Electric Dipole Moments of the Closed-shell Atoms

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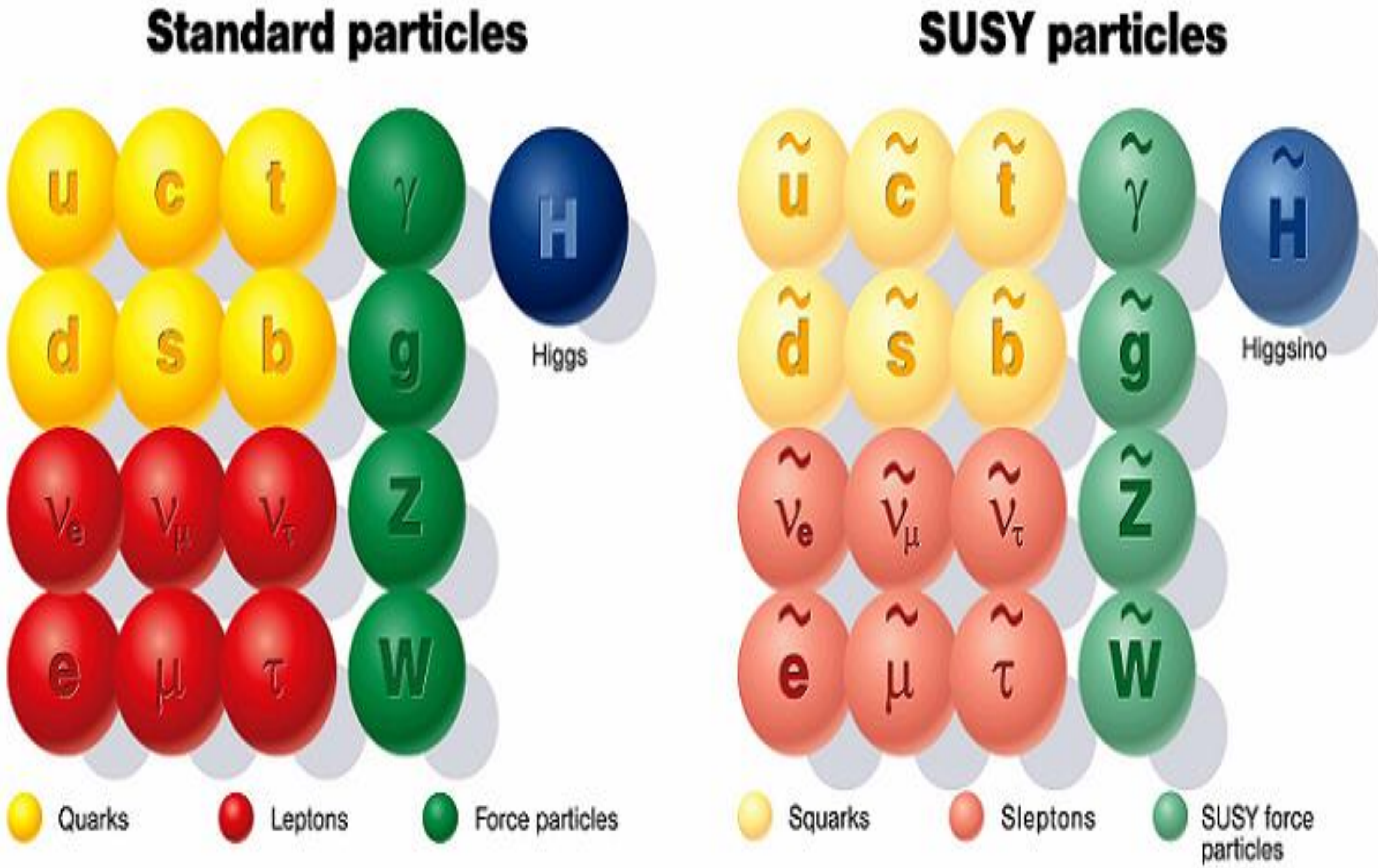
Outline

- Motivation
- Electric dipole moments (EDMs) of atoms
- Origins of atomic EDMs
- Experimental status
- Theoretical results and limit on Θ_{QCD}
- Summary and Outlook

Standard model (SM) versus SuperSymmetry (SUSY) model



Motivation

1. To learn about sizes of electrons and quarks

2. Accurate values of electron-quark, quark-quark, etc. coupling constants due to weak interactions

Baryogenesis problem:

No. baryons ≠ No. antibaryon $\left(\frac{n_b}{n_\gamma} \sim 10^{-10} \ \text{while} \ \frac{n_{\bar{b}}}{n_\gamma} \sim 10^{-20}\right)$

From Cosmology: $t < 10^{-6}$ sec $\Rightarrow \frac{n_b - n_{\bar{b}}}{n_b} \sim 10^{-8}$

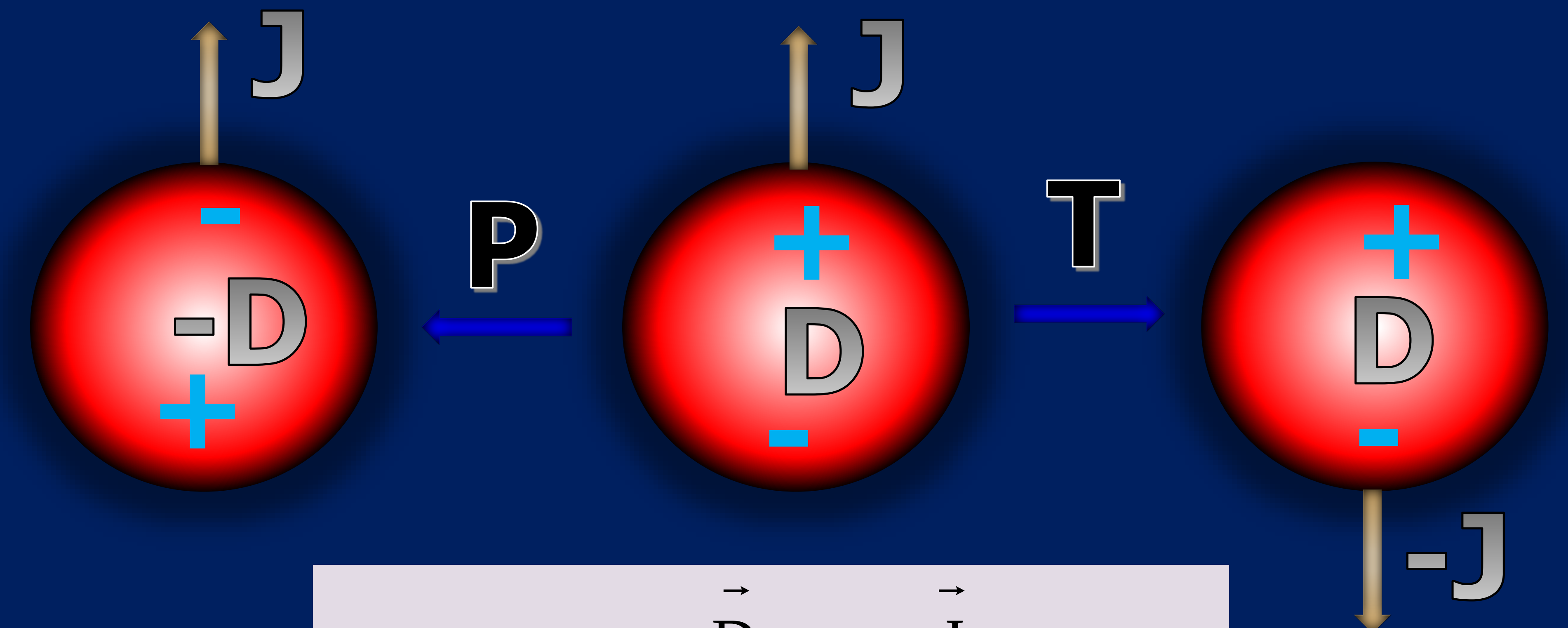
Sakharov's three conditions to explain baryogenesis:

