

# Electric Dipole moments signature of time reversal violation

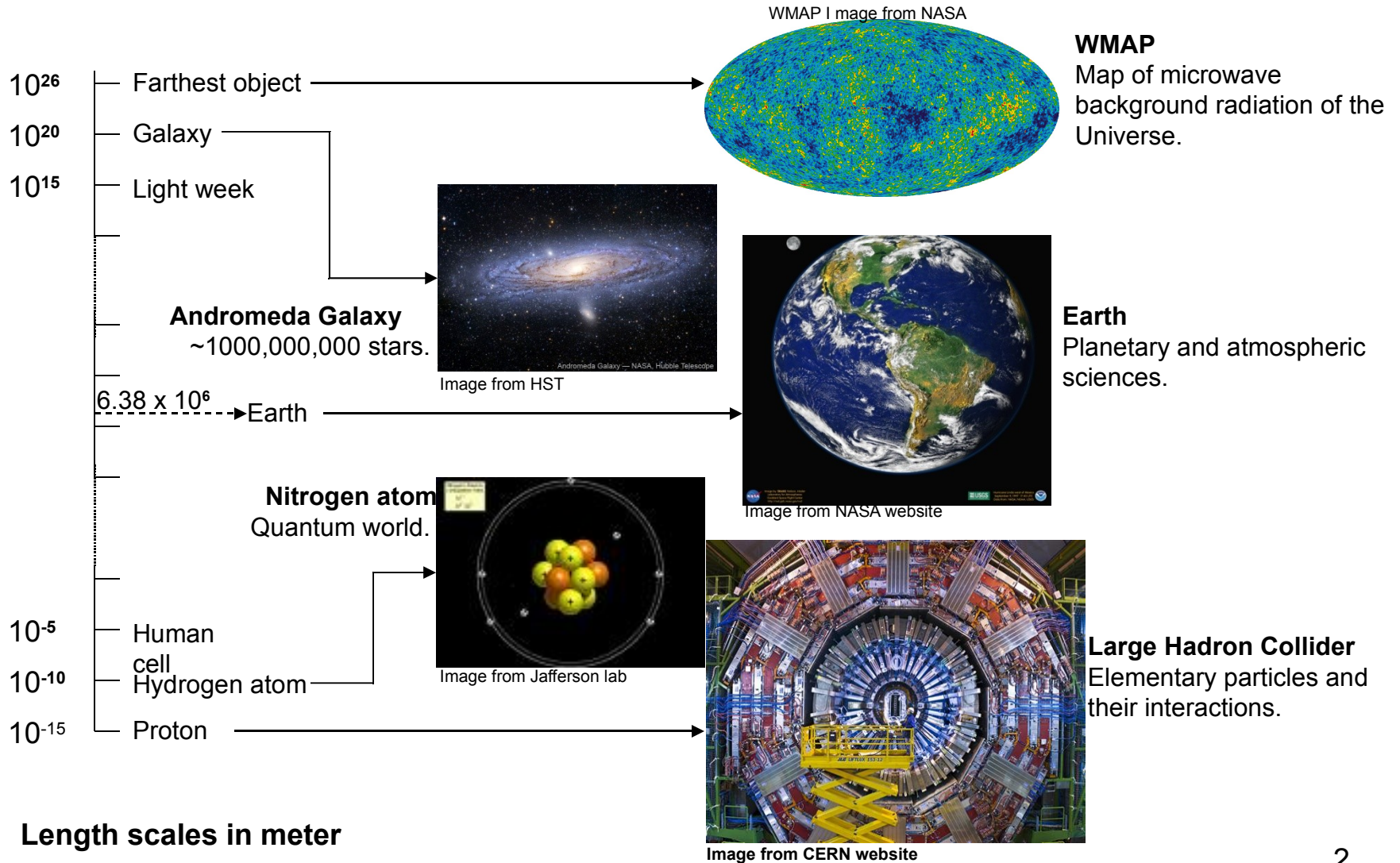
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Physical Research Laboratory



11 January, 2010

International school and conference on cold ions and atoms

# Science at different scales



# Symmetries in Nature

## continuous and discrete

### Continuous symmetries

Infinitesimal transformations are possible. Finite transformations are repeated operations.

Examples: rotation, translation in space and time, etc

### Discrete symmetries

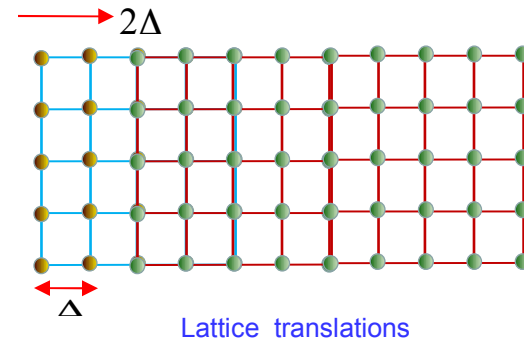
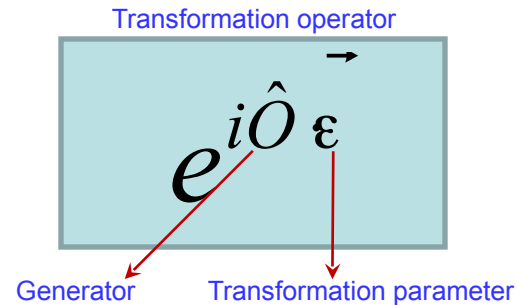
Infinitesimal transformations are not defined. Transformations are discrete operations.

Examples: crystal symmetries, reflection, charge conjugation, time reversal, etc

### Conservation laws

Dynamical variables which do not change under a symmetry transformation are conserved quantities.

Examples: rotation—angular momentum, translation—linear momentum, etc

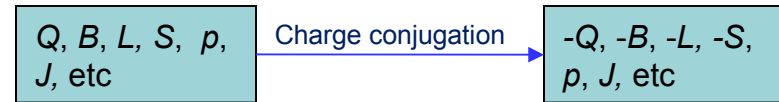


# CPT symmetries

## charge conjugation, parity and time reversal

### Charge conjugation

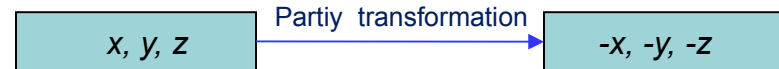
Transforms particle to antiparticle and leaves dynamical variables unchanged. Negates charge, baryon number, lepton number and strangeness.



Charge  $Q$ , baryon number  $B$ , lepton number  $L$ , strangeness  $S$ , linear momentum  $p$ , angular momentum  $J$ , etc.

### Parity/reflection

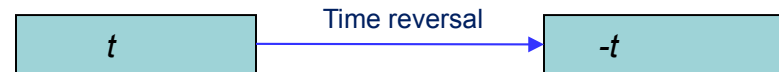
Mirror reflection about all the coordinates. Defines handedness of a system.



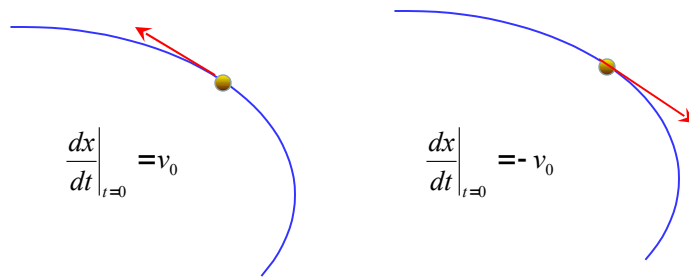
Coordinates undergo a change in sign and handedness changes.

### Time reversal

Change in direction of time or motion reversal.



Time changes sign.



Motion reversal without any **dissipative** forces.

### Motion under potential

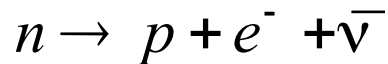
$$m \frac{d^2 x}{dt^2} = -\nabla U \xrightarrow{\text{CPT}} m \frac{d^2 x}{dt^2} = -\nabla U$$

Newton's equation of motion remain unchanged under parity and time reversal transformations.

