton mass.

There is analytical expression for the integral $h_{k,k'}$ and we can use experimental data on A and A_d and relation $C_{-2} = -\sqrt{2}C_1$ to find first three coefficient C_k.

$^2\Sigma_{1/2}$ molecules with known parameters of the spin-rotational Hamiltonian (MHz)

	I_1	I_2	B	γ	$A_{1\parallel}$	$A_{1\perp}$	$A_{2\parallel}$	$A_{2\perp}$
^{27}AlO	5/2	0	19242	150	871	714	0	0
^{27}AlS	5/2	0	8369	66	933	764	0	0
^{69}GaO	3/2	0	8217	839	1736	1356	0	0
^{71}GaO	3/2	0	8172	839	2207	1722	0	0
^{115}InO	9/2	0	9788	3831	1832	1070	0	0
Mg^{35}Cl	0	3/2	7339	67	0	0	61	24
Mg^{79}Br	0	3/2	4972	178	0	0	310	103
Mg^{81}Br	0	3/2	4944	177	0	0	334	111
^{87}SrF	9/2	1/2	7515	75	−576	−556	127	97
^{137}BaF	3/2	1/2	6480	81	2453	2401	67	59
^{171}YbF	1/2	1/2	7246	13	7822	7513	220	134
^{199}HgF	1/2	1/2			22621	21880		
^{201}HgF	3/2	1/2			−8054	−7760		

Parity non-conserving amplitudes at the crossings of the spin-rotational levels in the magnetic field

	I	κ_a	W_P Hz	B_{cross} Gs	|PNC| Hz	$\lvert D\langle\mathbf{n}\rangle\rvert$ $\frac{\text{kHz}}{\text{V/cm}}$
^{69}GaO	$\frac{3}{2}$	0.21	61	4950	4.4	30
				5290	3.6	7
				5430	2.0	36
^{71}GaO	$\frac{3}{2}$	0.22	61	4690	4.7	28
				5050	3.7	9
				5270	2.2	36
^{115}InO	$\frac{9}{2}$	0.30	180	4430	21	98
				4770	18	110
				4890	11	26
				5130	14	120
				5270	15	33
^{137}BaF	$\frac{3}{2}$	−0.06	160	3250	4.0	2.7
				3550	3.0	1.5
				3930	1.9	3.9
				4330	3.5	1.5
^{171}YbF	$\frac{1}{2}$	−0.07	730	3310	17	1.7
				3370	17	0.4
^{199}HgF	$\frac{1}{2}$	−0.08	2520	2650	79	10
				2690	58	11
				2730	58	11
				2890	37	4
				2930	37	4
^{201}HgF	$\frac{3}{2}$	−0.08	2560	1285	66	18
				1345	66	17

Conclusions

- There is need for high precision *top-of-the-art* calculations of the NSI amplitudes in Cs, Tl, and Bi. These calculations will lead to the more stringent tests of the standard model at low energies.

- Independent calculations of the PNC effects in Yb and Dy are highly desirable. The theory is very complicated here and current theoretical accuracy is not high. Experiments with both atoms are going!

- At present there are only few *ab initio* calculations of the parameters W_P and W_d for diatomic radicals. It is very important to do such calculations for relatively light molecules like GaO, or even AlS to check semiempirical results.