(i) Baryon number violation

(ii) C and CP violation

(iii) Departure from thermal equilibrium

Finite EDM implies P & T violations

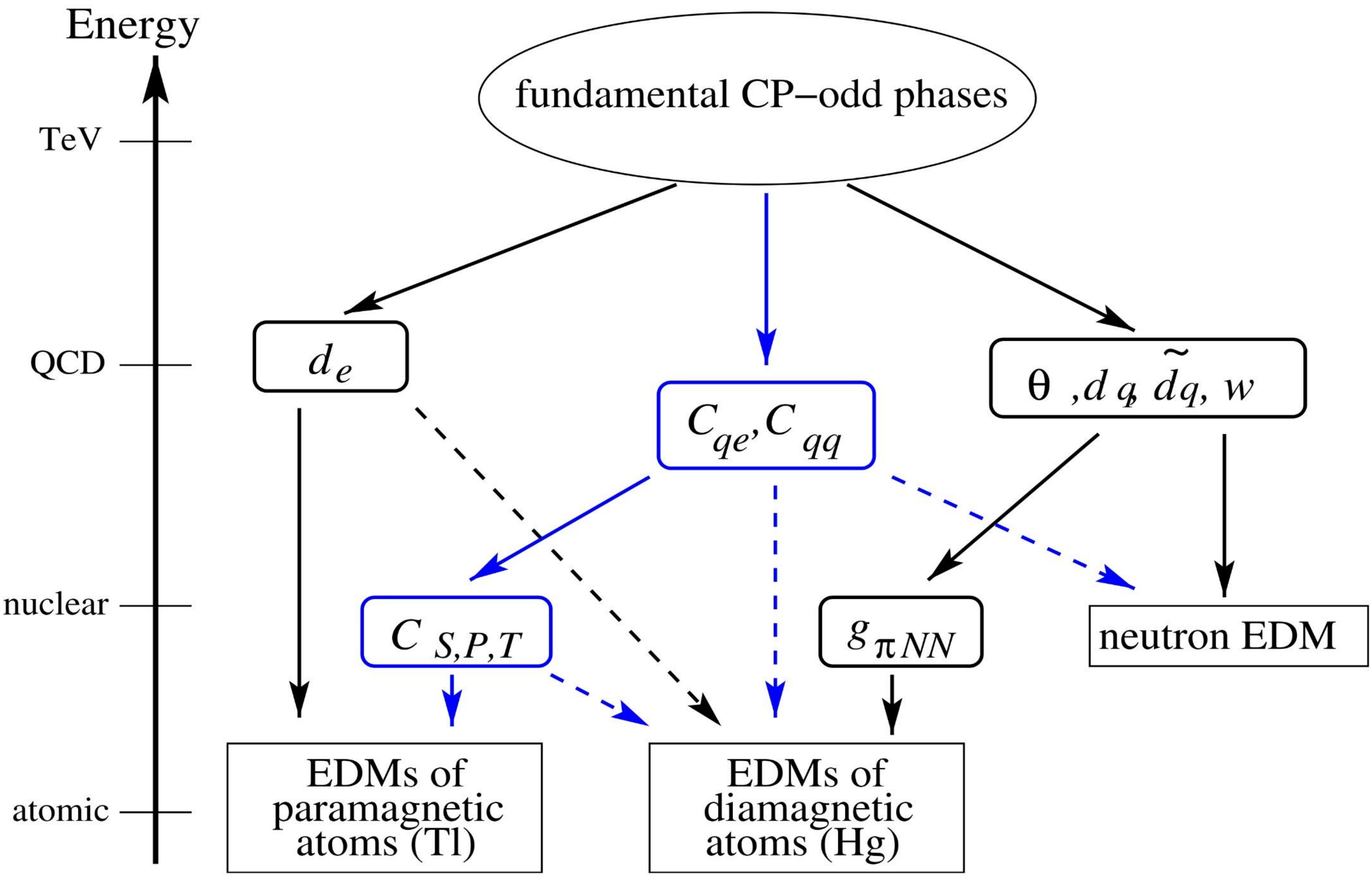


$$\vec{D} \quad \alpha \quad \vec{J}$$

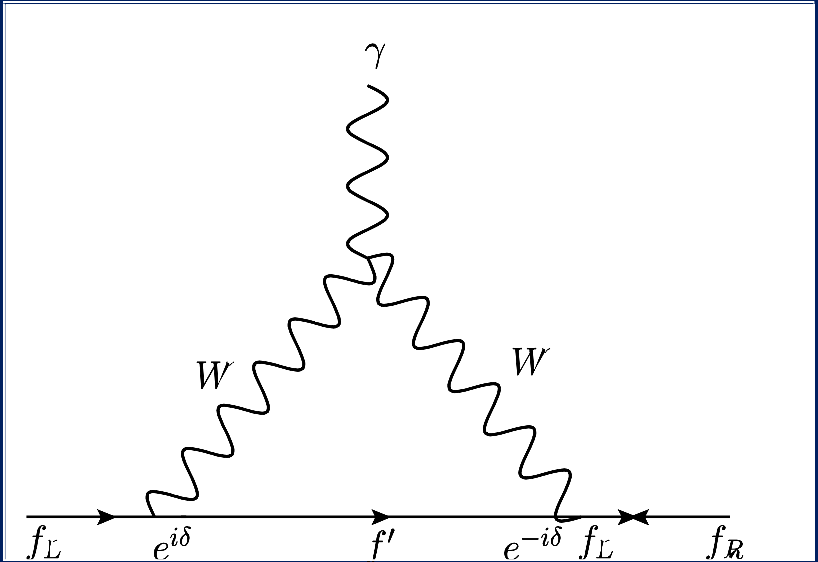
$$P: \qquad \vec{J} \rightarrow \vec{J} \qquad\qquad \vec{D} \rightarrow -\vec{D}$$

$$T: \qquad \vec{J} \rightarrow -\vec{J} \qquad\qquad \vec{D} \rightarrow \vec{D}$$

