Electric Dipole Moments of atomic Yb and Ra

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Many-body Hamiltonian

The relativistic many-body atomic Hamiltonian in the Born-Oppenheimer approximation is

$$H = \sum_i c\alpha_i \cdot p_i + \beta_i m_i c^2 + \sum_{i<j} \frac{e^2}{r_{ij}}$$

where α_i and β_i are the Dirac matrices, the last term is the electron-electron repulsion term and p_i is the momentum of the ith electron.

In the Hartree-Fock formalism,

$$H = \sum_i c\alpha_i \cdot p_i + \beta_i m_i c^2 + \sum_i U_{\mathrm{HF}}(r_i) + \underbrace{\left(\sum_{i<j} \frac{e^2}{r_{ij}} - \sum_i U_{\mathrm{HF}}(r_i) \right)}_{V_{es}}$$

$U_{\mathrm{HF}}(r)$ is the Hartree-Fock/Dirac-Fock potential

Hartree-Fock formalism

The Hartree-Fock equations are

$$\underbrace{\left(\sum_i c\alpha_i \cdot p_i + \beta_i m_i c^2 + \sum_i U_{\mathrm{HF}}(r_i)\right)}_{h_{\mathrm{HF}}} |\psi_a\rangle = \epsilon_a |\psi_a\rangle$$

where $|\psi_a\rangle$ are the single-electron wavefunctions that makeup the atom and ϵ_a are their energies. The potential $U_{\mathrm{HF}}(r_i)$ represents the average Coulomb interaction of an electron a with the other electrons in the atom.

- Effects of residual Coulomb interaction are treated as perturbations to the Hartree-Fock Hamiltonian.
- If atom has a non-zero EDM, the EDM interaction is treated as a perturbation in addition to V_{es}.

Slater-determinant formed from single-electron orbitals,

$$|\Psi\rangle = \frac{1}{N!}\begin{vmatrix} \psi_a(\boldsymbol{r}_1) & \psi_a(\boldsymbol{r}_2) & \psi_a(\boldsymbol{r}_3) & \cdots \\ \psi_b(\boldsymbol{r}_1) & \psi_b(\boldsymbol{r}_2) & \psi_b(\boldsymbol{r}_3) & \cdots \\ \psi_c(\boldsymbol{r}_1) & \psi_c(\boldsymbol{r}_2) & \psi_c(\boldsymbol{r}_3) & \cdots \\ \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots \end{vmatrix} \quad (1)$$

Dipole moment as an expectation value

The quantum mechanical definition of atomic EDM

$$D_a = \frac{\langle\tilde{\Psi}|\mathbf{D}|\tilde{\Psi}\rangle}{\langle\tilde{\Psi}|\tilde{\Psi}\rangle}$$

where D = e r is the electric dipole operator, expectation value of which is calculated with exact atomic wavefunctions.

where $|\tilde{\Psi}\rangle$ are the perturbed atomic exact states, given by

$$|\tilde{\Psi}\rangle = |\Psi_0\rangle + \lambda|\Psi_1\rangle$$

Then,

$$D_a/\lambda = \frac{\langle\Psi_0|\vec{D}|\Psi_1\rangle\langle\Psi_1|\vec{D}|\Psi_0\rangle}{\langle\Psi_0|\Psi_0\rangle}$$

Perturbed HF theory

A many-body atomic state is the Slater determinant of single-electron orbitals.

Hamiltonian perturbed by V_{es} as well as H_{EDM} is,

$$H' = H + \lambda H_{\text{EDM}}$$

where H_{EDM} may be due to any P, T violating interaction. The wavefunctions also get modified to

$$|\tilde{\psi}_a\rangle = |\psi_a^0\rangle + \lambda|\psi_a^1\rangle$$

Substitute them in the perturbed equation,

$$\left(h^0 + g^0 - \epsilon_a^0\rangle\right) |\psi_a^1\rangle = \left(-h_{\text{EDM}} - g^1\right) |\psi_a^0\rangle$$

This is the final form of the perturbed HF equation.

$$g^0|\psi_a^0\rangle = \sum_b \left[\langle\psi_b^0|v|\psi_b^0\rangle|\psi_a^0\rangle - \langle\psi_b^0|v|\psi_a^0\rangle|\psi_b^0\rangle\right]$$

HF
potential

The perturbed HF operator is

$$g^1|\psi_a^0\rangle = \sum_b \left[\langle\psi_b^0|v|\psi_b^1\rangle|\psi_a^0\rangle - \langle\psi_b^0|v|\psi_a^0\rangle|\psi_b^1\rangle\right] + \sum_b \left[\langle\psi_b^1|v|\psi_b^0\rangle|\psi_a^0\rangle - \langle\psi_b^1|v|\psi_a^0\rangle|\psi_b^0\rangle\right]$$

Contd..

