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Workshop on the original of P, CP and T Violation

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Parity and Time Reversal Violations in Atoms: Present Status and Future Prospects

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Parity and Time-Reversal Violations in Atoms: Present Status and Future Prospects

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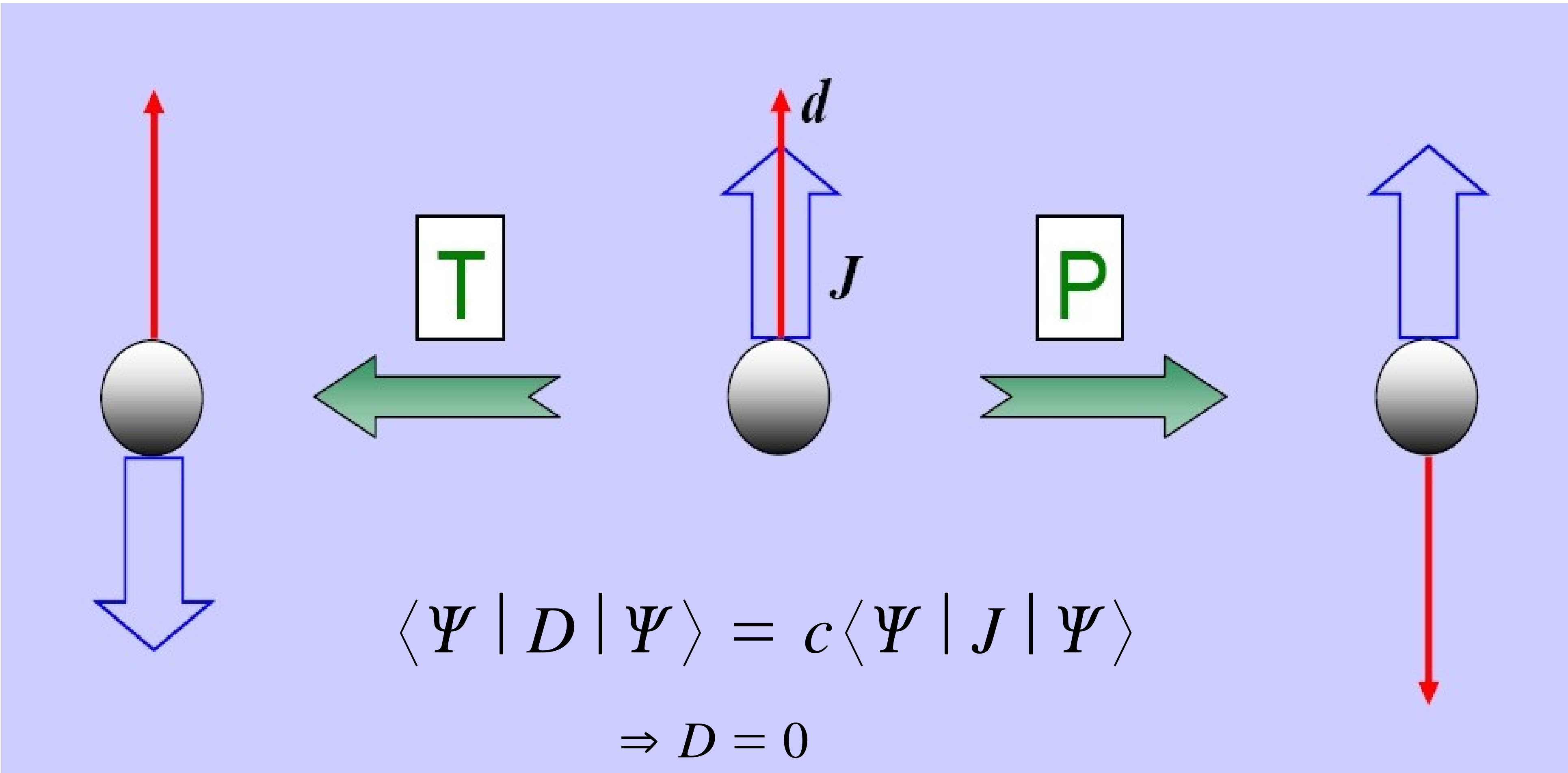
Outline of the talk

- Introduction to Atomic EDMs
- Theory of Atomic EDMs
- Measurement of Atomic EDMs
- Atomic EDM results and future improvements
- Conclusions



$$\langle \Psi \mid D \mid \Psi \rangle = c \langle \Psi \mid J \mid \Psi \rangle$$

$$\Rightarrow D = 0$$

Permanent EDM of a particle VIOLATES both P - & T -invariance.
T-violation implies CP-violation via CPT theorem.