Sources of EDMs in atoms

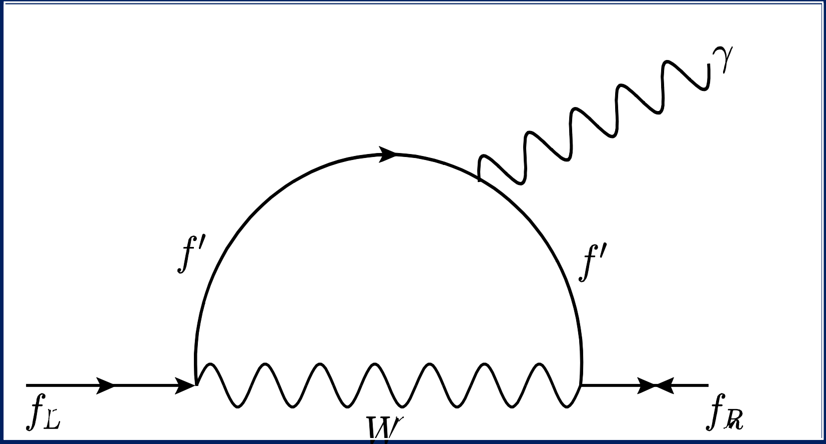


EDMs sensitive to beyond standard model (SM) physics

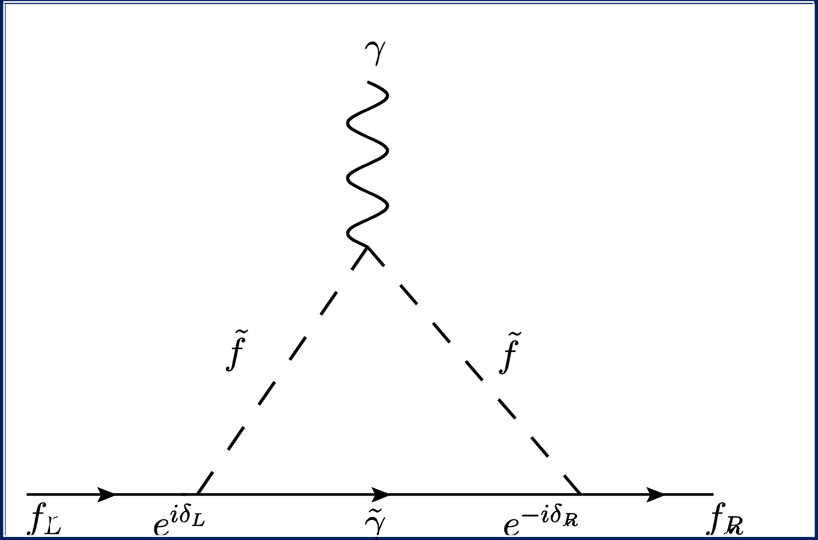


One phase factor

SM

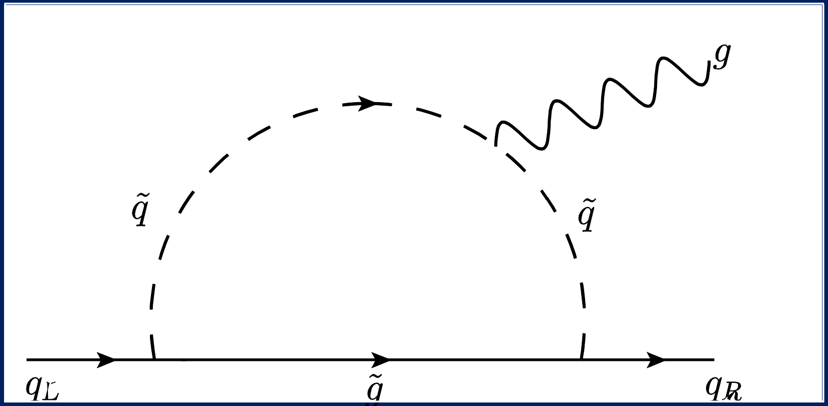


quark EDM



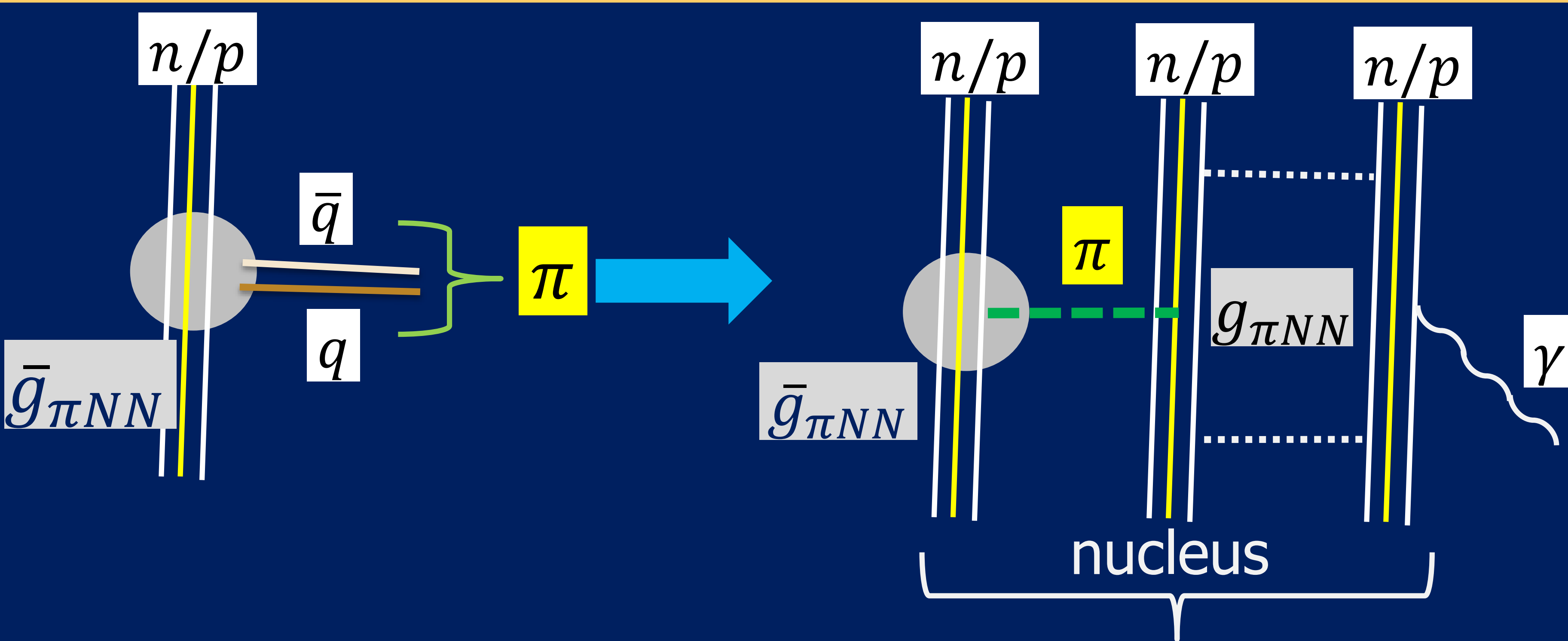
Extra phase factors

SUSY



quark chromo-EDM

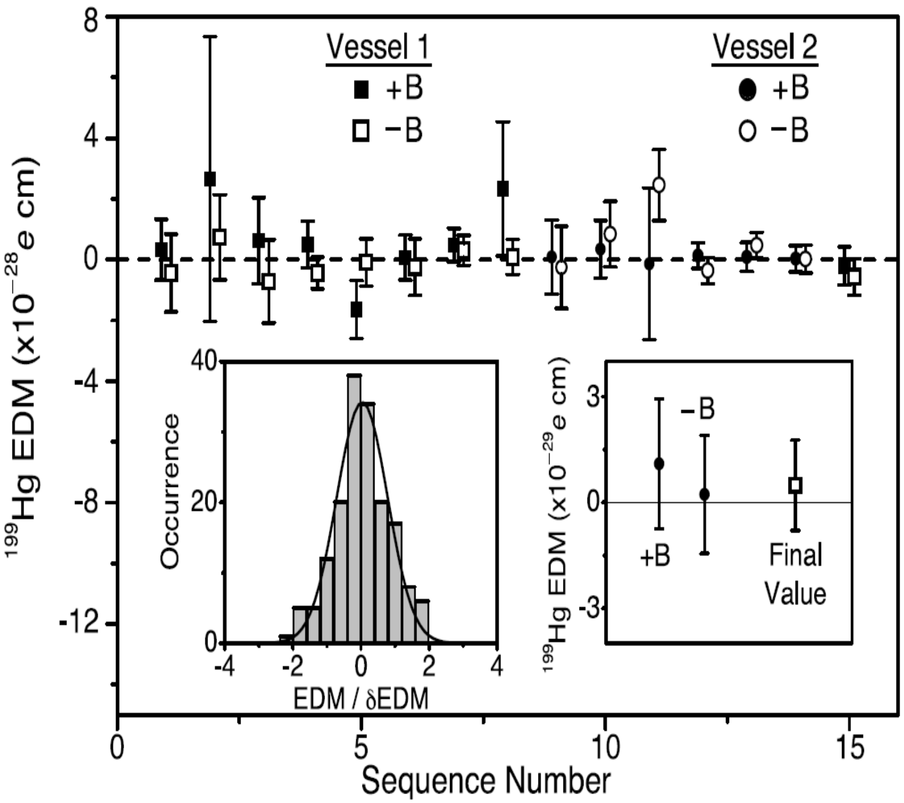
Nuclear EDM due to pion exchange

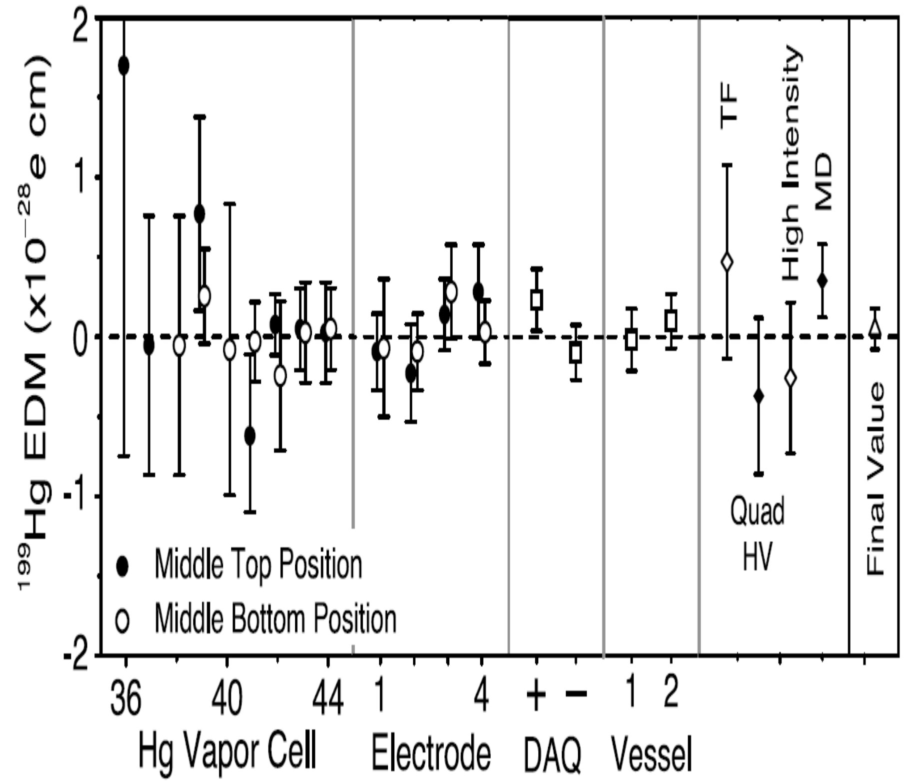


Possible sources:

a. **Higgsino contribution in SUSY**
b. **Higgs mediated two loop contributions**
