Electric dipole moments of hadrons in atoms, molecules and solids.

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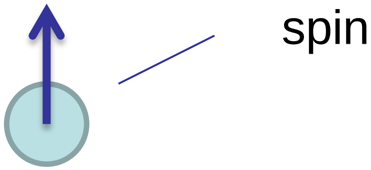
Neutron Electric Dipole Moment (EDM)



$$\vec{d} = 2d_n\vec{S}$$

Violates P
Violates T

$$\delta E = -\mu_n\vec{S}\cdot\vec{B} - 2d_n\vec{S}\cdot\vec{E}$$

NMR experiment

$$\omega = \mu_n B + d_n E$$

$$\omega = \mu_n B - d_n E$$

Charged particle, proton or nucleus

1) The particle inside an electrically neutral system.

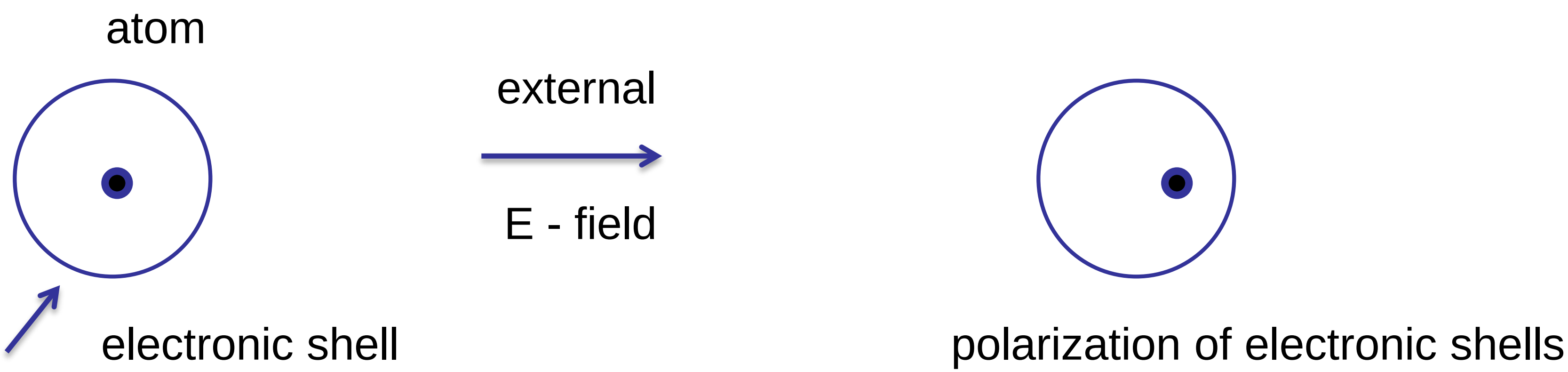
2) The particle in a storage ring.

(1) In principle the EDM story is the same as that for neutron.

$$\vec{d} = 2d_z\vec{S}$$

How to apply electric field to the particle?

Shielding of external electric field by electrons.



atom

external

E - field

electronic shell

polarization of electronic shells

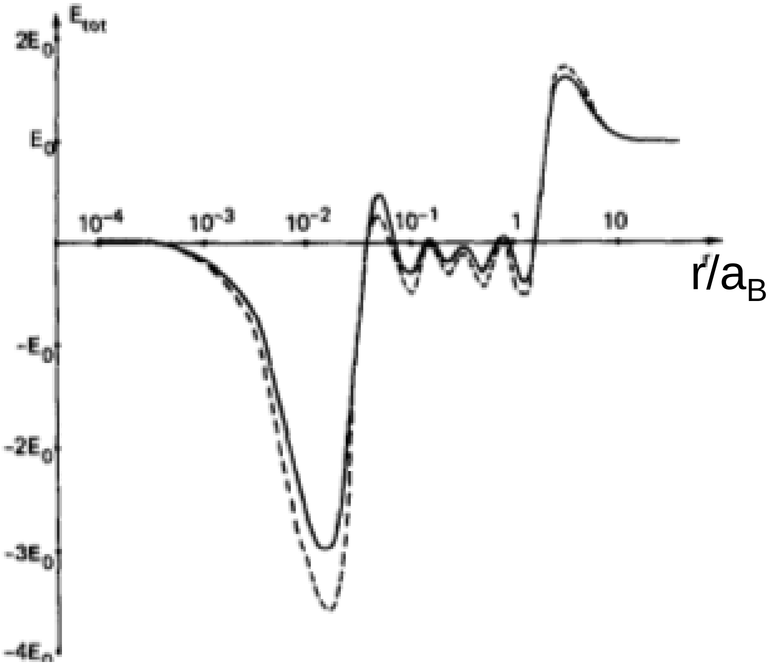
The total electric field acting on nucleus is zero.

$$\boxed{\vec{E} = \vec{E}_{ext} + \vec{E}_{polarization} = 0}$$

Total force acting on nucleus is zero.

