A Complete Analysis of Closed-shell Atomic EDMs: case study of Xe atom

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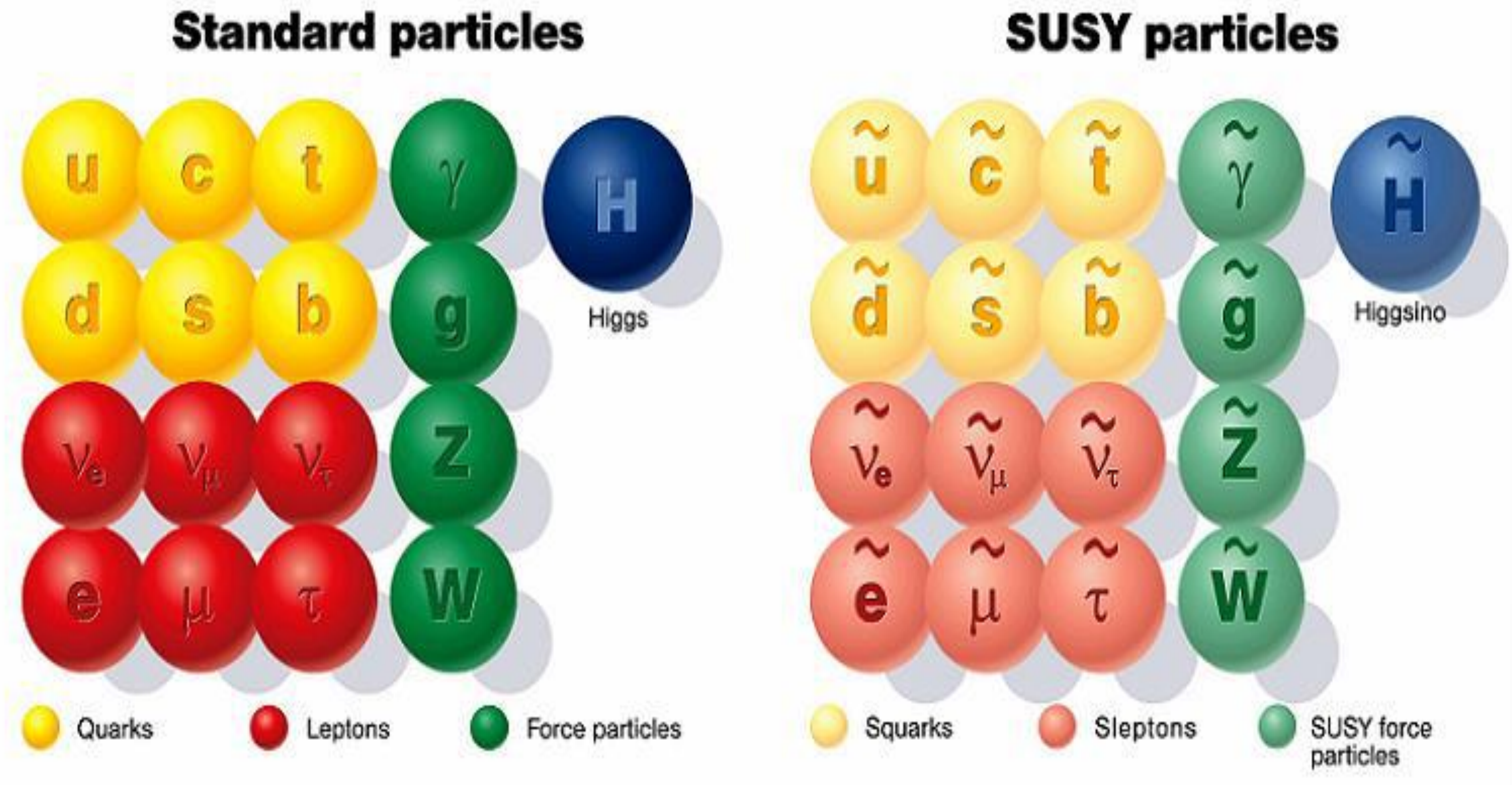
Outline

