Diamagnetic EDMs and Nuclear Structure

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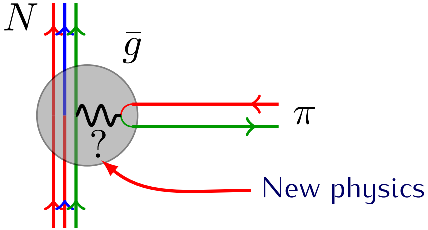
One Way Things Get EDMs

Starting at fundamental level and working up:

- Underlying fundamental theory generates three T-violating πNN vertices:



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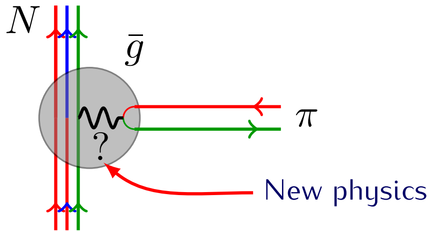
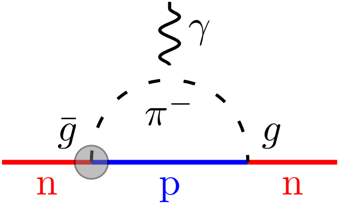
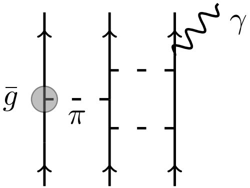


- Then neutron gets EDM, e.g., from chiral-PT diagrams like this:



How Diamagnetic Atoms Get EDMs

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



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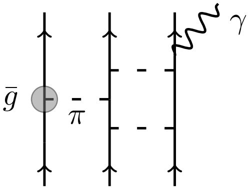

$$V_{PT} \propto \left\{ \left[\bar{g}_0 \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 - \frac{\bar{g}_1}{2} \left(\tau_1^z + \tau_1^z \right) + \bar{g}_2 \left(3\tau_1^z \tau_2^z - \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 \right) \right] \left(\boldsymbol{\sigma}_1 - \boldsymbol{\sigma}_2 \right)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

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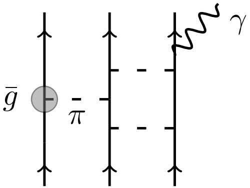

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- Finally, atom gets one from nucleus. Electronic shielding makes the relevant nuclear object the "Schiff moment" $\langle S \rangle \approx \langle \sum_p r_p^2 z_p + \ldots \rangle$ rather than the dipole moment $\langle D_z \rangle$.

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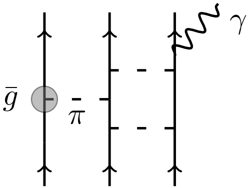

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> Job of nuclear theory: calculate dependence of $\langle S \rangle$ on the $\bar{g}$'s.

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.

Proof

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

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

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$$= H_0 + \sum_k (1/e_k) \vec{d}_k \cdot \vec{\nabla} V(\vec{r}_k)$$

K.E. + Coulomb → H_0

dipole perturbation → $\sum_k (1/e_k) \vec{d}_k \cdot \vec{\nabla} V(\vec{r}_k)$

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= & \; H_0 + i \sum_k (1/e_k) \left[\vec{d}_k \cdot \vec{p}_k , H_0 \right]
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How Does Shielding Work?

The perturbing Hamiltonian

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

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$$

So the net EDM is zero!

All is Not Lost, Though…

Th nucleus has finite size. Shielding is not complete, and nuclear T violation can still induce atomic EDM $\vec{d}$.

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

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

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Overall suppression of $\langle \vec{D} \rangle$ is only about 10^{-3}.

Theory for Heavy Nuclei

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

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Nuclear version: Mean-field theory with density-dependent interactions (called Skyrme interactions) built from delta functions and deriviatives of delta functions plus whatever corrections one can manage, e.g.

- projection of deformed wave functions onto states with good angular momentum
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Density functional still obtained largely through phenomenology.

