Closed-shell Atomic Electric Dipole Moments

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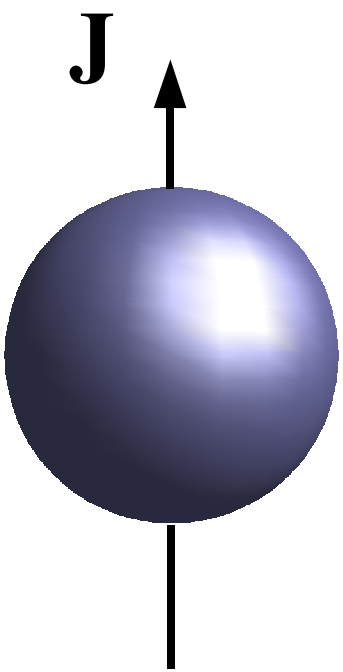
- An observation of EDM of a non-degenerate physical system is a direct unambiguous evidence of violation of P and T symmetries.



D = d **J** , **J** is the angular momentum of the physical system.

Quantity	Parity	Time-reversal
D	**D = – D**	**D = D**
J	**J = J**	**J = – J**

D ≠ 0 ⇒ P and T violation

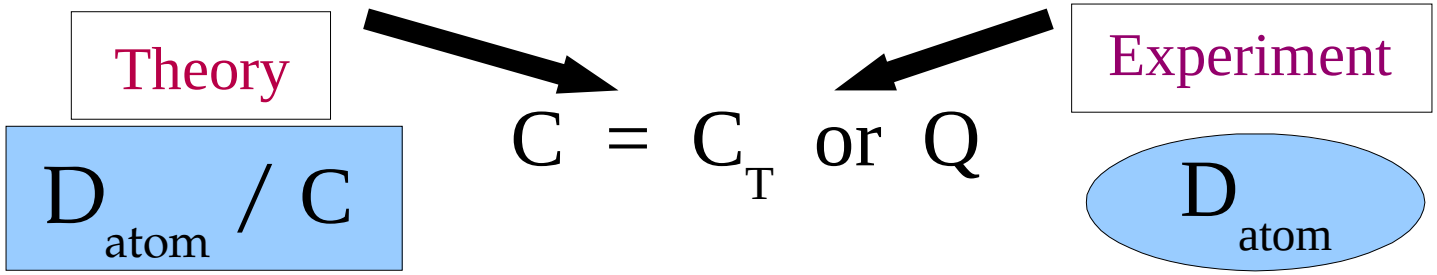
Atoms can have a non-zero EDM

EDM of a diamagnetic atom arises predominantly from,

- Nuclear Schiff moment ← nucleon-nucleon interactions ← quark-quark interactions and chromo EDMs.
- Electron-nucleus interactions ← electron-quark interactions .

EDMs are enhanced in atoms having,

- High nuclear charge (Z) ⇒ P, T – odd effects are dominant in heavy atoms.
- Close levels of opposite parity, $D_{atom} \sim 1 / \Delta E$



The atomic EDM is

$$D_{\text{atom}} = 2\sum_I \frac{\langle \Psi_a^{(0)} | D | \Psi_I^{(0)} \rangle \langle \Psi_I^{(0)} | H_{\text{EDM}} | \Psi_a^{(0)} \rangle}{E_0^{(0)} - E_I^{(0)}}$$

where $|\Psi_a^{(0)}\rangle$ = atomic state,
$H_{\text{EDM}} = \vec{P}$ and $\vec{T}$ violating Hamiltonian,
D = Electric dipole operator.

H_{EDM} is parameterized in terms of the P and T violating Coupling constants.

A new many-body theory to calculate D_a / C

- Knowledge of the Hamiltonian of the system
- Accurate relativistic electronwavefunctions

H_a = Dirac Hamiltonian for a many-electron atom

(unperturbed Hamiltonian)

$$= \sum_i \left(C\, \alpha_i \cdot p_i + m c^2 - Z e^2 / r_i \right) + \sum_{i<j} e^2 / r_{ij}$$

$h_0(i)$

Coulomb interaction (V_N)

$$H_a = t + g^0 \qquad t = h_0(i) + U_{DF}$$

$$g^0 = V_N - U_{DF} = \text{residual Coulomb interaction}$$

Perturbed atomic Hamiltonian

Hartree – Fock equation,

$$\left(t + g^0 - \epsilon_a^0\right)|\psi_a^0\rangle = 0$$

where

$$g^0|\psi_a^0\rangle = \sum_{b=1}^{N_{\rm occ}} \left[\langle\psi_b^0|v|\psi_b^0\rangle|\psi_a^0\rangle - \langle\psi_b^0|v|\psi_a^0\rangle|\psi_b^0\rangle\right]$$

