Many-Body Methods Applied to Parity Nonconserving Transitions in Atoms: The Weak Charge and Anapole Moment of ^{133}Cs

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I. Atomic Theory Considerations for PNC Calculations

a) Correlation effects in heavy alkali-metals atoms are large.

b) Relativistic effects in heavy alkali-metal atoms are important.

c) Precise *ab-initio* theory is essential in PNC studies.

Outline

- (Quick) Review of Relativistic MBPT
- 2nd- and 3rd-Order Energies
- 2nd- and 3rd-Order Matrix Elements
- All-order SDCC and SD Equations.
- SD Energies & Fine-Structure Intervals.
- SD Dipole Matrix Elements & Hyperfine Constants.
- Polarizabilities.

Dirac Hamiltonian

One-electron atoms:

$$h_0 = c\,\boldsymbol{\alpha}\cdot\boldsymbol{p} + \beta mc^2 + U(r) + V_{\rm nuc}\,.$$

$$h_0\phi_i = \epsilon_i\phi_i$$

The spectrum of h_0 consists of electron scattering states ($\epsilon_i > mc^2$), electron bound states ($mc^2 > \epsilon_i > 0$) and negative energy (positron) states ($-mc^2 > \epsilon_i$).

Many-electron atoms:

The *no-pair* Hamiltonian

is a many-electron generalization obtained from the field-theoretic Hamiltonian of QED by performing a contact transformation to eliminate the electron - photon interaction to order e^2.

The *no-pair* Hamiltonian[1] can be written

$$H = H_0 + V$$

$$H_0 = \sum_i \epsilon_i \, a_i^\dagger a_i$$

$$V = \frac{1}{2} \sum_{ijkl} v_{ijkl} \, a_i^\dagger a_j^\dagger a_l a_k - \sum_{ij} U_{ij} \, a_i^\dagger a_j \, ,$$

where,

1. sums are restricted to electron states only,
2. v_{ijkl} is a two-particle matrix element of Coulomb + Breit interactions,
3. U_{ij} compensates for including $U(r)$ in h_0.

[1] Brown, G.E. & Ravenhall, D.G. 1951 *Proc. R. Soc. London,* Ser. A **208**, 552-559.

MBPT (One Valence Electron)

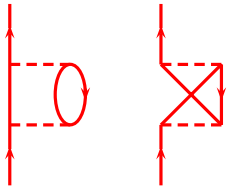
Choose $U = V_{\rm DHF}$, then $\Psi^{(0)} = \Psi_{\rm DHF}$

$$\Psi = \Psi^{(0)} + \Psi^{(1)} + \ldots$$

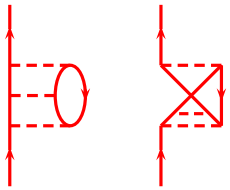
$$E = E^{(0)} + E^{(1)} + \ldots$$

$$E_v^{(0)} = \epsilon_v$$

$$E_v^{(2)} = -\sum_{bmn} \frac{v_{mnvb}\tilde{v}_{vbmn}}{\epsilon_m + \epsilon_n - \epsilon_v - \epsilon_b} + \sum_{abn} \frac{v_{vnab}\tilde{v}_{abvn}}{\epsilon_v + \epsilon_n - \epsilon_a - \epsilon_b}$$



$$E_v^{(3)} = \sum_{bmnrs} \frac{\tilde{v}_{vbmn}v_{mnrs}v_{rsvb}}{(\epsilon_v + \epsilon_b - \epsilon_m - \epsilon_n)(\epsilon_v + \epsilon_b - \epsilon_r - \epsilon_s)}$$