EDM and Degeneracy :

Consider the degeneracy of opposite parity states in a physical system

$$|\Psi\rangle = a\,|\Psi_e\rangle + b\,|\Psi_o\rangle$$

$$D = \langle \Psi | e\, r | \Psi \rangle \neq 0$$

EDM can be nonzero for degenerate states.

Examples : EDMs of Water, Ammonia etc.

P and T violations in non-degenerate systems implies nonzero EDM.

Sources of Atomic EDM

Elementary Particles	Nucleon	Nucleus	Coupling constant	Atomic
d_e			d_e	D_a *(open shell)*
			C_S	D_a *(open shell)*
e-q	e-n	e-N		
			C_T	D_a *(closed shell)*
d_q	d_n	d_N	Q	D_a *(closed shell)*
q-q	d_n, n-n	d_N	Q	D_a *(closed shell)*

P and T Violating Interactions in Atoms

1. Atomic EDM from Electron EDM

$$H_{PTV} = - d_e \sigma \cdot E^I$$ (Non-relativistic)

$$H_{PTV} = - d_e \beta \sigma \cdot E^I$$ (Relativistic) : (Sandars 1968)

$$E^I = -\nabla \{ \sum_i V_N(r_i) + \sum_{i<j} V_C(r_{ij}) \}$$

H_{PTV} can be expressed as an effective one-body Hamiltonian

$$H_{PTV} = \sum_j 2ic\, d_e \beta \gamma_5 p_j^2$$ (Das 1988)

2. Atomic EDM from e – N scalar-pseudoscalar (S-PS) interaction

$$H_{PTV} = \frac{G_F}{\sqrt{2}} J_S \times J_{PS}$$

$$H_{PTV} = \frac{i G_F C_S A}{\sqrt{2}} \sum_i \beta \gamma_5 \rho_N(r_i)$$ C_s is the e – N S-PS coupling constant

3. Atomic EDM from e – N Tensor-Pseduotensor (T-PT) interaction

$$H_{PTV} = i\sqrt{2}\, G_F\, C_T \sum_i \beta \alpha \cdot I \rho_N(r_i)$$

C_T is the e – N T-PT coupling constant

4. Atomic EDM from P and T violating interaction from the nucleus

Total charge density of the nucleus $\rho(\vec{r}) = \rho_0(\vec{r}) + \delta\rho(\vec{r})$

$\rho_0(\vec{r})$ Normal nuclear charge density;

$\delta\rho(\vec{r})$ Correction due to P- and T-violating interactions

EDM of the Nucleus $\vec{D}_N = e\int \vec{r}\,\delta\rho_N(\vec{r})\,d^3r$

P- and T-violating Nuclear electrostatic potential $\delta\phi(\vec{R}) = 4\pi\,\vec{Q}\cdot\vec{\nabla}\,\delta(\vec{R})$

Interaction of an electron with the above potential $H_{PTV} = -4\pi e\,\vec{Q}\cdot\vec{\nabla}\,\delta(\vec{R})$

Q : Schiff Moment ; depends on ρ_0 , $\delta\rho$ and related quantities

P and T Violating Coupling Constants

All the P- and T-violating interactions scale as Z^3 or Z^2.

The atomic EDM (D_a) experiments are therefore done on heavy atoms (Cs, Tl, Hg, etc).

The measured value of D_a in combination with the calculated value of D_a/C_{PTV} will give the C_{PTV}.