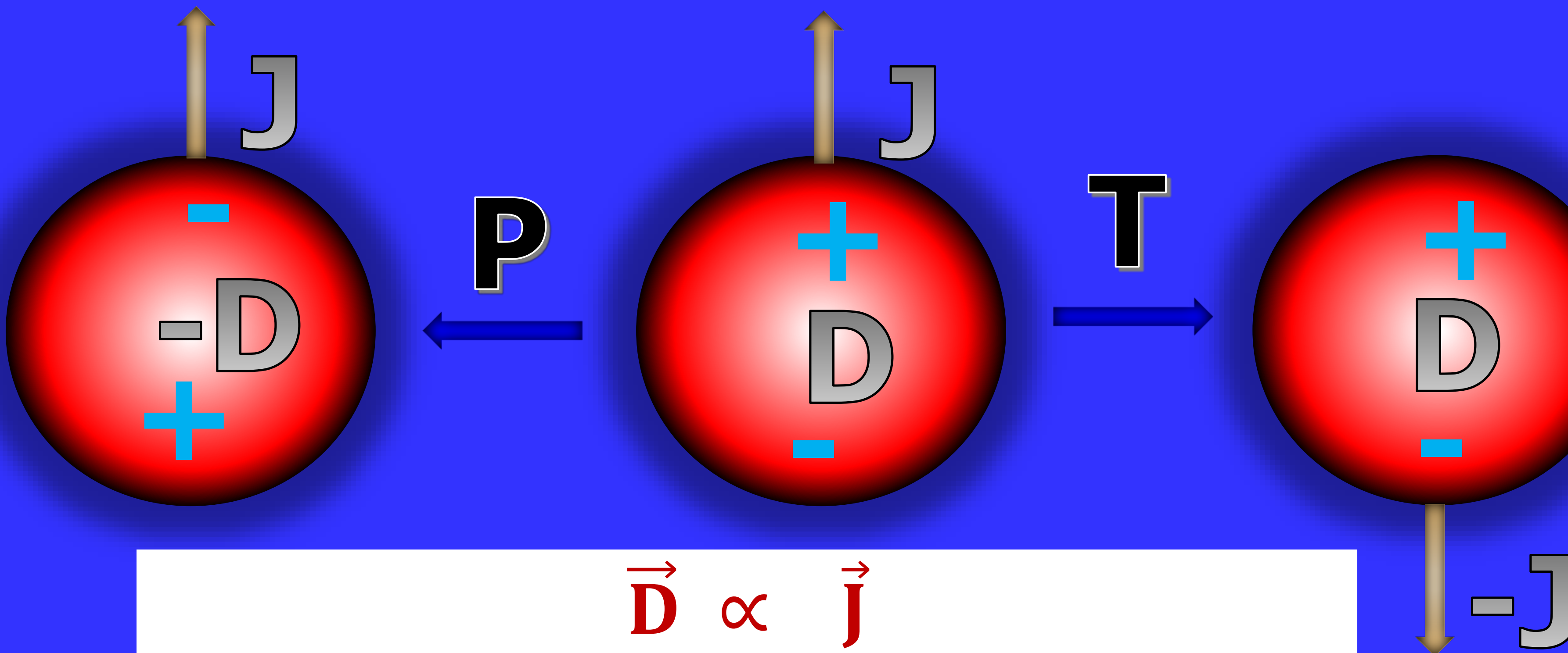
- Motivation.
- P,T-odd interactions leading to EDM.
- Experimental status in closed-shell atoms.
- Status of theoretical calculations.
- Less rigorously investigated P,T-odd interactions.
- New results for Xe atom.
- Conclusion.

Standard model (SM) vs. SuperSymmetry (SUSY) model



1. Prediction of different sizes for electrons and quarks.
2. Give different values for coupling constants for the electron-quark, quark-quark, etc. interactions.

Parity (P) & time-reversal (T) violations give EDM



$$\vec{D} \propto \vec{J}$$

P symmetry: $\vec{J} \to \vec{J}$ but $\vec{D} \to -\vec{D}$

T symmetry: $\vec{J} \to -\vec{J}$ but $\vec{D} \to \vec{D}$

P & T violation ⇒ EDM of system

T violation ⟺ CP violation

Experimental status (closed-shell atoms)

$D(^{129}Xe) = (0.7 \pm 3.3_{stat} \pm 0.1_{syst}) \times 10^{-27}\ e\text{-cm}$

$\Rightarrow |D(^{129}Xe)| < 4.1 \times 10^{-27}$ e cm (90% C.L.)

M. A. Rosenberry and T. E. Chupp, Phys. Rev. Lett. **86**, 22 (2001).

$D(^{199}Hg) = (2.20 \pm 2.75_{stat} \pm 1.48_{syst}) \times 10^{-30}\ e\text{-cm}$

$\Rightarrow |D(^{199}Hg)| < 7.4 \times 10^{-30}$ e cm (95% C.L.)

B. Graner, Y. Chen, E. G. Lindahl and B. R. Heckel, Phys. Rev. Lett. **116**, 161601 (2016).

$D(^{225}Ra) = (4.0 \pm 6.0_{stat} \pm 0.2_{syst}) \times 10^{-24}\ e\text{-cm}$

$\Rightarrow |D(^{225}Ra)| < 1.4 \times 10^{-23}$ e cm (95% C.L.)

M. Bishof, R. H. Parker, K. G. Bailey, J. P. Greene, R. J. Holt, M. R. Kalita, W. Korsch, N. D. Lemke, Z. –T. Lu, P. Mueller, T. P. O'Connor, J. T. Singh and M. R. Dietrich, Phys. Rev. C. **94**, 025501 (2016).

$D(^{171}Yb) = (-6.8 \pm 5.1_{stat} \pm 1.2_{syst}) \times 10^{-27}\ e\text{-cm}$

$\Rightarrow |D(^{171}Yb)| < 1.5 \times 10^{-26}$ e cm (95% C.L.)

T. Zheng, Y. Yang, S.Z. Wang, J. T. Singh, Z.X. Xiong, T. Xia and Z. T. Lu, Phys. Rev. Lett. **129**, 083001 (2022).

Other interested closed-shell atoms: Rn.

P,T-odd electron-nucleon Langrangians

Following Ann. Phys. (NY) 318, 119 (2005), we can write:

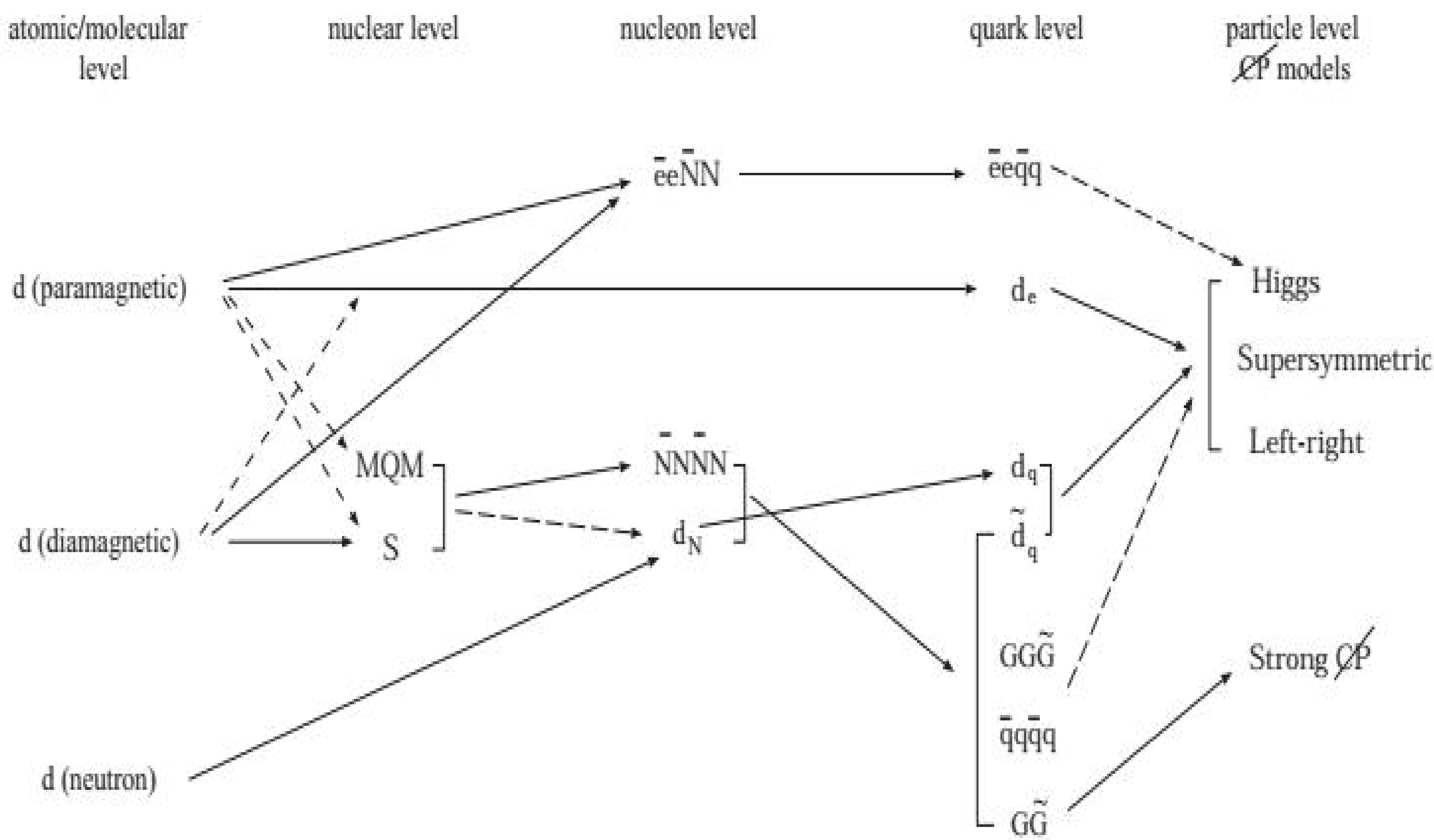
Effective Lagrangian: $L = L_e + L_q + L_{\pi NN} + L_{eN}$

where $L_e + L_q = -\frac{i}{2} \sum_{k=e,p,n} d_k \bar{\psi}_k (F\sigma) \psi_k$

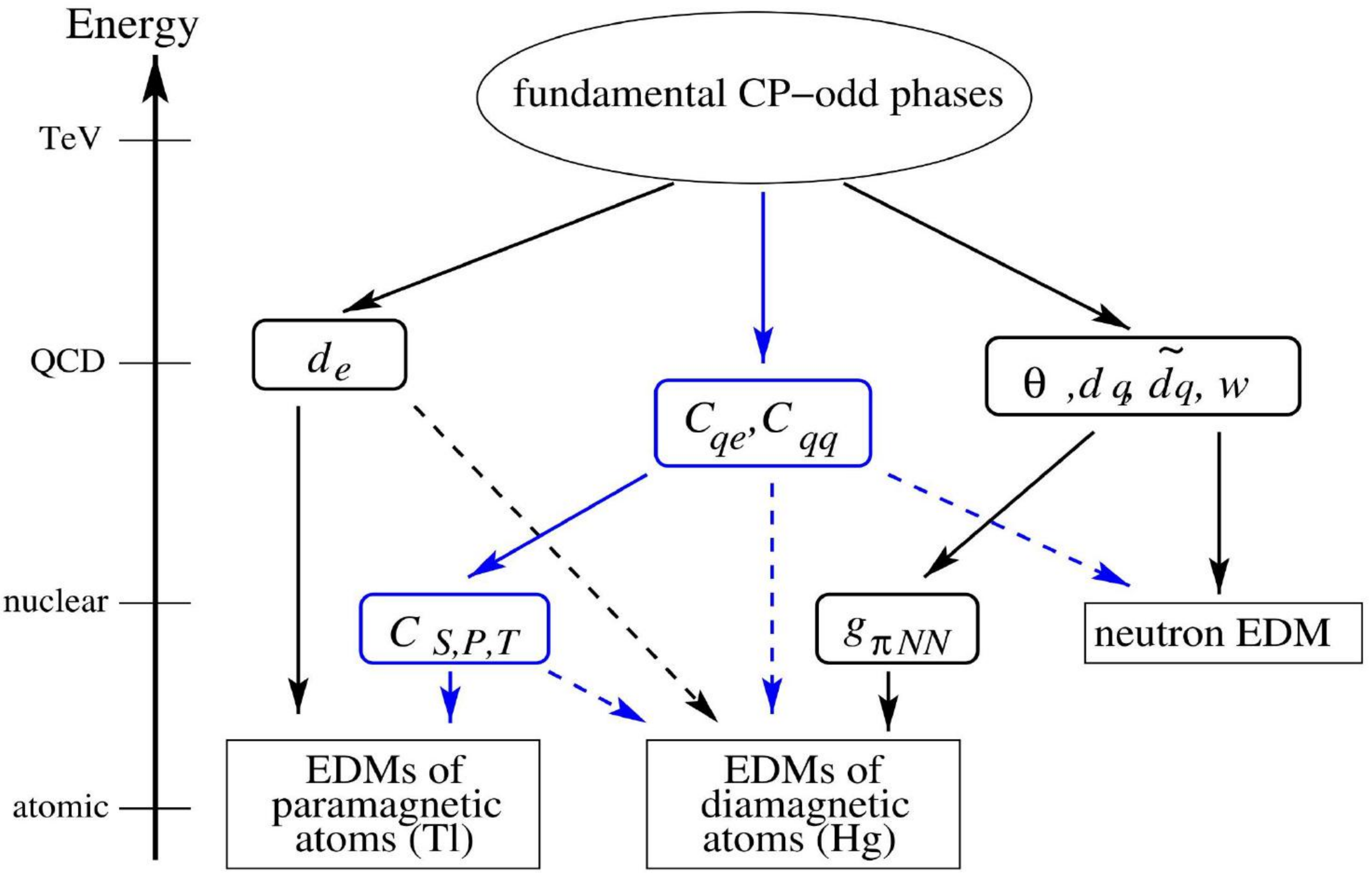
$$L_{\pi NN} = \bar{g}^{(0)}_{\pi NN} \overline{N} \tau^a N \pi^a + \bar{g}^{(1)}_{\pi NN} \overline{N} N \pi^0$$
$$+ \bar{g}^{(2)}_{\pi NN} (\overline{N} \tau^a N \pi^a - 3 \bar{g} \overline{N} \tau^3 N \pi^0)$$
$$\approx \bar{\theta} \frac{\alpha_s}{8\pi} \tilde{G} G$$