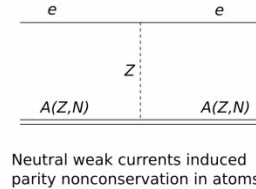
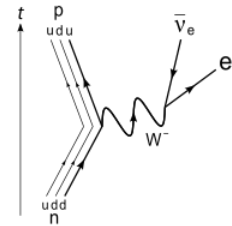
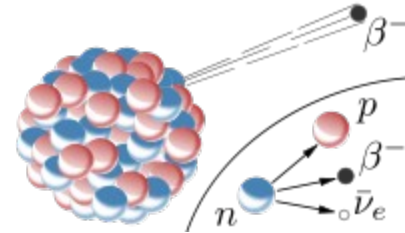
# Parity violation in beta decay equivalent to time reversal violation

## Parity violation in weak interaction

Weak interaction violates parity. First suggested to explain tau-theta puzzle and observed in beta decay of  $^{60}\text{Co}$



Arises from charged weak current interaction. Electroweak unification predicts a neutral weak current. Atoms are ideal candidate to observe neutral weak current.



**Elementary Particles**

|                          |                              |                            |                            |                |
|--------------------------|------------------------------|----------------------------|----------------------------|----------------|
| Quarks                   | u<br>up                      | c<br>charm                 | t<br>top                   | Force Carriers |
|                          | d<br>down                    | s<br>strange               | b<br>bottom                |                |
| Leptons                  | $\nu_e$<br>electron neutrino | $\nu_\mu$<br>muon neutrino | $\nu_\tau$<br>tau neutrino | Force Carriers |
|                          | e<br>electron                | $\mu$<br>muon              | $\tau$<br>tau              |                |
| I    II    III           |                              |                            |                            |                |
| Three Families of Matter |                              |                            |                            |                |

### Attention

**D. Budker**

Atomic and Molecular P- and P,T-Violation Experiments

18 Jan, 13:40 PM

**B. K. Sahoo**

Relativistic Many-Body Theory of Parity Nonconservation....

18 Jan, 14:30 PM

Lee, T. D., and C. N. Yang, Phys. Rev., 104, 254 (1956).

C. S. Wu, E. Ambler, R. W. Hayward, D. D. Hoppes, and R. P. Hudson, Phys. Rev. 105, 1413 (1957).

# Time reversal violations genesis

## Time reversal transformation

One dimensional time-dependent Schrodinger equation with real potential. Under time reversal transformation.

$$-\frac{\partial^2}{\partial x^2} + V(\vec{r}) \psi(\vec{r}) = i \frac{\partial}{\partial t} \psi(\vec{r})$$

## Invariance

To preserve invariance of equation of motion (Schrodinger equation), time reversal transformation implies complex conjugation

$$-\frac{\partial^2}{\partial x^2} + V(\vec{r}) \psi(\vec{r}) = i \frac{\partial}{\partial t} \psi(\vec{r})$$

## Time reversal violation

Complex potential, under time reversal transformation Schrodinger equation is modified. Classical analogue is dissipation.

$$e^{i\varphi} v(r, \theta) \xrightarrow{\text{time-reversal}} e^{-i\varphi} v(r, \theta)$$

**Time reversal violation is associated with phase of interaction**

# CP violation in kaon decay equivalent to time reversal violation

## $\kappa^0$ - meson

Bound state of down (d) and anti-strange ( $\bar{s}$ ) quarks. Strangeness and parity eigenvalues are 1 and -1. K-mesons are isospin doublets.

$$[\bar{K}^0 (s\bar{d}), \kappa^- (s\bar{u})], [K^0 (d\bar{s}), \kappa^+ (u\bar{s})]$$

Dominant decay channels, which conserve CP symmetry are:

$$|K_1^0\rangle \rightarrow \pi^0 + \pi^0; |K_1^0\rangle \rightarrow \pi^+ + \pi^-$$

$$|K_2^0\rangle \rightarrow \pi^0 + \pi^+ + \pi^-$$

## CP violation

Decay products which changes CP eigenvalue.

$$|K_2^0\rangle \rightarrow \pi^+ + \pi^-$$

From CPT invariance, *CP violation implies time reversal violation*.

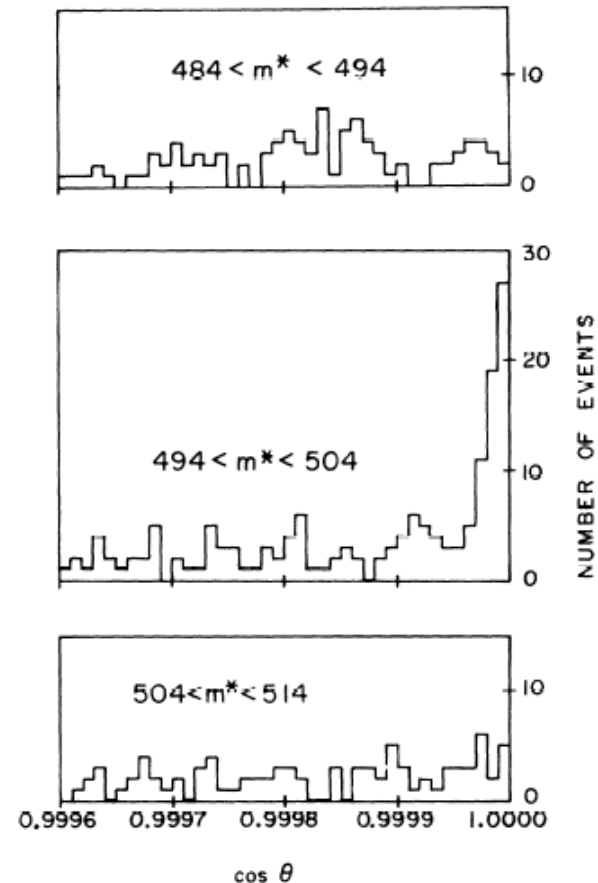


FIG. 3. Angular distribution in three mass ranges for events with  $\cos \theta > 0.9995$ .

# Importance of CP violation

## time reversal violation

### Important questions

•If Universe originates from big-bang, equal amounts of matter and antimatter are created. However, no signature of sizable antimatter presence is observed in the current epoch.

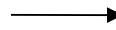
### How and where antimatter vanished ?

•If the standard model of particle physics can be fine tuned with extensions or opt for alternatives. So that deficiencies or short comings of standard model can be fixed.

### How to validate/check other models ?

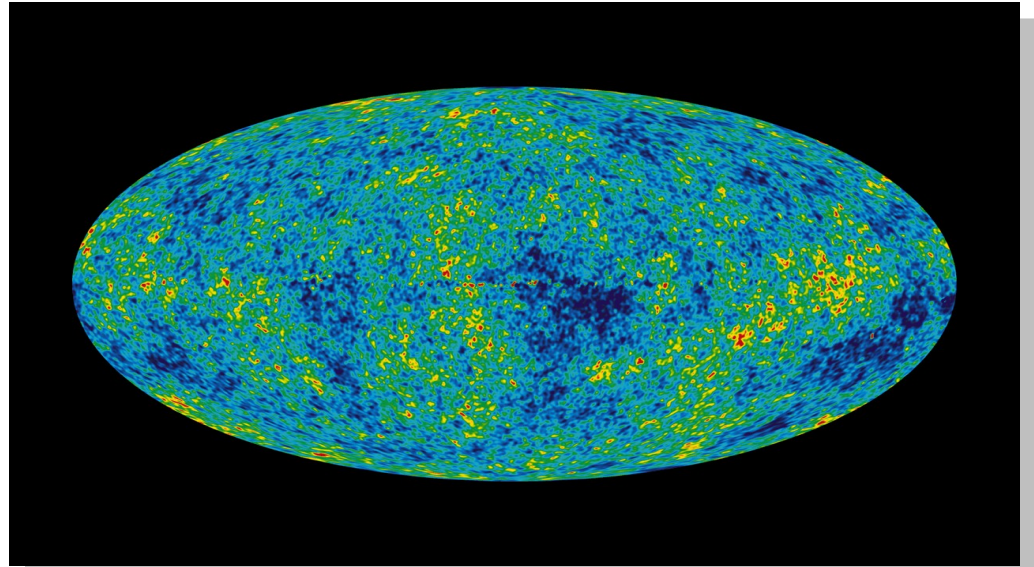
### Key to finding a solution

Phenomenon providing clues to answering these questions is time reversal violation.



