

Diamagnetic EDMs and Nuclear Structure

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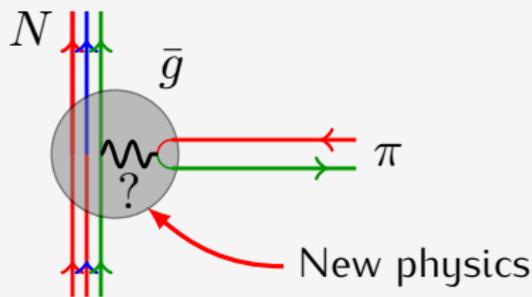
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October 9, 2013

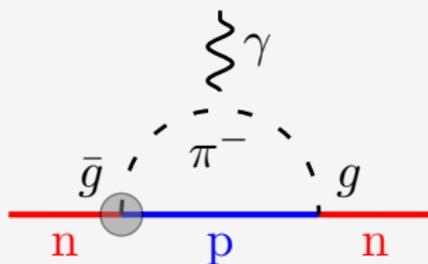
One Way Things Get EDMs

Starting at fundamental level and working up:

Underlying fundamental theory generates three T -violating πNN vertices:

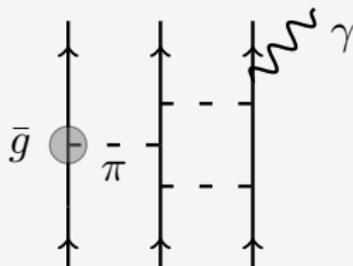


Then neutron gets EDM, e.g., from chiral-PT diagrams like this:



How Diamagnetic Atoms Get EDMs

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



$$V_{PT} \propto \left\{ \left[\bar{g}_0 \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 - \frac{\bar{g}_1}{2} (\tau_1^z + \tau_2^z) + \bar{g}_2 (3\tau_1^z \tau_2^z - \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2) \right] (\boldsymbol{\sigma}_1 - \boldsymbol{\sigma}_2) - \frac{\bar{g}_1}{2} (\tau_1^z - \tau_2^z) (\boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2) \right\} \cdot (\nabla_1 - \nabla_2) \frac{\exp(-m_\pi |\mathbf{r}_1 - \mathbf{r}_2|)}{m_\pi |\mathbf{r}_1 - \mathbf{r}_2|}$$

+ contact term

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

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

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

$$\begin{aligned} &= && H_0 && + \sum_k (1/e_k) \vec{d}_k \cdot \vec{\nabla} V(\vec{r}_k) \\ &= && H_0 && + i \sum_k (1/e_k) \left[\vec{d}_k \cdot \vec{p}_k, H_0 \right] \end{aligned}$$

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

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

So the net EDM is zero!

All is Not Lost, Though...

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:

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

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

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

Ughh! 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

$\langle S \rangle \propto Z^2$, so experiments are in heavy nuclei

but

can't solve Schrödinger eq'n for $A > 40$. Usually approximate, then account for omitted physics by modifying operators.

Paradigm: Density functional Theory

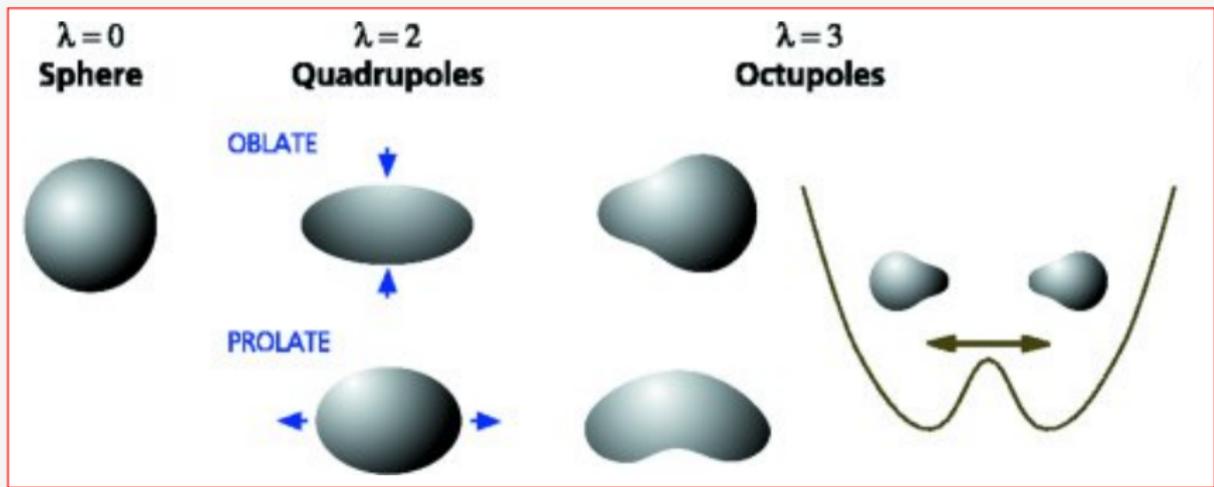
Höhenberg-Kohn-Sham: Can get exact density from Hartree calculation with effective interaction (density functional).

