Nuclear Schiff Moments and Atomic EDMs

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June 26, 2007
Theorem (T/EDM Connection)

Nondegenerate states have static electric dipole moments iff T and P are violated.

Handwaving Proof

Lack of degeneracy implies $\langle \vec{d} \rangle \propto \langle \vec{J} \rangle$ with the same proportionality constant in each $M$ substate. But $\langle \vec{J} \rangle$ and $\langle \vec{d} \rangle$ transform oppositely under time reversal of operators and state ($M \rightarrow -M$) if T is conserved. So if T is a good symmetry, the state cannot have an EDM. If not, the state will have one.

Of course, $T = CP$. 
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Of course, $\mathcal{T} = \mathcal{CP}$. 
EDMs Sensitive to New Physics

In standard model only one phase. Diagrams cancel to high order, e.g.:

\[ i \sin \delta \]

\[ f \quad W \quad f \]

\[ f' \quad f' \quad f \]

\[ \gamma \]

\[ + \]

\[ -i \sin \delta \]

Thus, EDMs are insensitive to standard-model \( C_P \) but sensitive to extra-standard-model \( C_P \). Limits from atoms and neutrons, have already made SUSY a difficult proposition.
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\[ f \rightarrow W \rightarrow f \]

\[ + \ldots \]

SUSY has many phases. Low-order diagrams uncanceled, e.g.:

\[ \gamma \]

\[ \tilde{f} \rightarrow \tilde{f} \]

\[ f \rightarrow e^{i\theta} \rightarrow f \]
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In standard model only one phase. Diagrams cancel to high order, e.g.:

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\[ f f W \gamma f' f' f f' \]
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Thus, EDMs are insensitive to standard-model $\mathcal{CP}$ but sensitive to extra-standard-model $\mathcal{CP}$. Limits from atoms and neutrons, have already made SUSY a difficult proposition.
How Do Things Get EDMs?

Starting at most fundamental level and moving up:
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- Underlying fundamental theory generates three $T$-violating $\pi NN$ vertices:

\[
\begin{array}{c}
N & g & \bar{q} & q \\
\end{array}
\]
How Do Things Get EDMs?

Starting at most fundamental level and moving up:

- Underlying fundamental theory generates three $T$-violating $\pi NN$ vertices:

- Then neutron gets EDM from diagrams like this:
How Do Atoms Get EDMs?

- Nucleus can get one from nucleon EDM or $T$-violating $NN$ interaction:

$$\begin{align*}
N & \quad N & \quad N \\
\bar{g} & \quad \pi & \quad g \\
\gamma & & \\
\end{align*}$$

Finally, atom gets one from nucleus. Electronic shielding makes the relevant nuclear object the "Schiff moment" $\langle \vec{S} \rangle \approx \langle \sum_p (\vec{r}_p - \vec{Z} \vec{D}) \rangle$ rather than dipole moment $\langle \vec{D} \rangle \equiv \langle \sum_p \vec{r}_p \rangle$. Nuclear-structure theory's place in the chain: calculating dependence of $\langle \vec{S} \rangle$ on the $\bar{g}$'s in heavy nuclei.
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- Nucleus can get one from nucleon EDM or T-violating $NN$ interaction:

$$W \propto \left\{ \bar{g}_0 \tau_1 \cdot \tau_2 - \frac{\bar{g}_1}{2} (\tau_1^z + \tau_2^z) + \bar{g}_2 (3\tau_1^z \tau_2^z - \tau_1 \cdot \tau_2) \right\} (\sigma_1 - \sigma_2)$$

$$- \frac{\bar{g}_1}{2} (\tau_1^z - \tau_2^z) (\sigma_1 + \sigma_2) \right\} \cdot (\nabla_1 - \nabla_2) \exp \left( \frac{-m_\pi |r_1 - r_2|}{m_\pi |r_1 - r_2|} \right)$$
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\[
\langle \vec{S} \rangle \approx \left\langle \sum_p \left( \vec{r}_p - \frac{1}{2} \vec{D} \right)^2 \left( \vec{r}_p - \frac{1}{2} \vec{D} \right) \right\rangle
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rather than dipole moment $\langle \vec{D} \rangle \equiv \langle \sum_p \vec{r}_p \rangle$. 
How Do Atoms Get EDMs?

