Calculating Schiff-Moments

in the Next Few Years

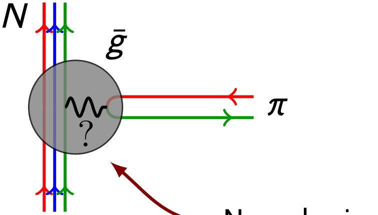
J. Engel

April 15, 2022

How Diamagnetic Atoms Get EDMs, Roughly

Because Standard-Model *CP* violation is so weak, an additional undiscovered source is required to explain why there is so much more matter than antimatter.

The source can work its way into nuclei through CP-violating πNN vertices (in chiral EFT)...



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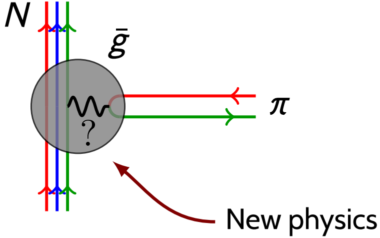
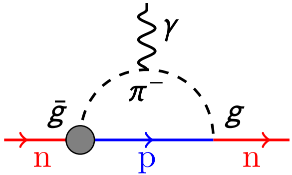


leading, e.g. to a neutron EDM…



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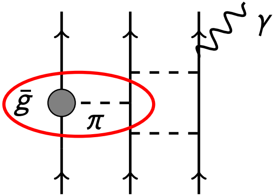

…and to a nuclear EDM from the nucleon EDM or a T-violating NN interaction:

$$V_{PT} \propto \bar{g}\,(\boldsymbol{\sigma}_1 \pm \boldsymbol{\sigma}_2)\cdot(\boldsymbol{\nabla}_1 - \boldsymbol{\nabla}_2)\,\frac{\exp\left(-m_\pi|\boldsymbol{r}_1 - \boldsymbol{r}_2|\right)}{m_\pi|\boldsymbol{r}_1 - \boldsymbol{r}_2|} + \text{contact terms/etc.}$$

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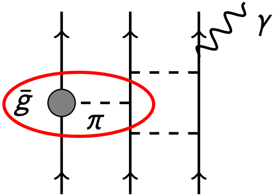

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Atoms get EDMs from nuclei. But electronic shielding replaces nuclear dipole operator with "Schiff operator,"

$$S \propto \sum_p \left(r_p^2 - \frac{5}{3} R_{\mathrm{ch}}^2 \right) z_p + \ldots\,,$$

making relevant nuclear quantity the Schiff moment:

$$\langle S \rangle = \sum_m \frac{\langle O|\, S\, |m\rangle \langle m|\, V_{PT}\, |O\rangle}{E_O - E_m} + c.c.$$

How Diamagnetic Atoms Get EDMs, Roughly

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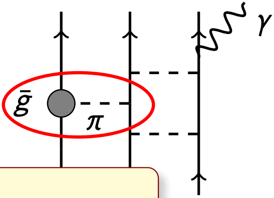


$V_{PT} \propto g$ … ns/etc.

Job of nuclear-structure theory: compute dependence of $\langle S \rangle$ on the three $\bar{g}$'s (and on the contact-term coefficients and nucleon EDM).

It's up to QCD/EFT to compute the dependence of the $\bar{g}$ vertices on fundamental sources of *CP* violation.

Atom … s

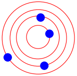
nuclea …

$$\sum_p \left(\quad \frac{\quad}{3} \quad \right)$$

making relevant nuclear quantity the Schiff moment:

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

Nuclear Models in One Slide



Starting point is always a mean field and potential

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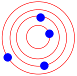

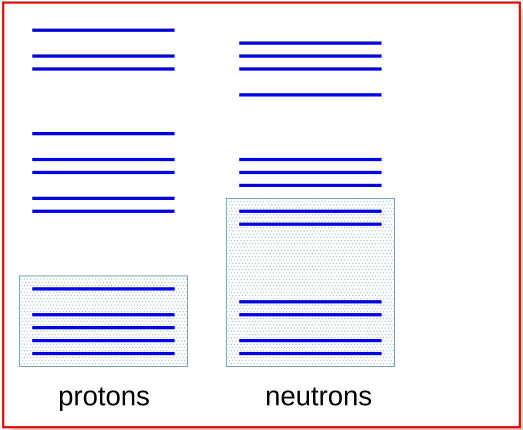

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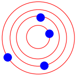