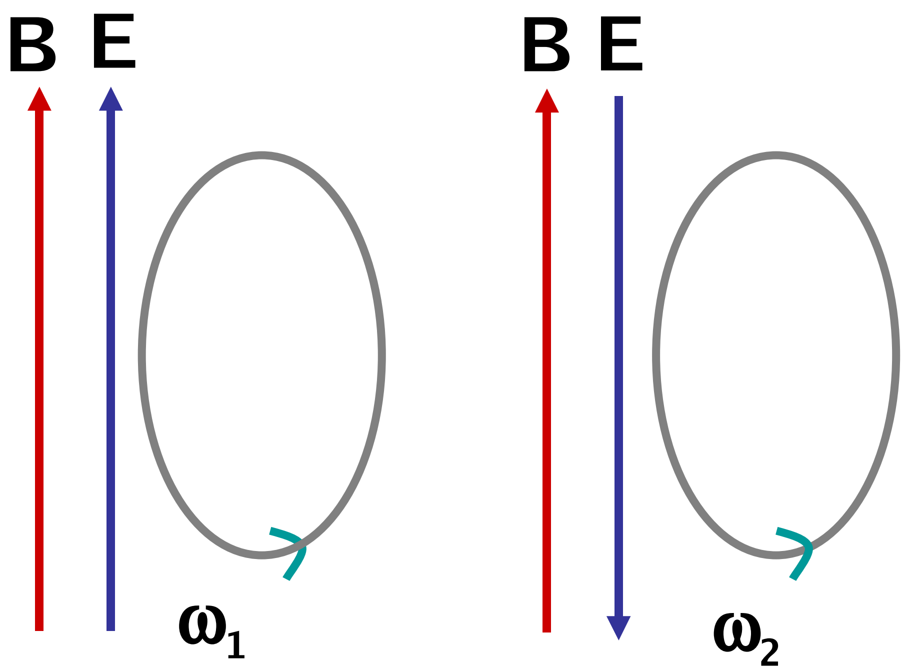
C_{PTV} is the P- and T-violating coupling constant : d_e, C_S, C_T and Q

Atomic experiment and theory are **BOTH** needed to extract the above coupling constants

EXPERIMENTS ON ATOMIC EDM

. . . Principle of Measurement

$$H_I = -\vec{D}_a \cdot \vec{E} - \vec{\mu} \cdot \vec{B}$$



$$\omega_1 = \frac{2\mu \cdot B + 2D_a \cdot E}{\hbar}$$

$$\omega_2 = \frac{2\mu \cdot B - 2D_a \cdot E}{\hbar}$$

$$\Delta\omega = \omega_1 - \omega_2 = \frac{4D_a \cdot E}{\hbar}$$

If the atomic EDM $D_a \sim 10^{-26}$ *e-cm* and E = 10^5 V/cm; $\Delta\omega \sim 10^{-5}$ Hz

Major source of error: $B_m = \dfrac{v \times E}{c^2}$

Theory of Atomic EDMs

The relativistic atomic Hamiltonian is,

$$H_a = \sum_i \{c\,\alpha_i \cdot p_i + \beta_i m c^2 + V_N(r_i)\} + \sum_{i<j} \frac{e^2}{r_{ij}}$$

Treating H_{EDM} as a first-order perturbation, the atomic wave function is given by

$$|\Psi\rangle = |\Psi^{(0)}\rangle + C_{PTV}\,|\Psi^{(1)}\rangle$$

The atomic EDM is given by $D_a = \langle \Psi | \, D \, | \Psi \rangle$

$$\frac{D_a}{C_{PTV}} = \langle \Psi^{(0)} | \, D \, | \Psi^{(1)} \rangle + \langle \Psi^{(1)} | \, D \, | \Psi^{(0)} \rangle$$

This ratio is calculated by relativistic atomic many-body theory

Unique many-body problem involving the interplay of the long range Coulomb interaction and short range P- and T-violating interactions.

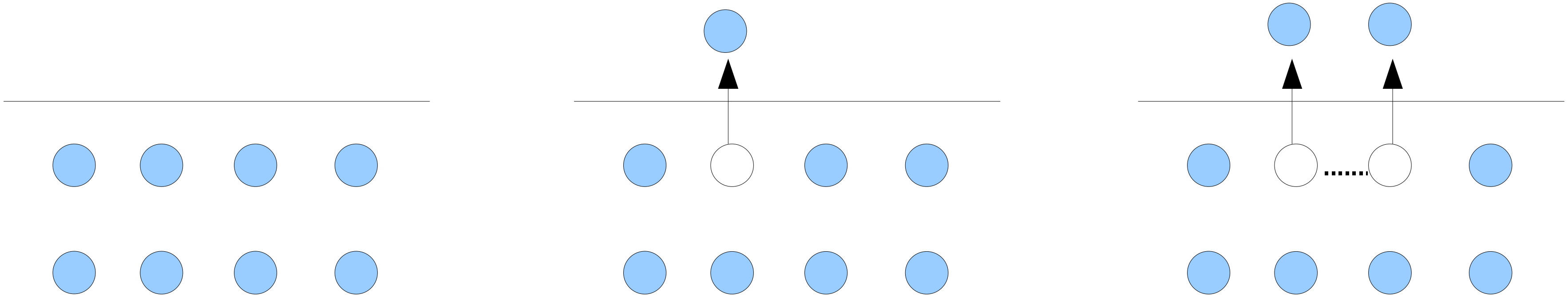
The accuracy depends on the precision to which $|\Psi^{(0)}\rangle$ and $|\Psi^{(1)}\rangle$ are calculated.