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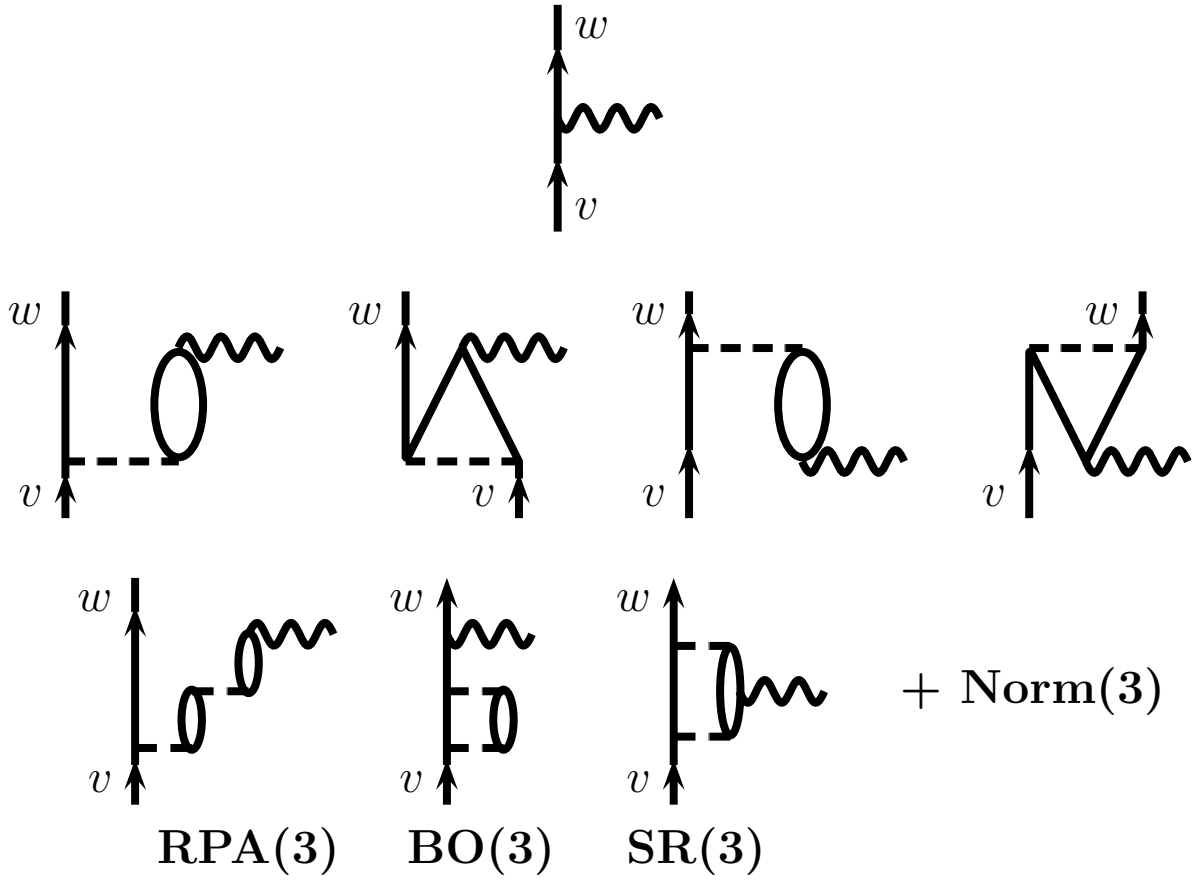
2nd- & 3rd-Order Energies

Valence State Energies for Alkali-Metal Atoms (a.u.).