$$L_{eN} = C_S^{(0)} \overline{e} i \gamma_5 e \overline{N} N + C_P^{(0)} \overline{e} e \overline{N} i \gamma_5 N$$
$$+ C_T^{(0)} \epsilon_{\mu\nu\alpha\beta} \overline{e} \sigma^{\mu\nu} e \overline{N} \sigma^{\alpha\beta} N + \cdots$$

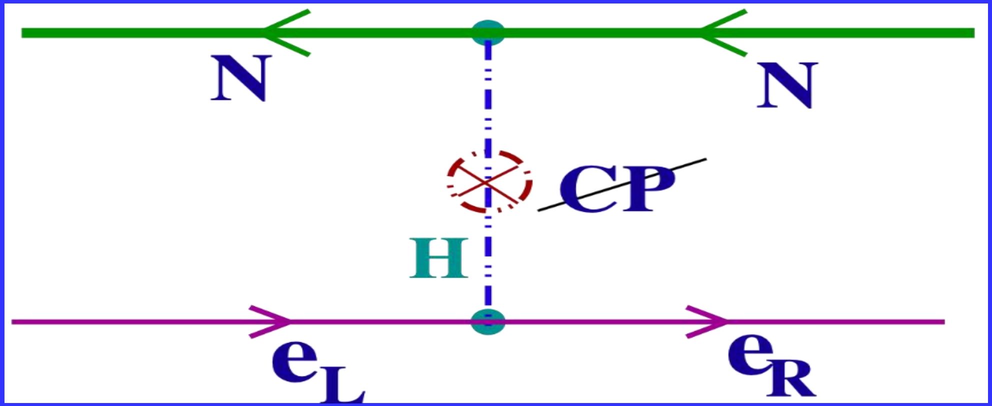
From particles to composite systems (vice-versa)



All possible sources



Atomic Hamiltonian due to T-PT (L_{eN} component)



Electron-nuclear P,T-odd Hamiltonian:

$$H_{P,T}^{e-N} = \frac{G_F}{\sqrt{2}} \left[i\, C_S^{e-N} \overline{N} N\, \bar{e}\, \gamma_5 e + i\, C_P^{e-N} \overline{N} \gamma_5 N\, \bar{e} e + \frac{G_F}{\sqrt{2}} i\, C_T^{e-N} \overline{N}\, \sigma_{\mu\nu} N\, \bar{e}\, \gamma^5 \sigma^{\mu\nu} e \right]$$

In the non-relativistic approximation T-PT e-N interaction:

$$H_{EDM}^{e-N} = \frac{i\, G_F}{\sqrt{2}} \sum_{e,N} C_T^{e-N} [\overline{\Psi}_N \sigma_{\mu\nu} \Psi_N][\overline{\Psi}_e \gamma^5 \Psi_e]$$

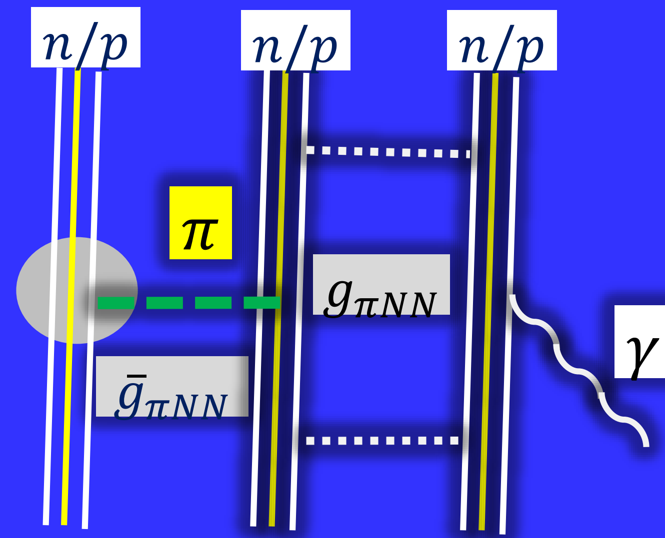
$$\simeq \sqrt{2}\, i\, G_F C_T \textstyle\sum_e \rho_N\,(r_e)\ \vec{I}_N \cdot\ \vec{\gamma}_e$$

