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High Performance Computational (HPC) Studies on Beyond the Standard Model of Particle Physics using Atoms

Members

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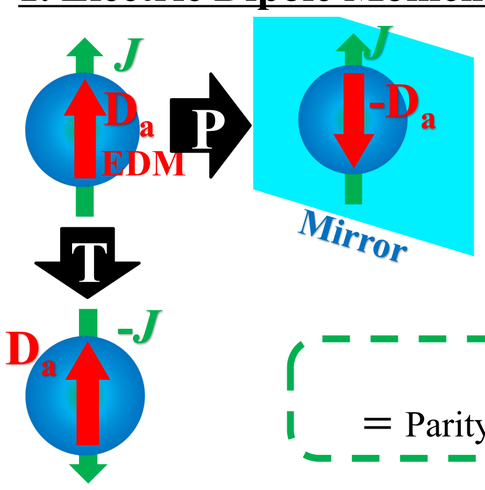
Background

1. Electric Dipole Moment(EDM) of Atom



The expectation value of the EDM (D) is can be represented by angular momentum (J).

Wigner–Eckart theorem

$$\langle\Psi|D|\Psi\rangle \propto \langle\Psi|J|\Psi\rangle$$

If the atom has P&T symmetry, EDM is **zero**

EDM of Atom is non-zero
= Parity and Time-reversal are violated (PTV)

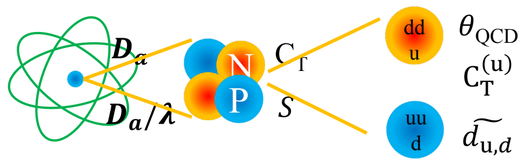
2. Why are EDMs of closed shell atom important ?

- Can give information on hadronic and semi-leptonic CP-violating (T-violating) quantities of the Standard and beyond Standard Model.

Hadronic sector :

Semi-leptonic sector :

θ_{QCD} (SM) ; $\widetilde{d_u} - \widetilde{d_d}$; $C_T^{(u)}$; $C_T^{(d)}$ (BSM)



- Evidence for new physics beyond the Standard Model
- Evidence for Time-reversal /CP violation and may be related to matter-antimatter asymmetry in the Universe.

Theory of Atomic EDM

- The physical quantity in quantum mechanics is given by the Hamiltonian of the interest system. The atomic Hamiltonian is given by

$$H_a = \sum_i^{N_e}\left[c\boldsymbol{\alpha_i}\cdot\boldsymbol{p_i} + \beta_i c^2 + V(r_i)\right] + \sum_{i<j}\frac{1}{r_{ij}} + \lambda H_{PTV}$$

- The original atomic Hamiltonian is P&T invariant, therefore we need to introduce the PTV interaction term in the Hamiltonian. The closed shell atoms has two important PTV-Interaction term

(1) Schiff-Momment (λ = S)

(2) Tensor-Pseudo Tensor (T-PT) interaction (λ=C_T)

(1) Nuclear Schiff-Moment (NSM)

P&T violation inside nucleus

The nuclear charge density : $\rho(r) = \rho_0(r) + \delta\rho(r)$

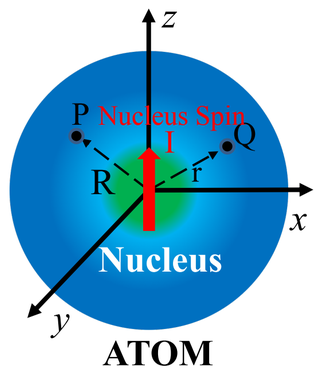
Nucleus has the EDM (N EDM) : d_N

Nuclear charge potential :

$$\delta\Phi(R) = \underbrace{\int_0^\infty \frac{e\delta\rho(r)}{|\boldsymbol{R}-\boldsymbol{r}|}d^3r}_{\text{Due to density distribution}} + \underbrace{\frac{1}{Z}(\boldsymbol{d}_N\cdot\nabla)\int_0^\infty \frac{e\rho(r)}{|\boldsymbol{R}-\boldsymbol{r}|}d^3r}_{\text{Due to N EDM}}$$

The PTV-interaction Hamiltonian

$$H_{PTV}^{NSM} = -e\delta\Phi(R) = -3e\frac{\vec{S}\cdot\vec{R}}{B}\rho(R)$$



Nuclear Schiff Moment

$$\vec{S} = S\frac{\vec{I}}{|I|} = S\,\vec{z}$$

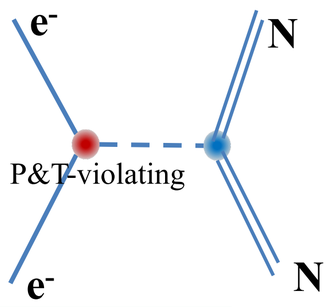
(2) Tensor-Pseudo Tensor (T-PT) interaction

T-PT interaction (QFT)

$$\mathcal{H}^{TPT} = \frac{iG_F C_T}{\sqrt{2}}\sum_{n,e}(\bar{\psi}_n\sigma_{\mu\nu}\psi_n)(\bar{\psi}_e\gamma_5\sigma_{\mu\nu}\psi_e)$$