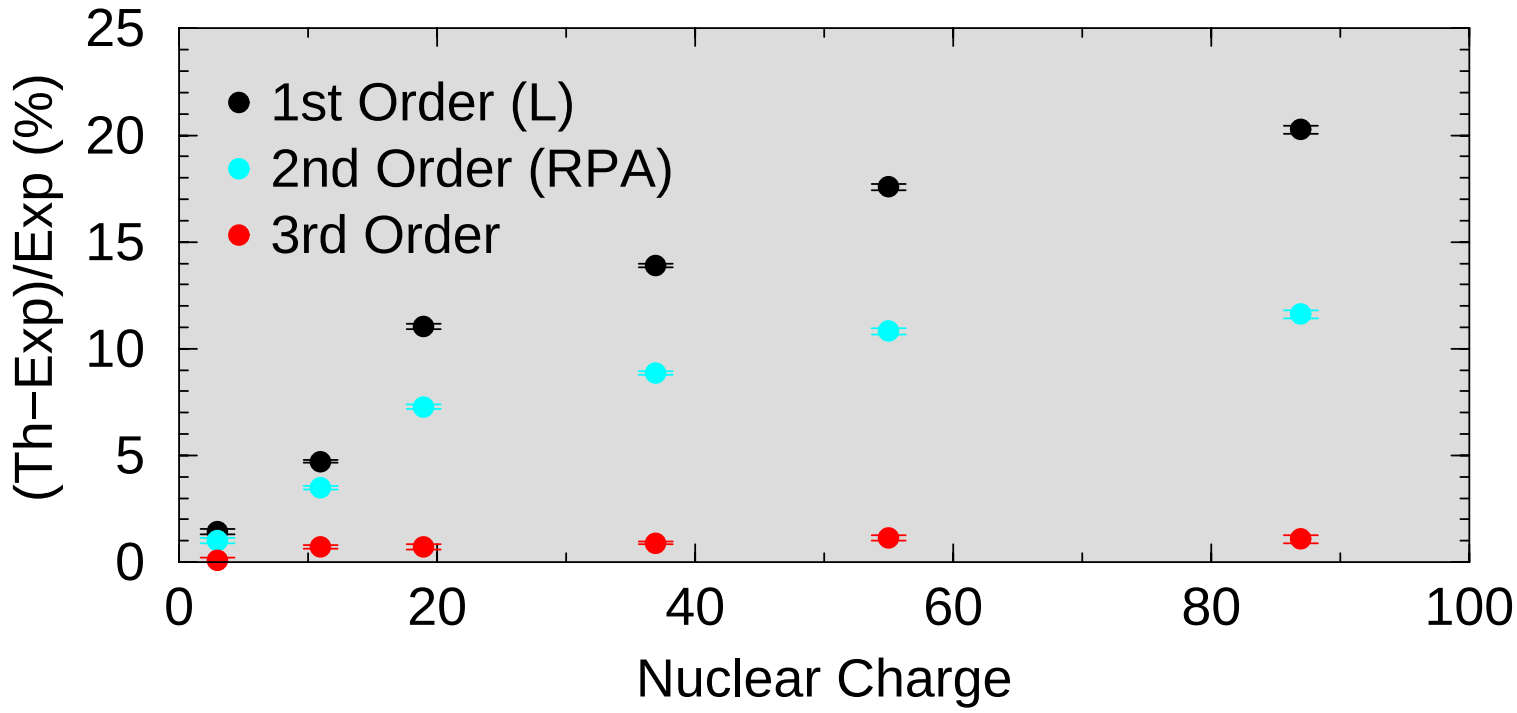
Term	Li $2s$	Na $3s$	K $4s$	Rb $5s$	Cs $6s$	Fr $7s$
DHF	-0.19632	-0.18203	-0.14749	-0.13929	-0.12737	-0.13108
$E^{(2)}$	-0.00165	-0.00593	-0.01246	-0.01507	-0.01782	-0.02174
$E^{(3)}$	-0.00012	-0.00032	0.00205	0.00309	0.00570	0.00770
Sum	-0.19809	-0.18829	-0.15790	-0.15127	-0.13949	-0.14512
NIST	-0.19814	-0.18886	-0.15952	-0.15351	-0.14310	-0.14967
Δ%	0.03	0.3	1.0	1.5	2.8	3.0

Lesson: It is necessary to go beyond 3rd-order MBPT to obtain energies accurate to better than 1% for heavy alkali-metal atoms.

1st-, 2nd-, & 3rd-order Matrix Elements



Dipole Matrix Elements for Alkali-Metal Atoms



Lesson: Third-order transition moments for heavy alkali-metal atoms are accurate to about 1%

Dipole Matrix Elements (Gauge)

Term	L	V	L	V
Cs	$6s_{1/2} - 6p_{1/2}$		$6s_{1/2} - 6p_{3/2}$	
1st	5.2777	5.0371	7.4265	7.0662
2nd	4.9747	4.9747	7.0137	7.0137
3rd	4.5402	4.5400	6.3892	6.3891
Fr	$7s_{1/2} - 7p_{1/2}$		$7s_{1/2} - 7p_{3/2}$	
1st	5.1438	4.8402	7.0903	6.6424
2nd	4.7741	4.7741	6.6268	6.6268
3rd	4.3236	4.3234	5.9450	5.9448

Lesson: "Dressed" third-order dipole matrix element are independent of gauge.

