Schiff Moments

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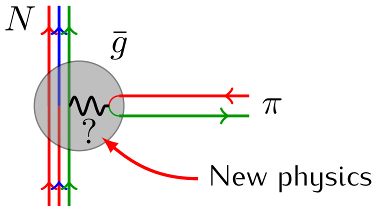
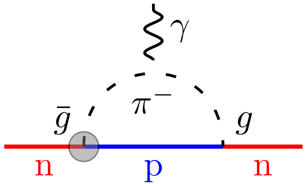
One Way Things Get EDMs

Starting at fundamental level and working up:

Underlying fundamental theory generates three T-violating πNN vertices:

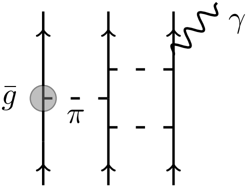


Then neutron gets EDM, e.g., from chiral-PT diagrams like this:



How Diamagnetic Atoms Get EDMs

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



$$V_{PT} \propto \left\{ \left[\bar{g}_0 \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 - \frac{\bar{g}_1}{2} \left(\tau_1^z + \tau_1^z \right) + \bar{g}_2 \left(3\tau_1^z \tau_2^z - \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 \right) \right] (\boldsymbol{\sigma}_1 - \boldsymbol{\sigma}_2) - \frac{\bar{g}_1}{2} \left(\tau_1^z - \tau_2^z \right) (\boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2) \right\} \cdot (\boldsymbol{\nabla}_1 - \boldsymbol{\nabla}_2) \frac{\exp\left(-m_\pi |\boldsymbol{r}_1 - \boldsymbol{r}_2|\right)}{m_\pi |\boldsymbol{r}_1 - \boldsymbol{r}_2|}$$

$$+ \text{ contact term}$$

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 $\bar{g}$'s (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

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

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

$$\begin{aligned}
|\tilde{0}\rangle &= |0\rangle + \sum_m \frac{|m\rangle\langle m| H_d |0\rangle}{E_0 - E_m} \\
&= |0\rangle + \sum_m \frac{|m\rangle\langle m| i\sum_k (1/e_k)\vec{d}_k \cdot \vec{p}_k |0\rangle (E_0 - E_m)}{E_0 - E_m} \\
&= \left(1 + i\sum_k (1/e_k)\vec{d}_k \cdot \vec{p}_k\right)|0\rangle
\end{aligned}$$

How Does Shielding Work?

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

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

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:

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

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

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

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}.

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Can other T-odd moments play a significant role?

$\langle D_{\mathrm{Nuc}} \rangle$ by

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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

but

Ab initio methods are making rapid progress, but

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

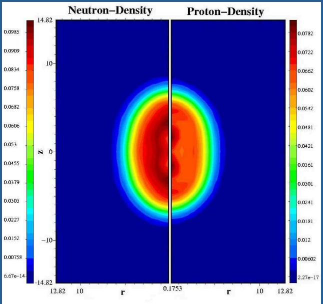
so

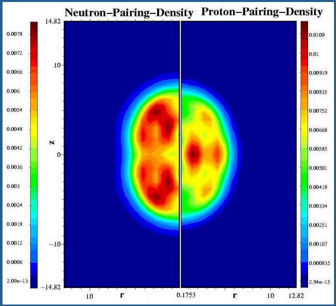
for the near future must rely on nuclear density-functional theory: Mean-field theory with phenomenological "density-dependent interactions" (Skyrme, Gogny, or successors) plus corrections, e.g.:

- 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)
- ...

Skyrme DFT

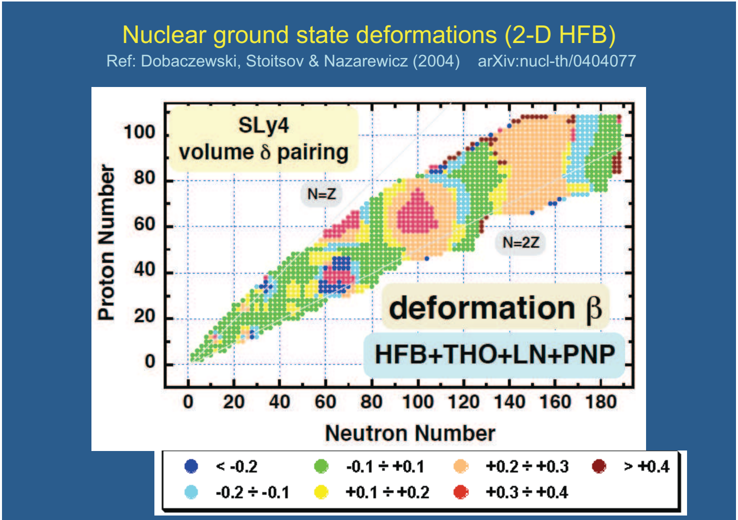
Zr-102: normal density and pairing density
HFB, 2-D lattice, SLy4 + volume pairing
Ref: Artur Blazkiewicz, Vanderbilt, Ph.D. thesis (2005)





HFB: $\beta_2^{(p)}$=0.43 exp: $\beta_2^{(p)}$=0.42(5) , J.K. Hwang et al., Phys. Rev. C (2006)

Applied Everywhere



Varieties of Recent Schiff-Moment Calculations

Need to calculate

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

where $H = H_{strong} + V_{PT}$.