With H_{EDM} as perturbation,

$$H = H_a + h_{EDM}$$

Coupled-perturbed Hartree-Fock equations

The perturbed Hartree-Fock equations are obtained by solving

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

where $|\Psi_a\rangle = |\Psi_a^0\rangle + |\Psi_a^1\rangle$

Expand

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

Substituting above, CPHF equations are,

$$C_{pa}\left(\epsilon_p^0 - \epsilon_a^0\right) + \sum_{bq}\left[\tilde{V}_{pqab}C_{qb}^* + \tilde{V}_{pbaq}C_{qb}\right] +$$

$$\langle p|h_{\mathrm{EDM}}|a\rangle = 0$$

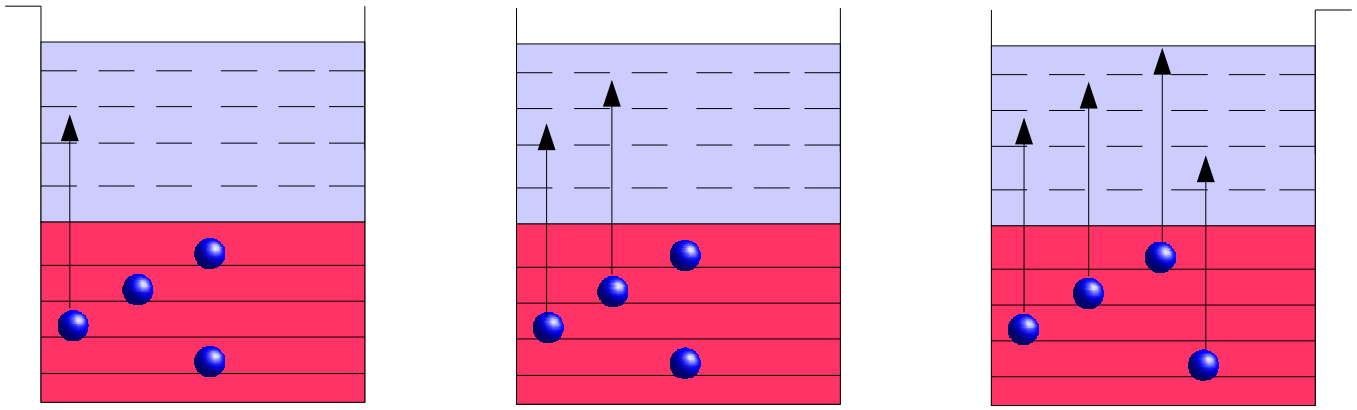
$V_{ijkl} = \langle ij \mid v \mid kl \rangle - \langle ij \mid v \mid lk \rangle$

$$D_{atom} = 2 \sum_{ap} \langle a | D | p \rangle C_{pa}^{(\infty, 1)}$$

CPHF theory :

- Solving for the coefficients allows one to treat the residual Coulomb interaction to all orders with correlations of 2-paritcle and 2-hole type only.
- Perturbations which depend on the coordinate of a single particle.

Coupled-cluster method



T_1 $\quad T_1^2, T_2$ $\quad T_1^2 T_2, T_2^2, T_4$

Continuum

Fermi level

$|\varphi_0\rangle$ = Hartree-Fock reference state

$|\Psi\rangle$ = Exact atomic state = $\exp(T^0)\,|\varphi 0\rangle$

$= (1 + T^0 + T^{0\,2}/2! + \ldots\ldots)\,|\varphi_0\rangle$

$T^0 = T_1^{\,0} + T_2^{\,0}$

Coupled-cluster equations

In Coupled-cluster theory,

$$|\Psi_a^0\rangle = e^{T^0}|\Phi_0\rangle$$

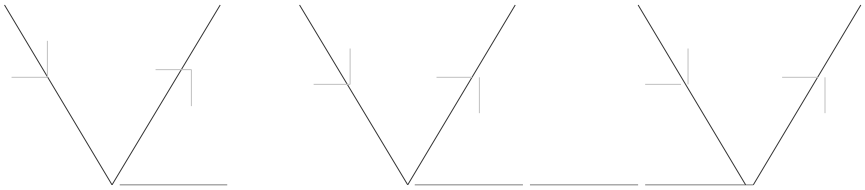
where $|\Phi_0\rangle$ is the reference state.