Hyperfine Matrix Elements

Cesium Hyperfine Constants (MHz)

Term	$6s_{1/2}$	$6p_{1/2}$	$6p_{3/2}$
A (1)	1423.77	160.92	23.92
A (2)	292.18	40.67	18.85
BO(3)	718.60	84.73	16.12
SR(3)	-7.97	5.43	-7.49
No(3)	-22.80	-1.20	-0.23
A (3)	687.83	88.96	8.40
Sum	2403.78	290.55	51.17
Expt.	2298.16	291.89	50.28
Δ%	4.6%	0.5%	1.8%

Lesson: (once again) One must go beyond 3rd-order to obtain matrix elements accurate to better than 1% for heavy alkali-metal atoms.

Coupled-Cluster Expansion

$$\Psi_v = \exp\{1 + S_1 + S_2 + \cdots + S_N\}\,\Psi_{\text{DHF}}$$

$$\approx \left\{1 + S_1 + S_2 + \frac{1}{2}S_1^2 + S_1 S_2 + \frac{1}{2}S_2^2 + \frac{1}{6}S_1^3 + + \frac{1}{2}S_1^2 S_2 + \frac{1}{24}S_1^4\right\}\Psi_{\text{DHF}}$$

$$S_1 = S_{1c} + S_{1v} = \sum_{ma} \rho_{ma} a_m^\dagger a_a + \sum_{m \neq v} \rho_{mv} a_m^\dagger a_v$$

$$S_2 = S_{2c} + S_{2v} = \frac{1}{2}\sum_{mnab} \rho_{mnab} a_m^\dagger a_n^\dagger a_b a_a + \sum_{mna} \rho_{mnvb} a_m^\dagger a_n^\dagger a_b a_v$$

Nonlinear terms account for about 10% of correlation energy in Cs and about 4% in Na. These nonlinear corrections are partially canceled by triples!

All-Order SD Approximation

$$\Psi_v = \Psi_{\rm DHF} + \delta\Psi$$

$$\delta\Psi = \left\{ \sum_{am} \rho_{ma}\, a_m^\dagger a_a + \frac{1}{2} \sum_{abmn} \rho_{mnab}\, a_m^\dagger a_n^\dagger a_b a_a \right.$$

$$\left. + \sum_{m\neq v} \rho_{mv}\, a_m^\dagger a_v + \sum_{bmn} \rho_{mnvb}\, a_m^\dagger a_n^\dagger a_b a_v \right\} \Psi_{\rm DHF}$$

$$E_c = E_c^{\rm DHF} + \delta E_c$$

$$E_v = E_v^{\rm DHF} + \delta E_v$$

Later, we will discuss triples!

Core Excitation Equations

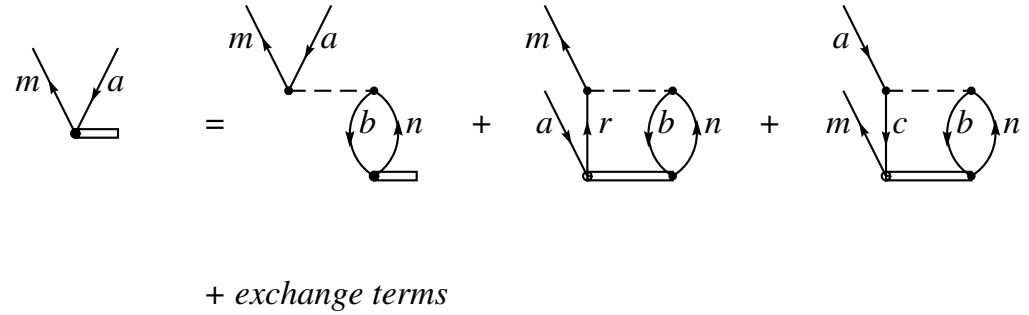
$$(\epsilon_a - \epsilon_m)\rho_{ma} = \sum_{bn} \tilde{v}_{mban}\rho_{nb} + \sum_{bnr} v_{mbnr}\tilde{\rho}_{nrab} - \sum_{bcn} v_{bcan}\tilde{\rho}_{mnbc}$$