Relativistic Wavefunctions of Atoms

Atoms of interest for EDM studies are relativistic many-body systems;

Wavefunctions of these atoms can be written in the mean field approximation as

$$|\Phi_0\rangle = Det\ \{\phi_1 \phi_2 \cdots \phi_N\}$$ (Relativistic Dirac-Fock wavefunction)



$|\Phi_0\rangle$ $T_1|\Phi_0\rangle$ $T_2|\Phi_0\rangle$

$$T_1 = \sum_{a,p} t_{ap} a^\dagger_p a_a \qquad T_2 = \sum_{a,b,p,q} t_{abpq} a^\dagger_p a^\dagger_q a_b a_a \qquad T = T_1 + T_2 + \cdots$$

Relativistic Coupled-cluster (CC) wavefunction; $|\Psi^{(0)}\rangle = \exp(T)\,|\Phi_0\rangle$

CC wfn. has electron correlation to all-orders of perturbation theory for any level of excitation.

In presence of EDM, $|\Psi\rangle = |\Psi^{(0)}\rangle + C_{PTV}|\Psi^{(1)}\rangle = \exp\{T + C_{PTV}T^1\}\,|\Phi_0\rangle$

First-order EDM Perturbed RCC wfn. satisfies : $(H_0 - E_0)|\Psi^{(1)}\rangle = -H_{PTV}|\Psi^{(0)}\rangle$

ATOMIC EDM RESULTS

D_a / C_{PTV} Has been calculated by semi-empirical and ab initio methods.

The calculation of this quantity by RCC theory.

D_a/d_e : Liu & Kelly Phys. Rev. A Rap. Comm. 1992

D_a/d_e, D_a/C_s : Nataraj et al. Phys. Rev. Lett. 2008

D_a/C_s : Sahoo et al. Phys. Rev. A Rap. Comm. 2008

D_a/C_T , D_a/Q : Latha et al. (Unpublished)

(Da/de)

Atom	Our Work	Others
Rubidium	25.74	25.68 (Shukla et al 1994)
Cesium	120.53	130.5 (Das 1988), 114 (Hartley et al 1990)
Thallium	- 395*	- 585 (Liu & Kelly 1992)

The best limit for de is from Thallium EDM experiment (Regan et al. Phys. Rev. Lett. 2002) and theory (Liu and Kelly)

$$d_e < 1.6 \times 10^{-27} e - cm$$

* Our work is in progress to improve the above limit.

(Da/C_S) in units of 10^{-18} e-cm

Atom	Our Work	Others
Rubidium	0.113 ± 0.001	0.119 (Shukla et al 1994)
Cesium	-0.801 ± 0.004	-0.72 ± 0.10 (Martensson & Lindroth 1991) -0.805 (Venugopal 1990)
Thallium	4.056 ± 0.137	7 ± 2 (Martensson & Lindroth 1991)

The current best limit for C_T is $< 1.3\times 10^{-8}$ by combining our calculated Da/C_T for Hg (Latha et al. 2008) and Hg EDM experiment (Romalis et al. Phys. Rev. Lett. 2001) at 95% C.L. $< 2.1 \times 10^{-28}\, e\, cm$

Da/Q has been calculated by Dzuba et al. Phys. Rev. A 2002 by using a hybrid method involving relativistic configuration interaction and relativistic many-body perturbation theory. Combining this with Hg EDM experiment :