Atomic Hamiltonian due to Schiff mom. ($L_{\pi NN}$)

Electron-Schiff moment int.

$$H_{int}(r) = e\vec{r}\cdot\left[\int_0^\infty d^3r'\left(\frac{\langle\vec{r}'\rangle}{Zr^3} - \frac{\vec{r'}}{r^3} + \frac{\vec{r'}}{\vec{r}'^3}\right)\rho_n(r')\right]$$

$$= \frac{S}{|I|}\frac{\vec{I}\cdot\vec{r}}{B}\rho_n(r) \text{ with } B = \int_0^\infty dr\, r^4\rho_n(r)$$



Schiff moment:

$$S = g_{\pi NN}\left[a_0\bar{g}_{\pi NN}^{(0)} + a_1\bar{g}_{\pi NN}^{(1)} + a_2\bar{g}_{\pi NN}^{(2)}\right] \approx [\, b_1\, d_n + b_2 d_p]$$

Where parity conserving $g_{\pi NN} \approx 13.5$ and a_0, a_1, a_2, b_1 and b_2 are determined using Skyrme interactions.

Relations with the particle physics parameters:

$$\bar{g}_{\pi NN}^{(0)} \approx -0.018(7)\bar{\theta} \quad \text{and} \quad \bar{g}_{\pi NN}^{(0)} \approx -1.02(\tilde{d}_u + \tilde{d}_d)$$

$$\bar{g}_{\pi NN}^{(1)} = 2\times 10^{-12}(\tilde{d}_u - \tilde{d}_d) \quad \text{and} \quad \bar{g}_{\pi NN}^{(2)} \approx 0$$

Only these two types of interactions are often taken into account while studying EDMs of closed-shell atoms.

↓

It is important to analyse contributions from all possible sources of CP violation to EDM of any atomic system.

Why some interactions contribute predominantly to EDM of an atomic system?

Atomic theory for EDM

EDM of a state $|\Psi_n\rangle$ given by: $D_a = \left[\frac{\langle\Psi_n|D|\Psi_n\rangle}{\langle\Psi_n|\Psi_n\rangle}\right]$

Mixed parity states: $|\Psi_n\rangle \simeq |\Psi_n^{(0)}\rangle + \lambda\,|\Psi_n^{(1)}\rangle$

$\mathrm{H} \equiv H_{at} + H_{EDM} = H_{at} + \lambda\, H_{odd}$ **with** $\lambda = S$ or $\langle\sigma_n\rangle C_T$

$$\Rightarrow D_a = \lambda\, R \cong 2\left[\frac{\left\langle\Psi_n^{(0)}\middle|D\middle|\Psi_n^{(1)}\right\rangle}{\left\langle\Psi_n^{(0)}\middle|\Psi_n^{(0)}\right\rangle}\right]$$

Inhomogeneous Eq^{n}:

$$(H_{at} - E_0^{(0)})|\Psi_n^{(1)}\rangle = -H_{EDM}|\Psi_n^{(0)}\rangle$$

Selection rules:

At the second-order perturbation:

$$\Rightarrow D_a(J) = \left[\frac{\left\langle \Psi_n^{(0)}(J) \middle| D^{(k=1)} \middle| \Psi_n^{(1)}(J') \right\rangle}{\left\langle \Psi_n^{(0)}(J) \middle| \Psi_n^{(0)}(J) \right\rangle} \right]$$

Diatomic (closed-shell) systems: $J = 0$

EDM contribution will be finite when rank of H_{EDM} is 1. For the case when rank of H_{EDM} is 0, finite EDM can be obtained after inducing atomic states due to the hyperfine interactions (one-more order).

Paramagnetic (one-valence shell) systems: $J = \frac{1}{2}; \frac{3}{2}; \ldots$

Interaction Hamiltonians due to electron EDM and electron-nucleus S-PS interaction have rank 0. They contribute predominantly to open-shell systems.

Other sources of EDMs to closed-shell atoms

At the second-order perturbation theory:

- Pseudoscalar-scalar (Ps-S) electron-nuclear interaction:

$$H_{PsS}^{e-N} = -\frac{G_F C_P}{2\sqrt{2} M_p c} \sum_{j=1}^{N} \gamma_0 \left(\nabla_j \rho\left(r_j\right) \langle \sigma_A \rangle \right)$$

$$\Rightarrow \quad H_{PsS}^{e-N} \propto \frac{G_F}{M_P} \quad \text{and} \quad H_{PsS}^{e-N} \propto \nabla_j \, \rho\left(r_j\right) \langle \sigma_A \rangle$$

- Interaction between electron EDM with nuclear magnetic field:

$$H_B^{d_e} = i \, c d_e \sum_{j=1}^{N} \left(\beta \, \alpha_j B_j \right)$$

where $B = \nabla \times A$ with $A = \frac{g_I \, I}{4\,\pi} \frac{[\,\mu \times r]}{|r|^3} \mu_N;$ $\quad \mu_N = \frac{|e|\hbar}{2\, M_p}$

Other sources of EDMs to closed-shell atoms

- d_e interacting with internal electric field (rank=0):

$$H_{de} = 2icd_e \sum_{j=1}^{N} \beta\gamma_j^5 \; p_j^2$$

$$\Rightarrow \; H_{de} \propto \frac{1}{M_P}$$ and two energy denominators.

