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 ($\equiv \mathrm{CP}$) violation played an important role in the early universe, causing excess of matter over antimatter.

What is the Source of T-Violation?

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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.

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:

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

$R^{-1}R$ $\qquad$ $R^{-1}R$

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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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Together with the first equation, this implies

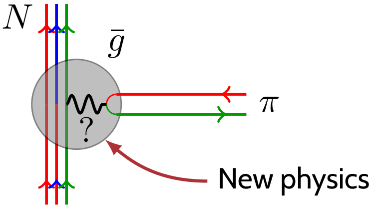
$$\boxed{\langle d_z \rangle = 0 \, .}$$

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 $\pi \mathrm{NN}$ vertices in chiral PT:



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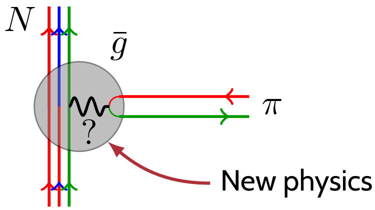

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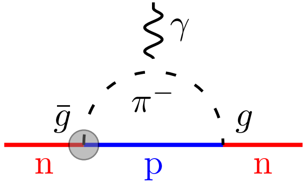
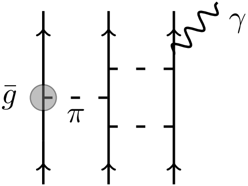


How Diamagnetic Atoms Get EDMs



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

$$V_{\mathrm{PT}} \propto \left\{ \left[\bar{g}_0 \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 - \frac{\bar{g}_1}{2} \left(\tau_1^z + \tau_1^z \right) + \bar{g}_2 \left(3\tau_1^z \tau_2^z - \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 \right) \right] \left(\boldsymbol{\sigma}_1 - \boldsymbol{\sigma}_2 \right) \right.$$

$$\left. - \frac{\bar{g}_1}{2} \left(\tau_1^z - \tau_2^z \right) \left(\boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2 \right) \right\} \cdot \left(\boldsymbol{\nabla}_1 - \boldsymbol{\nabla}_2 \right) \frac{\exp\left(-m_\pi |\boldsymbol{r}_1 - \boldsymbol{r}_2| \right)}{m_\pi |\boldsymbol{r}_1 - \boldsymbol{r}_2|}$$

$$+ \text{ contact term}$$

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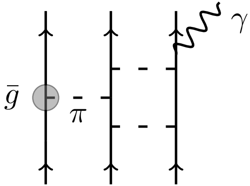

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Finally, atom gets one from nucleus. Electronic shielding makes relevant nuclear object the "Schiff moment" $\langle S \rangle \approx \langle \sum_p r_p^2 z_p + \ldots \rangle$.

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

How Does Shielding Work?

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 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

$$
\begin{aligned}
H &= \underbrace{\sum_k \frac{p_k^2}{2m_k} + \sum_k V(\vec{r}_k)}_{} - \sum_k \vec{d}_k \cdot \vec{E}_k \\
&= \quad H_0 \quad + \sum_k (1/e_k)\vec{d}_k \cdot \vec{\nabla} V(\vec{r}_k) \\
&= \quad H_0 \quad + i \sum_k (1/e_k) \left[\vec{d}_k \cdot \vec{p}_k, H_0\right]
\end{aligned}
$$

K.E. + Coulomb

dipole perturbation

How Does Shielding Work?

The perturbing Hamiltonian

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

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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&\quad \times \left(1 + i\sum_k (1/e_k)\vec{d}_k \cdot \vec{p}_k\right) |0\rangle \\
&= i\langle 0| \left[\sum_j e_j \vec{r}_j, \sum_k (1/e_k)\vec{d}_k \cdot \vec{p}_k\right] |0\rangle
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\end{aligned}$$

So the net EDM is zero!

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:

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

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

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

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 $A = 50$.
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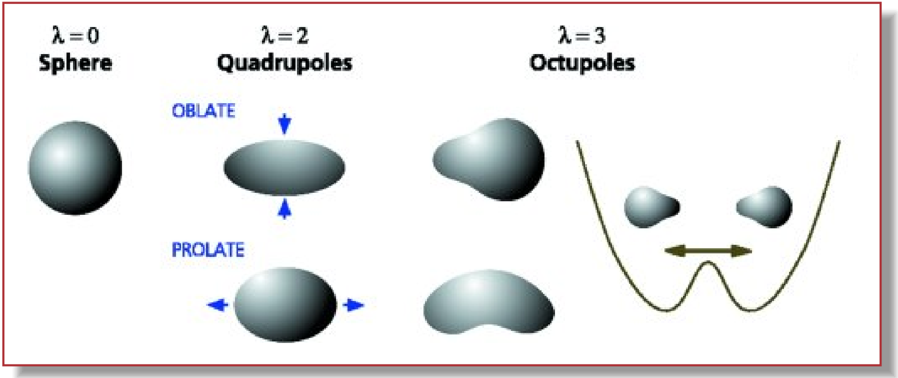
so