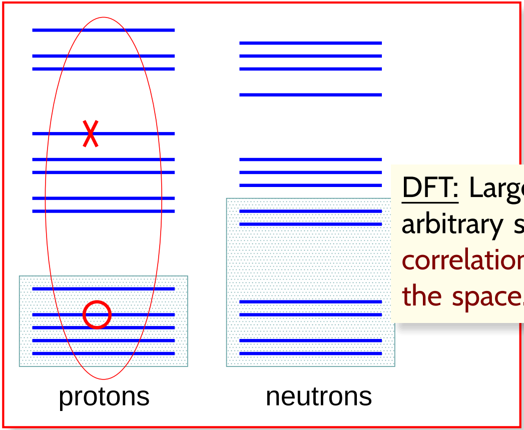

DFT: Large single-particle spaces in arbitrary single mean field; simple correlations and excitations within the space.

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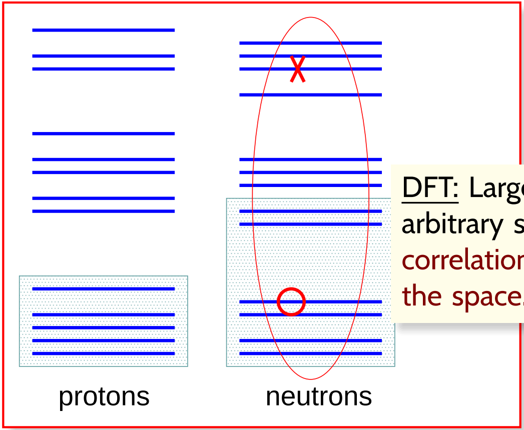

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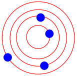

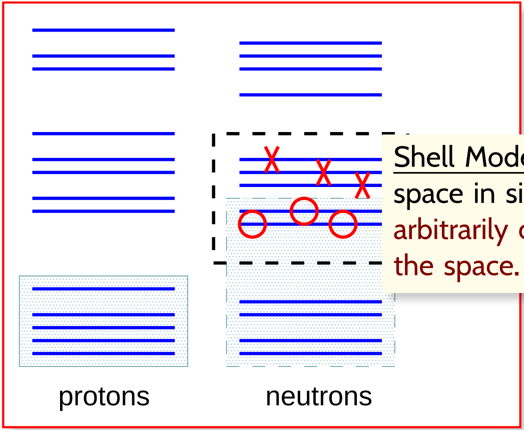

Shell Model: Small single-particle space in simple spherical mean field; arbitrarily complex correlations within the space.

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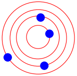

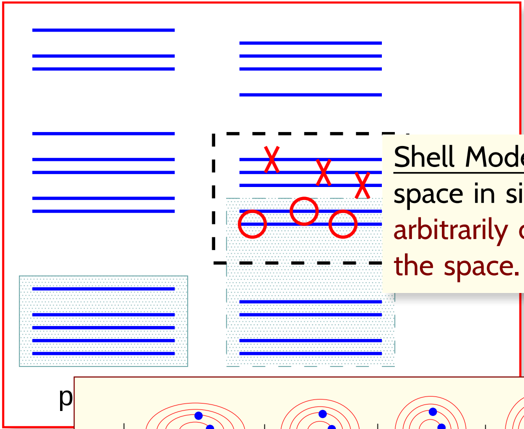

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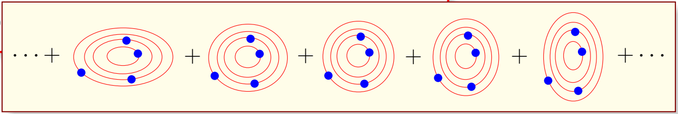

Generator-Coordinate Method (GCM): extension of DFT that mixes many mean-field states with different collective properties.