Expand the perturbed wavefunctions in terms of a complete set of unperturbed wavefunctions,

$$|\psi_a^1\rangle = \sum_p C_{pa} |\psi_p^0\rangle$$

C's are the mixing coefficients determined by solving perturbed HF equations.

Projecting the above equation by $\langle\psi_m^0|$,

$$\sum_p \langle\psi_m^0|\left(h^0 + g^0 - \epsilon_a^0\right)|\psi_p^0\rangle C_{pa} = \langle\psi_m^0|\left(-h_{\mathrm{EDM}} - g^1\right)|\psi_a^0\rangle$$

Substituting g^1 and expanding $|\psi_b^1\rangle = \sum_q C_{qb}|\psi_q^0\rangle$, the mixing coefficients are solutions of the linear alegebraic equations

$$C_{pa}\left(\epsilon_p^0 - \epsilon_a^0\right) + \sum_{bq}\left[\left(\langle pq|v|ab\rangle - \langle pq|v|ba\rangle\right)C_{qb}^*\right]$$

$$+\left[\left(\langle pb|v|aq\rangle - \langle pb|v|qa\rangle\right)C_{qb}\right] + \langle p|h_{\mathrm{EDM}}|a\rangle = 0$$

The zeroth order contribution

$$C_{pa}^{(0,1)} = -\frac{\langle p|h_{\mathrm{EDM}}|a\rangle}{\left(\epsilon_p^0 - \epsilon_a^0\right)}$$

These equations can be represented as a set of linear matrix equations,

$$\sum_{qb} A_{pa\ qb} C_{qb} = -B_{pa}$$

where

$$A_{pa\ qb} = \tilde{V}_{pq,ab} + \tilde{V}_{pb,aq} + \left(\epsilon_p^0 - \epsilon_a^0\right) \delta_{pq} \delta_{ab}$$