- 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 explicit sum over intermediate states.
- 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.
2. Polarization of core by last neutron and action of V_{PT}, treated as explicit corrections in quasiparticle RPA, which sums over intermediate states.

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

	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. $J_z = K$, average over angles gives:

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

Matrix elements (with more detailed notation):

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

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

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

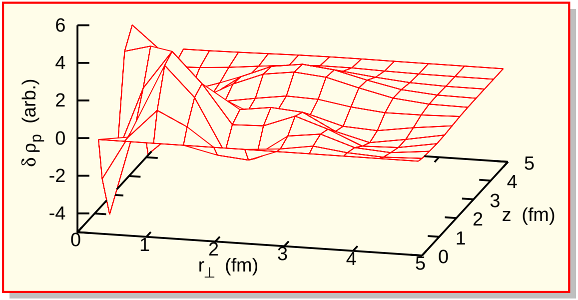
For expectation value in $J = \frac{1}{2}$ state:

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

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 limit of current technology[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...

What to Do About Discrepancy

- Authors of these papers need to revisit/recheck/interpolate between their results. (This will be done, at least to some extent.)
- Improve treatment further:
  - Variation after projection
  - Triaxial deformation

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

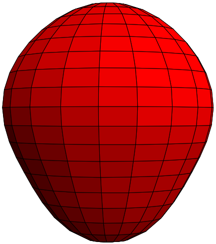
Still a ways off because of difficulties marrying generator coordinates to density functionals.

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.



Calculated ^{225}Ra density

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

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

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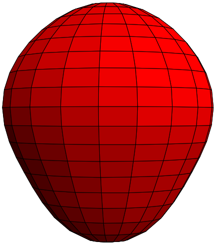

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Why is this? See next slide.

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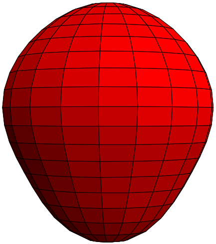

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Why is this? See next slide.

$\langle S \rangle$ 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)$

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

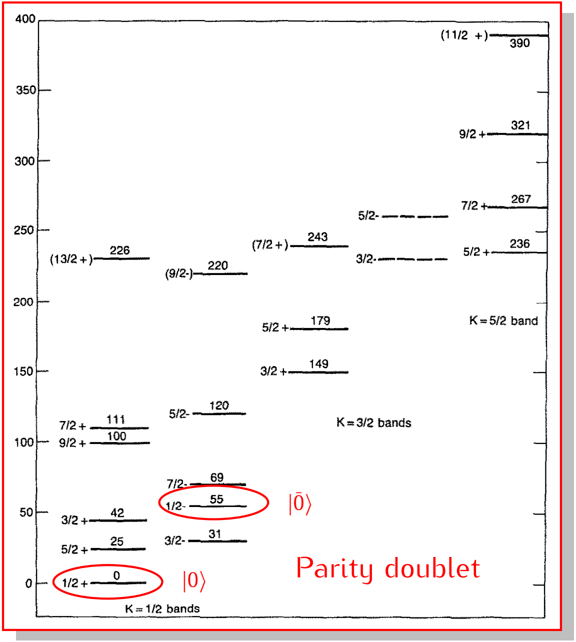
$$\langle S\rangle \approx \frac{\langle 0|\, S_z\, |\bar{0}\rangle \langle \bar{0}|\, V_{PT}\, |0\rangle}{E_0 - E_{\bar{0}}} + c.c.$$

And in the rigid-deformation limit

$\langle 0|O|\bar{0}\rangle \propto \langle$$|O|$$\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

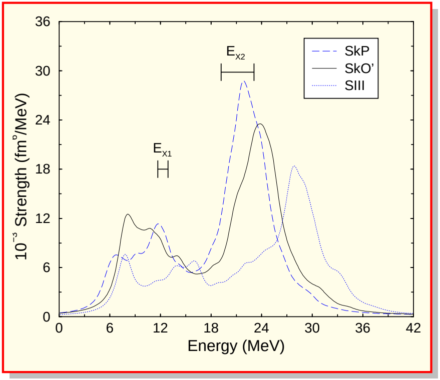
Judgment in review article from last year (based on spread in reasonable calculations):

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

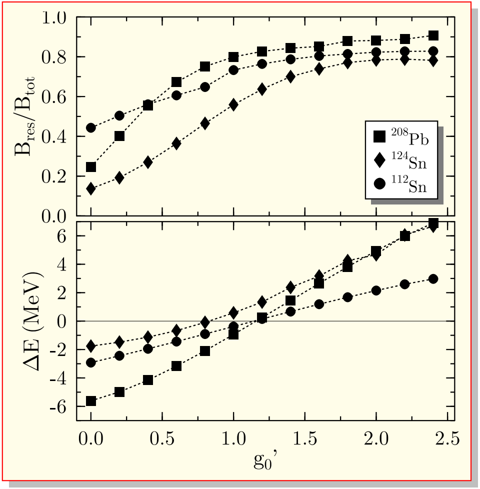
Improving many-body theory to handle soft deformation, though probably necessary, is tough. But can also try to optimize density functional.