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.:

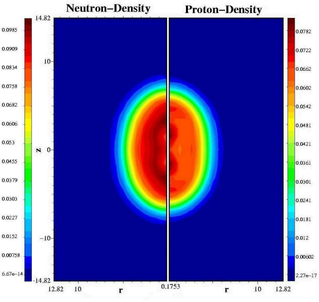
- projection of deformed wave functions onto states with good particle number, angular momentum
- inclusion of small-amplitude zero-point motion (RPA)
- mixing of mean fields with different character (GCM)
- ...

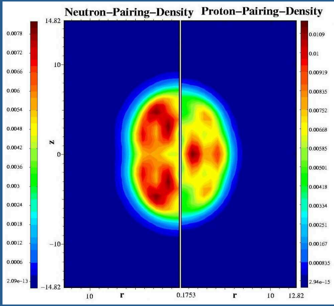
Nuclear Deformation



Skyrme DFT

Zr-102: normal density and pairing density
HFB, 2-D lattice, SLy4 + volume pairing
Ref: Artur Blazkiewicz, Vanderbilt, Ph.D. thesis (2005)





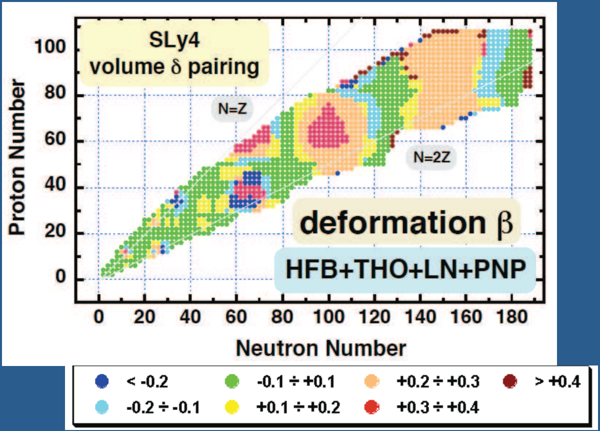
HFB: $\beta_2^{(p)}$=0.43

exp: $\beta_2^{(p)}$=0.42(5) , J.K. Hwang et al., Phys. Rev. C (2006)

Applied Everywhere

Nuclear ground state deformations (2-D HFB)

Ref: Dobaczewski, Stoitsov & Nazarewicz (2004) arXiv:nucl-th/0404077



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_{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.

^{199}Hg via Explicit RPA in Spherical Mean Field

1. Skyrme HFB (mean-field theory with pairing) in ^{198}Hg.

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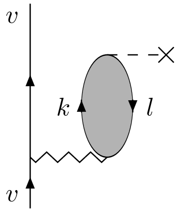
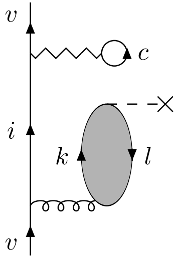
1. Skyrme HFB (mean-field theory with pairing) in ^{198}Hg.
2. Polarization of core by last neutron and action of V_{PT}, treated as explicit corrections in quasiparticle RPA, which sums over intermediate states.





v = last neutron

$\times$ = Schiff operator

Blob = core-particle ring sum

Looped line = V_{strong}

Sawtooth = V_{PT}

Results

$$\boxed{\langle S \rangle_{\mathrm{Hg}} \equiv a_0 \; g\bar{g}_0 + a_1 \; g\bar{g}_1 + a_2 \; g\bar{g}_2 \quad (\mathrm{e\ fm}^3)}$$

	a_0	a_1	a_2
SkM*	0.009	0.070	0.022
SkP	0.002	0.065	0.011
SIII	0.010	0.057	0.025
SLy4	0.003	0.090	0.013
SkO′	0.010	0.074	0.018
Dmitriev & Senkov RPA	0.0004	0.055	0.009