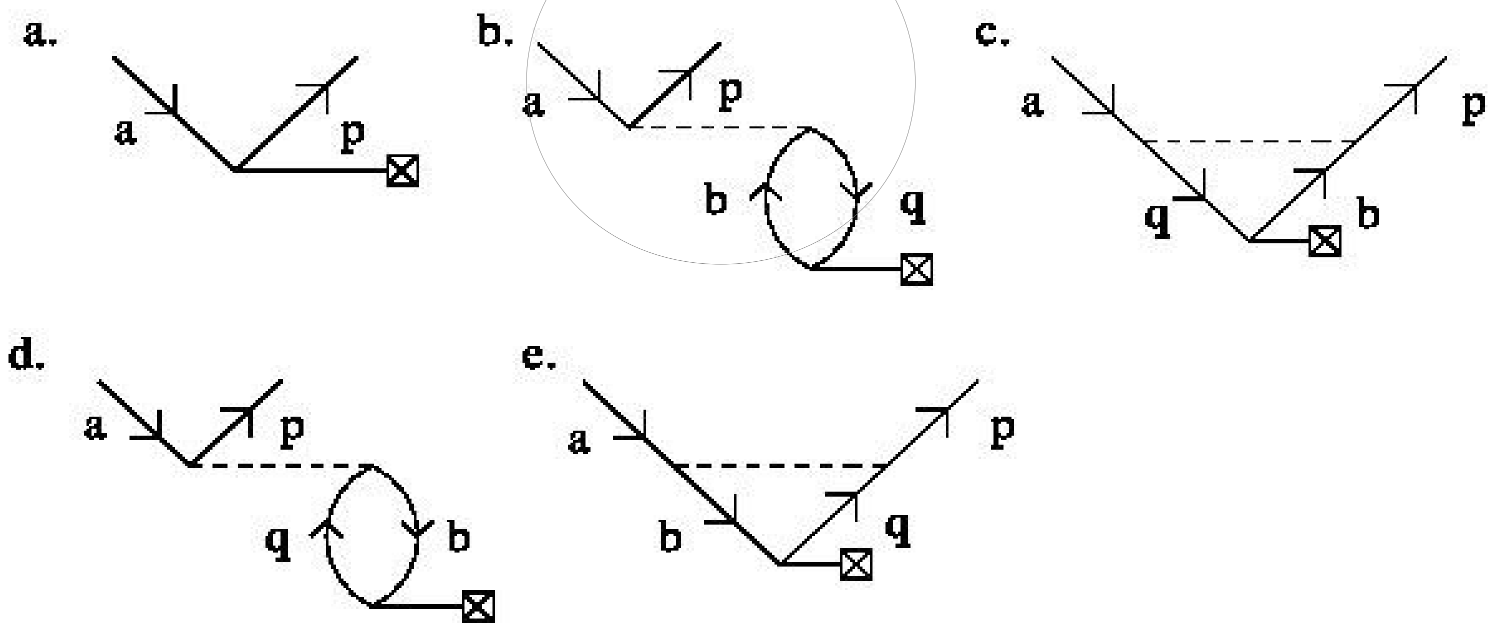
and

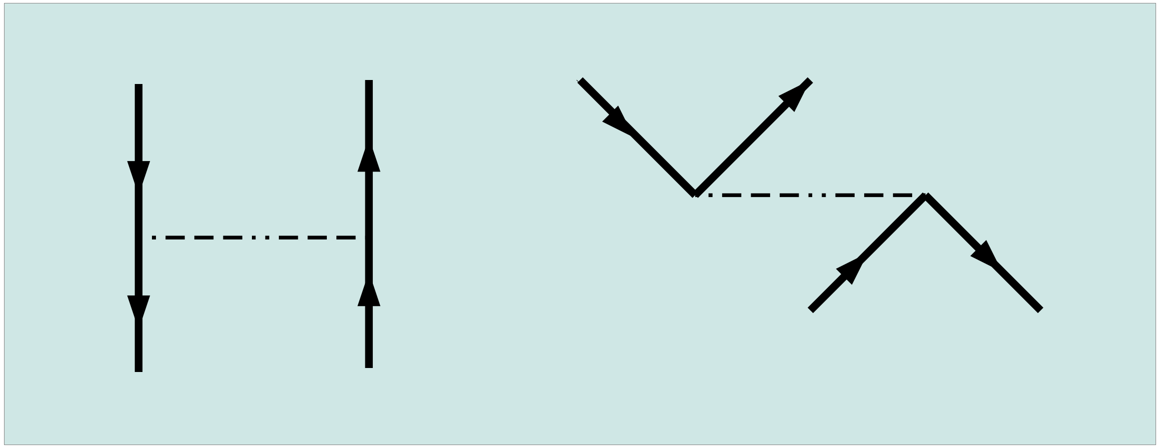
$$B_{pa} = \langle p | h_{\mathrm{EDM}} | a \rangle$$

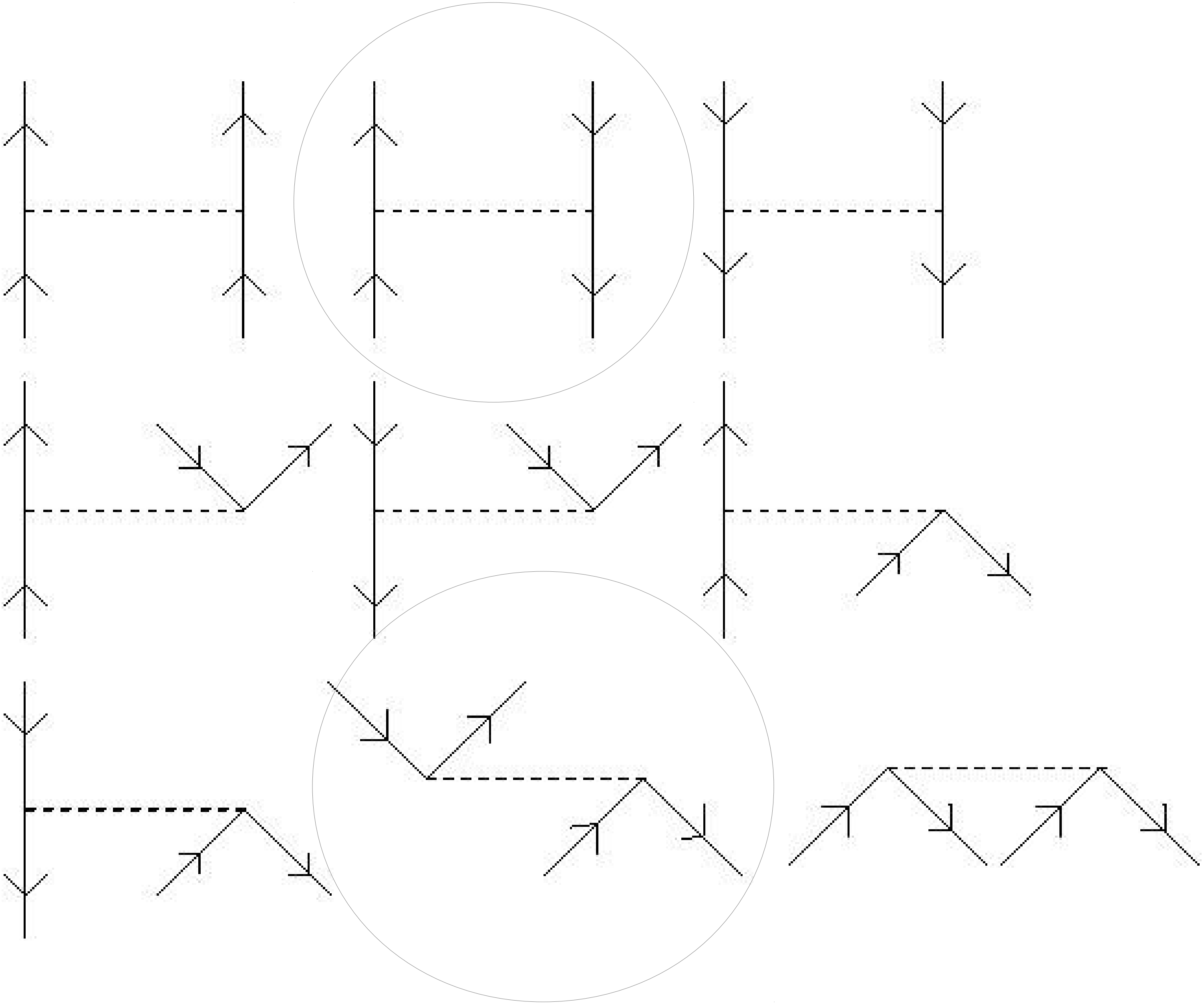
In the perturbed HF framework, the atomic EDM is