$$Q < 7.4\times 10^{-12}\, e\, fm^3$$

Limits for Hadronic T-violating coupling constants

P, T-violating term	Value	System
Neutron EDM d_n	$(17 \pm 8 \pm 6) \times 10^{-26} e$ cm	^{199}Hg
	$(1.9 \pm 5.4) \times 10^{-26} e$ cm	Neutron
	$(2.6 \pm 4.0 \pm 1.6) \times 10^{-26} e$ cm	Neutron
Proton EDM d_p	$(1.7 \pm 0.8 \pm 0.6) \times 10^{-24} e$ cm	^{199}Hg
	$(17 \pm 28) \times 10^{-24} e$ cm	TlF
$\eta_{np} i(G/\sqrt{2}) \bar{p} p \bar{n} \gamma_5 n$	$\eta_{np} = (2.7 \pm 1.3 \pm 1.0) \times 10^{-4}$	^{199}Hg
$\bar{g}^0_{\pi NN}$	$(3.0 \pm 1.4 \pm 1.1) \times 10^{-12}$	^{199}Hg
QCD phase $\bar{\theta}$	$(1.1 \pm 0.5 \pm 0.4) \times 10^{-10}$	^{199}Hg
	$(1.6 \pm 4.5) \times 10^{-10}$	Neutron
	$(2.2 \pm 3.3 \pm 1.3) \times 10^{-10}$	Neutron
CEDMs $\tilde{d}$ and	$e(\tilde{d}_d - \tilde{d}_u) = (1.5 \pm 0.7 \pm 0.6) \times 10^{-26} e$ cm	^{199}Hg
EDMs d of quarks	$e(\tilde{d}_d + 0.5\tilde{d}_u) + 1.3 d_d - 0.3 d_u$	
	$= (3.5 \pm 9.8) \times 10^{-26} e$ cm	Neutron
	$= (4.7 \pm 7.3 \pm 2.9) \times 10^{-26} e$ cm	Neutron

The above limits have been obtained by using the limit for the Schiff moment (Q) from atomic physics and combining with nuclear structure and QCD calculations.

Ongoing Atomic EDM Experiments and Theory

Experiments :

Rb:	Weiss, Penn State
Cs:	Gould, LBNL ; Heinzen, UT, Austin; Weiss, Penn State
Fr:	Sakemi, Tohoku
Ra*:	Jungmann, KVI, Netherlands

Hg:	Fortson, UW, Seattle
Xe:	Romalis, Princeton
Yb:	Takahashi, Univ. of Kyoto, Natarajan, IISc, Bangalore
Rn:	Chupp, Univ. of Michigan
Ra:	Holt and Lu, ANL

Theory : Flambaum, UNSW, Sydney ; Das, IIA, Bangalore; Angom, PRL, Ahmedabad

Improved accuracies in experiments and relativistic many-body theory for Rb, Cs and Fr could give new limits for d_e and C_S

New limits for C_T and Q are expected from Hg in the near future.

Molecular EDMs

The electron EDM enhancement factors in certain molecules can be several orders of magnitude larger than those in atoms.

Some of the current molecular EDM experiments that are underway are :

YbF : Hinds, Imperial College, London

PbO * : DeMille, Yale University

HfF^+ : Cornell, JILA, Colorado

The sensitivities of these experiments could be 2-3 orders of magnitude better than that of the current limit from Tl.