c. **Large $tan\ \beta$ contribution**
d. **Neutrino Yukawa coupling contribution, etc.**

Experimental result for ^{199}Hg





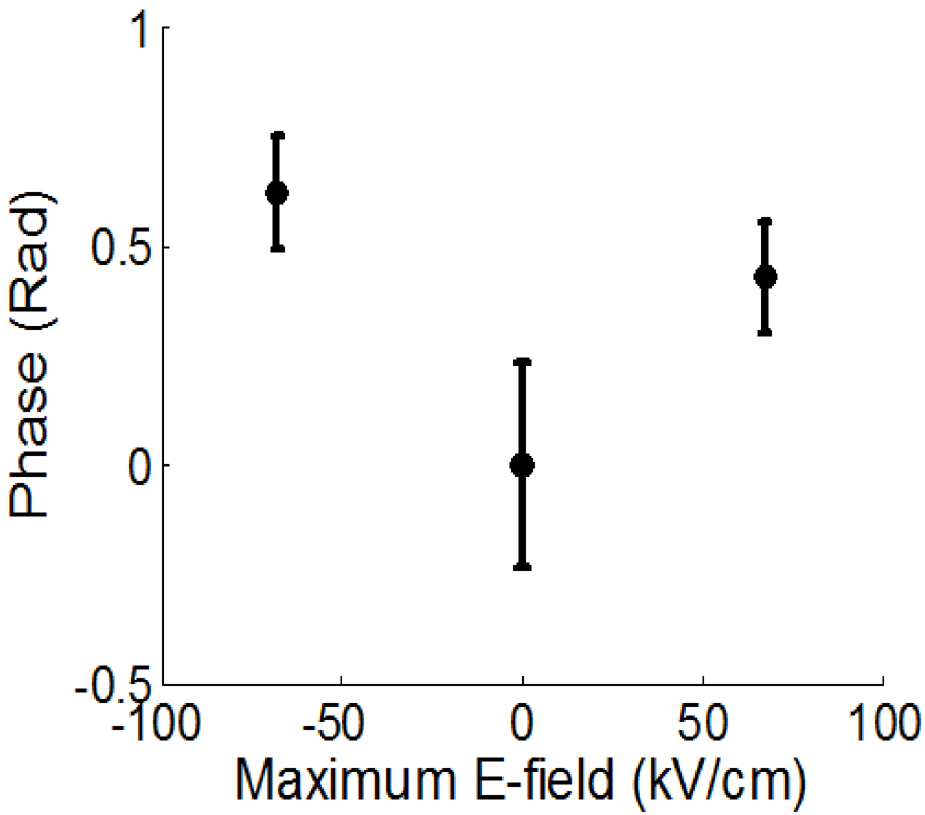
- $d(^{199}\mathrm{Hg}) = (0.49 \pm 1.29_{stat} \pm 0.76_{syst}) \times 10^{-29}\ e\,\mathrm{cm}$

  $\Rightarrow |d(^{199}\mathrm{Hg})| < 3.1 \times 10^{-29}$ e cm (95% C.L.)

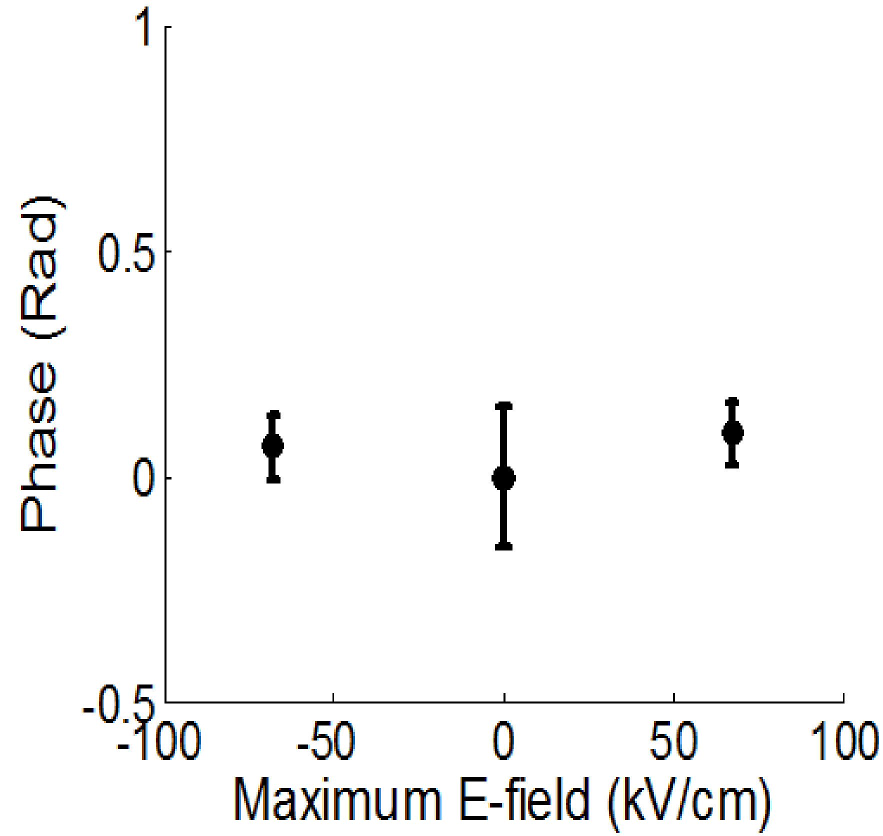
W. C. Griffith, M. D. Swallows, T. H. Loftus, M. V. Romalis, B. R. Heckel, E. N. Fortson
Phys. Rev. Lett. **102**, 101601 (2009).