T^0 represents single/double/triple ... excitations from the reference state.

The unperturbed coupled-cluster equations :

$$H_a|\Psi_a^0\rangle = E^0|\Psi_a^0\rangle$$

$$H_a e^{T^0}|\Phi_0\rangle = E^0 e^{T^0}|\Phi_0\rangle$$



T_1^0 T_2^0

$T_1^0 = \sum_{ap} t_{ap}\ a_p^\dagger a_a\ |\varphi_0\rangle$

$T_2^0 = \sum_{ap,bq} t_{ab}^{pq}\ a_p^\dagger\ a_q^\dagger\ a_b\ a_a\ |\varphi_0\rangle$

Acting by $\exp(-T^0)$ and projecting by singly and doubly excited determinantal states,

$$\langle \Phi_a^p | \; e^{-T^0} \;\; H_a^N \;\; e^{T^0} \; |\Phi_0\rangle = 0$$
$$\langle \Phi_{ab}^{pq} | \; e^{-T^0} \;\; H_a^N \;\; e^{T^0} \; |\Phi_0\rangle = 0$$

With H_{EDM} as perturbation,

$$H = H_a + h_{EDM} \qquad \text{And} \quad T = T^0 + T^1$$

Perturbed Coupled-cluster equations,

$$\langle \Phi_a^p | \left\{ \overline{H}_a^N T^1 \right\} |\Phi_0\rangle = -\langle \Phi_a^p | \, \overline{h}_{\rm EDM} | \Phi_0 \rangle$$
$$\langle \Phi_{ab}^{pq} | \left\{ \overline{H}_a^N T^1 \right\} |\Phi_0\rangle = -\langle \Phi_{ab}^{pq} | \, \overline{h}_{\rm EDM} | \Phi_0 \rangle$$

H_N is the normal ordered Hamiltonian, $H_N = \exp(-T^0) \, H_N(T^0)$.

Restricting $T^1 = T_1{}^1 + T_2{}^1$, set of equations, linear in T^1 and non-linear in T^0 are obtained. The working equations are

$$\langle \Phi_a^p | \{ \overline{H}_a^N T_1^1 \} + \{ \overline{H}_a^N T_2^1 \} | \Phi_0 \rangle = -\langle \Phi_a^p | \bar{h}_{\mathrm{EDM}} | \Phi_0 \rangle$$

$$\langle \Phi_{ab}^{pq} | \{ \overline{H}_a^N T_1^1 \} + \{ \overline{H}_a^N T_2^1 \} | \Phi_0 \rangle = -\langle \Phi_{ab}^{pq} | \bar{h}_{\mathrm{EDM}} | \Phi_0 \rangle$$

$$\mathrm{Datom} = 2 \langle \mathrm{Ref} | \overline{D}\, T^1 | \mathrm{Ref} \rangle$$

$$\overline{D} = \exp(-T^0)\, D \exp(T^0) .$$

Results for ^{199}Hg EDM

CPHF result (Martensson et.al, 1985) in e cm.	Hg EDM experiment (Romalis et.al, 2001) in e cm.	Present best limit for C_T
-6.0×10^{-20}	2.1×10^{-28}	3.3×10^{-9}

CC theory for EDMs ➔ CPHF effects + more

Our preliminary results show that the LCCEDM contribution reduces the HF contribution by 1.0 % with an unoptimised basis set.

- Polarizability of Hg and other atoms
- Unperturbed CC amplitudes

Diamagnetic atoms

EDM experiment on ^{199}Hg is in progress in University of Washington, Seattle.

The best limit (present) is

$$D(^{199}Hg) > 2.1 \times 10^{-28} \text{ e-cm}$$

A non-zero value of C_T would imply new physics beyond the Standard Model. To set limits on specific models of CP violation, the experimental results must be related to EDMs of fundamental particles.

Interpretation of EDM experimental result :

Atomic level

$$D_{Hg} = -2.8 \times 10^{-4}\ \text{fm}^2\ S_{Hg}$$

(Dzuba et al)

Nuclear level

$$S_{Hg} = -1.2\ \text{e fm}^3\ g_{\pi\,NN}$$

(Nuclear shell model calculation)

(Flambaum et. Al)

Quark level

$$g_{\pi NN} = 20\ \text{fm}^{-1}\ (d_d - d_u)$$

(Posepelov)

$g_{\pi NN}$ = CP-odd pion exchange constant,

d_d and d_u are quark chromo EDMs.