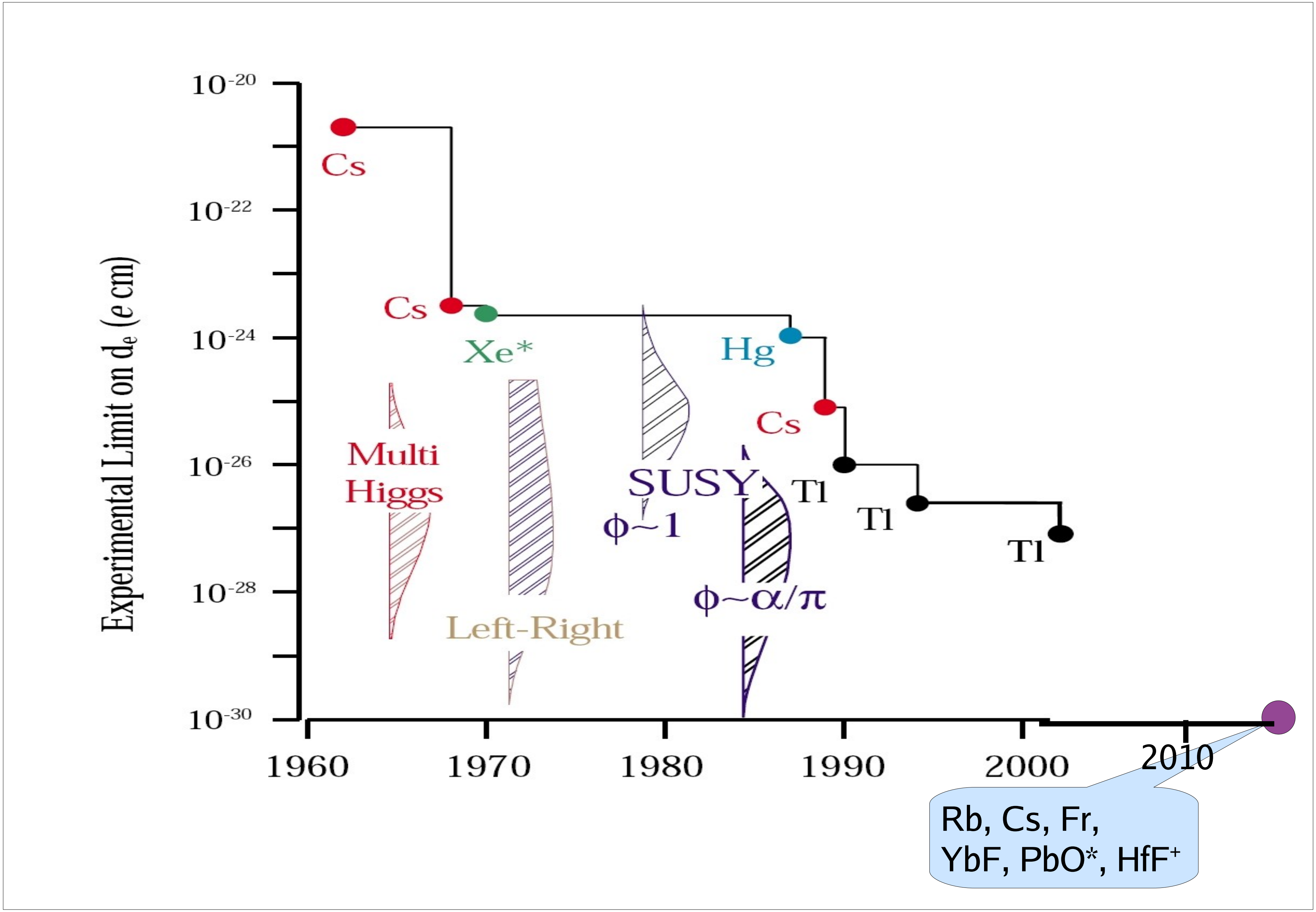
Molecular EDM calculations are currently in their infancy :

Petrov et al. Phys. Rev. A **72**, 022505 (2005)

Meyer et al. Phys. Rev. A **73**, 062108 (2006)

Nayak et al. Phys. Rev. A **75**, 022510 (2007)

Limits on d_e : Past, Present and Future



Conclusions

Atomic EDMs could serve as excellent probes of physics beyond the standard model.

Atoms are a rich source of T (or CP) violation : Can provide information on leptonic, semi-leptonic and hadronic T violations.

The current best atomic EDM limits come from Tl (d_e, C_s) and Hg (C_T, Q)

Several Atomic (Hg, Rb, Cs etc.) and Molecular (YbF, PbO*, HfF^+, etc) EDM experiments are underway. Results of some of these experiments could in combination with relativistic many-body calculations give improve the limits for the T violating coupling constants.

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Aside

METHOD OF CALCULATION

. . . Dirac - Fock Theory

For a relativistic N-particle system, we have a Dirac-Fock equation given by,

$$H_0 = \sum_I \{c\,\vec{\alpha}_I \cdot \vec{p}_I + (\beta_I - 1)\, m\, c^2 + V_N(r_I)\} + \sum_{I<J} \frac{e^2}{r_{IJ}}$$

We represent the ground state wave function Φ as an N×N Slater determinant,

$$\Phi_0 = \frac{1}{\sqrt{N!}} \begin{vmatrix} \phi_1(x_1) & \phi_1(x_2) & \phi_1(x_3) & \cdots & \phi_1(x_N) \\ \phi_2(x_1) & \phi_2(x_2) & \phi_2(x_3) & \cdots & \phi_2(x_N) \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ \phi_N(x_1) & \phi_N(x_2) & \phi_N(x_3) & \cdots & \phi_N(x_N) \end{vmatrix}$$

The single particle wave functions ϕ_ι's expressed in Dirac form as,

$$\phi_a = \frac{1}{r} \begin{pmatrix} P_a(r)\chi_{\kappa_a, m_a} \\ iQ_a(r)\chi_{-\kappa_a, m_a} \end{pmatrix}$$