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.

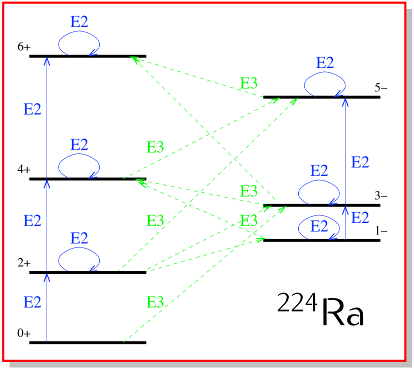


More generally, examine correlations between Schiff moment and lots of other observables.

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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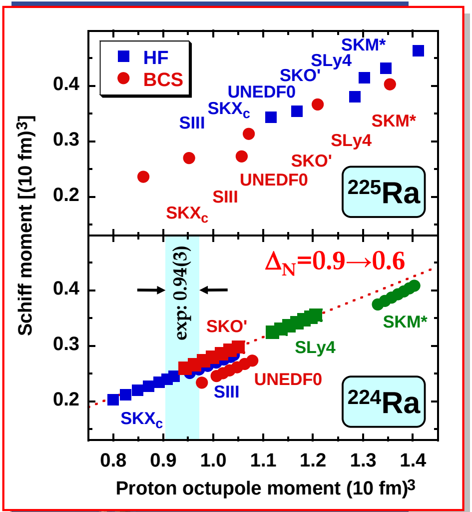

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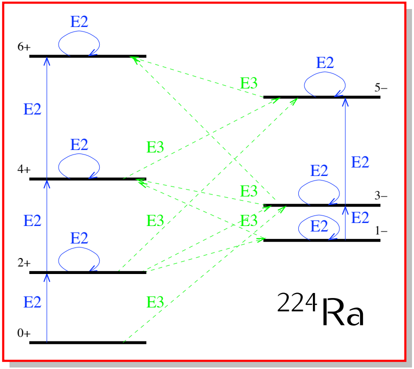

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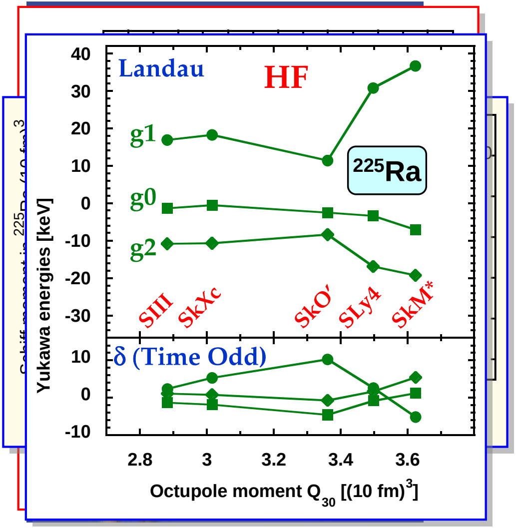

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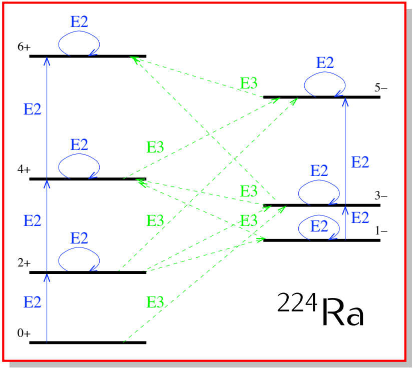

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More on Reducing Uncertainty in Ra

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.

Occurs in weak neutral current, but with large corrections from meson exchange.

p,p' reactions? Something else? Input would be really useful.

Finally: A Little on Contact Term in V_{PT}

First approximation: simply use the interaction as given. Something like this has been done with two-body weak currents in shell-model calculations of double-beta decay.

Ultimately need to renormalize the contact interaction to account for the omission of high-energy states in many-body calculation. Renormalization scheme that preserves local nature of interaction will be useful, should be feasible.

The Future

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

In tne near future, that work must be in nuclear DFT.

- In Hg, a GCM calculation eventually needed.

  And need correlation analysis, good proxies for Schiff distributions (e.g. isoscalar dipole distribution), V_{PT} distribution.

- In ocutpole-deformed nuclei, improved techniques probably won't change things drastically.

  But again, need correlation analysis. Have good proxy for $\langle S \rangle_{\text{int.}}$, need one for $\langle V_{PT} \rangle_{\text{int.}}$.

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THE END

Thanks for your kind attention.