Nuclear Models in One Slide

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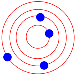

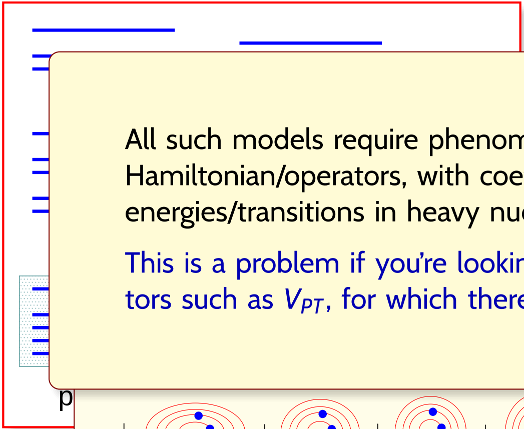

All such models require phenomenological Hamiltonian/operators, with coefficients fit to energies/transitions in heavy nuclei.

This is a problem if you're looking at operators such as V_{PT}, for which there are no data.

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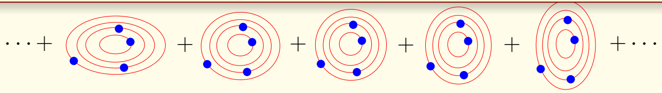

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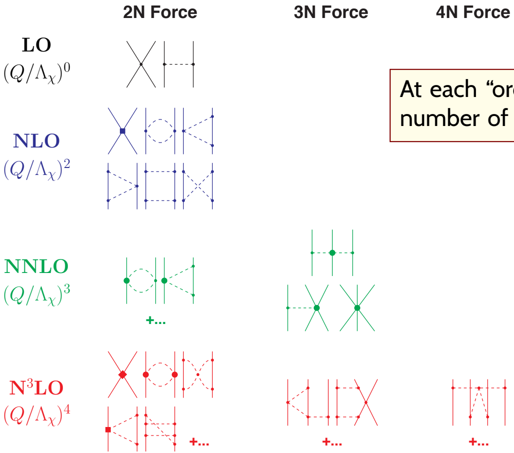
Ab Initio Nuclear Structure

Starts with chiral effective-field theory

Nucleons, pions sufficient below chiral-symmetry breaking scale.
Expansion of operators in powers of Q/Λ_χ.

$Q = m_\pi$ or typical nucleon momentum.



At each "order," only a finite number of operators exist.

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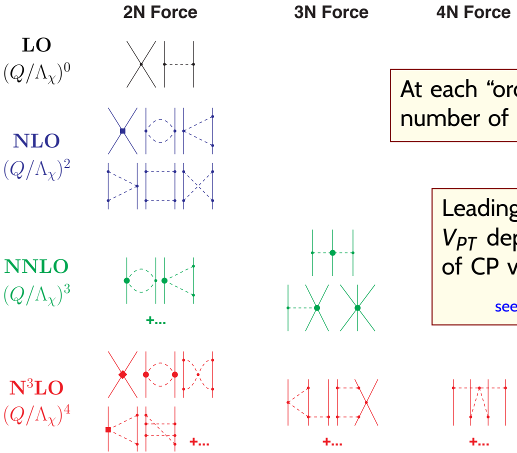


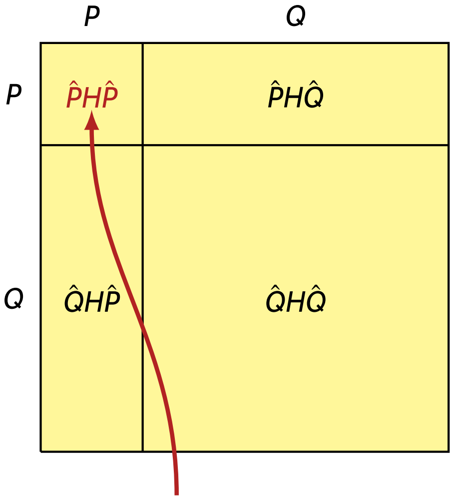
At each "order," only a finite number of operators exist.

Leading-order terms in V_{PT} depend on source of CP violation.

see Jordy's talk.

Ab Initio Many-Body Methods

Partition of Full Hilbert Space



Simpler calculation done here.

P = “reference” space
Q = the rest

Task: Find unitary transformation to make H block-diagonal in P and Q, with H_{eff} in P reproducing most important eigenvalues.