Conclusions

- Presence of EDMs is a direct evidence of T – violation.

- The knowledge of the T – PT coupling constants and the Schiff moment, Q gives deep insights into the CP violating interactions responsible for their existence at the fundamental level.

  The observable EDMs can be used to constrain the chromo EDMs of quarks predicted by the non-Standard Models.

Calculation of Electric quadrupole moment of Sr^+

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Electric Quadrupole moments in the context of Atomic Clocks :

The best clock must be

- Accurate
- Stable
- Reproducible

→ Clocks based on microscopic oscillators - Atomic Clocks

The resonant transitions between two non-degenerate energy levels of an atoms are extremely stable and can be most accurate. Two identical atoms have the same unperturbed transition and two clocks based on such transitions generate the same time – Property of reproducibility.

The basic atomic clock recipe

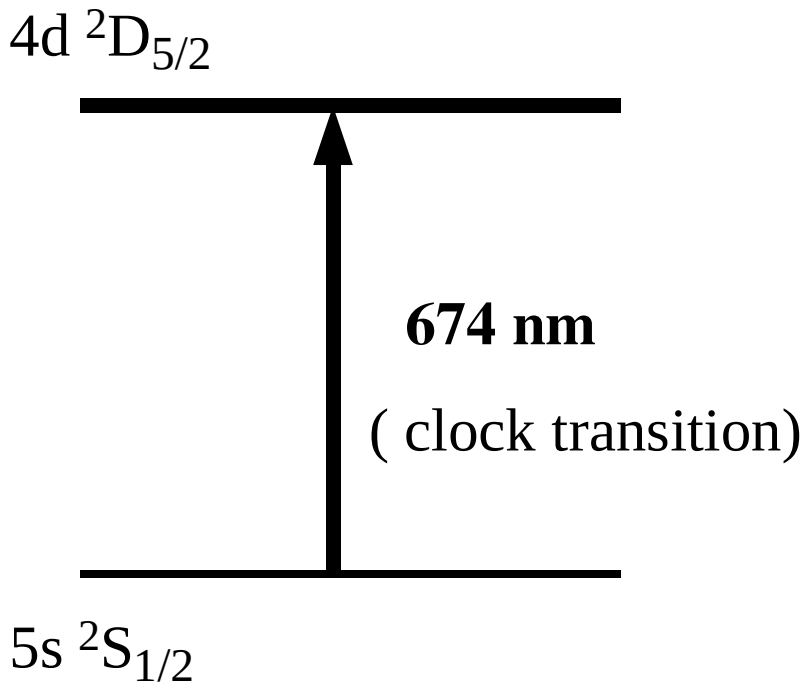
- Identify a transition between two non-degenerate atomic states
- Create an ensemble of such atoms
- Illuminate the ensemble with radiation from a tunable source – an oscillator operating near the transition frequency f_0 . At maximum absorption count the number of cycles of the oscillator.

  A certain number of cycles generate a standard interval of time.

The stability, accuracy and the reproducibility of the clock is determined by the matching of the osillator frequency with the resonance frequency of the atom, which is limited by :

- Environmental perturbations – External fields
- Collisions
- Doppler shifts
- Quantum projection noise, etc.

Sr : Z = 38 ;



The interaction of atomic electric quadrupole moment with external electric field gradient produces the electric quadrupole shift, proportional to the electric quadrupole moment (Θ) in that state. For Sr^+ the contribution to this shift comes only from $4d\ ^2D_{5/2}$ state.

The electric quadrupole moment in a state $|\Psi\rangle$ is

$$\Theta = \langle \Psi\ (J, M, \gamma) \,|\, \Theta_{zz} \,|\, \Psi\ (J, M, \gamma) \rangle$$

Where $\Theta_{ZZ} = -\, e/2\ \Sigma_j\ (\, 3\, Z_j^2 - r_j^2\,)$

The closed shell state is

$$|\Psi\rangle = \exp(\,T\,)\ \ |\Phi_0\rangle$$

Open shell state is obtained by an electron attachment to a closed-shell reference state.

$$|\Phi^{N+1}{}_k\rangle = a_k^{\dagger}\, |\Phi_0\rangle$$

$$\text{Exact state :}\quad |\Psi_k^{N+1}\rangle = \exp(\,T\,)\,\{1+S\}\ |\Phi_k^{N+1}\rangle$$