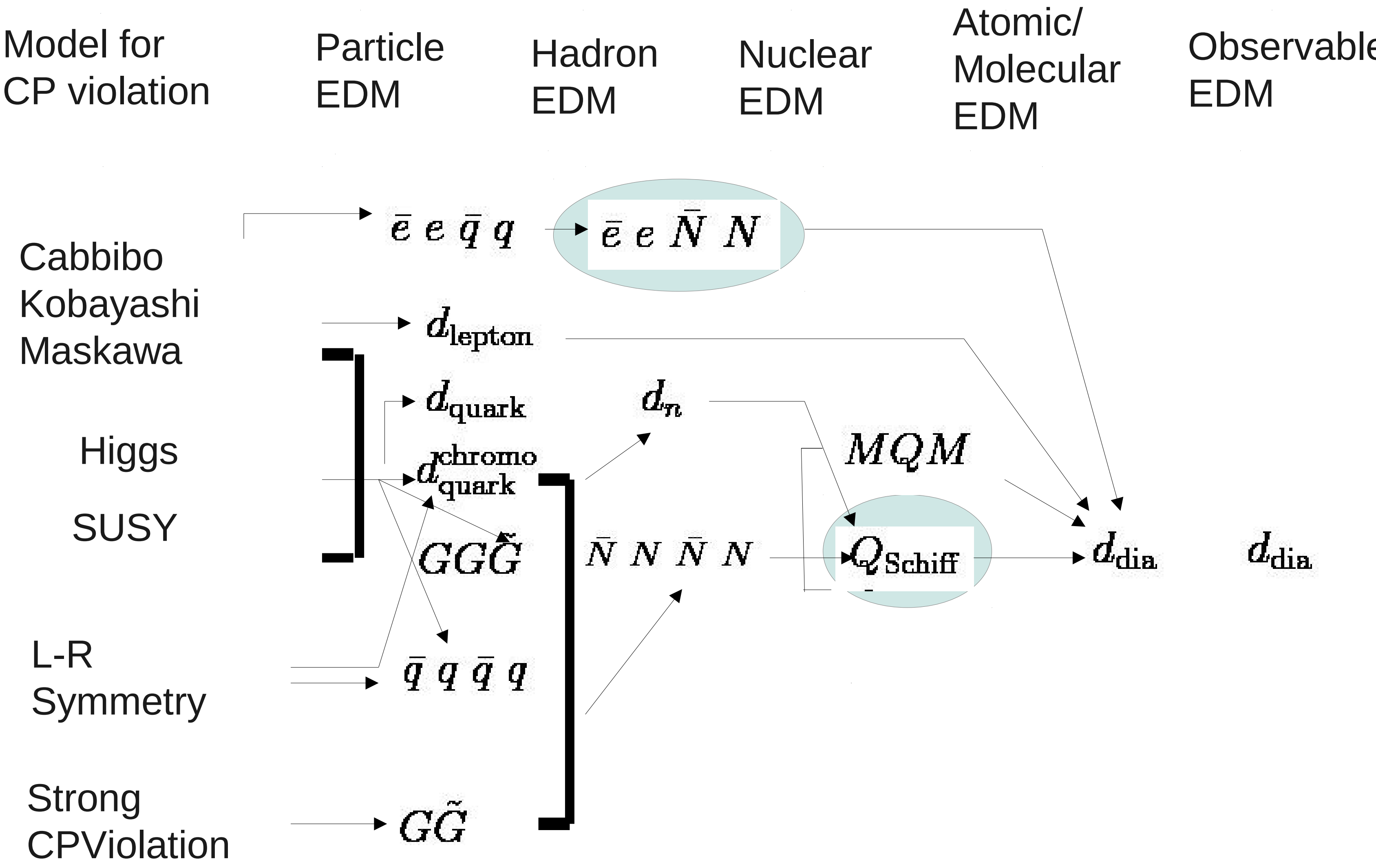
$$D_a = \sum_{ap} \langle a | d | p \rangle C_{pa}^{(\infty,1)} + C_{pa}^{*,(\infty,1)} \langle p | d | a \rangle$$