### Observable signature

Observable signature of time reversal violation is intrinsic electric dipole moment.



[http://map.gsfc.nasa.gov/media/080997/080997\\_5yrFullSky\\_WMAP\\_1280B.png](http://map.gsfc.nasa.gov/media/080997/080997_5yrFullSky_WMAP_1280B.png)



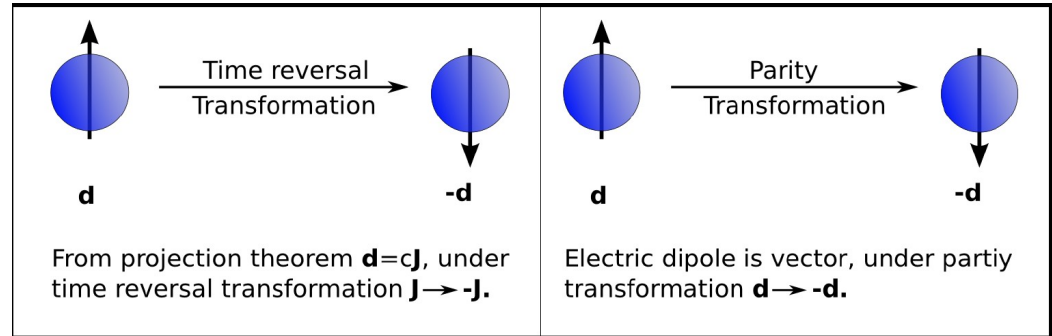
# Observing time reversal violation

## Electric dipole moments

### P and T reversal transformations

Finite electric dipole moment of non-degenerate quantum system is signature of parity and time reversal violations.

Permanent EDM of molecules arise from degenerate opposite parity states.



### Detecting electric dipole moments

EDM and magnetic moment couples to external static electric field and magnetic fields.

Observable signature, energy difference under reversal of electric field.

$$H_{\text{int}} = -d_a \cdot E - \mu \cdot B$$

$$\Delta E = 2d_a \cdot E = \omega$$

$$d_a = \frac{\omega}{2E} \quad \text{Electric dipole moment}$$

**Attention**  
**D. Budker**

Atomic and Molecular P- and P,T-Violation Experiments

18 Jan, 13:40 PM

# Measuring electric dipole moments not any particles

## Particles with EDM

Intrinsic EDM of electron and quarks are signature of fundamental physics. It probes phenomena at the high energy scales. For charge particles

$$F = qE_{\text{ext}}$$

Particle accelerates away. Neutron is an exception.

## Neutron EDM

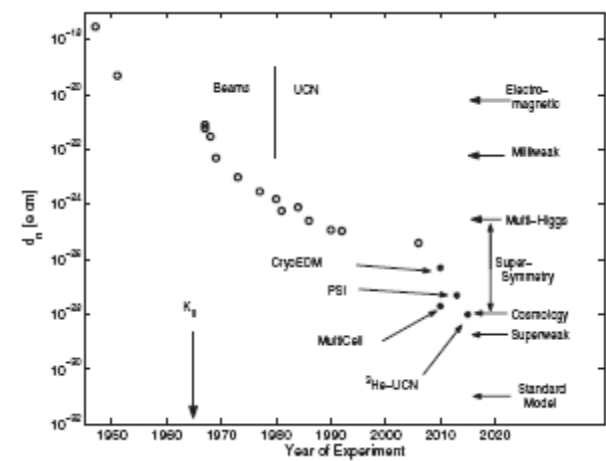
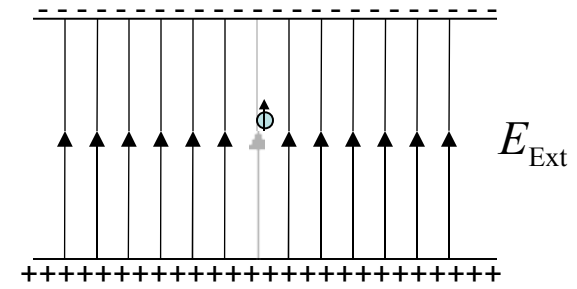
Current limit on neutron EDM.

$$|d_n| < 2.9 \times 10^{-26} \text{ e cm.}$$

## EDM of charged particles

To measure EDM of electron, composite charge neutral systems like atoms and molecules are ideal. These do not experience Coulomb force.

Charge particles with EDM in external fields



C. A. Baker, et al., Phys. Rev. Lett **97**, 131801 (2006),

S. K. Lamoreaux and R. Golub, Phys. G: Nucl. Part. Phys. **36**, 104002 (2009).

# Atomic electric dipole moments

## Can we measure it ?

### Schiff theorem

Non-relativistically, collection of point particles with electric dipole moments (EDMs) realigns to shield applied external electric field. This renders observable EDM to zero.

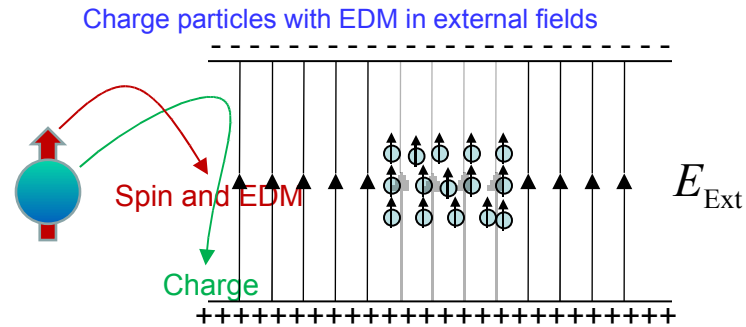
Interaction of EDMs with external/internal electric field.

$$H_{\text{EDM}} = \sum_i -d_i \sigma_i \cdot E_i$$

### Exceptions

EDM is observable due to

- Relativistic effects,
- Finite size of particles,
- Non-electrostatic interactions.



$$H_0 = \sum_i \frac{p_i^2}{2m_i} + \sum_{i \neq j} \frac{q_i q_j}{2r_{ij}} + \sum_i q_i V(r_i)$$

External/internal electric field

$$E_i = \nabla_i \sum_j \frac{q_j}{2r_{ij}} + V(r_i)$$

$$H_{\text{EDM}} = \sum_i \frac{d_i}{q_i} \sigma_i \cdot \nabla_i H_0$$

EDM of the system

$$W_{\text{EDM}} = \langle \psi | \sum_i \frac{d_i}{q_i} \sigma_i \cdot \nabla_i H_0 | \psi \rangle = 0$$

L. I. Schiff, Phys. Rev. **132**, 2194 (1963),

P. G. H. Sandars, Contemporary Physics **42**, 97 (2001).

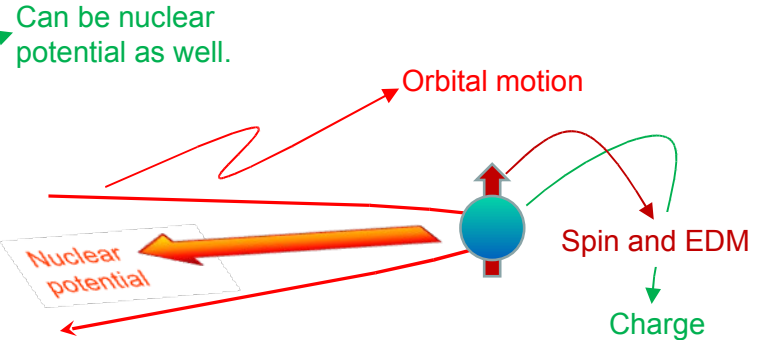
# Defying Schiff theorem I

## relativistic effects

### Relativistic description

Relativistic Hamiltonian of an electron in central potential

$$H_D = \beta mc^2 + c\alpha \cdot p - eV(r).$$



Can be nuclear potential as well.