Experimental result for ^{225}Ra

3 mCi Run (October 2014)



6 mCi Run (December 2014)



$d_{\text{E-squared syst}} \leq 0.5 \times 10^{-22}$ e-cm

$d_{\text{E-squared syst}} \leq 0.05 \times 10^{-22}$ e-cm

R. H. Parker, M. R. Dietrich, M. R. Kalita, N. D. Lemke, K. G. Bailey, M. Bishof, J. P. Greene, R. J. Holt, W. Korsch, Z. –T. Lu, P. Mueller, T. P. O'Connor and J. T. Singh, Phys. Rev. Lett. **114**, 233002 (2015).

Lagrangians of the interactions

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

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

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

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

Schiff theorem

$$H_{int}(r) = \int d^3r' \left[\frac{e\,\rho_q(r')}{|\vec{r}-\vec{r}'|} + \frac{\vec{d}_N \cdot \vec{\nabla}}{Z}\left(\frac{\rho_d(r')}{|\vec{r}-\vec{r}'|}\right)\right]$$

Multiple expansion: $$\frac{1}{|\vec{r}-\vec{r}'|} = \sum_l \frac{r_<^l}{r_>^{l+1}} P_l(\cos\theta)$$

To have P & T terms: $l = 1$ for the first term
and $l = 0$ for the second term

$$\Rightarrow H_{int}\,(r) = \int d^3r' \left[-e\,\rho_q(r')\left(\vec{r}' \cdot \vec{\nabla}\frac{1}{|\vec{r}|}\right) + \frac{\vec{d}_N \cdot \vec{\nabla}}{Z|\vec{r}|}\rho_d(r')\right]$$

For point nuclei; cancelation is exact.

Finite contributions

When: $l = 3$ for first term and $l = 2$ for second term

$$H_{int}(r) = -\frac{1}{6}\int d^3r'\, e\,\rho_q(r')\, r_i' r_j' r_k' \nabla_i \nabla_j \nabla_k \frac{1}{|\vec{r}|}$$

$$+\frac{\vec{d}_N \cdot \vec{\nabla}}{Z} \nabla_i \nabla_j \frac{1}{\vec{r}} \int d^3r' \;\; \rho_N(r') r_i r_j$$

$$\Rightarrow H_{int}\,(r) = H_{int}^{octupole}(r) \quad + \quad H_{int}^{Schiff}(r)$$

Finite when: $|\vec{I}| \geq 3/2$ for the first term
and $|\vec{I}| \geq 1/2$ for the second term

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

where $B = \int d^3\, r\, \rho_n(r) r^4$

Nuclear parameterization of NSM

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

$$\approx \left[\, b_1\, d_n + b_2 d_p\right]$$

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:

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

$$\bar{g}^{(1)}_{\pi NN} = 2 \times 10^{-12}\left(\tilde{d}_u - \tilde{d}_d\right)$$

and

$$\bar{g}^{(2)}_{\pi NN} \approx 0$$

Tensor-pseudotensor (T-PT) interaction in atoms

T-PT interaction between the quarks and electrons lead to the nucleon-electron T-PT interaction and EDM in atoms:

$$H_{TPT}^{e-q} = \frac{iG_F C_T^{e-q}}{\sqrt{2}} [\bar{\Psi}_q \, \sigma_{\mu\nu} \, \Psi_q \,][\bar{\Psi}_e \, \gamma^5 \, \sigma^{\mu\nu} \, \Psi_e]$$

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

$$= \frac{i\,G_F}{\sqrt{2}} \sum\nolimits_{N,e} C_T^{e-N} \left[\Psi_N^+ \, \vec{\alpha}_i \vec{\alpha}_j \Psi_\mathrm{N}\right]_{i\neq j} \left[\Psi_e^+ \, \vec{\alpha}_i \vec{\alpha}_j \Psi_\mathrm{e}\right]_{i\neq j}$$

$$= \frac{iG_F}{\sqrt{2}} \sum\nolimits_{e,N} \; C_T^{e-N} \left[\, i \;\; \Psi_N^+ \, \beta \, \epsilon_{ijk} \, \sigma_N^k \Psi_N\right] \left[\Psi_e^+ (-1) \epsilon^{ijk} \gamma_i \Psi_e\right]$$

$$= \; \sqrt{2} \, i \; G_F C_T \sum\nolimits_e \rho_N \, (r_e) \quad \vec{I}_N \cdot \, \vec{\gamma}_e$$

As in the non-relativistic limit:

$$\left(\alpha_i \alpha_j\right)_{i\neq j} \; = \; \left(\sigma_i \; \sigma_j\right)_{i\neq j} = i \; \epsilon_{ijk} \sigma^k = i \; \epsilon_{ijk} \, \gamma^5 \alpha^k$$

Calculations for Xe

	α_d	$D_a^{T-PT}(10^{-20}\langle\sigma\rangle C_T)$	$D_a^{NSM}\left(\frac{10^{-17}S}{\lvert e\rvert fm^3}\right)$
DF	26.918	4.485	2.459
MBPT(2)	23.388	3.927	2.356
MBPT(3)	18.693	4.137	2.398
RPA	26.987	5.400	3.331
LCCSD	27.484	5.069	3.055
CCSD	27.744	4.85	2.89
CCSDpT	27.78(5)	4.85(6)	2.89(4)
Experiment	27.815(27)		

Y. Singh, B. K. Sahoo and B. P. Das, Phys. Rev. A **89**, 050502(R) (2014).

$D_a^{expt} < 4.1 \times 10^{-27}\ e-cm$ Phys. Rev. Lett. **86**, 22 (2002).

Calculations for Rn

	α_d	$D_a^{T-PT}(10^{-20}\langle\sigma\rangle C_T)$	$D_a^{NSM}\ (\frac{10^{-17}S}{\lvert e\rvert fm^3})$
DF	34.42	4.485	2.459
MBPT(2)	29.57	3.927	2.356
MBPT(3)	18.10	4.137	2.398
RPA	35.00	5.400	3.331
LCCSD	35.08	5.069	3.055
CCSD	35.27	4.85	2.89
CCSDpT	35.28(9)	4.85(6)	2.89(4)

B. K. Sahoo Y. Singh and B. P. Das, Phys. Rev. A **90**, 050501(R) (2014).

Calculations for Hg

	α_d	$D_a^{T-PT}(10^{-20}\langle\sigma\rangle C_T)$	$D_a^{NSM}\left(\frac{10^{-17}S}{\lvert e\rvert fm^3}\right)$
DF	40.95	-2.39	-1.20
MBPT(2)	34.18	-4.48	-2.30
MBPT(3)	22.98	-3.33	-1.72
RPA	44.98	-5.89	-2.94
LCCSD	33.91	-4.52	-2.24
CCSD	34.98	-4.02	-2.00
CCSDpT	34.07(40)	-4.30(20)	-2.12(10)
CI+MBPT	32.99	-5.1	-2.6 (F & D 2009)
PRCC	33.59	-4.3	-5.07 (Latha et al 2009)
Experiment	33.91(34)		

Y. Singh and B. K. Sahoo, Phys. Rev. A **91**, 030501(R) (2015).

$D_a^{expt} < 3.1 \times 10^{-29}\ e - cm$ Phys. Rev. Lett. **102**, 101601 (2009).

