Time-Reversal Violation, EDMs, and Schiff Moments

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Time-Reversal Invariance is Violated

- Violation is seen in decay of $K$-mesons (direct) and $B$-mesons (through CP violation).

- And we strongly believe that $T (\equiv CP)$ violation played an important role in the early universe, causing excess of matter over antimatter.
What is the Source of T-Violation?

K and B phenomena almost certainly due to a phase in the $3 \times 3$ CKM matrix, which connects $(d, s, b)$ to flavor eigenstates that couple to $W$ and $Z$. But this violation is too weak to cause baryogenesis, which must arise outside the standard model, e.g. through supersymmetry, heavy neutrinos, Higgs sector...

To complicate things more, there’s the strong CP problem. In short...

We need to see T-violation outside mesonic systems to understand its sources. EDM’s are not sensitive to CKM T-violation, but are to other sources. They’ve already put extreme pressure on supersymmetry.
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Connection Between EDMs and T Violation

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

$$\langle \text{g.s.}: J, M | \ d_z | \text{g.s.}: J, M \rangle = - \langle \text{g.s.}: J, -M | \ d_z | \text{g.s.}: J, -M \rangle.$$
Connection Between EDMs and $T$ Violation

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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

$$ \langle \text{g.s.} : J, M | d_z | \text{g.s.} : J, M \rangle = + \langle \text{g.s.} : J, -M | d_z | \text{g.s.} : J, -M \rangle . $$

$T^{-1}T$
Connection Between EDMs and T Violation

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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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\]

Together with the first equation, this implies

\[
\langle d_z \rangle = 0.
\]

If \( T \) is violated, argument fails because \( T \) takes \( |g : JM\rangle \) to states with \( J, -M \), but different energy.
One Way Things Get EDMs

Starting at fundamental level and working up:

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

Then neutron gets EDM from chiral-PT diagrams like this:
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How Diamagnetic Atoms Get EDMs

Nucleus gets one from nucleon EDM and $T$-violating $NN$ interaction:

$$\nu_{PT} \propto \left\{ \left[ \bar{g}_0 \tau_1 \cdot \tau_2 - \frac{\bar{g}_1}{2} (\tau_1^z + \tau_2^z) + \bar{g}_2 (3\tau_1^z\tau_2^z - \tau_1 \cdot \tau_2) \right] (\sigma_1 - \sigma_2) \right. - \frac{\bar{g}_1}{2} (\tau_1^z - \tau_2^z) (\sigma_1 + \sigma_2) \right\} \cdot (\nabla_1 - \nabla_2) \exp \left( -\frac{m_\pi |r_1 - r_2|}{m_\pi |r_1 - r_2|} \right) + \text{contact term}$$
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+ contact term

Finally, atom gets one from nucleus. Electronic shielding makes relevant nuclear object the “Schiff moment” $\langle S \rangle \approx \langle \sum_p r_p^2 z_p + \ldots \rangle$.

Job of nuclear theory: calculate dependence of $\langle S \rangle$ on the $\bar{g}_i$ (and on the contact term and nucleon EDM).
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.*
How Does Shielding Work?

**Proof**

Consider an atom with non-relativistic constituents (with dipole moments \( \vec{d}_k \)) held together by electrostatic forces. The atom has a “bare” edm \( \vec{d} \equiv \sum_k \vec{d}_k \) and a Hamiltonian

\[
H = \sum_k \frac{p_k^2}{2m_k} + \sum_k V(\vec{r}_k) - \sum_k \vec{d}_k \cdot \vec{E}_k
\]

\[
= H_0 + \sum_k \frac{1}{e_k} \vec{d}_k \cdot \vec{\nabla} V(\vec{r}_k)
\]

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

**K.E. + Coulomb**

**dipole perturbation**
How Does Shielding Work?

The perturbing Hamiltonian

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

shifts the ground state \(|0\rangle\) to

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

The induced dipole moment $\vec{d}'$ is

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

So the net EDM is zero!
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$$
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$$

$$
= i \langle 0 | \left[ \sum_j e_j \vec{r}_j, \sum_k \left( \frac{1}{e_k} \vec{d}_k \cdot \vec{p}_k \right) \right] | 0 \rangle
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$$

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$$

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Recovering from Shielding

The nucleus has finite size. Shielding is not complete, and nuclear T violation can still induce atomic EDM $D_A$.