Orbital motion

Spin and EDM

Charge

Covariant form of electron EDM and external field interaction

$$H_{\text{EDM}} = -d_e \beta \sigma \cdot E.$$

In terms of total Hamiltonian

$$H_{\text{EDM}} = \left[ -d_e \beta \sigma \cdot \vec{\nabla}, H_D \right] + 2i \frac{d_e}{e} c \beta \gamma_5 p^2.$$

Expectation of second term is non zero

$$\langle \psi | \frac{d_e}{e} \beta \sigma \cdot \vec{\nabla}, H_D | \psi \rangle = 0,$$

$$\langle \psi | 2i \frac{d_e}{e} c \beta \gamma_5 p^2 | \psi \rangle > d_e$$

### Enhancement

Derivation can be extended to atoms higher Z and there is an enhancement of atomic EDM.

$$D_A \propto Z^3 \alpha^2,$$

Incomplete cancellation arises from the spin-orbit coupling (magnetic interaction)

$$2i \frac{d_e}{e} c \beta \gamma_5 p^2.$$

P. G. H. Sandars, Phys. Lett. 14, 194 (1965)

# Defying Schiff theorem II

## finite size effects

### Schiff moment

Emerges when charge and electric dipole moment distributions are different within the nucleus. Then

$$W_{\text{EDM}} = - D_N \sigma_N \cdot \int d^3x (\rho_d - \rho_c) \langle \psi | E(x) | \psi \rangle$$

The above dipole interaction energy is zero if nuclear charge and dipole distributions are the same. Unequal distributions can arise from

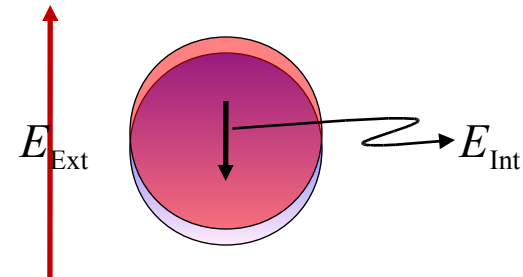
- Electric dipole moment of quarks,
- CP violating quark-quark interactions.

It is also referred to as the local dipole moment of the nucleus.

$$W_{\text{EDM}} = - eS \cdot \left[ \nabla, \delta(r_e) \right]$$

This is point nucleus limit. More precise treatment is to consider finite nucleus.

Charge distribution gradient within nucleus



$$\phi(R) = - \frac{3S \cdot R}{B} \rho_N(R)$$

**Schiff potential**

$$B = \int \rho_N(R) R^4 dR$$

**Nuclear Schiff moment**

# Atomic electric dipole moments choosing one

## Elementary particles to atoms

Atomic EDM arise from parity and time reversal phenomena at elementary particle physics level. These could be

- Quark or electron electric dipole moments,
- Quark-quark, quark-electron, electron-electron P and T odd interactions,

## Choice of atoms

Different atoms are sensitive to parity and time reversal violations in various sectors

- Paramagnetic atoms—leptonic sector,
- Diamagnetic atoms—leptonic and hadronic sectors,

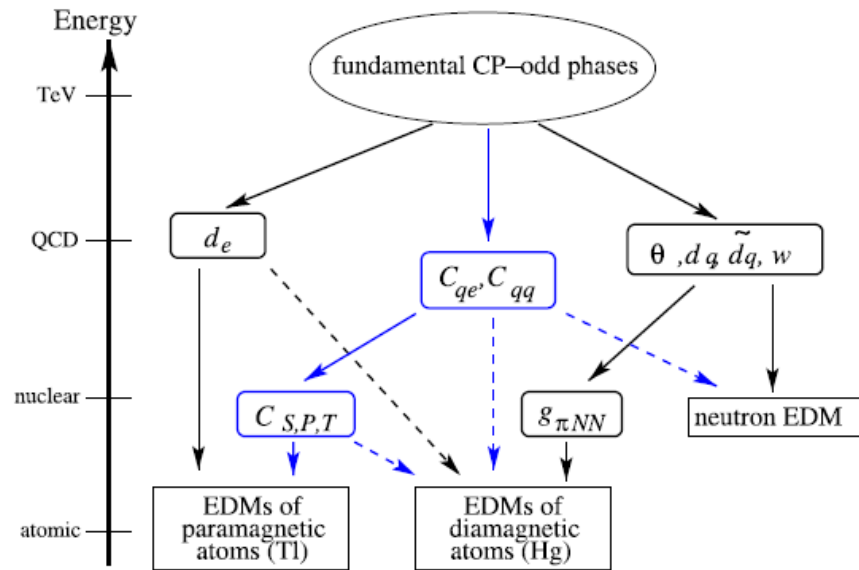
## Electron electric dipole moment

Standard model predictions

$$d_e < 10^{-38} e \text{ cm}$$

C. Jarlskog, Phys. Rev. Lett. **55**, 1039 (1985),

W. Bernreuther and M. Suzuki, Rev. Mod. Phys. **63**, 313 (1991).



M. Pospelov, A. Ritz, Ann. Phys. **318**, 119 (2005).

# Electron electric dipole moment limits

## Current limit

Thallium experimental results provide the best limit on electron EDM.

- Atomic beam experiment,
- Enhancement factor is -585,
- Main systematic error is motional magnetic field.

$$d_e = (6.9 \pm 7.4) \times 10^{-28} e \text{ cm}$$

Equivalent to the upper limit

$$|d_e| < 1.6 \times 10^{-27} e \text{ cm}$$

B. C. Regan, E. D. Commins, C. J. Schmidt, D. DeMille, PRL **88**, 071805 (2002).

## Other atoms

Theoretically, alkali metal atoms have less complications and are preferred choice.

| Atom | Experimental result  |
|------|--|
| Rb   |  |
| Cs   | J. M. Amini, et al, PRA 75, 063416 (2007)<br>$d_e = (-1.5 \pm 5.5 \pm 1.5) \times 10^{-26} e \text{ cm}$ |
| Fr   | S. A. Murthy, et al, PRL <b>63</b> , 965(1989)<br>-----<br>Z-T. Lu, et. al, PRL 79, 994 (1997)           |

| Atom  | Experimental result |
|---|---------------------|
| 81 <sup>2</sup> P <sup>o</sup> <sub>1/2</sub> Tl  | 25.74               |
| 120.53  |                     |
| Limit from atomic PNC experiments, charge asymmetry ~ 10 <sup>-6</sup> cm = 10 <sup>-9</sup> angstrom |                     |
| H. S. Nataraj, et. Al. PRL 101, 033002 (2008)   |                     |
| H. S. Nataraj, et. Al. PRL 101, 033002 (2008)   |                     |
| 910 ± ~5%   |                     |
| T. M. R. Byrnes, et al Phys. Rev. A 59, 3082 (1999),  |                     |

# CP violation parameters

## Hadronic sector

### CPT theorem

Combined discrete symmetries CPT is a good symmetry.  
Result obtained from local field theory.

T reversal violation, then *imply CP violation*.

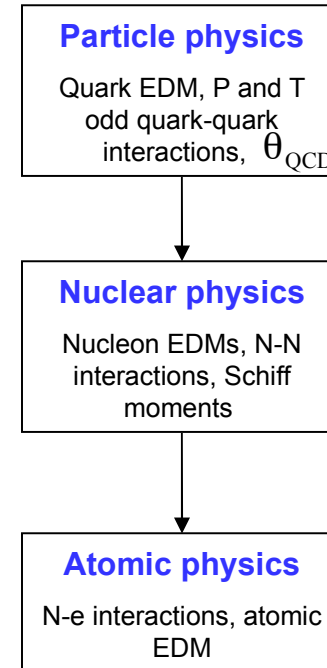
### Current experiments

Diamagnetic or closed-shell atoms like Yb, Hg, Xe, Ra and Rn are candidate atoms to probe CP violation in hadronic sector.