Calculations for Ra

	α_d	$D_a^{T-PT}(10^{-20}\langle\sigma\rangle C_T)$	$D_a^{NSM}\left(\frac{10^{-17}S}{\vert e\vert fm^3}\right)$
DF	204.13	-3.46	-1.85
MBPT(2)	230.67	-11.00	-5.48
MBPT(3)	189.53	-10.59	-5.30
RPA	296.85	-16.66	-8.12
LCCSD	251.88	-13.84	-8.40
CCSD	247.76	-10.04	-6.79
CCSDpT	241.40(60)	-10.01(30)	-6.79(15)
CI+MBPT	229.9	-18.0	-8.8 (F & D)

Y. Singh and B. K. Sahoo, Phys. Rev. A **92,** 022502 (2015).

$D_a^{expt} < 5.0 \times 10^{-22}\ e - cm$ Phys. Rev. Lett. **114**, 233002 (2015).

Extracting limits

Experimental limit on Hg EDM is the best till date:

$D_a^{expt} < 3.1 \times 10^{-29}\, e - cm$ Phys. Rev. Lett. **102**, 101601 (2009).

Our calculations: Phys. Rev. A **91**, 030501(R) (2015)

$S < 3.1 \times 10^{-29}\, |e| fm^3$ **and** $C_T < 3.1 \times 10^{-29}$

Nuclear calculations: $S = [1.9\, d_n + 0.2\, d_p]$

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

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

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

In combination: $|\bar{\theta}| < 1.1 \times 10^{-9}$

$|\tilde{d}_u - \tilde{d}_d| < 2.8 \times 10^{-26}\, e - cm$ $d_n < 7.6 \times 10^{-26}\, e - cm$

Consequence due to small $\bar{\theta}$ value

The value of $\bar{\theta}$ can be between 0 and 2π. However, its extremely tiny value is due to some unknown reason.

With the symmetries of SM, it cannot be explained. This is known as Strong CP problem.

Plausible explanation:

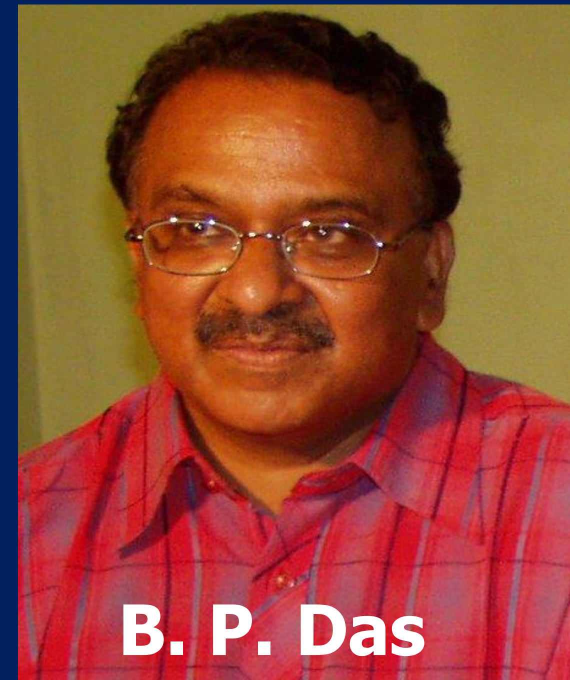
It may be due to extra contributions than known in SM such as possible existence of Axions which are predicted by beyond SM.

Summary and outlook

- Motivation to study EDM in the diamagnetic atoms are discussed.
- Origin of atom EDMs at the elementary level are mentioned.
- Dipole polarizabilities and EDMs due to both the T-PT and NSM interactions for the experimentally interested atoms are calculated accurately.
- Theoretical results can be further improved using a biorthogonal CC method.

Thank You

Acknowledgement



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Lagrangians of the interactions

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

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

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

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

P &T Violating Interaction Potential

A finite EDM of nucleus can manifest itself in the atom through interactions with the electrons.

The electron-nucleus interaction potential is given by:

$$H_{int}(r) = \int d^3r' \left[\frac{e\,\rho_q(r')}{|\vec{r} - \vec{r}'|} + \frac{\vec{d}_N \cdot \vec{\nabla}}{Z} \left(\frac{\rho_d(r')}{|\vec{r} - \vec{r}'|} \right) \right]$$

where $\int \rho_q(r) d^3r = Z$

and $\vec{d}_N = |\vec{d}_N| \frac{\vec{I}}{|\vec{I}|} = \int e\,\vec{r}\,\rho_d(r)\,d^3r$

Thus, $\rho_q(r_i)$ and $\rho_d(r_i)$ are the normalized electric charge and dipole moment densities of the nucleus.

Finite contributions

Next terms: $l = 3$ for the first term
and $l = 2$ for the second term

$$H_{int}(r) = -\frac{1}{6}\int d^3r'\, e\,\rho_q(r')\, r_i' r_j' r_k' \nabla_i \nabla_j \nabla_k \frac{1}{|\vec{r}|}$$

$$+\frac{\vec{d}_N\cdot\vec{\nabla}}{Z}\nabla_i \nabla_j \frac{1}{\vec{r}}\int d^3r' \;\; \rho_N(r') r_i r_j$$

$$\Rightarrow H_{int}\,(r) = H_{int}^{octupole}(r) \quad + \quad H_{int}^{Schiff}(r)$$

Finite when: $|\vec{I}| \geq 3/2$ for the first term
and $|\vec{I}| \geq 1/2$ for the second term

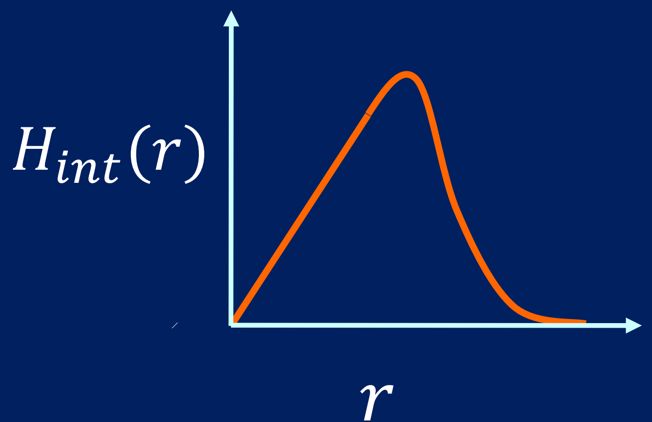
Enhancements: (a) Finite size nucleus
(b) Relativistic effects

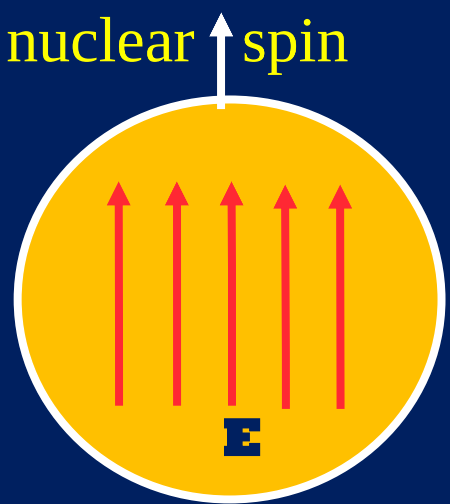
$\Big\}$ **Heavy atoms**

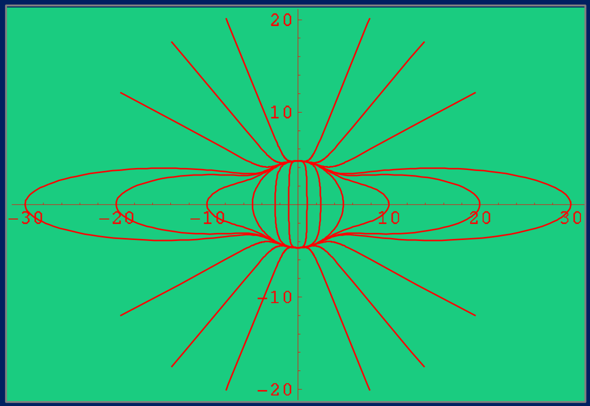
Electric field due to NSM

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

$$= \frac{\vec{S}\cdot\vec{r}}{B}\,\rho_n(r) \qquad \text{where} \quad B = \int d^3r\,\rho_n(r)r^4$$







$$H_{int}(r_i) = -\vec{d}_i\cdot\vec{E}(r_i) \qquad \text{Thusly,} \quad \left[\frac{\vec{d}_i\cdot\vec{\nabla}_i}{q_i}, H_{atom}\right] = 0$$