Post-screening nucleus-electron interaction proportional to Schiff moment:

$$\langle S \rangle \equiv \left\langle \sum_p e_p \left( r_p^2 - \frac{5}{3} \langle R_{ch}^2 \rangle \right) z_p \right\rangle + \ldots$$
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$$

If, as you'd expect, $\left\langle S \right\rangle \approx R_{Nuc}^2 \left\langle D_{Nuc} \right\rangle$, then $D_A$ is down from $\left\langle D_{Nuc} \right\rangle$ by

$$
O \left( \frac{R_{Nuc}^2}{R_A^2} \right) \approx 10^{-8}.
$$

Fortunately, the large nuclear charge and relativistic wave functions offset this factor by $10Z^2 \approx 10^5$.

Overall suppression of $D_A$ is only about $10^{-3}$. 

Theory for Heavy Nuclei

$\langle S \rangle$ largest for large $Z$, so experiments are in heavy nuclei.

Ab initio methods are making rapid progress, but

- Interaction (from chiral EFT) has problems beyond $A = 50$.
- Many-body methods not quite ready to tackle soft nuclei such as $^{199}$Hg, or even those with rigid deformation such as $^{225}$Ra.
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so

for now we must rely on nuclear density-functional theory: mean-field theory with phenomenological “density-dependent interactions” (Skyrme, Gogny, or successors) plus corrections, e.g.:

- projection of deformed wave functions onto states with good particle number, angular momentum
- inclusion of small-amplitude zero-point motion (RPA)
- mixing of mean fields with different character (GCM)
- ...

...
Nuclear Deformation

\[ \lambda = 0 \]
Sphere

\[ \lambda = 2 \]
Quadrupoles

OBLATE

\[ \lambda = 3 \]
Octupoles

PROLATE
Zr-102: normal density and pairing density
HFB, 2-D lattice, SLy4 + volume pairing

HFB: $\beta_2^{(p)}=0.43$  \hspace{1cm} \text{exp: } \beta_2^{(p)}=0.42(5), \text{ J.K. Hwang et al., Phys. Rev. C (2006)}
Nuclear ground state deformations (2-D HFB)
Varieties of “Recent” Schiff-Moment Calculations

Need to calculate

\[ \langle S \rangle \approx \sum_m \frac{\langle 0 | S | m \rangle \langle m | V_{PT} | 0 \rangle}{E_0 - E_m} + \text{c.c.} \]

where \( H = H_{\text{strong}} + V_{PT} \).

- \( H_{\text{strong}} \) represented either by Skyrme density functional or by simpler effective interaction, treated on top of separate mean field.
- \( V_{PT} \) either included nonperturbatively or via the explicit sum over intermediate states above.
- Nucleus either forced artificially to be spherical or allowed to deform.
1. Skyrme HFB (mean-field theory with pairing) in $^{198}$Hg.
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2. Polarization of core by last neutron and action of $V_{PT}$, treated as explicit corrections in quasiparticle RPA, which sums over intermediate states.

$\nu =$ last neutron
$\times =$ Schiff operator
Blob = core-particle
ring sum
Looped line = $V_{\text{strong}}$
Sawtooth = $V_{PT}$
\[ \langle S \rangle_{Hg} \equiv a_0 \, \overline{g} g_0 + a_1 \, \overline{g} g_1 + a_2 \, \overline{g} g_2 \ (e \text{ fm}^3) \]

<table>
<thead>
<tr>
<th></th>
<th>( a_0 )</th>
<th>( a_1 )</th>
<th>( a_2 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>SkM*</td>
<td>0.009</td>
<td>0.070</td>
<td>0.022</td>
</tr>
<tr>
<td>SkP</td>
<td>0.002</td>
<td>0.065</td>
<td>0.011</td>
</tr>
<tr>
<td>SIII</td>
<td>0.010</td>
<td>0.057</td>
<td>0.025</td>
</tr>
<tr>
<td>SLy4</td>
<td>0.003</td>
<td>0.090</td>
<td>0.013</td>
</tr>
<tr>
<td>SkO'</td>
<td>0.010</td>
<td>0.074</td>
<td>0.018</td>
</tr>
<tr>
<td>Dmitriev &amp; Senkov RPA</td>
<td>0.0004</td>
<td>0.055</td>
<td>0.009</td>
</tr>
</tbody>
</table>