Nuclear version: Mean-field theory with density-dependent interactions (named after Skyrme) built from delta functions and derivatives of delta functions, plus corrections, e.g.:

- ▶ projection of deformed wave functions onto states with good angular momentum
- ▶ mixing of several mean fields
- ▶ ...

Density functional still largely phenomenological.

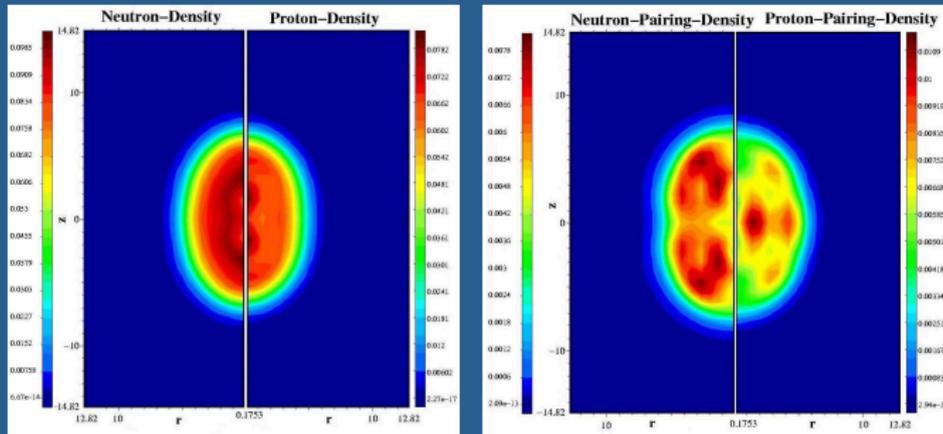
Nuclear Deformation



Deformed Skyrme Mean-Field Theory

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

Ref: Artur Blazkiewicz, Vanderbilt, Ph.D. thesis (2005)

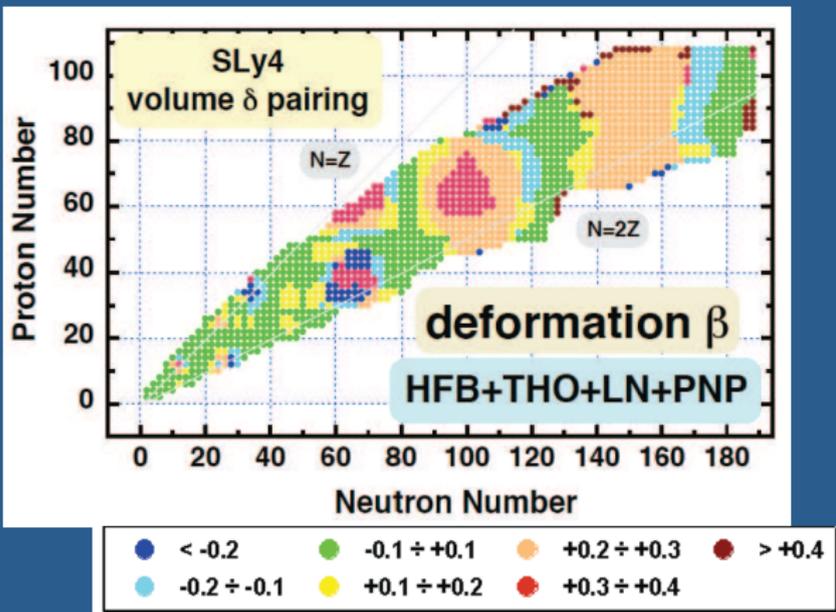


HFB: $\beta_2^{(p)}=0.43$

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

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

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

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:

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

Matrix elements (with more detailed notation):

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

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

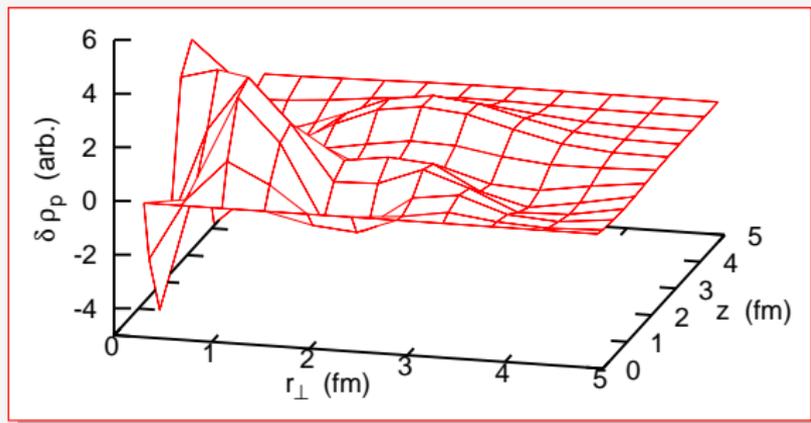
For expectation value in $J = \frac{1}{2}$ state:

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

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 odd nuclei, that's the limit of current technology¹. V_{PT} included nonperturbatively and calculation done in one step. Includes more physics than RPA (deformation), plus economy of approach. Otherwise more or less equivalent.



Oscillating PT -odd density distribution indicates delicate Schiff moment.

¹Has some “issues”: doesn'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	$E_{\text{exc.}}$	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 their results.
- ▶ Improve treatment further:
 - ▶ Variation after projection
 - ▶ Triaxial deformation

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

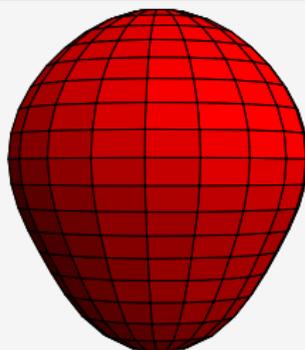
Still a ways off because of difficulties marrying generator coordinates to density functionals.

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:

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

$\langle S \rangle$ 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:

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

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

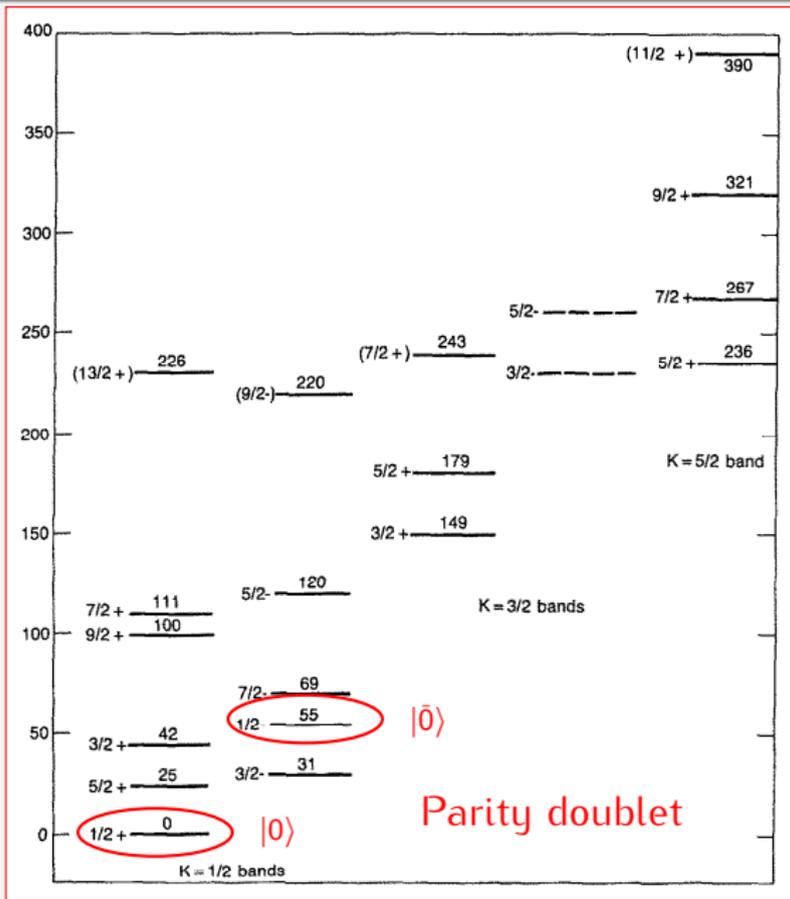
$$\langle S \rangle \approx \frac{\langle 0 | S_z | \bar{0} \rangle \langle \bar{0} | V_{PT} | 0 \rangle}{E_0 - E_0} + c.c.$$