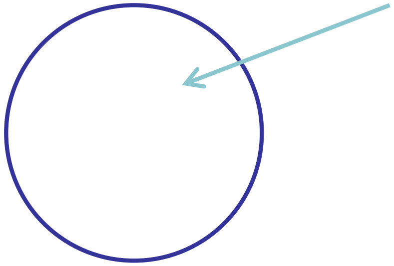
Schiff Theorem.

Screening of the external electric field in Tl, 81 electron



V. A. Dzuba et al.
Phys. Lett A **118**, 177 (1986).

However, this does not imply that the TP-odd effects are nonobservable.



Atomic nucleus

$\rho_0(r)$ - spherically symmetric charge density.

$\delta\rho$ - *TP* odd density perturbation.

$$\int \rho_0(r)dV = Z$$

$$EDM : \vec{d} = \int \vec{r}\,\delta\rho(r)dV$$

Schiff theorem claims that total force acting on the nucleus is zero.

$$\int E_{tot}(r)\rho_0(r)dV = 0$$

Since E_{tot}(r) varies inside nucleus one can, in principles, probe $\delta\rho$ (r) since spatial distribution of $\delta\rho$ (r) is different from ρ_0 (r).

Exact word identity

How to account Schiff's theorem exactly to avoid the problem of non-exact compensations in approximate calculation?

Exclude the dipole component of the nucleus electrostatic potential.

$$\delta\rho_{TP}(R) = \int \frac{\delta\rho(r)dV}{|R-r|} \rightarrow \int \frac{\delta\rho(r)dV}{|R-r|} + \frac{1}{Z}\vec{d}\vec{\nabla}_R \int \frac{\rho_0(r)dV}{|R-r|}$$

Expanding $\frac{1}{|R-r|}$ in powers of r

$$\frac{1}{|R-r|} = \frac{1}{R} - r_\mu \partial_\mu \frac{1}{R} + \frac{1}{2} r_\mu r_\nu \partial_\mu \partial_\nu \frac{1}{R} - \frac{1}{6} r_\mu r_\nu r_\alpha \partial_\mu \partial_\nu \partial_\alpha \frac{1}{R} \ldots$$

$$\partial^2 \frac{1}{R} = \Delta \frac{1}{R} = 4\pi\delta(r)$$

$$\delta\varphi_{TP} = 4\pi\vec{S}\cdot\vec{\nabla}\rho(r)$$

$$\vec{S}_{\mu} = \frac{q}{10}\left\{\int \delta\rho_{TP}(r)r^{2}r_{\mu}dV - \frac{5}{3}r_{q}^{2} < r_{\mu} >\right\} = S\frac{\vec{I}}{I}$$

q is charge of the “valence” nucleon, I is spin of the nucleus.

$$< r_{\mu} >= \int r_{\mu}\delta\rho_{TP}(r)dV$$

$$r_{q}^{2} = \frac{1}{Z}\int \rho_{0}r^{2}dV$$

The above story is almost correct. On top of the story one has to account for relativistic wave function of electron inside nucleus.

Interaction with electrons.

$$\boxed{H_{TP} = e\delta\varphi_{TP} = -4\pi\,|e|\,S_\mu \partial_\mu \delta(r)}$$

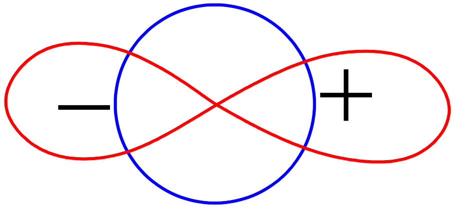
Matrix element of the interaction is nonzero between s- and p-states of the external atomic electron.

$$\boxed{< s\,|\,H_{TP}\,|\,p > \;\propto\; Z^2 S R}$$

R ~ 1-5 is the relativistic factor.

One power of Z comes from $|\psi^{(0)}|^2$ and another power of Z comes from $\vec{\nabla}$.

$$\boxed{\psi = \psi_s + \alpha\psi_p}$$

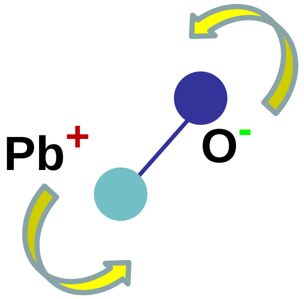


constructive interference

This leads to **atomic EDM**, for example ^{199}Hg.