Range of variation here doesn’t look too bad. But these calculations are not the end of the story…
Deformation and Angular-Momentum Restoration

If deformed state $|\Psi_K\rangle$ has good intr. $J_z = K$, one averages over angles to get:

$$|J, M\rangle = \frac{2J + 1}{8\pi^2} \int d\Omega \, D^J_{MK} (\Omega) R(\Omega) \, |\Psi_K\rangle$$

Matrix elements (with more detailed notation):

$$\langle J, M| S_m | J', M' \rangle \propto \int \int \sum_n d\Omega \, d\Omega' \times (\text{some D-functions})$$

$$\times \langle \Psi_K| R^{-1} (\Omega') S_n R(\Omega) |\Psi_K\rangle$$

rigid defm.  $\Omega \approx \Omega'$ (Geometric factor)  $\times \langle \Psi_K| S_z |\Psi_K\rangle$

For expectation value in $J = \frac{1}{2}$ state:

$$\langle S \rangle = \langle S_z \rangle_{J=\frac{1}{2}, M=\frac{1}{2}} \Rightarrow \begin{cases} \langle S \rangle_{\text{intr.}} & \text{spherical nucleus} \\ \frac{1}{3} \langle S \rangle_{\text{intr.}} & \text{rigidly deformed nucleus} \end{cases}$$

Exact answer somewhere in between.
Deformed Mean-Field Calculation Directly in $^{199}$Hg

Deformation actually small and soft – perhaps worst case scenario for mean-field. But in heavy odd nuclei, that's the best that has been done$^1$. $V_{PT}$ included nonperturbatively and calculation done in one step. Includes more physics than RPA (deformation), plus economy of approach. Otherwise should be more or less equivalent.

Oscillating PT-odd density distribution indicates delicate Schiff moment.

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$^1$Has some “issues”: don’t get ground-state spin correct, limited for now to axially-symmetric minima, which are sometimes a little unstable, true minimum probably not axially symmetric …
Results of “Direct” Calculation

Like before, use a number of Skyrme functionals:

<table>
<thead>
<tr>
<th></th>
<th>$E_{gs}$</th>
<th>$\beta$</th>
<th>$E_{exc.}$</th>
<th>$a_0$</th>
<th>$a_1$</th>
<th>$a_2$</th>
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<tbody>
<tr>
<td>SLy4</td>
<td>HF</td>
<td>-1561.42</td>
<td>-0.13</td>
<td>0.97</td>
<td>0.013</td>
<td>-0.006</td>
</tr>
<tr>
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<td>HF</td>
<td>-1562.63</td>
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<td>0</td>
<td>0.012</td>
<td>0.005</td>
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<tr>
<td>SV</td>
<td>HF</td>
<td>-1556.43</td>
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<td>0.68</td>
<td>0.009</td>
<td>-0.0001</td>
</tr>
<tr>
<td>SLy4</td>
<td>HFB</td>
<td>-1560.21</td>
<td>-0.10</td>
<td>0.83</td>
<td>0.013</td>
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</tr>
<tr>
<td>SkM*</td>
<td>HFB</td>
<td>-1564.03</td>
<td>0</td>
<td>0.82</td>
<td>0.041</td>
<td>-0.027</td>
</tr>
<tr>
<td>Fav. RPA</td>
<td>QRPA</td>
<td>–</td>
<td>–</td>
<td>–</td>
<td>0.010</td>
<td>0.074</td>
</tr>
</tbody>
</table>

Hmm…
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Ultimate goal: mixing of many mean fields, aka “generator coordinates”

Still a ways off because of difficulties marrying generator coordinates to density functionals.
Schiff Moment with Octupole Deformation

Here we treat always $V_{PT}$ as explicit perturbation:

$$\langle S \rangle = \sum_{m} \frac{\langle 0 | S | m \rangle \langle m | V_{PT} | 0 \rangle}{E_0 - E_m} + c.c.$$ 

where $|0\rangle$ is unperturbed ground state.
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Ground state has nearly-degenerate partner $|\bar{0}\rangle$ with same opposite parity and same intrinsic structure, so:

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Why is this? See next slide.
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Why is this? See next slide.