- Nucleus can get one from nucleon EDM or T-violating NN interaction:

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Nuclear-structure theory’s place in the chain: calculating dependence of \( \langle \hat{S} \rangle \) on the \( \tilde{g}'s \) in heavy nuclei.
Hartree-Fock-Bogoliubov calculations with phenomenological density-dependent Skyrme interaction
State of Art in Heavy Nuclei

Hartree-Fock-Bogoliubov calculations with phenomenological density-dependent Skyrme interaction

\[ H_{\text{Sk}} = b_0 \left(1 + x_0 \hat{P}_\sigma\right) \delta(r_1 - r_2) \]
\[ + b_1 \left(1 + x_1 \hat{P}_\sigma\right) \left[(\nabla_1 - \nabla_2)^2 \delta(r_1 - r_2) + h.c.\right] \]
\[ + b_2 \left(1 + x_2 \hat{P}_\sigma\right) (\nabla_1 - \nabla_2) \cdot \delta(r_1 - r_2)(\nabla_1 - \nabla_2) \]
\[ + b_3 \left(1 + x_3 \hat{P}_\sigma\right) \delta(r_1 - r_2)\rho^\alpha\left(\frac{r_1 + r_2}{2}\right) \]
\[ + ib_4 (\sigma_1 + \sigma_2) \cdot (\nabla_1 - \nabla_2) \times \delta(r_1 - r_2)(\nabla_1 - \nabla_2) , \]

where

\[ \hat{P}_\sigma = \frac{1 + \sigma_1 \cdot \sigma_2}{2} , \]

\( b_i, x_i, \alpha \) adjusted to fit masses, radii, etc.
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Corrections to HFB are the frontier.
EDM Work Thus Far

In normal (non-octupole-deformed) nuclei, e.g., $^{199}\text{Hg}$, the best work has been approximations to HFB with

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$T$-violating interaction
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In octupole-deformed-nuclei, where Schiff moments are enhanced, treating $W$ as an explicit perturbation is easier.
$W$ probes spin density. Interaction should have good spin response. M. Bender et al. fit some time-odd terms of SkO$'$ to Gamow-Teller resonance energies and strengths.
Strength distribution of isoscalar analog of Schiff operator measured in $^{208}\text{Pb}$.
Testing SkO' and other Skyrme interactions

Strength distribution of isoscalar analog of Schiff operator measured in $^{208}$Pb.

How do Skyrme interactions do?
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How do Skyrme interactions do?
This is the nucleus with the best experimental limit.

\[ \langle S_z \rangle_{\text{Hg}} \equiv a_0 \, g \, g_0 + a_1 \, g \, g_1 + a_2 \, g \, g_2 \, (\text{e fm}^3) \]
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Is the spread a measure of uncertainty? Hard to know without intense focus on Skyrme functionals and related observables.
Nuclear Deformation

\[ \lambda = 0 \]

Sphere
Nuclear Deformation

$$\lambda = 0$$
Sphere

$$\lambda = 2$$
Quadrupoles

OBLATE

PROLATE
Here we need to treat $W$ as explicit perturbation:

$$\langle \vec{S} \rangle = \sum_m \frac{\langle 0 | \vec{S} | m \rangle \langle m | W | 0 \rangle}{E_0 - E_m} + c.c.$$  

where $|0\rangle$ is unperturbed ground state.
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where \( |0\rangle \) is unperturbed ground state.

Ground state has nearly-denerate partner \( |\bar{0}\rangle \) with same opposite parity and same intrinsic structure, so:

\[
\langle \vec{S} \rangle \rightarrow \frac{\langle 0 | \vec{S} | \bar{0} \rangle \langle \bar{0} | W | 0 \rangle}{E_0 - E_{\bar{0}}} + \text{c.c.} \propto \frac{\langle \vec{S} \rangle_{\text{intr.}} \langle W \rangle_{\text{intr.}}}{E_0 - E_{\bar{0}}}
\]
Schiff Moment with Octupole Deformation

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$\langle \vec{S} \rangle$ is large because $\langle \vec{S} \rangle_{\text{intr.}}$ is collective and $E_0 - E_0$ is small.
Spectrum of $^{225}\text{Ra}$
Testing Skyrme Interactions Again

Binding and Separation Energies

\[ \delta E \text{ (\%)} \]

\[ S_{2n} \text{ (MeV)} \]

Expt.
SIII
SkM*
SLy4
SkO'

Neutron Number N

124 128 132 136 140 144 148
Testing Skyrme Interactions Again

Binding and Separation Energies

Single-Particle Energies

Expt.
SIII
SkM*
SLy4
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124 128 132 136 140 144 148

$S_{2n}$ (MeV)

0.0
-0.2
-0.4
-0.6
-0.8

$\delta E$ (%)
More Interaction Testing...

Octupole, Dipole, Schiff Stuff
Hartree-Fock calculation (Dobaczweski et al.) with SkO' gives

\[ \langle S_z \rangle_{\text{Ra}} = -1.5 \, g_0 + 6.0 \, g_1 - 4.0 \, g_2 \text{ (e fm}^3\text{)} \]

Larger by over 100 than in $^{199}$Hg!
Hartree-Fock calculation (Dobaczweski et al.) with SkO' gives

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What can we do to reduce it?
The Future

Can improve calculations in all heavy nuclei via

- More exact Schiff operator
- Parity- and angular-momentum projection
- Particle-hole correlations

But, as in $\beta\beta$ decay, uncertainties may not shrink much.