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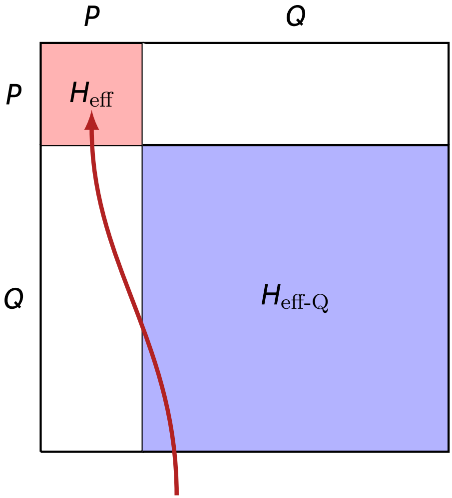

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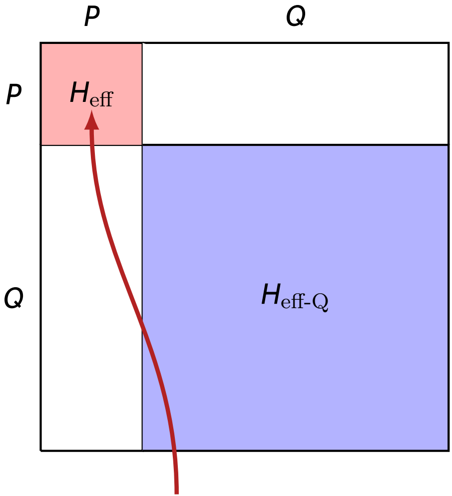

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Must must apply same unitary transformation to transition operator.

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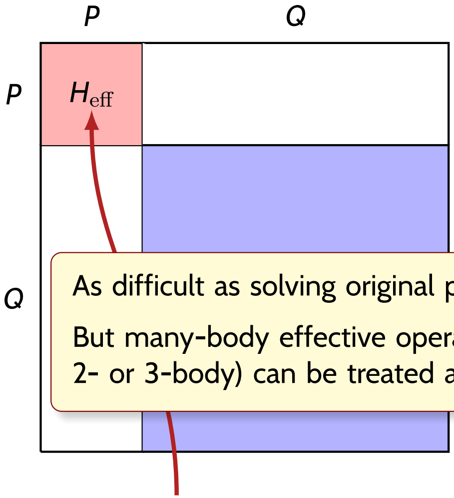

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operator.

As difficult as solving original problem.

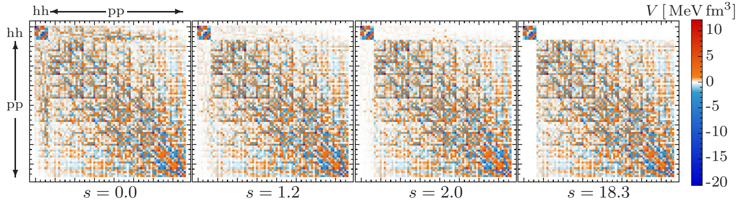
But many-body effective operators (beyond 2- or 3-body) can be treated approximately.

Simpler calculation done here.

In-Medium Similarity Renormalization Group

One way to determine the transformation

Flow equation for effective Hamiltonian.
Gradually decouples reference space.



from H. Hergert

$$\frac{d}{ds}H(s) = [\eta(s), H(s)]\,, \qquad \eta(s) = [H_d(s), H_{od}(s)]\,, \qquad H(\infty) = H_{\text{eff}}$$

Trick is to keep all 1- and 2-body terms in H at each step *after normal ordering* (**IMSRG-2**, includes most important parts of 3, 4-body … terms).

If reference space is a single state, end up with g.s. energy. If, e.g., it is a valence space, get effective shell-model interaction and operators.

Reference State with Collective Correlations

Background: Generator Coordinate Method

Construct set of mean fields by constraining coordinate(s), e.g. quadrupole moment $\langle Q_0 \rangle$. Then diagonalize H in space of symmetry-restored quasiparticle vacua with different $\langle Q_0 \rangle$.

Reference State with Collective Correlations

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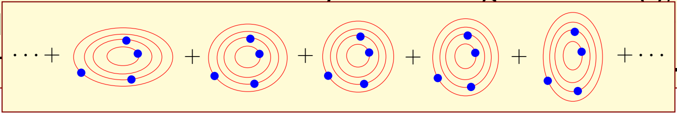
Construct set of mean fields by constraining coordinate(s), e.g.
quad
symm .