Kinetic energy commutes with the $\vec{\nabla}$ operator: $\langle H_{int}(r_i)\rangle = 0$

EDM of an atomic state

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

$$= \frac{2}{\left\langle \Psi_n^{(0)} \middle| \Psi_n^{(0)} \right\rangle}\left[\sum_{k \neq n} \frac{\left\langle \Psi_n^{(0)} \middle| D \middle| \Psi_k^{(0)} \right\rangle \left\langle \Psi_k^{(0)} \middle| H_{int} \middle| \Psi_n^{(0)} \right\rangle}{E_n^{(0)} - E_k^{(0)}}\right]$$

$R = S$ or $R = \langle \sigma_n \rangle C_T$

Accuracy test: $H_{int} \equiv D \Rightarrow \alpha_n$

Bloch's prescription

According to the Bloch's prescription, the Fock space is divided into model (P) and orthogonal (Q) space.

$$P = |\Phi_0\rangle\langle\Phi_0| \qquad \text{and} \qquad Q = 1 - P$$

$$|\Psi\rangle = \Omega \; |\Phi_0\rangle$$

In perturbation approach:

$$\Omega = \Omega^{(0)} + \Omega^{(1)} + \Omega^{(2)} + \cdots = \sum_n \Omega^{(n)} \qquad \text{with} \quad \Omega^{(0)} = 1$$

Amplitude solving equation:

$$[\Omega^{(k)}, H_0]P = QV\,\Omega^{(k-1)}P - \sum_{m=1}^{(k-m)} PV_{int}\,\Omega^{(k-1)}\,P$$

Energy equation: $H^{eff} = PH\Omega P \; = P\,(H_0 + V_{int})\Omega P$

Double sources of perturbation

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

Let wave function is approximated as

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

In perturbation approach for this case:

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

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

Amplitude equation:

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

All order many-body methods

Random phase approximation (RPA):

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

Configuration interaction (CI) method:

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

Coupled-cluster (CC) method:

$$\begin{aligned}\left|\Psi_n^{(0/1)}\right\rangle &= C_0|\Phi_n\rangle + C_I\,|\Phi_I\rangle + C_{II}\,|\Phi_{II}\rangle + \cdots \\ &= |\Phi_n\rangle + T_I\,|\Phi_n\rangle + T_{II}\,|\Phi_n\rangle + \frac{1}{2}\,T_I^2\,|\Phi_n\rangle + \cdots \\ &= e^{T_I+T_{II}+\cdots}\,|\Phi_n\rangle = e^{T}\,|\Phi_n\rangle\end{aligned}$$

Advantage of truncated CC method over truncated CI method

EDM and polarizability calculations

MBPT(n) method:

$$X = 2 \frac{\sum_{k=0}^{m=k+1,n} \left\langle \Phi_0 \middle| \Omega^{(m-k-1,0)+} D \Omega^{(k,1)} \middle| \Phi_0 \right\rangle}{\sum_{k=0}^{m=k+1,n-1} \left\langle \Phi_0 \middle| \Omega^{(m-k-1,0)+} \Omega^{(k,0)} \middle| \Phi_0 \right\rangle}$$

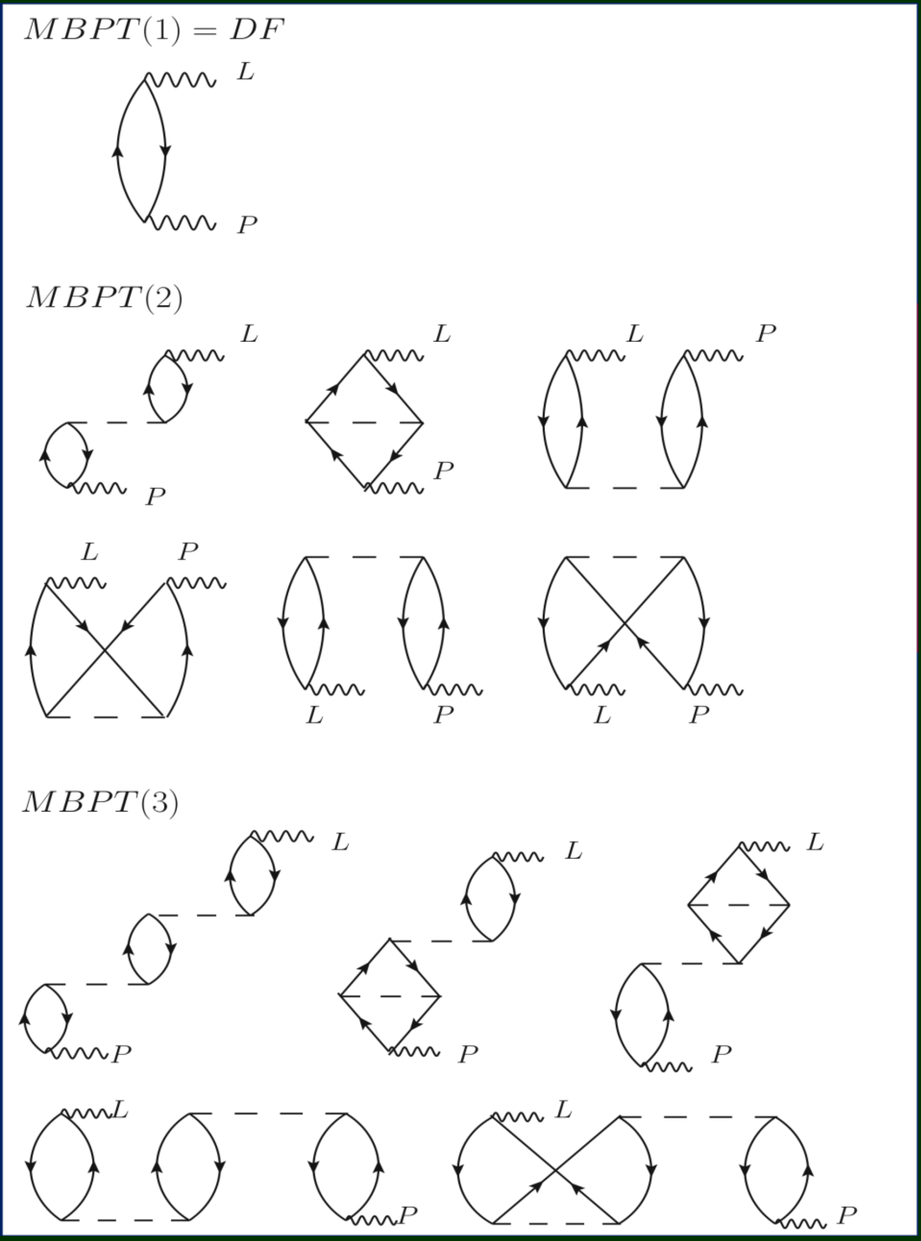
RPA method:

$$X = 2 \left\langle \Phi_0 \middle| \Omega^{(0,0)+} \mathrm{D} \Omega_{RPA}^{(1)} \middle| \Phi_0 \right\rangle = \left\langle \Phi_0 \middle| \mathrm{D} \Omega_{RPA}^{(1)} \middle| \Phi_0 \right\rangle$$