- Scalar-pseudoscalar (S-Ps) electron-nuc. Interac. (rank=0):

$$H_{SPs}^{e-N} = i\frac{G_F C_S}{\sqrt{2}} A \sum_{j=1}^{N} \beta\,\gamma_j^5\,\rho(r_j)$$

$$\Rightarrow \; H_{SPs}^{e-N} \propto \frac{G_F}{M_P}$$ and two energy denominators.

At third-order (mag. dip. hyperfine induced):

$$\Rightarrow D_a \cong 2\left[\frac{\langle\Psi_0^{(0,0)}|D|\Psi_0^{(1,1)}\rangle + \langle\Psi_0^{(1,0)}|D|\Psi_0^{(0,1)}\rangle}{\langle\Psi_0^{(0,0)}|\Psi_0^{(0,0)}\rangle}\right]$$

Double/Triple sources of perturbation

In this case: $H = H_0 + V_{int}^{(1)} + V_{int}^{(2)}$

Let wave function is approximated as

$$|\Psi\rangle = |\Psi^{(0)}\rangle + |\Psi^{(\prime)}\rangle \approx |\Psi^{(0)}\rangle + |\Psi^{(1)}\rangle$$
$$E = E^{(0)} + E^{(\prime)} \approx E^{(0)}$$

In perturbation approach for this case:

$$\Omega = \Omega^{(0,0)} + \Omega^{(1,0)} + \Omega^{(0,1)} + \Omega^{(0,2)} + \Omega^{(1,1)} + \cdots = \sum_{n,m} \Omega^{(\mathrm{n,m})}$$

with $\Omega^{(0,0)} = 1,$ $\Omega^{(1,0)} = \mathrm{V}_{\mathrm{int}}^{(1)}$ **and** $\Omega^{(0,1)} = \mathrm{V}_{\mathrm{int}}^{(2)}$

Amplitude equation:

$$[\Omega^{(\beta,\alpha)}, H_0]P = QV_{int}^{(1)}\Omega^{(\beta-1,\delta)}P + Q\,V_{int}^{(2)}\Omega^{(\beta,\delta-1)}P$$
$$- \sum_{m=1}^{\beta-1}\sum_{l=1}^{\delta-1}\left(\Omega^{(\beta-m,\delta-1)}PV_{int}^{(1)}\Omega^{(m-1,l)}P - \Omega^{(\beta-m,\delta-l)}PV_{int}^{(2)}\Omega^{(m,l-1)}P\right)$$

All order many-body methods

Configuration interaction (CI) method:

$$\left|\Psi_n^{(0/1)}\right\rangle = C_0|\Phi_n\rangle + C_I\,|\Phi_I\rangle + C_{II}\,|\Phi_{II}\rangle + \cdots$$

Random phase approximation (RPA):

$$\left|\Psi_n^{(0)}\right\rangle \to |\Phi_n\rangle \quad \text{and} \quad \left|\Psi_n^{(1)}\right\rangle \to \Omega_{I,CP}^{(\infty,1)}|\Phi_n\rangle = \Omega_{RPA}^{(1)}|\Phi_n\rangle$$

Coupled-cluster (CC) method:

$$\left|\Psi_n^{(0/1)}\right\rangle = C_0|\Phi_n\rangle + C_I\,|\Phi_I\rangle + C_{II}\,|\Phi_{II}\rangle + \cdots$$

$$= |\Phi_n\rangle + T_I^{(0/1)}\,|\Phi_n\rangle + T_{II}^{(0/1)}\,|\Phi_n\rangle + \frac{1}{2}\,{T_I^{(0/1)}}^2|\Phi_n\rangle + \cdots$$

$$= e^{T_I^{(0/1)}+T_{II}^{(0/1)}+\cdots}\,|\Phi_n\rangle = e^{T^{(0)}(+T^{(1)})}\,|\Phi_n\rangle$$

Advantage of truncated CC method over truncated CI method.

D_a in $S \times 10^{-20}\ |e| fm^3$

	^{129}Xe	^{223}Rn	^{171}Yb	^{199}Hg	^{225}Ra
DHF	0.288	2.459	-0.42	-1.20	-1.86
MBPT(2)	0.266	2.356	-1.42	-2.30	-5.48
MBPT(3)	0.339	2.398	-1.34	-1.72	-5.30
RPA	**0.375**	**3.311**	**-1.91**	**-2.94**	**-8.12**
CI+MBPT			**-2.12**	**-2.6**	**-8.8**
MCDF			**-2.15**	**-2.22**	
CCSD	**0.333(4)**	**2.78(4)**	**-1.51(4)**	**-1.8(3)**	**-6.22(6)**

$D_a^{expt} < 7.4 \times 10^{-30}\ e - cm$ $\qquad$ $S < 4.2 \times 10^{-13}\ |e| fm^3$

Eur. Phys. J. A 53, 54 (2017) (review).

$D_a\ in\ C_T\langle\sigma\rangle \times 10^{-20}$ e-cm

	^{129}Xe	^{223}Rn	^{171}Yb	^{199}Hg	^{225}Ra
DHF	0.447	4.485	-0.71	-2.39	-3.46
MBPT(2)	0.405	3.927	-2.49	-4.48	-11.00
MBPT(3)	0.515	4.137	-2.34	-3.33	-10.59
RPA	**0.562**	**5.400**	**-3.39**	**-5.89**	**-16.66**
CI+MBPT			**-2.12**	**-5.1**	**-18.0**
MCDF			**-2.51**	**-4.84**	
CCSD	0.475(4)	4.46(6)	-2.04(6)	-3.4(5)	-9.93(8)

Atomic probe: $C_T < 7.0 \times 10^{-10}$ **SM:** $C_T = 0$

Eur. Phys. J. A 53, 54 (2017) (review).