$$(\epsilon_a + \epsilon_b - \epsilon_m - \epsilon_n)\rho_{mnab} = v_{mnab} + \sum_{cd} v_{cdab}\rho_{mncd} + \sum_{rs} v_{mnrs}\rho_{rsab}$$

$$+ \left[\sum_{r} v_{mnrb}\rho_{ra} - \sum_{c} v_{cnab}\rho_{mc} + \sum_{rc} \tilde{v}_{cnrb}\tilde{\rho}_{mrac}\right] + \left[\ a \leftrightarrow b \quad m \leftrightarrow n\ \right]$$

$$\delta E_c = \frac{1}{2}\sum_{abmn} v_{abmn}\tilde{\rho}_{mnab}$$

15,000,000 ρ_{mnab} coefficients for Cs ($\ell = 6$).



Brueckner-Goldstone Diagrams for the core SD equations.

Valence Equations

$$(\epsilon_v - \epsilon_m + \delta E_v)\rho_{mv} = \sum_{bn} \tilde{v}_{mbvn}\rho_{nb} + \sum_{bnr} v_{mbnr}\tilde{\rho}_{nrvb} - \sum_{bcn} v_{bcvn}\tilde{\rho}_{mnbc}$$

$$(\epsilon_v + \epsilon_b - \epsilon_m - \epsilon_n + \delta E_v)\rho_{mnvb} = v_{mnvb} + \sum_{cd} v_{cdvb}\rho_{mncd} + \sum_{rs} v_{mnrs}\rho_{rsvb}$$

$$+ \left[\sum_{r} v_{mnrb}\rho_{rv} - \sum_{c} v_{cnvb}\rho_{mc} + \sum_{rc} \tilde{v}_{cnrb}\tilde{\rho}_{mrvc}\right] + \left[\begin{array}{c} v \leftrightarrow b \\ m \leftrightarrow n \end{array}\right]$$

$$\delta E_v = \sum_{ma} \tilde{v}_{vavm}\rho_{ma} + \sum_{mab} v_{abvm}\tilde{\rho}_{mvab} + \sum_{mna} v_{vbmn}\tilde{\rho}_{mnvb}$$

1,000,000 ρ_{mnvb} coefficients for each state (Cs)

Perturbation Expansion of SD Energy

- δE_c agrees with MBPT through third-order.
- $\delta E_v^{(3)}$ disagrees with $E_v^{(3)}$ from MBPT.

Add a limited class of triple excitations to the SD wave function

$$\frac{1}{6}\sum_{abmnr}\rho_{mnrvab}a_m^\dagger a_n^\dagger a_r^\dagger a_v a_b a_a\,\Psi_{\text{DHF}}$$

$$\delta E_{\text{extra}} = \frac{1}{2}\sum_{mnab}\tilde{v}_{abmn}\rho_{mnvvab}$$

- $\delta E_v + \delta E_{\text{extra}}$ includes the entire third-order MBPT valence correlation energy

Lithium Energy Levels

Summary for lithium $2s$ and $2p$ states (a.u.)

