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 $\alpha_i$ and $\beta_i$ are the Dirac matrices, the last term is the electron-electron repulsion term and $p_i$ is the momentum of the $i$th electron.

In the Hartree-Fock formalism,

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

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

The Hartree-Fock equations are

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

where $\left| \psi_a \right\rangle$ are the single-electron wavefunctions that makeup the atom and $\epsilon_a$ are their energies. The potential $U_{HF}(r_i)$ 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,

\[ |\Psi\rangle = \frac{1}{N!} \begin{vmatrix} \psi_a(r_1) & \psi_a(r_2) & \psi_a(r_3) & \cdots \\ \psi_b(r_1) & \psi_b(r_2) & \psi_b(r_3) & \cdots \\ \psi_c(r_1) & \psi_c(r_2) & \psi_c(r_3) & \cdots \\ \vdots & \vdots & \vdots & \ddots \\ \vdots & \vdots & \vdots & \ddots \end{vmatrix} \quad (1) \]
Dipole moment as an expectation value

The quantum mechanical definition of atomic EDM

\[ D_a = \frac{\langle \tilde{\Psi} | D | \tilde{\Psi} \rangle}{\langle \tilde{\Psi} | \tilde{\Psi} \rangle} \]

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,

\[ \frac{D_a}{\lambda} = \frac{\langle \Psi_0 | \tilde{D} | \Psi_1 \rangle \langle \Psi_1 | \tilde{D} | \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle} \]
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,

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

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

$$|\tilde{\psi}_a\rangle = |\psi_0^a\rangle + \lambda |\psi_1^a\rangle$$

Substitute them in the perturbed equation,

$$(h^0 + g^0 - \epsilon^0_a) |\psi_1^a\rangle = (-h_{EDM} - g^1) |\psi_0^a\rangle$$

This is the final form of the perturbed HF equation.
The perturbed HF operator is

\[ g^1 |\psi^0_a\rangle = \sum \left[ \langle \psi^0_{b^*} | v | \psi^1_{b^*} \rangle |\psi^0_a\rangle - \langle \psi^0_{b^*} | v | \psi^0_a \rangle |\psi^1_{b^*}\rangle \right] \]

\[ + \sum \left[ \langle \psi^1_{b^*} | v | \psi^0_{b^*} \rangle |\psi^0_a\rangle - \langle \psi^1_{b^*} | v | \psi^0_a \rangle |\psi^0_{b^*}\rangle \right] \]
Expand the perturbed wavefunctions in terms of a complete set of unperturbed wavefunctions,

\[ |\psi_1^a\rangle = \sum_p C_{p\alpha} |\psi_p^0\rangle \]

C's are the mixing coefficients determined by solving perturbed HF equations.
Projecting the above equation by $\langle \psi_m^0 |$, 

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

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 algebraic equations

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

$$+ \left[ (\langle pq | v | ab \rangle - \langle pq | v | ba \rangle) C_{qb} \right] + \langle p | h_{EDM} | a \rangle = 0$$

The zeroth order contribution

$$C_{pa}^{(0,1)} = -\frac{\langle p | h_{EDM} | a \rangle}{(\epsilon_p^0 - \epsilon_a^0)}.$$
These equations can be represented as a set of linear matrix equations,

\[ \sum_{q_b} A_{pa \ q_b} C_{q_b} = -B_{pa} \]

where

\[ A_{pa \ q_b} = \tilde{V}_{pq,ab} + \tilde{V}_{pb,aq} + (\epsilon_p^0 - \epsilon_a^0) \delta_{pq} \delta_{ab} \]

and

\[ B_{pa} = \langle p|h_{\text{EDM}}|a \rangle \]

In the perturbed HF framework, the atomic EDM is

\[ D_a = \sum_{ap} \langle a|d|p \rangle C^{(\infty,1)}_{pa} + C^*_{pa}^{(\infty,1)} \langle p|d|a \rangle \]
Perturbed HF diagrams
Tensor-pseudotensor EDM interaction

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

\[ H_{\text{EDM}} = iC_T G_F \sqrt{2} \sum_i (\gamma_i \cdot I) \rho_N(r) \]

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

$D_{\text{atom}} / C_T$

EXPERIMENTS

$D_{\text{atom}}$

$C_T, S, C_S$
Yb$^{171}$:

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

Xe$^{129}$:

\[ \text{1s}^2 \text{ 2s}^2 \text{ 2p}^6 \text{ 3s}^2 \text{ 3p}^6 \text{ 4s}^2 \text{ 4p}^6 \text{ 3d}^{10} \text{ 5s}^2 \text{ 4d}^{10} \text{ 5p}^6 \]

Ra$^{225}$:

\[ \text{1s}^2 \text{ 2s}^2 \text{ 2p}^6 \text{ 3s}^2 \text{ 3p}^6 \text{ 4s}^2 \text{ 4p}^6 \text{ 3d}^{10} \text{ 5s}^2 \text{ 4d}^{10} \text{ 5p}^6 \text{ 4d}^{10} \text{ 4f}^{14} \text{ 6s}^2 \text{ 6p}^6 \text{ 5d}^{10} \text{ 7s}^2 \]
EDM results for Yb and Ra

Tensor-pseudotensor electron-nuclear interaction

<table>
<thead>
<tr>
<th>System</th>
<th>Zeroth order EDM in units of $10^{-20} \text{C}_T \sigma \text{ e cm}$</th>
<th>All-order EDM in units of $10^{-20} \text{C}_T \sigma \text{ e cm}$</th>
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<tbody>
<tr>
<td>Ytterbium</td>
<td>-0.71</td>
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<td>Xenon</td>
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<td>Mercury</td>
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EDM arising from Schiff moment

<table>
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<tr>
<th>System</th>
<th>Zeroth order EDM in units of $10^{-17} \text{ S/(e fm}^3\text{)}$ e cm</th>
<th>All-order EDM in units of $10^{-17} \text{ S/(e fm}^3\text{)}$ e cm</th>
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<tbody>
<tr>
<td>Ytterbium</td>
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</table>
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.