. . . Coupled Cluster Theory

The coupled cluster wave function for a closed shell atom is given by,

$$|\Psi_0\rangle = e^{T^{(0)}} |\Phi_0\rangle$$

Since the system considered here has only one valence electron, it reduces to

$$|\Psi_v\rangle = e^{T^{(0)}}\{1+S^{(0)}\}|\Phi_v\rangle$$

Where, $T^{(0)} = T_1^{(0)} + T_2^{(0)} + \cdots$ and $S^{(0)} = S_1^{(0)} + S_2^{(0)} + \cdots$

The RCC operator amplitudes can be solved in two steps; first we solve for closed shell amplitudes using the following equations:

$$\langle \Phi_0 | \overline{H}_0 | \Phi_0 \rangle = E_g \quad \text{and} \quad \langle \Phi_0^* | \overline{H}_0 | \Phi_0 \rangle = 0$$

Where, $\overline{H}_0 = e^{-T^{(0)}} H_0 e^{T^{(0)}}$

The open shell operators can be obtained by solving the following two equations :

$$\langle \Phi_v | \overline{H}_{op} \{1 + S_v^{(0)}\} | \Phi_v \rangle = -\Delta E_v$$

$$\langle \Phi_v^* | \overline{H}_{op} \{1 + S_v^{(0)}\} | \Phi_v \rangle = -\Delta E_v \langle \Phi_v^* | \{S_v^{(0)}\} | \Phi_v \rangle$$

Where, ΔE_v is the negative of the ionization potential of the valence electron v.

The total atomic Hamiltonian in the presence of EDM as a perturbation is given by,

$$|\Psi_v\rangle = e^{(T^{(0)} + d_e T^{(1)})} \{1 + S^{(0)} + d_e S^{(1)}\} |\Phi_v\rangle$$

The effective (one-body) perturbed EDM operator is given by,

$$\langle \Phi_v | \overline{H}_{op} \{1 + S_v^{(0)}\} | \Phi_v \rangle = -\Delta E_v$$

Thus, the modified atomic wave function is given by,

$$|\Psi_v\rangle = e^{(T^{(0)} + d_e T^{(1)})} \{1 + S^{(0)} + d_e S^{(1)}\} |\Phi_v\rangle$$

The perturbed cluster amplitudes can be obtained by solving the following equations self consistently :

$$\langle \Phi_0^* | \overline{H}_N^{(0)} T^{(1)} + \overline{H}_{EDM}^{eff} | \Phi_0 \rangle = 0$$

$$\langle \Phi_v^* | (\overline{H}_N^{(0)} - \Delta E_v) S_v^{(1)} + (\overline{H}_N^{(0)} T^{(1)} + \overline{H}_{EDM}^{eff}) \{ 1 + S_v^{(0)} \} | \Phi_v \rangle = 0$$

Where, $H_N = H_0 - \langle \Phi_0 | H_0 | \Phi_0 \rangle$

The atomic EDM is given by,

$$\langle D_a \rangle = \frac{\langle \Psi_v | D_a | \Psi_v \rangle}{\langle \Psi_v | \Psi_v \rangle}$$

Particle Physics Model	Electron EDM (e-cm)
Standard Model	$< 10^{-38}$
Super-symmetric Model	$10^{-24} – 10^{-28}$
Left-Right Symmetric Model	$10^{-25} – 10^{-30}$
Multi-Higgs Model	$10^{-25} - 10^{-29}$

ATOMIC EDM DUE TO THE ELECTRON EDM

(NON-RELATIVISTIC CASE)

The interaction between the electron spin and internal electric field exerted by the nucleus and the other electrons gives,

$$-d_e \sigma \cdot E^I$$ where, $$E^I = -\nabla \{ \sum_i V_N(r_i) + \sum_{i<j} V_C(r_{ij}) \}$$

The total atomic Hamiltonian is then,

$$H = \sum_i \{ \frac{p_i^2}{2\mathrm{m}} - \frac{Ze}{r_i} \} + \sum_{i<j} \frac{e^2}{r_{ij}} - d_e \sum_i \sigma_i \cdot E_i^I$$

Using perturbation theory, we can write, $H = H_O + H^/$

where,

$$H_O = \sum_i \{ \frac{p_i^2}{2\mathrm{m}} - \frac{Ze}{r_i} \} + \sum_{i<j} \frac{e^2}{r_{ij}}; \qquad H^/ = -d_e \sum_i \vec{\sigma}_i \cdot \vec{E}_i^I; \qquad H_O | \Psi_\alpha^O \rangle = E_O | \Psi_\alpha^O \rangle$$