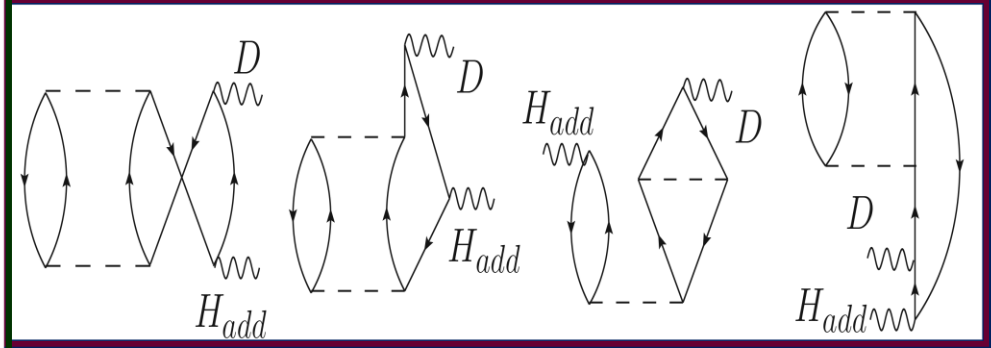
CC method:

$$X = 2 \left\langle \Phi_0 \middle| \left[e^{T^{(0)}+} D e^{T^{(0)}} \right] T^{(1)} \middle| \Phi_0 \right\rangle$$

MBPT(n) method



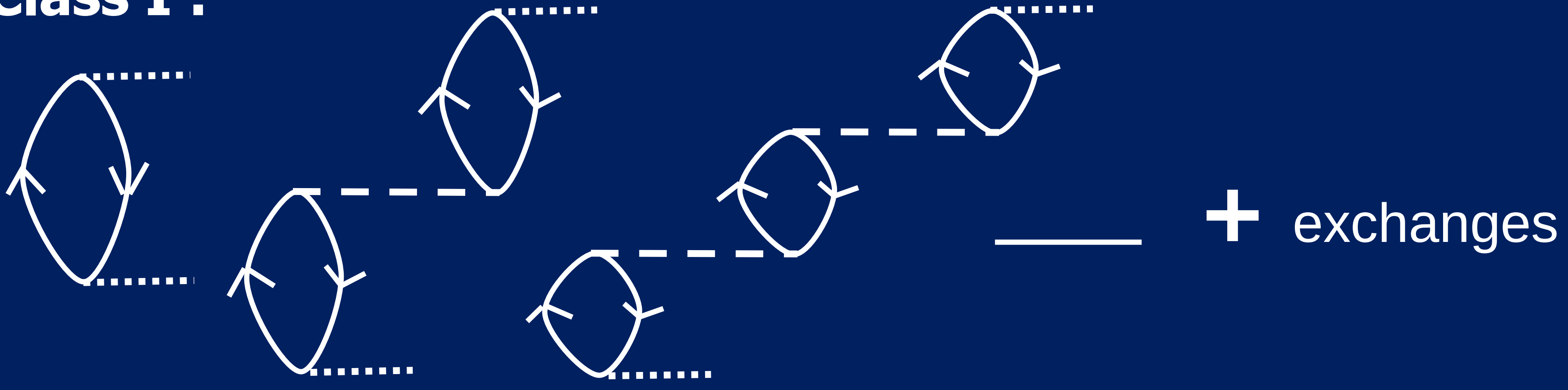
Non-core polarized diagrams:



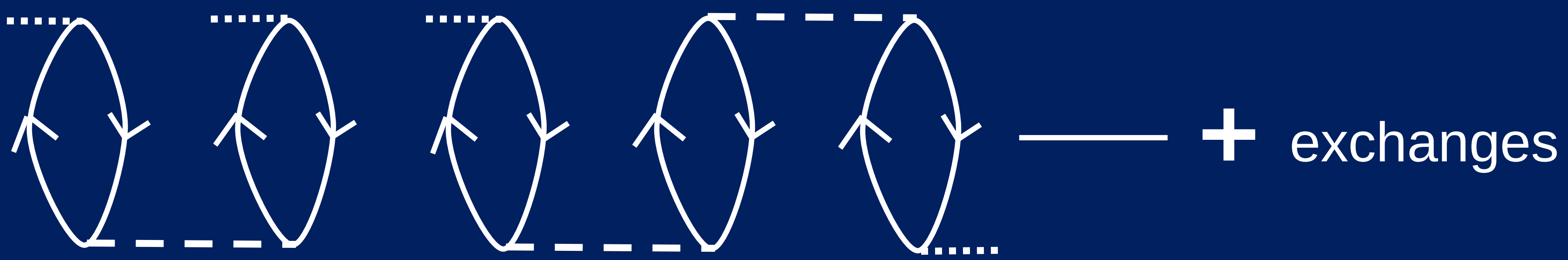
More than 120 diagrams in MBPT(3)

RPA/CPHF/TDF diagrams

Class I :



Class II :



Non-CP correlation contributions are missing.

Intermediate contributions

Y. Singh, B. K. Sahoo and B. P. Das, Phys. Rev. A 89, 030502(R) (2014).

TABLE III: Contributions from various matrix elements and from various angular momentum symmetry groups at the DF, lowest order CPHF (denoted by MBPT(l-CPHF)), CPHF and CCSD$_p$T methods to the α in ea_0^3, $\bar{\eta} = 10^{20} \times \eta$ and $\bar{\zeta} = 10^{17} \times \zeta$ values. Here the summation indices n and m represent for the occupied and unoccupied orbitals, respectively.

Excitation(s)	DF			MBPT(l-CPHF)			CPHF			CCSD$_p$T		
$(a \to p)$	α	$\bar{\eta}$	$\bar{\zeta}$	α	$\bar{\eta}$	$\bar{\zeta}$	α	$\bar{\eta}$	$\bar{\zeta}$	α	$\bar{\eta}$	$\bar{\zeta}$
$5p_{1/2} - 7s$	0.248	0.030	0.007	0.336	0.056	0.016	0.380	0.062	0.016	0.352	0.050	0.014
$5p_{1/2} - 8s$	0.517	0.090	0.022	0.690	0.159	0.045	0.769	0.172	0.045	0.733	0.145	0.039
$5p_{1/2} - 9s$	0.237	0.106	0.025	0.284	0.166	0.044	0.301	0.174	0.044	0.309	0.157	0.041
$5p_{3/2} - 7s$	0.844	$\sim$0	0.015	1.136	0.005	0.036	1.314	0.007	0.036	1.202	0.001	0.031
$5p_{3/2} - 8s$	1.558	$\sim$0	0.043	2.056	0.014	0.093	2.351	0.018	0.093	2.261	0.024	0.082
$5p_{3/2} - 9s$	0.583	$\sim$0	0.044	0.678	0.012	0.081	0.745	0.015	0.081	0.809	0.017	0.076
$5p_{1/2} - 7d_{3/2}$	2.267	$\sim$0	$\sim$0	2.200	−0.003	−0.008	2.407	−0.006	−0.008	2.259	−0.011	−0.008
$5p_{1/2} - 8d_{3/2}$	3.454	$\sim$0	$\sim$0	2.595	−0.013	−0.020	2.882	−0.022	−0.020	2.925	−0.028	−0.018
$5p_{3/2} - 7d_{5/2}$	5.667	$\sim$0	$\sim$0	5.747	−0.027	−0.018	6.365	−0.039	−0.018	5.827	−0.031	−0.018
$5p_{3/2} - 8d_{5/2}$	7.054	$\sim$0	$\sim$0	5.749	−0.048	−0.037	6.267	−0.071	−0.037	6.207	−0.057	−0.035