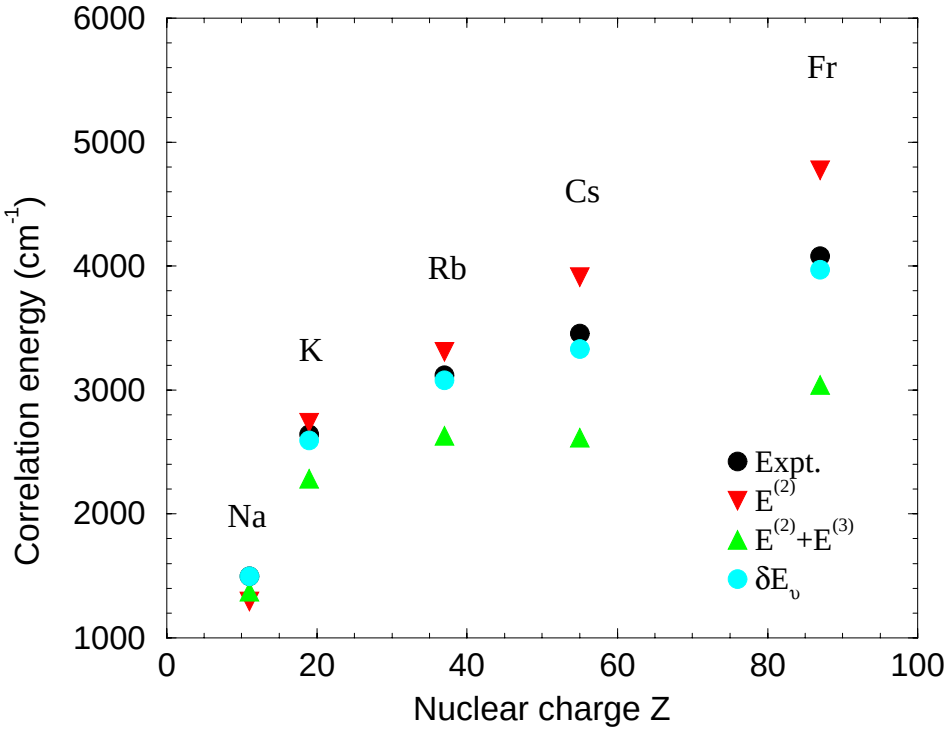
Term	$2s_{1/2}$	$2p_{1/2}$	$2p_{3/2}$
DHF	-0.196320	-0.128638	-0.128636
δE_{SD}	-0.001853	-0.001606	-0.001606
δE_{extra}	0.000011	0.000010	0.000010
Breit + RM + MP	0.000019	0.000009	0.000008
Total	-0.198143	-0.130226	-0.130225
Expt.	-0.198142	-0.130236	-0.130235

Sodium Energy Levels

Summary for sodium $3s$ and $3p$ states (cm^{-1})

Term	$3s$	$3p_{1/2}$	$3p_{3/2}$
DHF	-39951.6	-24030.4	-24014.1
δE_{SD}	-1488.8	-463.9	-461.6
$\delta E_{\mathrm{extra}}$	-9.2	-1.5	-1.6
Breit	1.2	1.4	0.1
RM+MP	1.0	0.5	0.5
Theory	-41447.3	-24493.9	-24476.7
Expt.	-41449.4	-24493.3	-24476.1

Energy Comparisons for Alkali-Metal Atoms



SD Energies for Heavy Atoms

Energies for cesium and francium cm^{-1}

Cs	$6s$	$7s$	$8s$	$9s$
Theory	31262	12801	7060	4479
Expt.	31407	12871	7089	4496
Cs	$6p_{1/2}$	$7p_{1/2}$	$8p_{1/2}$	$9p_{1/2}$
Theory	20204	9621	5687	3760
Expt.	20228	9641	5698	3769
Fr	$7s$	$8s$	$9s$	$10s$
Theory	32735	13051	7148	4522
Expt.	32849	13106	7168	4538
Fr	$7p_{1/2}$	$8p_{1/2}$	$9p_{1/2}$	$10p_{1/2}$
Theory	20583	9712	5724	3782
Expt.	20612	9736	*5738*	*3795*

SD Fine Structure Intervals

		Theory	Expt.
Rb	$5p_{3/2} - 5p_{1/2}$	236.5	237.6
	$6p_{3/2} - 6p_{1/2}$	76.5	77.5
	$7p_{3/2} - 7p_{1/2}$	34.8	35.1
	$8p_{3/2} - 8p_{1/2}$	18.6	18.9
Cs	$6p_{3/2} - 6p_{1/2}$	552.2	554.1
	$7p_{3/2} - 7p_{1/2}$	178.6	181.0
	$8p_{3/2} - 8p_{1/2}$	81.4	82.6
	$9p_{3/2} - 9p_{1/2}$	43.9	44.7
Fr	$7p_{3/2} - 7p_{1/2}$	1676	1687
	$8p_{3/2} - 8p_{1/2}$	536	545
	$9p_{3/2} - 9p_{1/2}$	244	*250*
	$10p_{3/2} - 10p_{1/2}$	132	*136*