When there is an external electric field, induced electric dipole moment arises.

$$e\vec{r}$$

Total electric dipole moment operator of an atom is then given by,

$$\vec{D}_a = \sum_i \left\{ d_e \vec{\sigma}_i + e\vec{r}_i \right\}$$

The atomic EDM is,

$$\langle D_a \rangle = \langle \Psi_\alpha | D_a | \Psi_\alpha \rangle$$

Using perturbation theory,

$$|\Psi_\alpha\rangle = |\Psi_\alpha^O\rangle + d_e |\Psi_\alpha^1\rangle + d_e^2 |\Psi_\alpha^2\rangle + \cdots$$

As d_e is small, d_e^2 term can be neglected.

Assume, the applied field is in the ***z*** direction. $d_e \vec{\sigma}_z$ is even under parity, where as, $e\vec{z}$ term is odd under parity.

$|\Psi_\alpha^O\rangle$ and $|\Psi_\alpha^1\rangle$ are of opposite parity, then the non-vanishing terms of the EDM are:

$$\langle D_a \rangle = \underbrace{d_e \langle \Psi_\alpha^O | \sum_i \vec{\sigma}_{z_i} | \Psi_\alpha^O \rangle}_{D^O} + \underbrace{d_e\, e \{ \langle \Psi_\alpha^O | \sum_i \vec{z}_i | \Psi_\alpha^1 \rangle + \langle \Psi_\alpha^1 | \sum_i \vec{z}_i | \Psi_\alpha^0 \rangle \}}_{D^1}$$

From the Time-independent Non-degenerate perturbation theory, we have,

$$| \Psi_\alpha^1 \rangle = \sum_{I \neq \alpha} | \Psi_I^O \rangle \frac{\langle \Psi_I^O | H^/ | \Psi_\alpha^O \rangle}{E_\alpha^O - E_I^O}$$

$$H^/ = -d_e \vec{\sigma} \cdot \vec{E}_i$$

$$\langle D_a \rangle = \langle D^O \rangle + \langle D^1 \rangle$$

$$\langle D^1 \rangle = -d_e \langle \Psi_\alpha^O | \sum_i \vec{\sigma}_{z_i} | \Psi_\alpha^O \rangle \qquad \langle D^O \rangle = d_e \langle \Psi_\alpha^O | \sum_i \vec{\sigma}_{z_i} | \Psi_\alpha^O \rangle$$

$$\Rightarrow \quad \langle D_a \rangle = 0$$

(Sandars 1968)

Hence, in the non-relativistic scenario, even though the electron is assumed to have a tiny EDM, when all the interactions in the atom are considered, the total atomic EDM becomes zero.

ATOMIC EDM DUE TO THE ELECTRON EDM

(RELATIVISTIC CASE)

The total atomic Hamiltonian, including intrinsic electron EDM is,

$$H = \sum_i \{ c\alpha_i \cdot p_i + (\beta_i - 1) mc^2 - \frac{Ze}{r_i} \} + \sum_{i<j} \frac{e^2}{r_{ij}} - d_e \sum_i \beta_i \sigma_i \cdot E_i^I$$

H_0 $\quad$ $H^{/}$

The expectation value of atomic EDM in the presence of applied electric field is given by,

$$\langle D_a \rangle = d_e \langle \Psi_\alpha^O | \sum_i \beta_i \sigma_{z_i} | \Psi_\alpha^O \rangle + d_e\, e \{ \langle \Psi_\alpha^O | \sum_i z_i | \Psi_\alpha^1 \rangle + \langle \Psi_\alpha^1 | \sum_i z_i | \Psi_\alpha^0 \rangle \}$$

D^O $\quad$ D^1

Finally, the expression for Atomic EDM reduces to,

$$\langle D_a \rangle = \frac{4 c d_e}{\hbar} \sum_{I \neq \alpha} \frac{\langle \Psi_\alpha^O | \vec{z} | \Psi_I^O \rangle \langle \Psi_I^O | i \beta \gamma_5 p^2 | \Psi_\alpha^O \rangle}{E_\alpha^O - E_I^O}$$

$$\Rightarrow \quad \langle D_a \rangle \neq 0$$

Hence, in the relativistic scenario, the total atomic EDM is non-zero.

(Sandars 1968)