The effect is enhanced for heavy elements, and the effect is obviously enhanced in strong electric field.

Diatomic molecule is a “quantum lever” to enhance electric field.

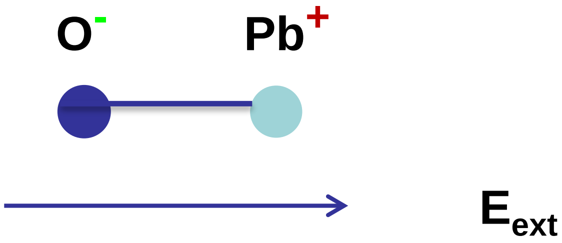


Rotational interval

$$\frac{\hbar^z}{2I} \sim 10^{-4} eV, \qquad I = m_0 r^2 \qquad r \sim 3a_B \sim \overset{o}{\mathrm{A}}$$

Hence an external electric field E_{ext} ~ 10 kV/cm is sufficient to fully polarize the molecule.

$$\boxed{eE_{ext} r \sim \frac{\hbar^2}{2I} \sim 10^{-4} eV.}$$



This polarization results in the huge internal molecular electric field

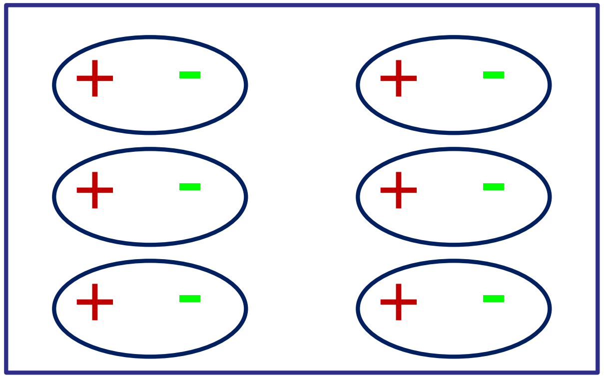
$$\boxed{E_{\text{int}} \sim \frac{e}{(1\overset{o}{\text{A}})^2} \sim 10^9 V/cm}$$

acting on Pb electrons.

The lever gain is $\dfrac{10^9}{10^4} = 10^5.$

This is the idea of experiments with diatomic molecules.

Ferroelectric is a next logical step on this way. This is a “semiquantum lever”.



solid

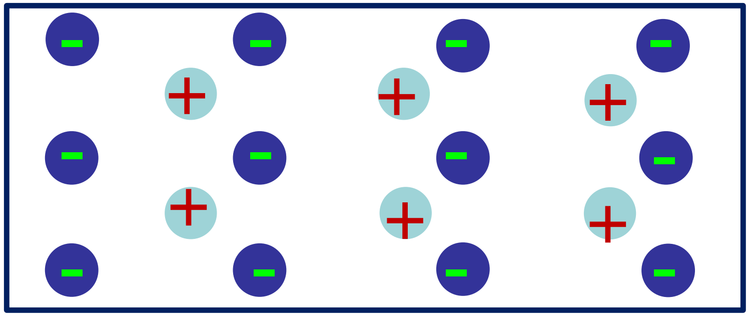
A.J.Leggett, PRL **41**, 586 (1978).
T.N. Mukhamedjanov, *O.P. Sushkov* PRA **72**, 034501 (2005).
J.A. Ludlow and *O.P. Sushkov* JPhys B **46**, 085001 (2013).