### Estimating CP violation parameter

CP violation parameters are obtained after combining the experimental results with the theoretical results.

|                    |                           |                   |                                   |                        |
|--------------------|---------------------------|-------------------|-----------------------------------|------------------------|
| Experiment result  | $d_a = \frac{\omega}{2E}$ | $\longrightarrow$ | $\lambda = \frac{\omega}{2E\eta}$ | CP violation parameter |
| Theoretical result | $d_a = \lambda\eta$       |                   |                                   |                        |





# Mercury EDM experiment recent results

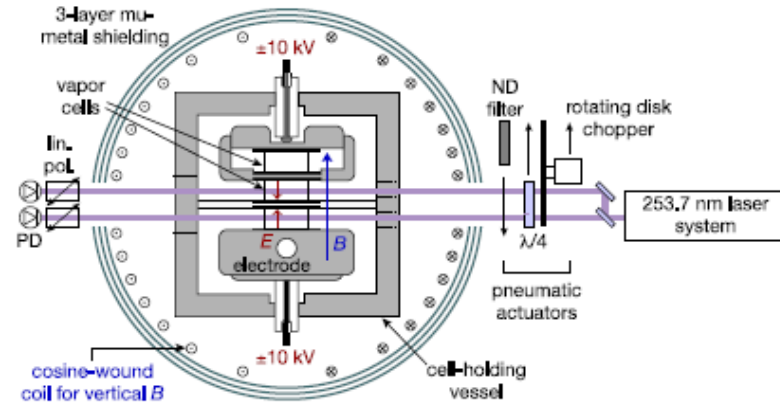
## Most precise EDM experiment

Hg EDM experiment results is the best result so far. Result from the current generation is

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

Limit from this experimental result is

$$|d(^{199}\text{Hg})| < 3.1 \times 10^{-29} \text{ e cm}$$



## CP violation parameter bounds

Bounds on CP violation parameters obtained after combining the experimental data with earlier theoretical results.

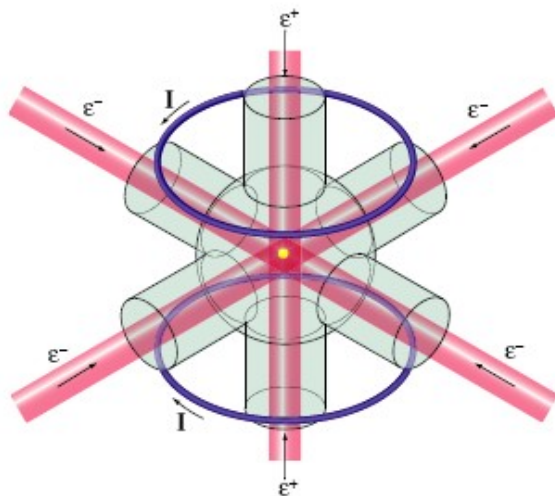
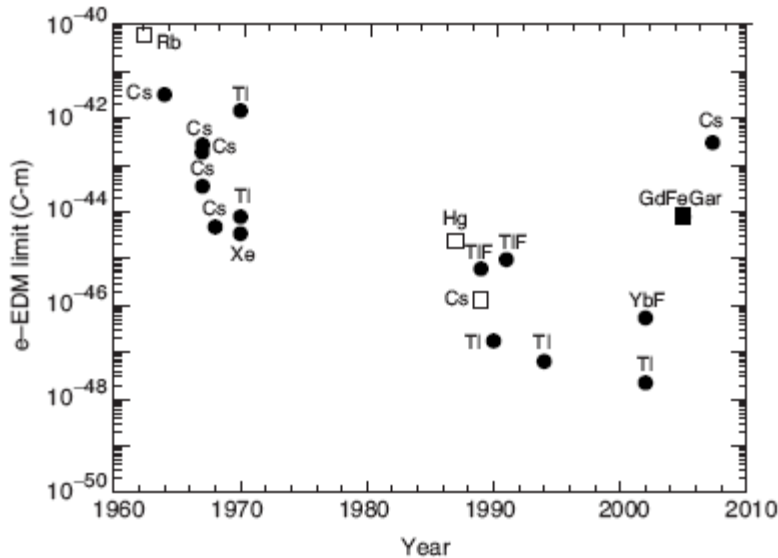
## Our recent calculations provide new bounds

| Parameter                  | $^{199}\text{Hg}$ bound | Hg theory | Best alternate limit           |
|----------------------------|-------------------------|-----------|--------------------------------|
| $\tilde{d}_q(\text{cm})^a$ | $6 \times 10^{-27}$     | [15]      | n: $3 \times 10^{-26}$ [3]     |
| $d_p(\text{e cm})$         | $7.9 \times 10^{-25}$   | [16]      | TIF: $6 \times 10^{-23}$ [17]  |
| $C_S$                      | $5.2 \times 10^{-8}$    | [18]      | TI: $2.4 \times 10^{-7}$ [19]  |
| $C_P$                      | $5.1 \times 10^{-7}$    | [18]      | TIF: $3 \times 10^{-4}$ [1]    |
| $C_T$                      | $1.5 \times 10^{-9}$    | [18]      | TIF: $4.5 \times 10^{-7}$ [1]  |
| $\tilde{\theta}_{QCD}$     | $3 \times 10^{-10}$     | [20]      | n: $1 \times 10^{-10}$ [3]     |
| $d_n(\text{e cm})$         | $5.8 \times 10^{-26}$   | [16]      | n: $2.9 \times 10^{-26}$ [3]   |
| $d_e(\text{e cm})$         | $3 \times 10^{-27}$     | [21, 22]  | TI: $1.6 \times 10^{-27}$ [18] |

<sup>a</sup>For  $^{199}\text{Hg}$ :  $\tilde{d}_q = (\tilde{d}_u - \tilde{d}_d)$ , while for n:  $\tilde{d}_q = (0.5\tilde{d}_u + \tilde{d}_d)$ .

# Ultracold atomic gases

## next generation experiments



### Ultracold atoms

Low atomic velocities reduce the systematic error from motional magnetic field

$$\vec{B}_{\text{mot}} = \frac{\vec{v} \times \vec{E}}{c^2}$$

It couples to the magnetic moment of atom and mimics EDM signal. Recall

$$H_{\text{int}} = -d_a \cdot \vec{E} - \vec{\mu} \cdot \vec{B}$$

Interaction of motional magnetic field with atom

$$- \vec{\mu} \cdot \frac{\vec{v} \times \vec{E}}{c^2}$$

Changes sign when electric field E is reversed like the EDM interaction term.

### Measurement scheme

There are various proposed schemes

- Quantum non-demolition measurement of cold atoms (Yb),
- Measurement using a cold atom fountain (Cs),
- Optical lattices (Cs, Rb).

# Candidate atoms and where

## Proposed experiments

| Atom | Proposed Lab   |
|------|--|
| Rb   | Penn State University<br>F.Fang and D.S. Weiss, <i>OL</i> <b>34</b> , 169 (2009).  |
| Cs   | LBNL<br>J. M. Amini, et al, <i>PRA</i> <b>75</b> , 063416 (2007).  |
| Yb   | Kyoto University<br>M. Takeuchi M, et. al, <i>PRA</i> <b>75</b> , 063827 (2008).<br>IISc<br>V. Natarajan, <i>EPJD</i> <b>32</b> , 33 (2005). |
| Fr   | RCNP, Osaka University<br>Sakemi et. al.<br>JILA<br>Z-T. Lu, et. al, <i>PRL</i> <b>79</b> , 994 (1997).                                      |

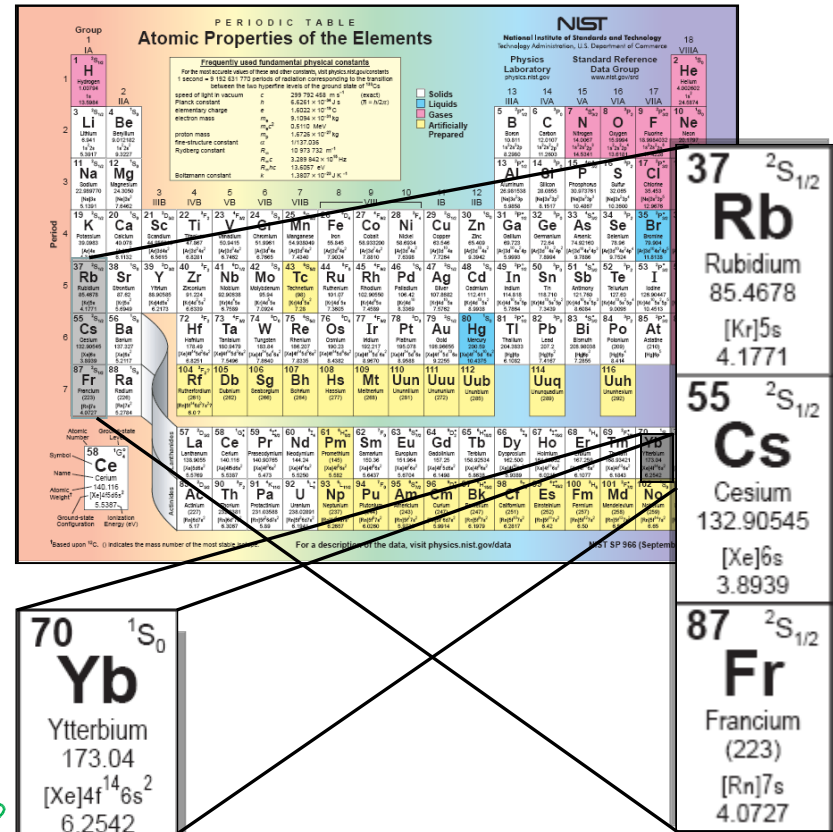
## What to expect

For Cs and Rb atoms trapped in a one dimensional, 1.064 μm, optical lattice.