- Spin-dependent two-body operators for which no data exist pose problems because
  - The operators are two-body and spin-dependent
  - There are no data
  - Skyrme interactions are limited.

Need more related data: isoscalar-dipole distributions, spin-multipole distributions, ... (like in $\beta\beta$)

Underlying theory of heavy nuclei still needs work.

Reducing uncertainty for Schiff, $\beta\beta$ ... will take concerted effort of more than a few people!

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But, as in ββ decay, uncertainties may not shrink much. Spin-dependent two-body operators for which no data exist pose problems because
- The operators are two-body and spin-dependent
- There are no data
- Skyrme interactions are limited.
- Need more related data: isoscalar-dipole distributions, spin-multipole distributions,… (like in ββ)
- Underlying theory of heavy nuclei still needs work.

Reducing uncertainty for Schiff, ββ…will take concerted effort of more than a few people! Is it worthwhile?
The Future

Can improve calculations in all heavy nuclei via

- More exact Schiff operator
- Parity- and angular-momentum projection
- Particle-hole correlations

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THE END
What Do EDMs Have to Do With $T$

Consider nondegenerate ground state $|g.s. : J, M\rangle$. Symmetry under rotations $R_y(\pi)$ for vector operator like $\vec{d} \equiv \sum_i e_i \vec{r}_i$,

$$\langle g.s. : J, M | \vec{d} | g.s. : J, M \rangle = -\langle g.s. : J, -M | \vec{d} | g.s. : J, -M \rangle.$$
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$R^{-1}R$
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$T$ takes $M$ to $-M$, like $R_y(\pi)$. But $\vec{d}$ is odd under $R_y(\pi)$ and even under $T$, so for $T$ conserved

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If $T$ is violated, argument fails because $T$ can take $|\text{g.s.} : JM\rangle$ to $|\text{ex.} : J, -M\rangle$, a state in a different multiplet.
Unfortunately for atomic experiments:

Theorem (Schiff)

The nuclear dipole moment causes the atomic electrons to rearrange themselves so that they develop a dipole moment opposite that of the nucleus. In the limit of nonrelativistic electrons and a point nucleus the electrons’ dipole moment exactly cancels the nuclear moment, so that the net atomic dipole moment vanishes!
Shielding by Electrons

Proof

Consider atom with nonrelativistic constituents (with dipole moments $\mathbf{d}_k$) held together by electrostatic forces. The atom has a “bare” edm $\mathbf{d} \equiv \sum_k \mathbf{d}_k$ and a Hamiltonian

$$H = \sum_k \frac{p_k^2}{2m_k} + \sum_k V(\mathbf{r}_k) - \sum_k \mathbf{d}_k \cdot \mathbf{E}_k$$
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$$= H_0 + \sum_k \left( \frac{1}{e_k} \mathbf{d}_k \cdot \nabla V(\mathbf{r}_k) \right)$$

K.E. + Coulomb  \hspace{1cm} \text{dipole perturbation}
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$$= H_0 + \sum_k \left( \frac{1}{e_k} \right) \vec{d}_k \cdot \vec{\nabla} V(\vec{r}_k)$$

$$= H_0 + i \sum_k \left( \frac{1}{e_k} \right) \left[ \vec{d}_k \cdot \vec{p}_k, H_0 \right]$$

K.E. + Coulomb
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The perturbing Hamiltonian

\[ H_d = i \sum_k \left( \frac{1}{e_k} \right) \left[ \vec{d}_k \cdot \vec{p}_k, H_0 \right] \]

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\]
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\[
= |0\rangle + \sum_m |m\rangle \langle m| i \sum_k \left( \frac{1}{e_k} \right) \vec{d}_k \cdot \vec{p}_k |0\rangle \left( E_0 - E_m \right) \frac{1}{E_0 - E_m}
\]

\[
= \left( 1 + i \sum_k \left( \frac{1}{e_k} \right) \vec{d}_k \cdot \vec{p}_k \right) |0\rangle
\]
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The induced dipole moment $\vec{d}'$ is

$$\vec{d}' = \langle \bar{0} | \sum_j e_j \vec{r}_j | \bar{0} \rangle$$
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$$\vec{d}' = \langle \tilde{0} | \sum_j e_j \vec{r}_j | \tilde{0} \rangle$$

$$= \langle 0 | \left( 1 - i \sum_k (1/e_k) \vec{d}_k \cdot \vec{p}_k \right) (\sum_j e_j \vec{r}_j)$$

$$\times \left( 1 + i \sum_k (1/e_k) \vec{d}_k \cdot \vec{p}_k \right) |0 \rangle$$

So the net EDM is zero!
Shielding by Electrons

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$$
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