Nuclear Deformation

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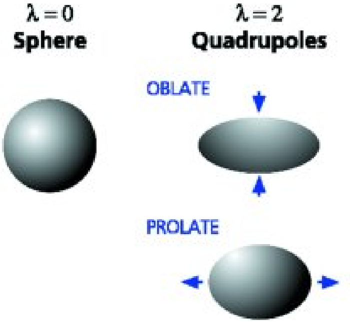

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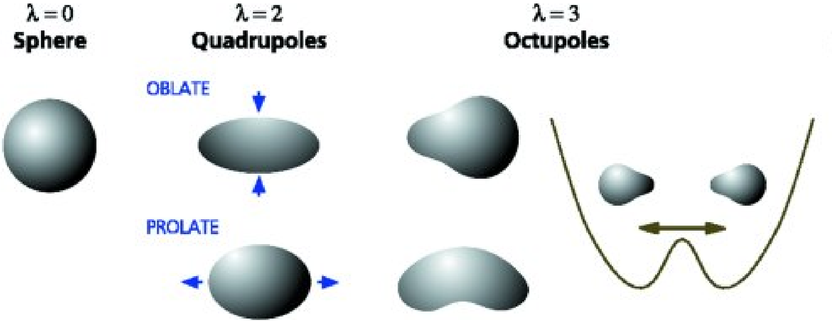
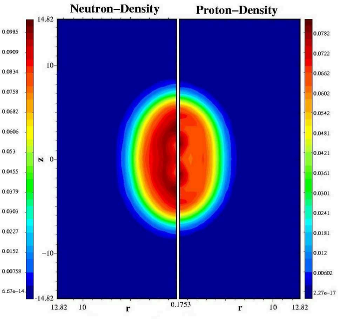
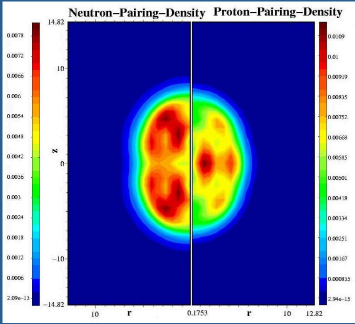


Deformed Skyrme Mean-Field Theory

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





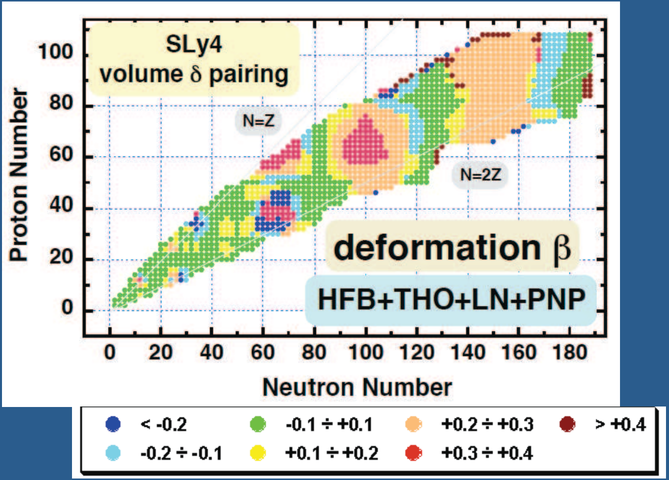
HFB: $\beta_2^{(p)}$=0.43

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

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

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

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

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

- H_{strong} represented either by Skyrme density functional or by simpler effective interaction, treated non-self-consistently.
- V_{PT} either included nonperturbatively or via explicit sum over intermediate states.
- Nucleus either forced artificially to be spherical or allowed to deform.

Spherical Calc.: ^{198}Hg + Polarization by Last Neutron

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

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

	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
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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 has good intr. $J_z = K$, averaging over angles gives:

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

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Matrix elements;

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

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

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

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

Exact answer somewhere in between.

Deformed 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 technology[1]. V_{PT} included nonperturbatively and calculation done in one step. Includes more physics (deformation) than RPA calculations, plus an economy of approach. Otherwise more or less equivalent.

[1] Has some "issues": doen't get ground sate spin correct, limited for now to axially-symmetric minima, which are sometimes a little unstable, true minimum probably not axially symmetric ...