The PTV-interaction Hamiltonian

$$H^{TPT} = i\sqrt{2}G_F C_T\sum_i \beta\alpha\cdot I\rho_N(r_i)$$



I : Nuclear Spin, G_F : Fermi constant, C_T : T-PT coupling constant

Theoretical method

- **The Atomic EDM**

$$H_a = \sum_i^{N_e}\left[c\boldsymbol{\alpha_i}\cdot\boldsymbol{p_i} + \beta_i c^2 + V(r_i)\right] + \sum_{i<j}\frac{1}{r_{ij}} + \lambda H_{PTV}$$

First order perturbation theory

$$|\Psi\rangle = |\Psi^{(0)}\rangle + \lambda|\Psi^{(1)}\rangle \qquad H_0|\Psi^{(0)}\rangle = E_0|\Psi^{(0)}\rangle$$
$$(H_0 - E_0)|\Psi^{(1)}\rangle = (E_1 - H_{PTV})|\Psi^{(0)}\rangle$$

The atomic EDM

$$D_a = \langle\Psi|D|\Psi\rangle \Rightarrow D_a/\lambda = 2\langle\Psi^{(0)}|D|\Psi^{(1)}\rangle$$

The accuracy of the atomic EDM depends on the zeroth order atomic state ($|\Psi^{(0)}\rangle$)

Dirac-Fock(DF) Method

DF Approximation

Each orbital ($|\phi_i\rangle$) is a four component spinor. ($i = 1,\cdots,N$) The atomic state is expressed by the $N\times N$ Slater determinant : $|\Phi_0\rangle = \mathrm{Det}\{\phi_1\phi_2\cdots\phi_N\}$

Each orbital ($|\phi_i\rangle$) is solution of following equation.

Dirac-Fock equation (the differential equation)

$$t|\phi_i\rangle + \sum_j\{\langle\phi_j|v|\phi_j\rangle|\phi_i\rangle - \langle\phi_j|v|\phi_i\rangle|\phi_i\rangle\} = \epsilon_i|\phi_i\rangle$$

Coupled Cluster Method (CCM)

The DF is called the Mean field approximation. Because, it does not consider the *electron correlation effects* (due to the residual interaction).

$$\boldsymbol{H_a} = \boldsymbol{T} + \boldsymbol{V_{DF}} + (\mathbf{V} - \mathbf{V_{DF}})$$

DF — Residual interaction

The exact atomic wave-function can be represented by DF state ($|\Phi_0\rangle$) plus a set of all particle-hole states ($|\Phi_{ij\cdots}^{ab\cdots}\rangle$) with reference to the DF state.

$$|\Psi\rangle = e^T|\Phi_0\rangle = e^{T_1+T_2+\cdots}|\Phi_0\rangle$$

$$|\Psi\rangle = |\Phi_0\rangle + T_1|\Phi_0\rangle + T_2|\Phi_0\rangle + \tfrac{1}{2!}T_1^2|\Phi_0\rangle + T_1T_2|\Phi_0\rangle + \tfrac{1}{2!}T_2^2|\Phi_0\rangle + \cdots$$

Cluster amplitudes ($t_{ij\cdots}^{ab\cdots}$) represent the probability amplitude of particles-holes excitation due to the residual interaction. These are given by CCM equations.

The CCM Equations

$$t_i^a : \langle\Phi_i^a|(H_N e^T)_c|\Phi_0\rangle = 0 \qquad t_{ij}^{ab} : \langle\Phi_{ij}^{ab}|(H_N e^T)_c|\Phi_0\rangle = 0$$

These equations are solved, using the iterative **Jacobi method**.

$$X_i^{(k+1)} = (b_i - \textstyle\sum_{j\neq i} a_{ij}X_j^k)/a_{ii}$$ X refers to the *t* amplitudes.

The solution of the above equations and the computation of the matrix elements of A (a_{ij}) and the evaluation of X are obtained by parallelization (**MPI**). The coupled-cluster equations are computationally intensive and memory intensive

Atomic EDM in RCCSD

The Atomic Hamiltonian

$$H_a = \sum_i\{c\alpha_i\cdot p_i + \beta_i mc^2\} + \sum_{i<j}\frac{e^2}{r_{ij}} + \lambda H_{PTV}$$

Cluster amplitude : $T = T^{(0)} + \lambda T^{(1)}$

$|\Psi^{(1)}\rangle = e^{T^{(0)}}T^{(1)}|\Psi_0\rangle$

The EDM calculation targets in our study

	NSM&T-PT	eEDM
Atom	Xe	Fr
Molecule	HgYb	YbF, HgF BaF

The CCM Equation for $T^{(0)}$ and $T^{(1)}$

$$\langle\Phi_0^*|(H_N^{DC}e^{T^{(0)}})_{con}|\Phi_0\rangle = 0 \;,\; \langle\Phi_0^*|e^{-T^{(0)}}H_0^{DC}e^{T^{(0)}}T^{(1)}|\Phi_0\rangle = \langle\Phi_0^*|e^{-T^{(0)}}De^{T^{(0)}}|\Phi_0\rangle$$

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

Atomic EDM by CCSD

$$\frac{\langle D\rangle}{\lambda} = 2\langle\Phi_0|e^{T^{(0)\dagger}}De^{T^{(0)}}T^{(1)}|\Phi_0\rangle_{con}$$
$$= \langle\Phi_0|[D + DT^{(0)} + T^{(0)\dagger}D + T^{(0)\dagger}DT^{(0)} + \tfrac{1}{2}DT^{(0)2} + \tfrac{1}{2}T^{(0)\dagger 2}D\cdots]T^{(1)}|\Phi_0\rangle_{con}$$