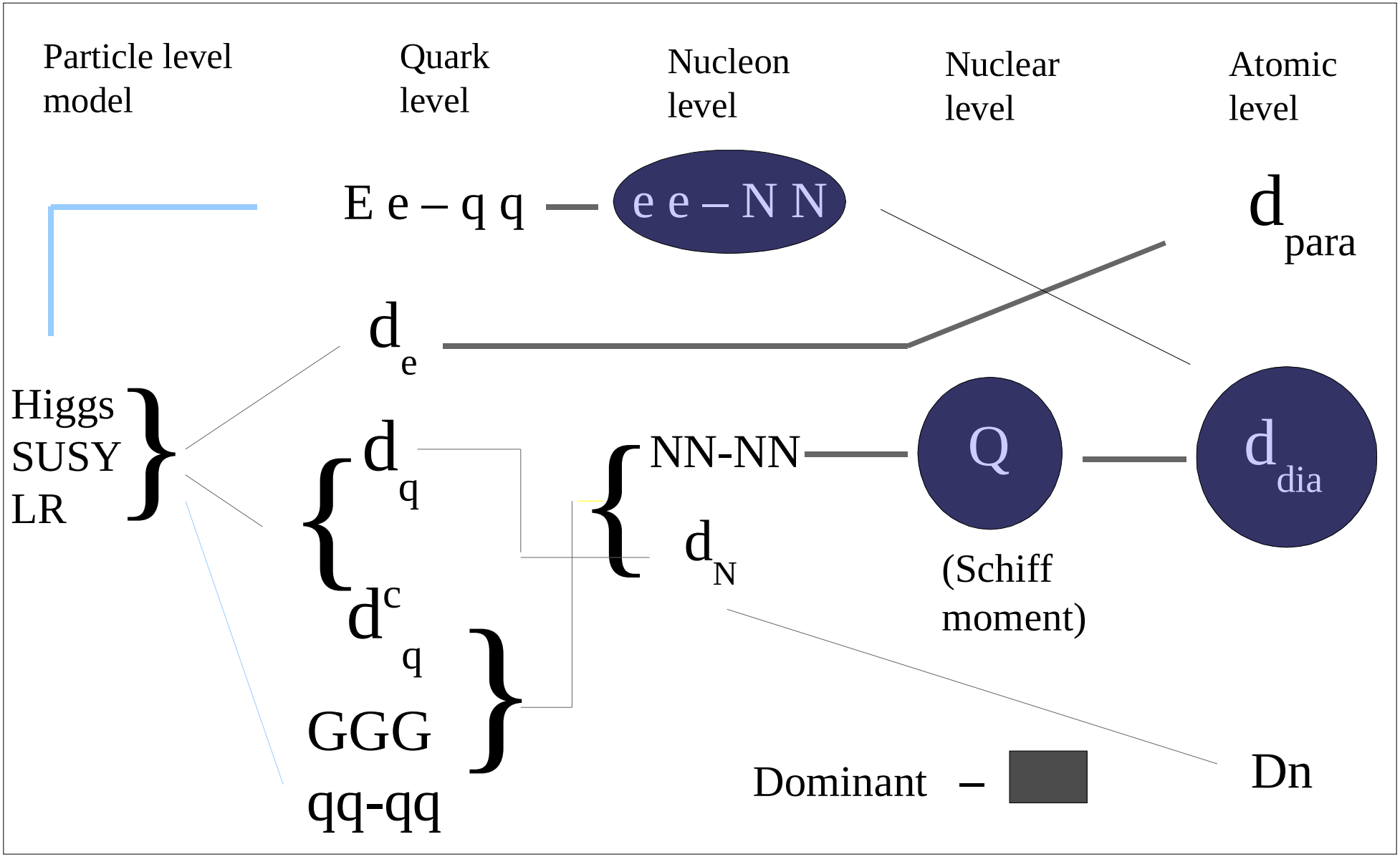
And S = cluster operator for valence to valence and valence to virtual excitations.

Results

	Present work in e - a_0^2	MCDF method Itano. et. Al	Experiment Barwood et.al
$4d\ ^2D_{5/2}$	2.94	3.02	2.6 ± 0.3

(Accepted for publication in Physical Review Letters)

Sources of an atomic EDM



T violation is less understood than parity violation and atoms are rich sources of T or CP violation arising from various sectors.