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):

$$\langle J, M|\, S_m\, |J', M'\rangle \propto \int\!\!\int \sum_n d\Omega\, d\Omega' \,\times\, (\text{some D-functions})$$
$$\times\, \langle \Psi_K|\, R^{-1}(\Omega')\, S_n\, R(\Omega)\, |\Psi_K\rangle$$

$$\xrightarrow[\Omega\approx\Omega']{\text{rigid defm.}} (\text{Geometric factor}) \times \underbrace{\langle \Psi_K|S_z|\Psi_K\rangle}_{\langle S\rangle_{\text{intr.}}}$$

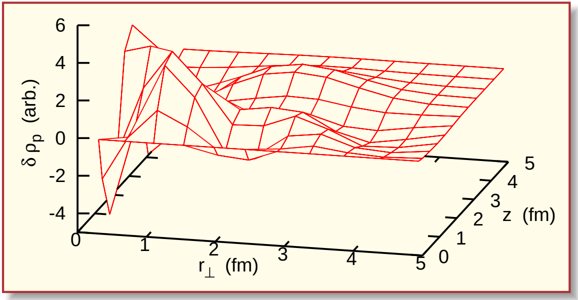
For expectation value in $J = \frac{1}{2}$ state:

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

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.

[1] Has some "issues": doen'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:

		E_{gs}	β	$E_{exc.}$	a_0	a_1	a_2
SLy4	HF	-1561.42	-0.13	0.97	0.013	-0.006	0.022
SIII	HF	-1562.63	-0.11	0	0.012	0.005	0.016
SV	HF	-1556.43	-0.11	0.68	0.009	-0.0001	0.016
SLy4	HFB	-1560.21	-0.10	0.83	0.013	-0.006	0.024
SkM*	HFB	-1564.03	0	0.82	0.041	-0.027	0.069
Fav. RPA	QRPA	–	–	–	0.010	0.074	0.018

Hmm...

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Ultimate goal: mixing of many mean fields, aka "generator coordinates"

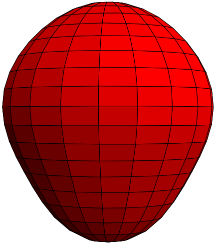
Still a ways off because of difficulties marrying generator coordinates to density functionals.

Schiff Moment with Octupole Deformation

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

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

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



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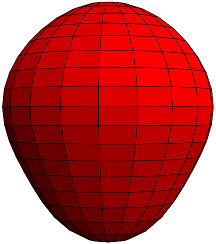

Calculated ^{225}Ra density

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

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

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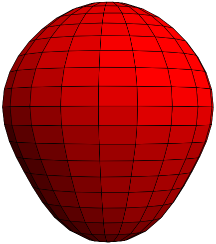

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$$\langle S \rangle \longrightarrow \frac{\langle 0 | S | \bar{0} \rangle \langle \bar{0} | V_{PT} | 0 \rangle}{E_0 - E_{\bar{0}}} + \text{c.c.} \quad \propto \quad \frac{\langle S \rangle_{\text{intr.}} \langle V_{PT} \rangle_{\text{intr.}}}{E_0 - E_{\bar{0}}}$$

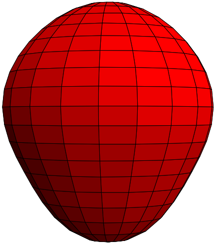
Why is this? See next slide.

Schiff Moment with Octupole Deformation

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

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

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



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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 $|$$\rangle$ is asymmetric, it breaks parity.

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

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

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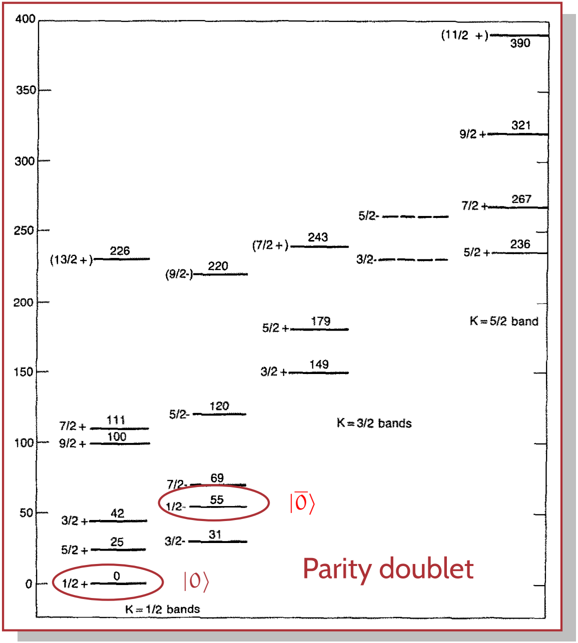
And in the rigid-deformation limit

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

again like angular momentum.