Perturbed HF diagrams








Model for CP violation
Particle EDM
Hadron EDM
Nuclear EDM
Atomic/ Molecular EDM
Observable EDM
Cabbibo Kobayashi Maskawa
Higgs
SUSY
L-R Symmetry
Strong CPViolation
$\bar{e}\ e\ \bar{q}\ q$
$\bar{e}\ e\ \bar{N}\ N$
d_{lepton}
d_{quark}
$d_{\text{quark}}^{\text{chromo}}$
$GG\tilde{G}$
$\bar{q}\ q\ \bar{q}\ q$
$G\tilde{G}$
d_n
$\bar{N}\ N\ \bar{N}\ N$
MQM
Q_{Schiff}
d_{dia}
d_{dia}

Tensor-pseudotensor EDM interaction

$H_{T\text{-}PT} = \bar{N}\sigma^{\mu\nu}N \cdot \bar{e}\sigma_{\mu\nu}\gamma^5 e$ (T-PT - tensor-pseudotensor)

$$H_{\mathrm{EDM}} = iC_T G_F \sqrt{(2)} \sum_i (\gamma_i \cdot I)\, \rho_N(r)$$

where $\rho_N(r)$ is the nuclear density, I is the nuclear spin, C_T is the T-PT coupling constant and G_F is the Fermi coupling constant.

THEORY

D_{atom}/C_T

EXPERIMENTS

D_{atom}

C_T, S, C_S

${}_{70}Yb^{171}$:

$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 4p^6\ 3d^{10}\ 5s^2\ 5p^6\ 4d^{10}\ 4f^{14}\ 6s^2$

${}_{54}Xe^{129}$:

$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 4p^6\ 3d^{10}\ 5s^2\ 4d^{10}\ 5p^6$

${}_{88}Ra^{225}$:

$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 4p^6\ 3d^{10}\ 5s^2\ 4d^{10}\ 5p^6\ 4d^{10}\ 4f^{14}\ 6s^2\ 6p^6\ 5d^{10}\ 7s^2$

EDM results for Yb and Ra

Tensor-pseudotensor electron-nuclear interaction

System	Zeroth order EDM in units of 10^{-20} $C_T \sigma\, e$cm	All-order EDM in units of 10^{-20} $C_T \sigma\, e$ cm
Ytterbium	-0.71	- 3.38
Xenon	0.45	0.56
Radium	-3.47	-16.59
Mercury	-2.38	- 5.85

EDM arising from Schiff moment

System	Zeroth order EDM in units of 10^{-17} S/(e fm^3) e cm	All-order EDM in units of 10^{-17} S/(e fm^3) e cm
Ytterbium	-0.42	-1.91
Xenon	0.29	0.38
Radium	-1.84	-8.09
Mercury	-1.19	-2.91

Conclusions

- Perturbed HF is one of the important milestones in many-body calculations.
- Calculations with more accurate theories of EDM have shown that beyond the HF level, the perturbed HF gives a substantial contribution
- Perturbed HF captures only selected effects arising from the residual Coulomb interaction.
- More effects of Coulomb interaction need to be incorporated through coupled-cluster kind of methods.