- No of atoms—Cs  $5 \times 10^8$  and Rb  $10^{10}$ ,
- External field—exceeding  $10^5$  V/cm,
- Integration time—approx 100 hours,
- Precision—less than  $5 \times 10^{-30}$  e-cm.

200-fold improvement over the current experimental limit.

D. S. Weiss, F. Fang, J. Chen, *BAPS J.008* (2003).



$$\Delta E = 2d_a \cdot E = \omega$$

### Attention

Y. Takahashi

Quantum simulator Using ytterbium

18 Jan, 11:50 PM

# Atomic theory calculations enhancement factor

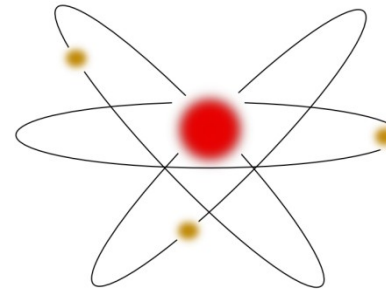
## Atomic EDM from Schiff moment

Electrons within atoms interact with the nuclear Schiff moment and induces finite atomic EDM.

Atomic EDM arising from the nuclear Schiff moment

$$d_a = 2 \sum_I \frac{\langle \Psi_0 | D | \Psi_I \rangle \langle \Psi_I | H_{\text{PTV}} | \Psi_0 \rangle}{E_0 - E_I} = S\eta$$

$$H_{\text{PTV}} = -\vec{\phi}(R) = \frac{3S \cdot R}{B} \rho_N(R)$$



*Though this be madness, yet there is method in it.*  
(Hamlet)

## Atomic theory

Considerations for accurate calculations

- Dipole—dominant contribution from large  $r$ ,
- Schiff moment—significant at small  $r$ ,
- Energy—contribution all radial ranges.

## Key points

- Complexity—multiple perturbations,
- Route to bounds—atomic-nuclear-particle,
- Many-body physics—heavy atoms,

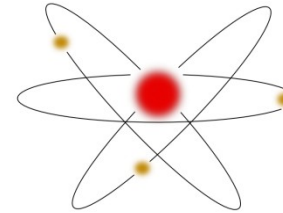
**Accurate wavefunction at all  $r$  ranges**

# Atomic wavefunctions mean field

## Atomic orbitals

For atoms with high nuclear charge relativistic effects are important. Dirac-Hamiltonian is an appropriate choice,

$$H_{\text{DC}} = \sum_i \left[ \alpha_i \cdot p_i + \beta c^2 - V_n(r_i) \right] + \sum_{i < j} \frac{1}{|r_i - r_j|}$$

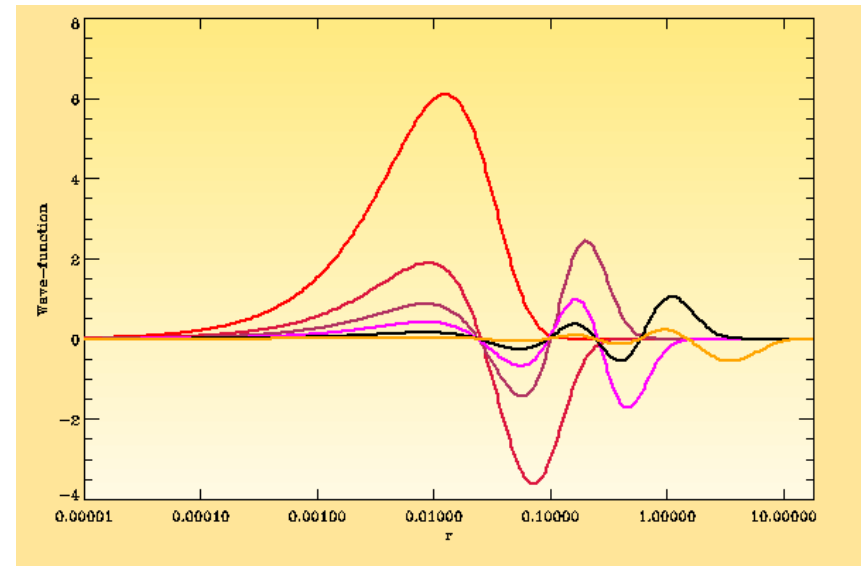


## Challenge

Accurate description of the electron-electron correlations

$$\sum_{i < j} \frac{1}{|r_i - r_j|}$$

Starting point is the mean field calculations, Dirac-Fock for the present calculations. Then obtain many electron wavefunctions as direct product.



Single electron radial wave functions (1-6s) of atomic Ytterbium.

# Many body perturbation theory diagrammatics

## Residual Coulomb interaction

Consider Helium atom, which has two electrons.

$$H = \sum_{i=1}^2 \frac{p_i^2}{2m} + \frac{Ze^2}{r_{1e}} + \frac{1}{r_{12}}$$

Where, linear momentum states are eigenstates for free particles; angular momentum are eigen states with the nuclear potential.

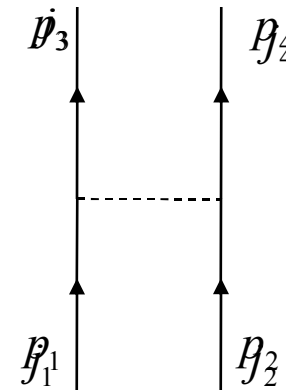
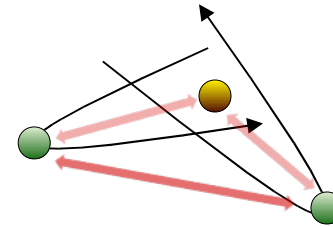
In actual many-body calculations, residual Coulomb interaction

$$\sum_{i<j} \frac{1}{|r_i - r_j|} = \sum_i U_{DF}(r_i)$$

Is the perturbative interaction.

## Complications in EDM calculations

Two more perturbative Hamiltonians: CP violating interaction Hamiltonian and electric dipole moment coupling to external field



$$H_{PTV} \quad \text{and} \quad D \cdot E_{\text{ext}}$$

# Correlations effects many-body effects

## Electron-electron correlation effects

To define Hilbert space, single particle states are separated into core and virtual.

- Core: states occupied in reference/unperturbed state,
- Virtual: states not occupied in reference/unperturbed state.

Hilbert space consist of reference and occupied replaced with virtual states.