Spectrum of ^{225}Ra



^{225}Ra Results

Hartree-Fock calculation with our favorite interaction SkO' gives

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

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

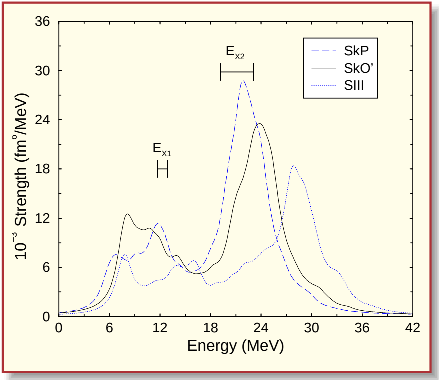
Judgment in 2013 review article (based on spread in reasonable calculations):

Nucl.	Best value			Range		
	a_0	a_1	a_2	a_0	a_1	a_2
^{199}Hg	0.01	± 0.02	0.02	0.005 – 0.05	-0.03 – +0.09	0.01 – 0.06
^{129}Xe	-0.008	-0.006	-0.009	-0.005 – -0.05	-0.003 – -0.05	-0.005 – -0.1
^{225}Ra	-1.5	6.0	-4.0	-1 – -6	4 – 24	-3 – -15

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

Reducing Uncertainty: Hg

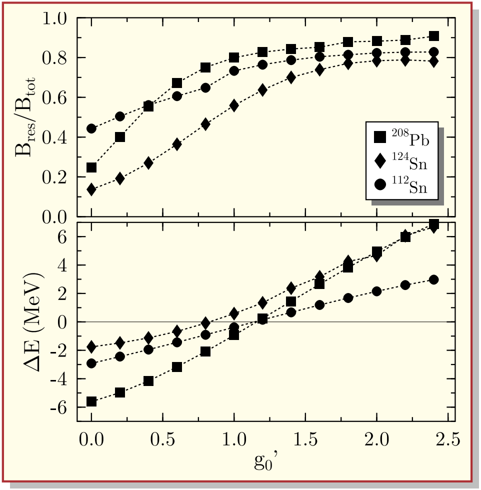
Improving many-body theory to handle soft deformation, though probably necessary, is tough. But can also try to optimize density functional.



Isoscalar dipole operator contains $r^2 z$ just like Schiff operator. Can see how well functionals reproduce measured distributions, e.g. in ^{208}Pb.

More on Reducing Uncertainty in Hg

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.

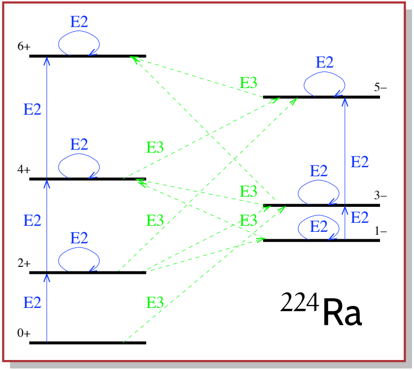


More generally, examine correlations between Schiff moment and lots of other observables.

Reducing Uncertainty: Ra

Important new developments here.

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



Gaffney et al., Nature

Transitions in ^{225}Ra to be measured soon?

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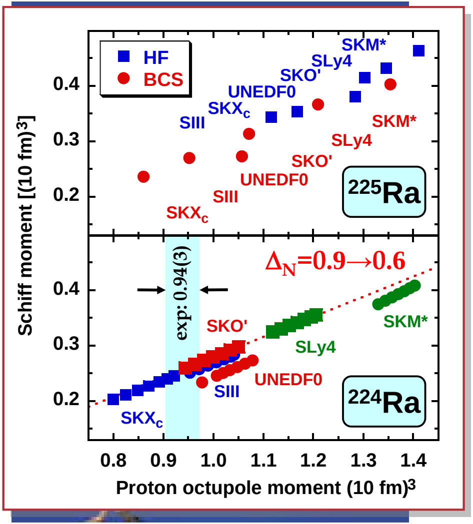

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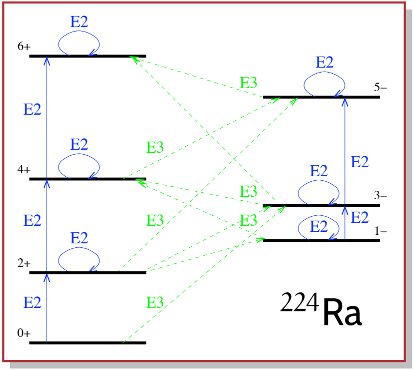