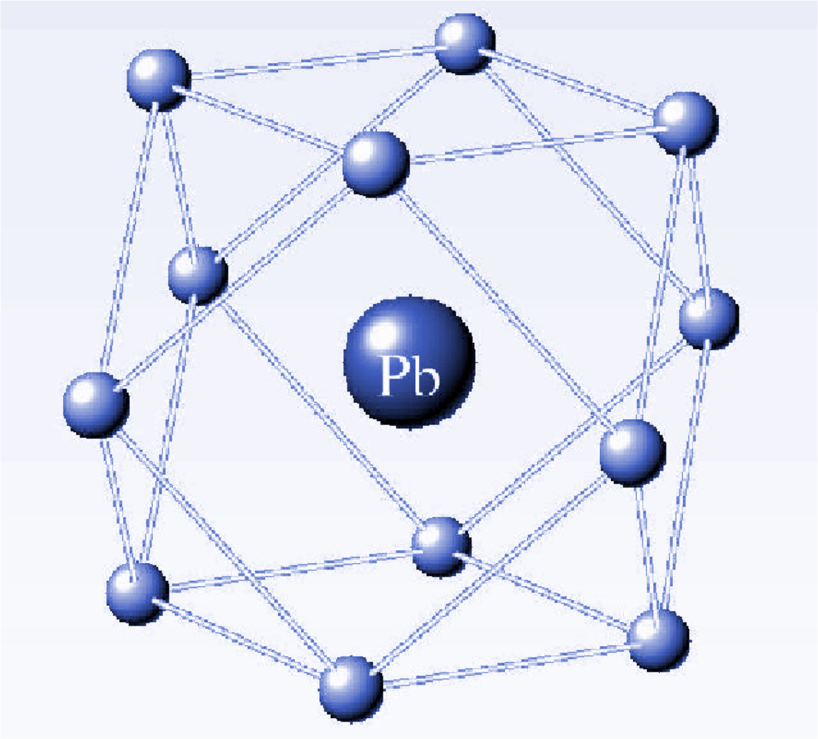
$PbTiO_3$

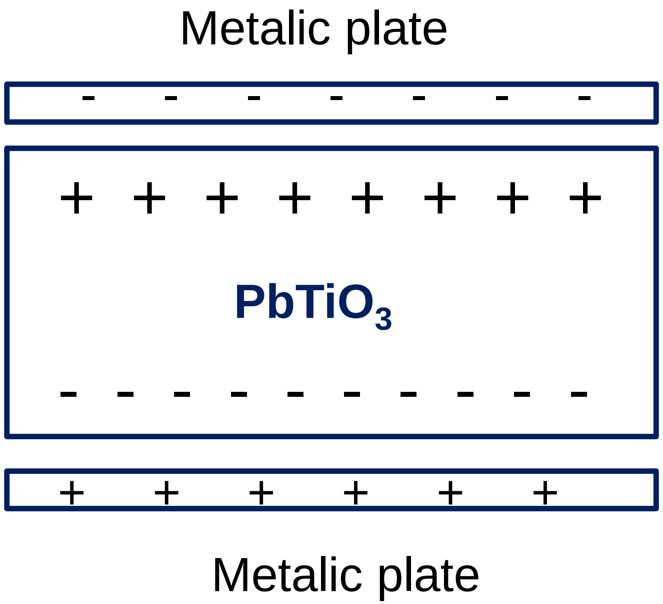
1) Pb, Z = 82.
2) a very strong ferroelectric.

A **2D model**, do not show Ti.

The lever gain = ∞






Metalic plate

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$PbTiO_3$

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Metalic plate

Of course, there is no electric field inside the solid.
However, each Pb^{2+} ion is shifted by **$x \approx 0.4$Å** with respect to the Oxygen cage.
This is equivalent to atomic electric field ~10^9V/cm.

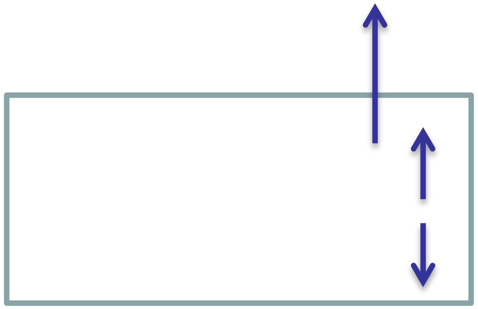
Wave functions of electrons localised at oxygen ions can be expanded in terms of Pb atomic orbitals.

$$| s > \rightarrow | 7s > + \beta_s \, | 6p_x >$$

$$| P > \rightarrow | 6p_x + \beta_p \, | 7s >$$

both β_s and β_p are proportional to x.

^{209}Pb NMR frequency shift



- direction of electric polarization

spin up, spin down

$$\Delta\varepsilon \approx -0.6 * 10^6 \frac{S}{e a_b^3} eV$$

Advantages:

1) large Z,
2) large effective internal electric field,
3) macroscopic density,
4) possibility of polarization of nuclear spins using optical pumping with UV created PB^{3+} paramagnetic centers.

Barium hexaferrite $BaFe_{12}O_{19}$

Multiferroic with high electric and magnetic critical temperatures

J. Scott, private comminication

Substitution of magnetic Fe by nonmagnetic Ga or Al.
So far $BaFe_3Ga_9O_{19}$
Quantum ferroelectric with T≈0.
Hyperbolic dynamics instead of usual diffusive dynamics.

(i) Replacement of Ba by Pb.
(ii) Full substitution of Fe.

Expected ordering temperature ~ 10K.

(i) Possibility of electric re-polarization
(ii) Semiconductor, gap ≈ 1eV. Transparent for infrared. Different possibilities for optical pumping.

Conclusions

The ferroelectric gain in EDM type of experiments is very significant.

$PbTiO_3$ is the best solid from the point of view of the magnitude of the effect. Nevertheless quantum ferroelectrics might be very interesting, they can give more flexibility.

Thank you!