## Size extensivity

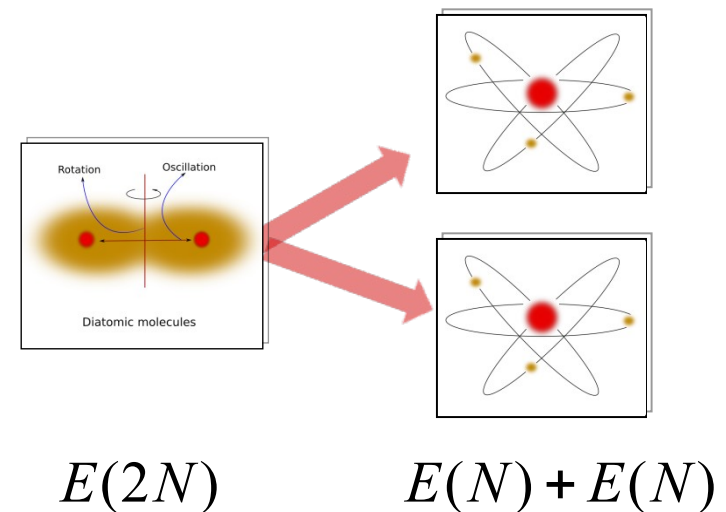
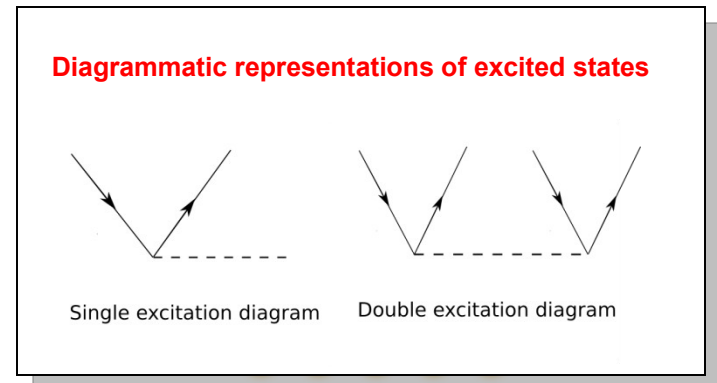
A key point in many-body theory is: total energy of the system depend linearly dependent on number of constituent particles.

$$E(n) \propto n$$

Which implies

$$E(N) = \sum_i E(n_i) : \sum_i n_i = N$$

Coupled-cluster theory satisfies this condition.



# Coupled-cluster theory accurate many-body theory

## Many-body perturbation to Coupled-cluster

Order by order calculation with many-body theory, even with diagrams, is tedious beyond third order. Number of diagrams runs into thousands.

Coupled-cluster theory is equivalent to selected summation or grouping of diagrams to all orders.

Wave operator is an exponential.

Further, it couples excitations of various orders.

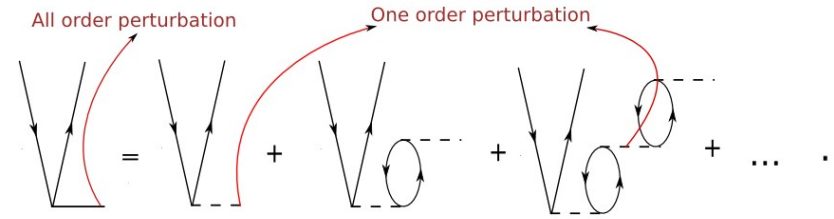
**Working equations are coupled Nonlinear equations**

$$|\Psi\rangle = e^T |\Phi_0\rangle$$

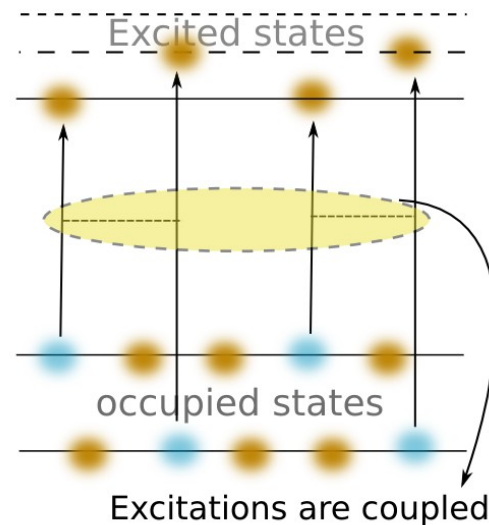
## Coupled-cluster equations

$$\langle \Phi_a^p | H_N + [H_N, T] + [H_N, [H_N, T]] + \dots | \Phi_0 \rangle = 0$$

$$\langle \Phi_{ab}^{pq} | H_N + [H_N, T] + [H_N, [H_N, T]] + \dots | \Phi_0 \rangle = 0$$



Coupled-cluster singles



**Attention**

**B. K. Sahoo**

Relativistic Many-Body Theory of Parity Nonconservation....

18 Jan, 14:30 PM



# Perturbed Coupled-cluster theory

## accurate many-body theory

### Perturbing coupled-cluster wave function

Electric dipole moment expression consist of summing over a set of intermediate atomic states

$$d_a = 2 \sum_I \frac{\langle \Psi_0 | D | \Psi_I \rangle \langle \Psi_I | H_{PTV}^{\text{Schiff}} | \Psi_0 \rangle}{E_0 - E_I} = S\eta$$

Reframe or modify the expression in terms of perturbed atomic state

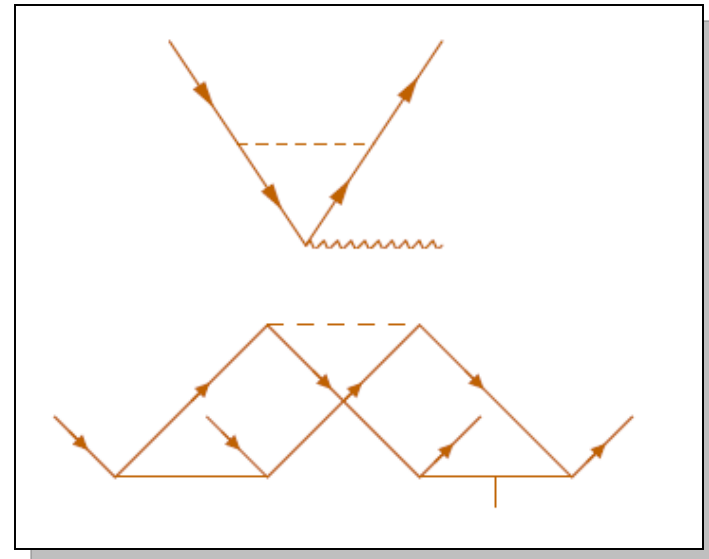
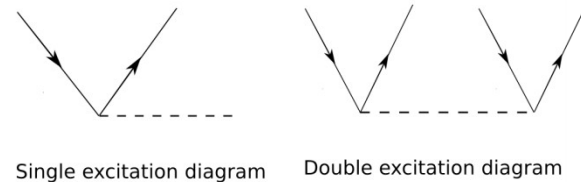
$$d_a = 2 \langle \tilde{\Psi}_0 | D | \tilde{\Psi}_0 \rangle$$

$$|\tilde{\Psi}_0\rangle = \sum_I \frac{|\Psi_I\rangle \langle \Psi_I | H_{PTV}^{\text{Schiff}} | \Psi_0 \rangle}{E_0 - E_I}$$

Perturbed coupled-cluster expression

$$|\tilde{\Psi}_0\rangle = e^{T^{(0)} + \lambda T^{(1)}} |\Phi_0\rangle$$

### Diagrammatic representations of excited states



# Particle physics implications parameter bounds

## Route via nuclear physics

Connecting atomic physics results to nuclear physics parameters

- Method—Skyrme potential, pion dominated interaction,
- Many-body effects—core-polarization,

$$S(^{199}\text{Hg}) = g_{\pi NN} \left[ 0.01 \bar{g}_{\pi NN}^{(0)} + 0.007 \bar{g}_{\pi NN}^{(1)} + 0.02 \bar{g}_{\pi NN}^{(2)} \right] \text{e fm}^3$$

J. H. de Jesus and J. Engel, Phys. Rev. C 72, 045503 (2005)

$\theta_{\text{QCD}}$  bound

Consider iso-scalar contributes maximally then  
[R. J. Crewther, P. Di Vecchiaa, G. Venezianoa  
and E. Witten, Phys. Lett. B 88, 123 (1979)]

$$\bar{g}_{\pi NN}^{(0)} = 0.027 \theta_{\text{QCD}}$$

$$\theta_{\text{QCD}} < 1.7 \times 10^{-10}$$

## Key points

- Least contribution—iso-vector component,
- Dominant contribution—iso-tensor component,
- Perturbation—P and T violating.