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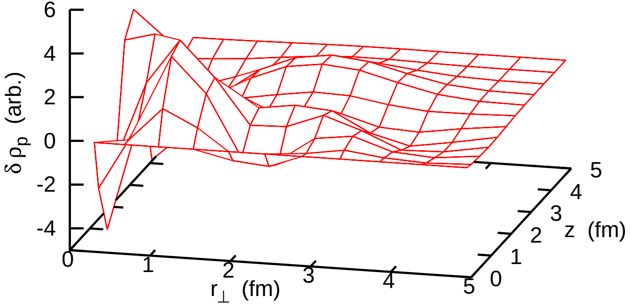

Induced change in density distribution indicates delicate Schiff moment.

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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

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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

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

Schiff Moment with Octupole Deformation

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

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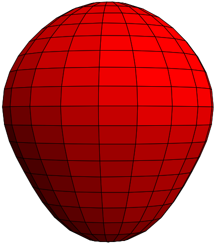
where $|0\rangle$ is unperturbed ground state.



Calculated ^{225}Ra density

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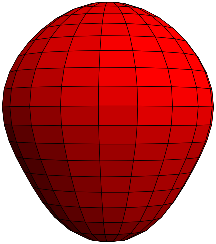

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Ground state has nearly-degenerate partner $|\bar{0}\rangle$ with same opposite parity and same intrinsic structure, so:

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

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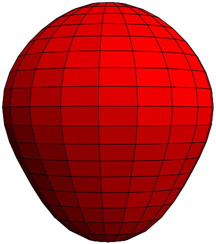

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S is large because $\langle S\rangle_{\text{intr.}}$ is collective and $E_0 - E_{\bar{0}}$ is small.

A Little on Parity Doublets

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

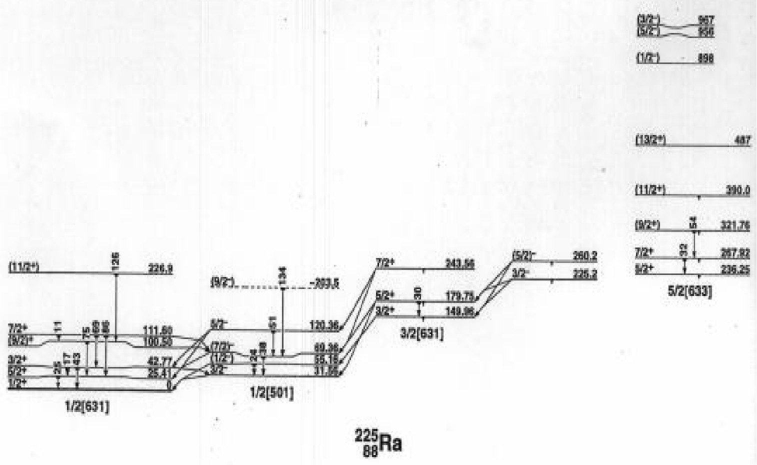
$$S \approx \frac{\langle 0| \, S_z \, |\bar{0}\rangle \, \langle \bar{0}| \, V_{PT} \, |0\rangle}{E_0 - E_{\bar{0}}} + c.c.$$

And in the rigid-deformation limit

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

again like angular momentum.

Spectrum of ^{225}Ra



^{225}Ra Results

Hartree-Fock calculation with our favorite interaction SkO′ gives

$$S_{\mathrm{Ra}} = -1.5\ g\bar{g}_0\ + 6.0\ g\bar{g}_1\ - 4.0\ g\bar{g}_2\ \ (\mathrm{e\ fm}^3)$$

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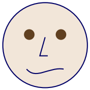
Variation a factor of 2 or 3.



Current “Assessment” of Uncertainties

Judgment in upcoming 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	0.01	0.02	0.005 – 0.02	-0.03 – 0.09	0.01 – 0.03
^{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 — 20	-2 – -15

Uncertainties pretty large, particularly for g_1 in ^{199}Hg (range includes zero). How can we reduce them?