$\langle S \rangle$ is large because $\langle S \rangle_{\text{intr.}}$ is collective and $E_0 - E_{\bar{0}}$ is small.
A Little on Parity Doublets

When intrinsic state $|\bullet\rangle$ is asymmetric, it breaks parity.

In the same way we get good $J$, we average over orientations to get states with good parity:

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These are nearly degenerate if deformation is rigid. So with $|0\rangle = |+\rangle$ and $|\bar{0}\rangle = |-\rangle$, we get

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$$|\pm\rangle = \frac{1}{\sqrt{2}} (|\bullet\rangle \pm |\bar{\bullet}\rangle)$$

These are nearly degenerate if deformation is rigid. So with $|0\rangle = |+\rangle$ and $|\bar{0}\rangle = |-\rangle$, we get

$$\langle S \rangle \approx \frac{\langle 0 | S_z | \bar{0} \rangle \langle \bar{0} | V_{PT} | 0 \rangle}{E_0 - E_{\bar{0}}} + c.c.$$  

And in the rigid-deformation limit

$$\langle 0 | O | \bar{0} \rangle \propto \langle \bullet | O | \bar{\bullet} \rangle = \langle O \rangle_{\text{intr.}}$$

again like angular momentum.
Spectrum of $^{225}$Ra

Parity doublet

$|0\rangle$  $|\bar{0}\rangle$
Hartree-Fock calculation with our favorite interaction SkO’ gives

\[ \langle S \rangle_{Ra} = -1.5 \, g \bar{g}_0 + 6.0 \, g \bar{g}_1 - 4.0 \, g \bar{g}_2 \, (e \, fm^3) \]

Larger by over 100 than in $^{199}$Hg!

Variation a factor of 2 or 3. But, as you’ll see, we should be able to do better!
Current “Assessment” of Uncertainties

Judgment in 2013 review article (based on spread in reasonable calculations):

<table>
<thead>
<tr>
<th>Nucl.</th>
<th>Best value</th>
<th>Range</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$a_0$</td>
<td>$a_1$</td>
</tr>
<tr>
<td>$^{199}$Hg</td>
<td>0.01</td>
<td>$\pm$ 0.02</td>
</tr>
<tr>
<td>$^{129}$Xe</td>
<td>-0.008</td>
<td>-0.006</td>
</tr>
<tr>
<td>$^{225}$Ra</td>
<td>-1.5</td>
<td>6.0</td>
</tr>
</tbody>
</table>

Uncertainties pretty large, particularly for $a_1$ in $^{199}$Hg (range includes zero). How can we reduce them?
Reducing Uncertainty: Hg

Improving many-body theory to handle soft deformation, though probably necessary, is tough. But can also try to optimize density functional.

Isoscalar dipole operator contains $r^2z$ just like Schiff operator. Can see how well functionals reproduce measured distributions, e.g. in $^{208}$Pb.
$V_{PT}$ probes spin density; functional should have good spin response. Can adjust relevant terms in, e.g. SkO', to Gamow-Teller resonance energies and strengths.

More generally, examine correlations between Schiff moment and lots of other observables.
Reducing Uncertainty: Ra

Important new developments here.

\[ \langle S \rangle_{\text{intr.}} \text{ correlated with octupole moment, which will be extracted from measured E3 transitions.} \]

Gaffney et al., Nature

Transitions in \(^{225}\text{Ra}\) to be measured soon?
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Gaffney et al., Nature
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Transitions in $^{225}$Ra to be measured soon?

Gaffney et al., Nature
More on Reducing Uncertainty in Ra

What about matrix element of $V_{PT}$?

In one-body approximation

$$V_{PT} \approx \vec{\sigma} \cdot \vec{\nabla} \rho.$$  

The closest simple one body operator is

$$O_{AC} = \vec{\sigma} \cdot \vec{r}.$$  

**Q:** Can we measure $\langle 0 | O_{AC} | O \rangle$ or something like it?

Doesn’t occur in electron scattering, but does occurs in weak neutral current. Neutrino scattering on Ra?
The Future

Calculations have become sophisticated, but we still have a lot of work to do.

In the near future, that work involve nuclear DFT.

- In Hg, need to decide which, if either, $\alpha_1$ is correct and eventually account for “softness” of nucleus. And need correlation analysis, good proxies for Schiff distributions (e.g. isoscalar dipole distribution), $V_{PT}$ distribution.
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THE END.

Thanks for your kind attention.