And in the rigid-deformation limit

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

again like angular momentum.

Spectrum of ^{225}Ra



^{225}Ra Results

Hartree-Fock calculation with our favorite interaction SkO' gives

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

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

Variation a factor of 2 or 3.



Current "Assessment" of Uncertainties

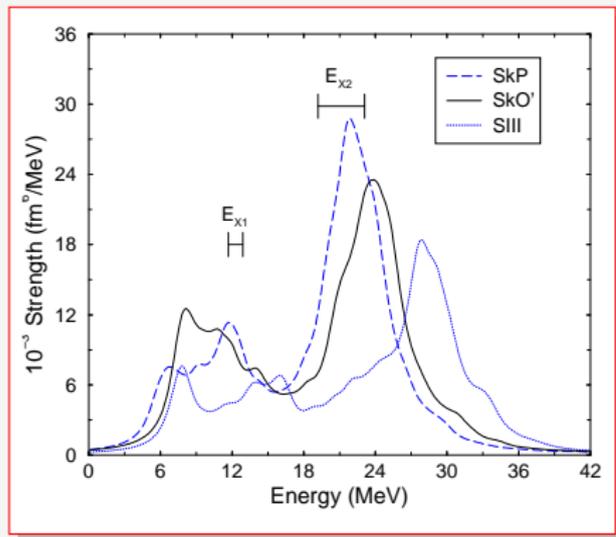
Judgment in recent review article (based on spread in reasonable calculations):

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 g_1 in ^{199}Hg (range includes zero). How can we reduce them?

Grounding the Calculations: Hg

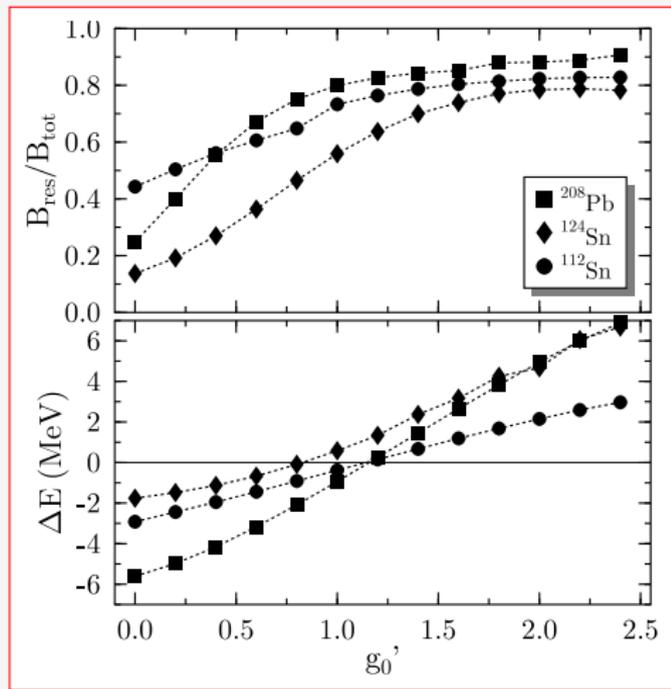
Improving many-body theory to handle soft deformation, though probably necessary, is tough. But can also try to optimize density functional.