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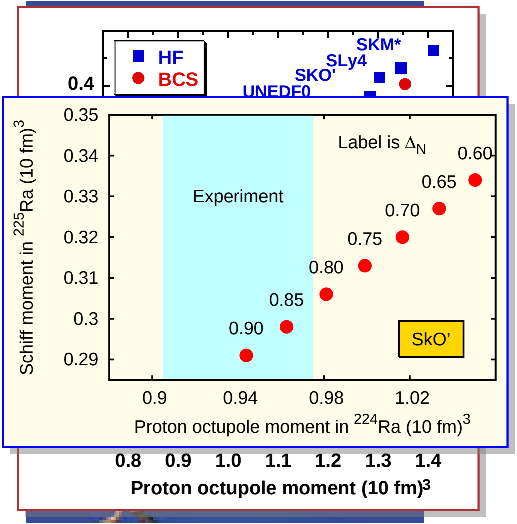

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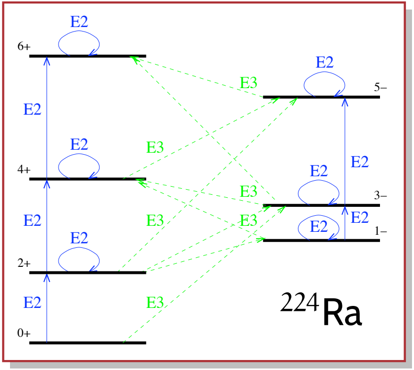

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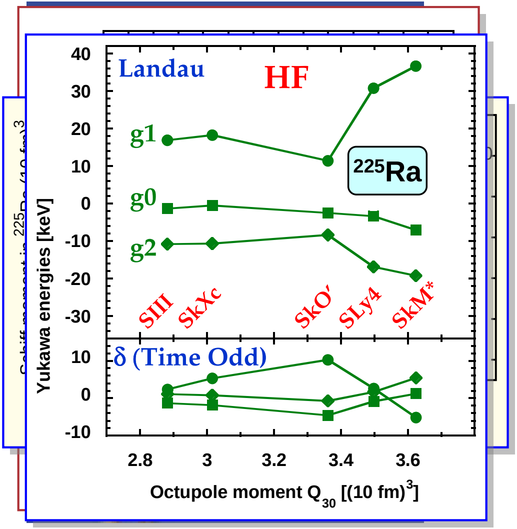

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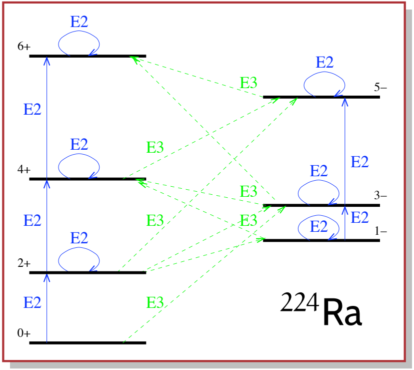

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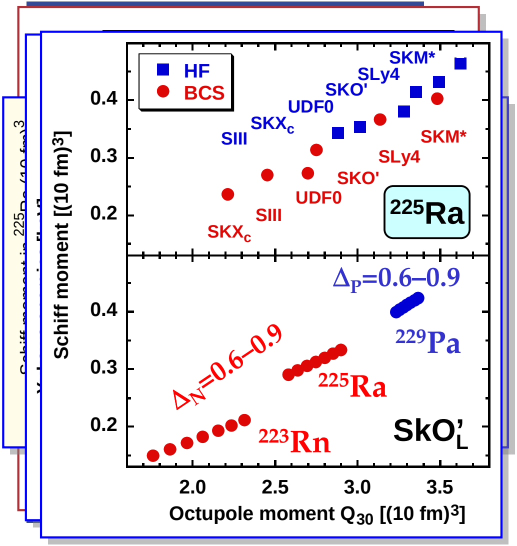

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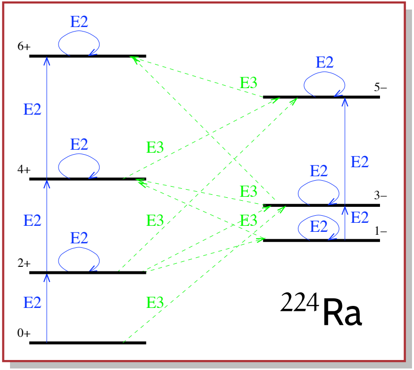

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More on Reducing Uncertainty in Ra

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 $\langle \bar{0} | \, O_{AC} \, | O \rangle$ 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, a_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.