Limits on T-violating quantities

Nuclear calculations for ^{199}Hg: $S = [1.9\, d_n + 0.2\, d_p]$

Phys. Rev. Lett. 91, 212303 (2003).

$$S = 13.5[0.01\bar{g}^{(0)}_{\pi NN} \pm 0.02\bar{g}^{(1)}_{\pi NN} + 0.02\bar{g}^{(2)}_{\pi NN}]\, |e| fm^3$$

Prog. Part. Nuc. Phys, 71, 21 (2013).

Atomic Expt+Theory

$d_n < 3.0 \times 10^{-27}\ e - cm$

$d_p < 2.1 \times 10^{-26}\ e - cm$

$|\tilde{d}_u - \tilde{d}_d| < 2.7 \times 10^{-27}\ e - cm$

$|\bar{\theta}| < 1.1 \times 10^{-10}$

Phys. Rev. D 95, 013002 (2017).

Standard Model (SM)

$d_n \sim 10^{-32}\ e - cm$

$d_p \sim 10^{-32}\ e - cm$

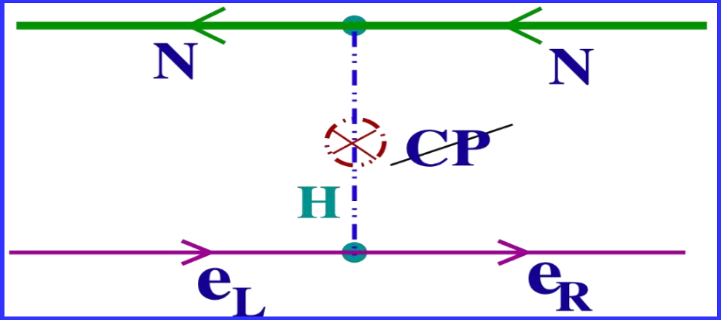
$d_u, d_d \sim 10^{-34}\ e - cm$

$0 \le \bar{\theta} \le 2\pi$

Strong CP problem.

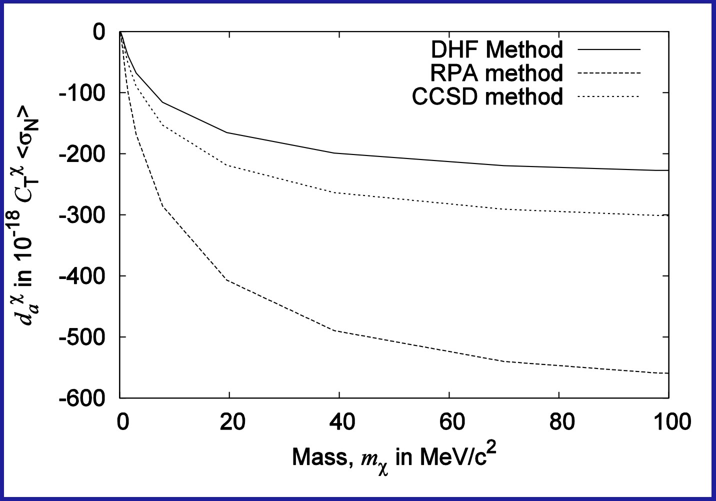
T-PT interaction due to a light dark matter

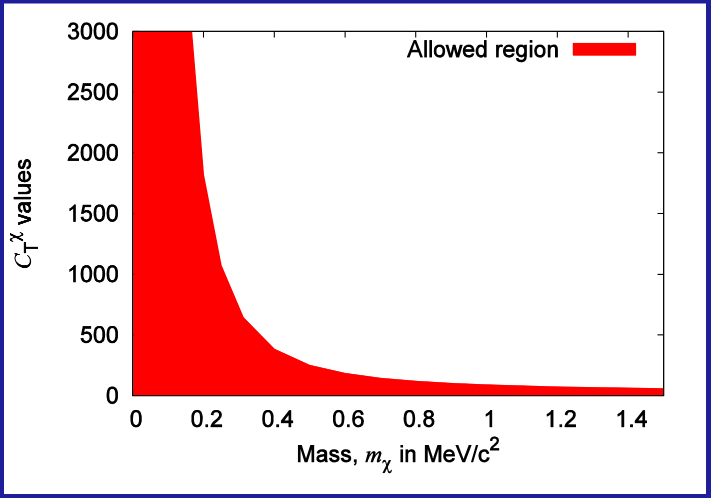
$$V_\chi(r,r') = \frac{e^{-m_\chi c|r-r'|}}{4\pi\,|r-r'|}$$



$$H_{EDM}^{e-N}(r) = \frac{i\,G_F}{\sqrt{2}} \sum_{e,N} C_T^{e-N} [\bar{\Psi}_N(r')\sigma_{\mu\nu}\Psi_N(r')] V_\chi(r,r') [\bar{\Psi}_e(r)\gamma^5\Psi_e(r)]$$

$$= \sqrt{2}\, i\, G_F C_T \sum_e \rho_N^\chi(r_e) \quad \vec{I}_N \cdot \vec{\gamma}_e$$