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

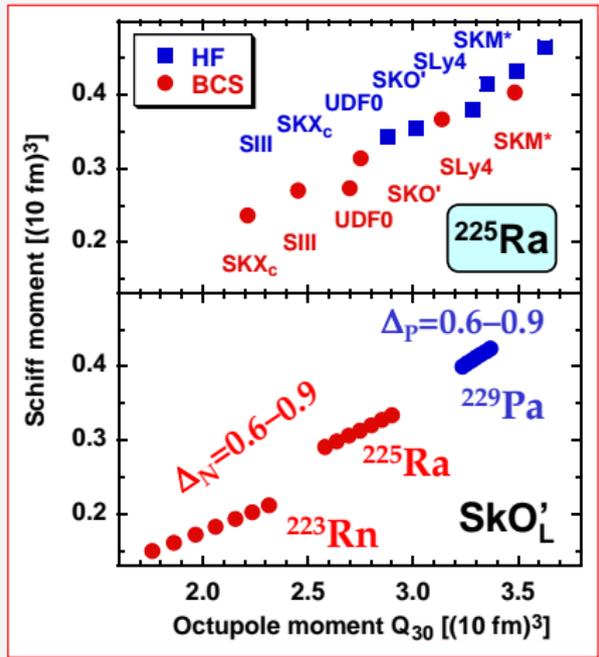
More on Grounding Hg Calculation

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.

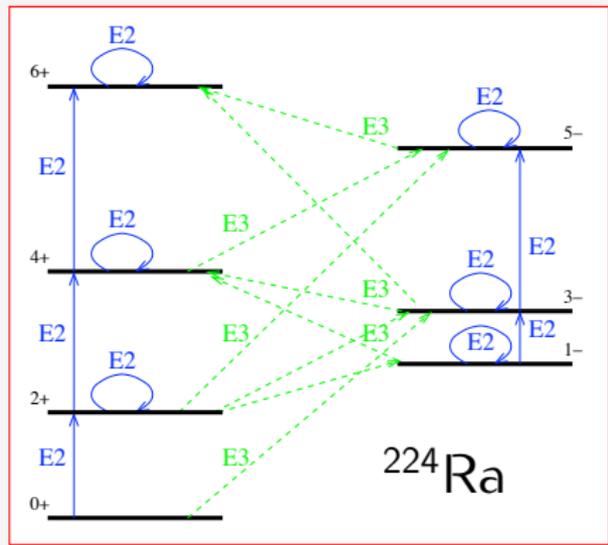


Grounding the Calculations: Ra

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.

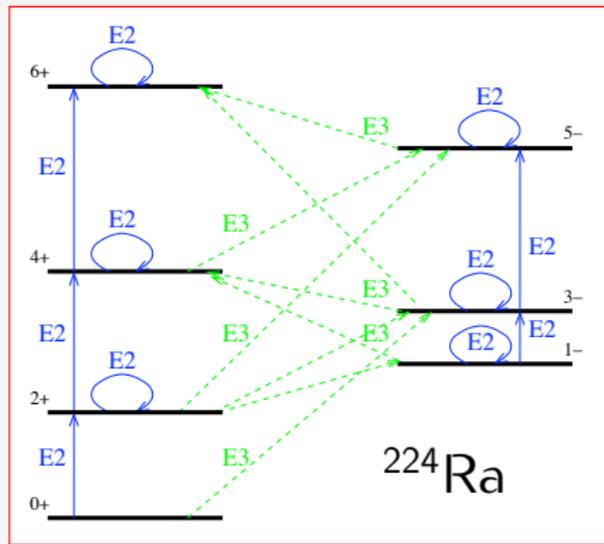
Grounding the Calculations: Ra

Imp

Schiff moment $[(10 \text{ fm})^3]$



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



Gaffney et al., Nature

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

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.

Calculations have become sophisticated, but we still have a lot of work to do. Octupole-deformed nuclei are more under control than ^{199}Hg .

THE END

Thanks for your kind attention.