SD Matrix Elements

$$\langle w|\left[\sum_{ij} z_{ij}\, a_i^\dagger a_j\right]|v\rangle = \left(z_{wv} + \sum_{i=a}^{t} Z_{wv}^{(i)}\right)/(N_w N_v)$$

$$Z_{wv}^{(a)} = \sum_{am} z_{am}\tilde{\rho}_{wmva} + \text{c.c.} \quad \text{(RPA)}$$

$$Z_{wv}^{(b)} = -\sum_{a} z_{av}\rho_{wa} + \text{c.c.}$$

$$Z_{wv}^{(c)} = \sum_{m} z_{wm}\rho_{mv} + \text{c.c.} \quad \text{(BO)}$$

$$\cdots \quad \text{(16 similar terms)}$$

$$Z_{wv}^{(t)} = -\sum_{abmn} \rho^*_{mnba} z_{mv}\tilde{\rho}_{nwab} + \text{c.c.}$$

Matrix elements are complete through 3rd order!

Dipole Transitions

Matrix Elements for heavy alkali metals (a.u.)

	K	Rb	Cs	Fr
$np_{1/2}$–$ns_{1/2}$	$n=4$	$n=5$	$n=6$	$n=7$
SD	4.098	4.221	4.478	4.256
Expt.	4.102(5)	4.231(3)	4.489(7)	4.277(8)
$np_{3/2}$–$ns_{1/2}$	$n=4$	$n=5$	$n=6$	$n=7$
SD	5.794	5.956	6.298	5.851
Expt.	5.800(8)	5.977(4)	6.324(7)	5.898(15)

SD Hyperfine Matrix Elaments

^{23}Na hyperfine constants A (MHz)

	$3s_{1/2}$	$3p_{1/2}$	$3p_{3/2}$
DHF	623.5	63.39	12.59
MBPT	860.9	91.40	19.80
SD	888.1	94.99	18.84
Expt.	885.81	94.44(13)	18.534(12)

Polarizabilities

For a valence s state:

$$\begin{aligned}
\alpha_v &= \frac{1}{3}\sum_m \left(\frac{|\langle v||z||mp_{1/2}\rangle|^2}{E_{mp_{1/2}} - E_v} + \frac{|\langle v||z||mp_{3/2}\rangle|^2}{E_{mp_{3/2}} - E_v} \right) \\
\alpha_c &= \frac{2}{3}\sum_{ma} \frac{|\langle a||z||m\rangle|^2}{E_m - E_a} \\
\alpha_{vc} &= \frac{1}{3}\sum_a \frac{|\langle a||z||v\rangle|^2}{E_a - E_v}
\end{aligned}$$

SD Results for Polarizabilities

Static polarizabilities (a.u.) of alkali-metal atoms.

	Na	K	Rb	Cs	Fr
$\alpha_v^{\rm main}$	162.06	284.70	308.43	383.8	294.0
$\alpha_v^{\rm tail}$	0.08	0.07	0.14	0.2	1.4
α_c	0.95	5.46	9.08	15.8	20.4
α_{vc}	-0.02	-0.13	-0.26	-0.5	-0.9
α^{SD}	163.07	290.10	317.39	399.3	314.9
Recom.	162.6(0.3)	290.2(0.8)	318.6(0.6)	399.9(1.9)	317.8(2.4)
Expt.	162.7(0.8)	293.6(6.1)	319.9(6.1)	403.6(8.1)	

Summary

The SD theory gives:

- Removal energies: 1–100 cm^{-1}
- Fine-structure intervals: 0.5%
- Transition Amplitudes: 0.3 – 1%
- Hyperfine constants: 0.1 – 1%
- Polarizabilities: 0.1 – 1%
- Applications to PNC in Cs and Fr (Next Lecture)