B. K. Sahoo, Phys. Rev. D 95, 013002 (2017).

Contributions from all possible interactions in Xe atom

	This work			Others	
	DHF	RPA	RCCSD		
T-PT ($\langle\sigma_A\rangle C_T \times 10^{-20} ecm$)	0.45	0.57	0.52	0.41	[a]
				0.57	[b]
SM ($\frac{S}{e\, fm^3} \times 10^{-17} ecm$)	0.29	0.38	0.34	0.38	[b]
d_e-B ($d_e \times 10^{-4} ecm$)	0.67	0.79	0.75	1.0	[a]
				1.05	[c]
Ps-S ($\langle\sigma_A\rangle C_P \times 10^{-23} ecm$)	1.28	1.63	1.50	1.6	[b]
Hfs+d_e ($d_e \times 10^{-4} ecm$)	10.16		11.21	-8.0	[a]
				-9.37	[c]
Hfs+SPS ($C_S/A \times 10^{-23} ecm$)	3.55		4.03	0.71(18)	[d]

[a] V. V. Flambaum, Zh. Eksp. Teor. Fiz. 89, 1505 (1985); [b] Dzuba et al, Phys. Rev. A 80, 032120 (2009); [c] Martensson and Oester, Phys. Scr. 36, 444 (1987); [d] Fleig and Jung, Phys. Rev. A 103, 012807 (2021).

Reason for large discrepancy for d_e int. with nuc. mag. field

	This work			Others	
	DHF	RPA	RCCSD		
d_e-B ($d_e \times 10^{-4} ecm$)	0.67	0.79	0.75	1.0	[a]
				1.05	[c]

- Interaction between electron EDM with nuclear magnetic field:

$$H_B^{d_e} = i\, c d_e \sum_{j=1}^{N} \left(\beta\, \alpha_j B_j\right)$$

where $B = \nabla \times A$ with $A = \frac{g_I\, I}{4\,\pi} \frac{[\,\mu \times r]}{|r|^3} \mu_N;\qquad \mu_N = \frac{|e|\hbar}{2\, M_p}$

$$\int_0^\infty dr\ \ldots \rightarrow \int_0^R dr\ \ldots + \int_R^\infty dr\ \ldots$$

Value is very sensitive for different choices of nuclear radius *R*.

Reason for large discrepancy for S-Ps interaction

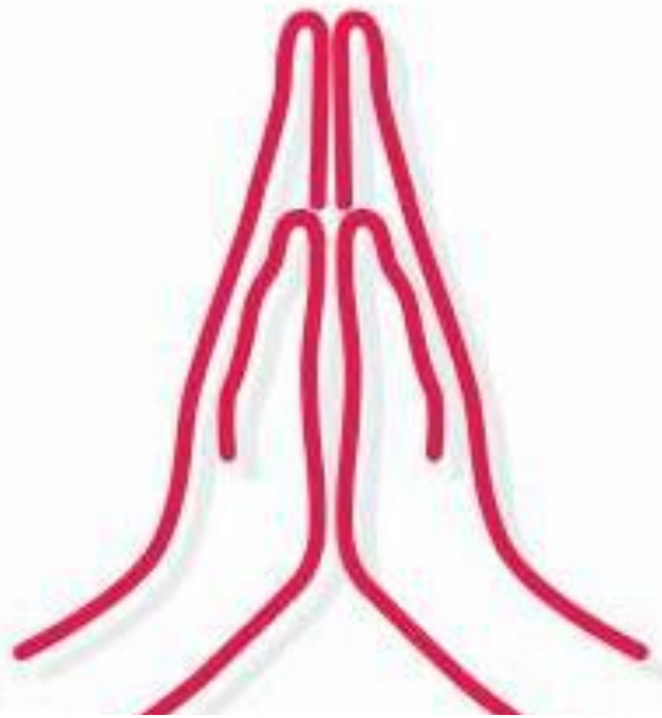
Calculations with	20s, 20p, 20d, 19f, 18g			35s, 35p, 35d, 19f, 18g			
	DHF	**RPA**	**RCCSD**	**DHF**	**RPA**	**RCCSD**	**Expt.**
Dip. Pol. α_d (in au)	26.87	26.97	27.50	26.87	26.97	28.84	27.815(27)
T-PT ($\langle\sigma_A\rangle C_T \times 10^{-20} ecm$)	0.45	0.57	0.52	0.45	0.57	0.52	
SM ($\frac{S}{e\, fm^3} \times 10^{-17} ecm$)	0.29	0.29	0.34	0.29	0.38	0.34	
d_e-B ($d_e \times 10^{-4} ecm$)	0.67	0.79	0.72	0.67	0.79	0.75	
Ps-S ($\langle\sigma_A\rangle C_P \times 10^{-23} ecm$)	1.28	1.68	1.50	1.28	1.63	1.50	
Hfs+d_e ($d_e \times 10^{-4} ecm$)	0.84		0.45	10.16		11.21	
Hfs+SPS ($C_S/A \times 10^{-23} ecm$)	0.07		0.04	3.55		4.03	

$$D_a^{2nd} = \sum_m \frac{\langle\Psi_0|D\,|\,\Psi_m\rangle\langle\Psi_m|H_{EDM}|\Psi_0\rangle}{(E_0 - E_m)}$$

$$D_a^{3rd} = \sum_{m,n} \frac{\langle\Psi_0|D\,|\,\Psi_m\rangle\langle\Psi_m|H_{hf}|\Psi_n\rangle\langle\Psi_n|H_{EDM}|\Psi_0\rangle}{(E_0 - E_m)(E_0 - E_n)}$$

Conclusion

- ✓ Atomic EDMs can offer sensitive probe of physics beyond the SM of particle physics.
- ✓ Earlier we had studied EDMs of closed-shell atoms only considering two major sources.
- ✓ Contributions from additional sources to EDM of Xe are investigated.
- ✓ Hyperfine-induced contributions are differing significantly from the earlier works.



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