$(\tilde{d}_u - \tilde{d}_d)$  bound

Consider iso-vector contributes maximally then  
[M. Pospelov, Phys. Lett. B 530, 123 (2002)]

$$g_{\pi NN}^{(1)} = \frac{2(\tilde{d}_u - \tilde{d}_d)}{10^{-14}}$$

$$(\tilde{d}_u - \tilde{d}_d) < 3.2 \times 10^{-27} \text{e cm}$$

# Experiments with polar molecules

## larger polarization

### Diatomic polar molecules

Electronic clouds of heavy atoms like Pb, Tl, Yb and Hg are strongly polarized/distorted when it form molecules with Fluorine or Oxygen.

$$\frac{\langle W_{\text{EDM}} \rangle_{\text{molecule}}}{\langle W_{\text{EDM}} \rangle_{\text{atom}}} \approx \frac{5 \times 10^8}{E_{\text{ext}}}$$

For moderate field of 5000 kV/cm, molecular interaction energy is 100,000 time larger. A huge gain.

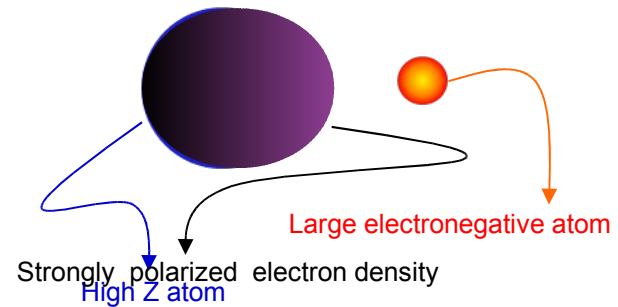
### Candidate molecules

| Molecule/ion   | Results or ongoing experiments                                      |
|--|---|
| PbO  | Yale<br>D. DeMille, et al, Phys. Rev. A 61, 052507 (2000) .         |
| YbF  | University of Sussex<br>J. J. Hudson, et al, PRL 89, 023003 (2002). |
| HfF <sup>+</sup> , HfH <sup>+</sup> , PtH <sup>+</sup> | JILA<br>Russell Stutz, Eric Cornell , BAPS J1.047 (2004)            |

### Attention

**E. A. Cornell**

How round is the electron? Looking for an asymmetry of 10<sup>-15</sup> femtometers  
20 Jan, 9:30 AM



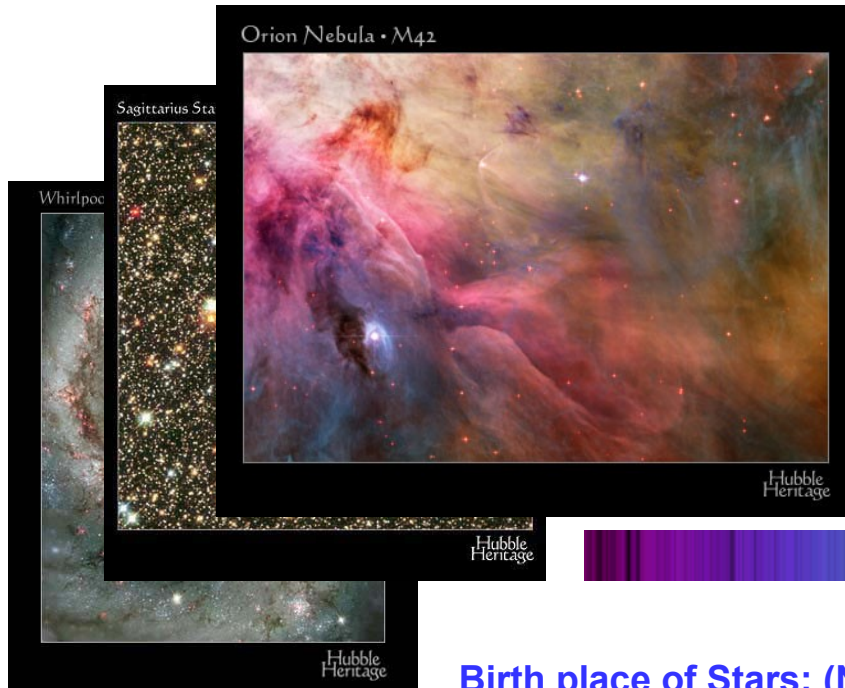
|  |  |   |   |
|--|--|---|---|
| 70<br><b>Yb</b><br>Ytterbium<br>173.04<br>[Xe]4f <sup>14</sup> 6s <sup>2</sup><br>6.2542 | 80<br><b>Hg</b><br>Mercury<br>200.59<br>[Xe]4f <sup>14</sup> 5d <sup>10</sup> 6s <sup>2</sup><br>10.4375 | 81<br><b>Tl</b><br>Thallium<br>204.3833<br>[Hg]6p<br>6.1082 | 82<br><b>Pb</b><br>Lead<br>207.2<br>[Hg]6p <sup>2</sup><br>7.4167 |
|--|--|---|---|

|  |  |
|--|--|
| 7<br><b>N</b><br>Nitrogen<br>14.0067<br>1s <sup>2</sup> 2s <sup>2</sup> 2p <sup>3</sup><br>14.5341 | 8<br><b>O</b><br>Oxygen<br>15.9994<br>1s <sup>2</sup> 2s <sup>2</sup> 2p <sup>4</sup><br>13.6181 |
|--|--|

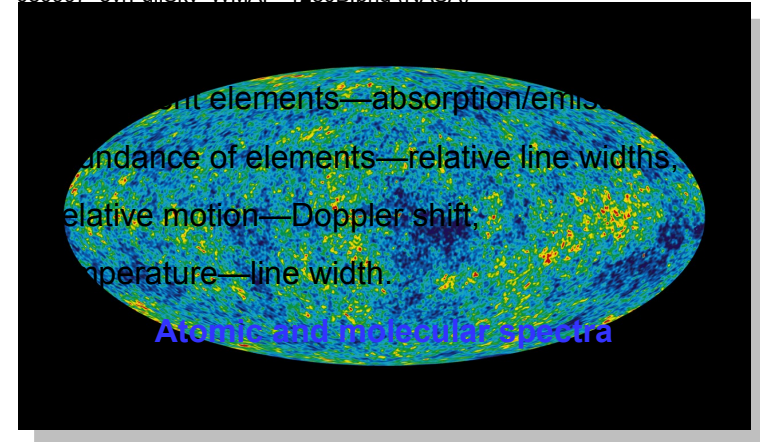
# Atomic/molecular physics probing cosmos

## The Universe

- ~13,700,000,000 yrs young,
- ~80,000,000,000 galaxies,
- Stable protons ~3 minutes after Big-bang,
- Molecular clouds and stars (galaxies) observable components.



080997\_5yrFullSky\_WMAP\_1280B.png (NASA)



## Implications: Helium discovery

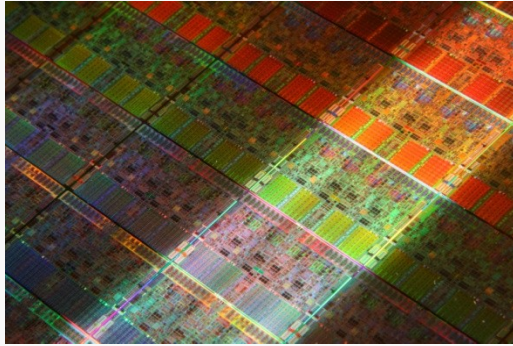
- Pierre Janssen—16 August 1868,
- Solar spectra during eclipse—He absorption line,
- Observation location—Guntur, India,
- Name—derived from Helios, Greek sun god.

**Unique signature of elements and molecules**

**Birth place of Stars: (Not bollywood ) Spectacular molecular clouds**

# A revolution what one PC can do

## Intel i7 940 processor



Latest Intel processor

- 2.93GHz clock frequency,
- Quad core,
- 8 processing threads,
- SPECfp2006 31.3

Average performance  
~  $5.8 \times 10^9$  FLOPS

## Quantum many-body calculations

### Performance required

Solving  $\sim 10^7$  nonlinear equations

Each term require  $\sim 10^7$  integrations

One iteration  $\sim 48$  hours

Complete calculation  
 $\sim 560$  hours (40 days)

### Cluster computing

#### Solution

Harness the power of several processors and parallelize applications. Possible options are shared memory, distributed memory and hybrid of these two.



# Conclusions

## implications of atomic EDMs

- Energy range—higher than achievable with LHC,
- Physics—sensitive to a wide variety of CP violation phenomena,
- Neutral systems—atoms and molecules are the only systems,
- Complimentarity—atomic EDMs explore slightly different parameter space

**Thank you**