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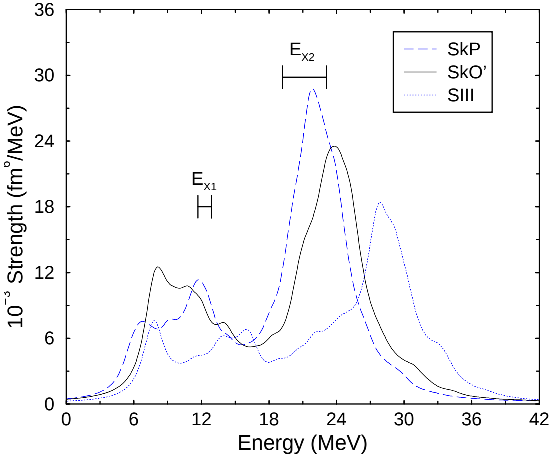
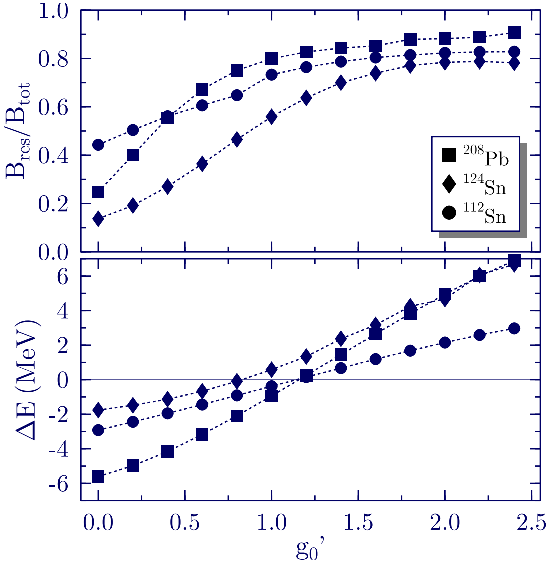


Isoscalar dipole operator contains $r^2 z$ just like Schiff operator. Can see how well functionals reproduce measured distributions, e.g. in ^{208}Pb.

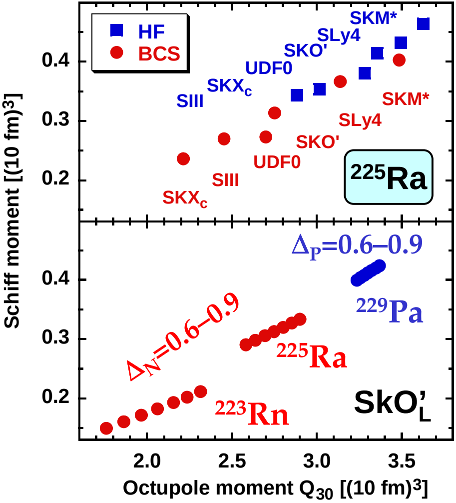
More on Grounding Hg Calculation

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

Here there have been important recent developments.



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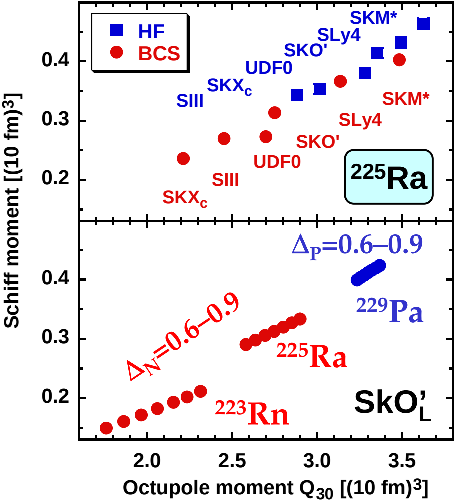

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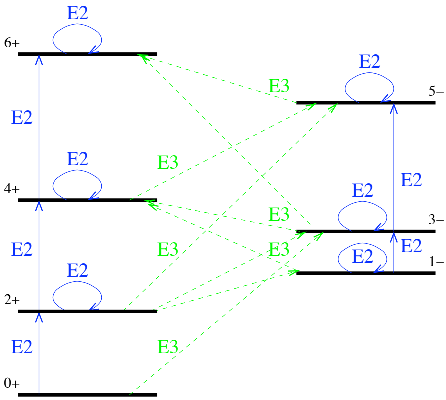

This is ^{224}Ra; transitions in ^{225}Ra will be measured soon.

THE END

Thanks for your kind attention.