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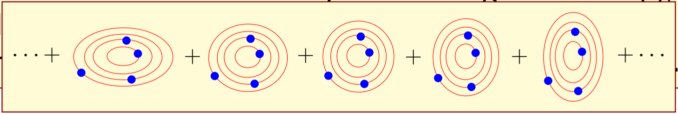
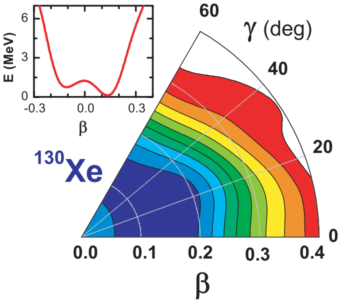
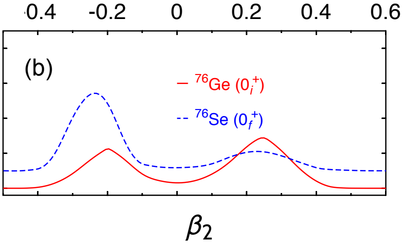


Potential energy surface



Li et al.: Potential energy surface for ^{130}Xe

Collective squared wave functions



Rodríguez and Martínez-Pinedo: Wave functions in ^{76}Ge,Se peaked at two different deformed shapes.

Reference State with Collective Correlations

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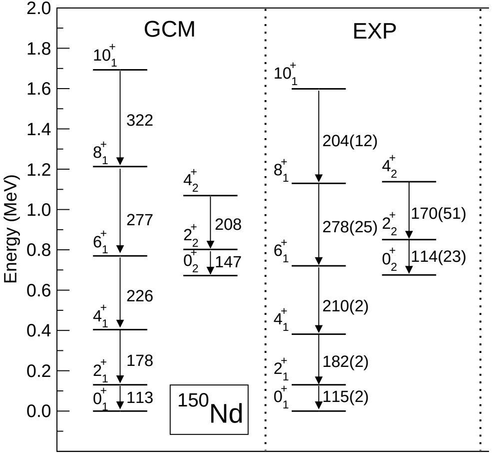
Construct … e(s), e.g.
quad
symr

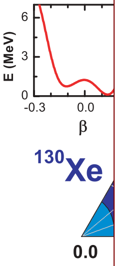
$\cdots +$ … $+ \cdots$

GCM in DFT



P. Ring et al, 2011

Potent



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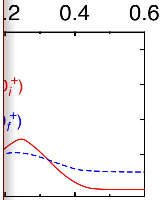

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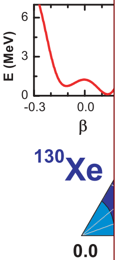

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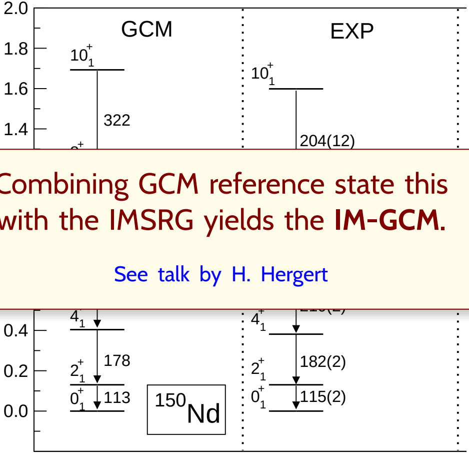

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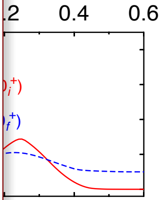
Combining GCM reference state this with the IMSRG yields the **IM-GCM**.

See talk by H. Hergert



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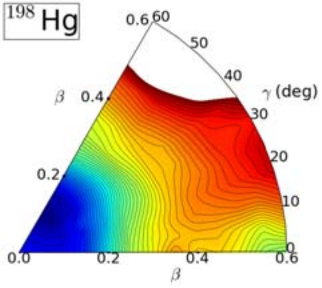
^{199}Hg: A Challenging Nucleus

^{198}Hg has a very soft oblate minimum.



Prassa et al., EPJ Web Conf. **252** 02007 (2021).

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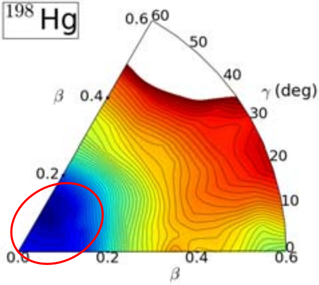

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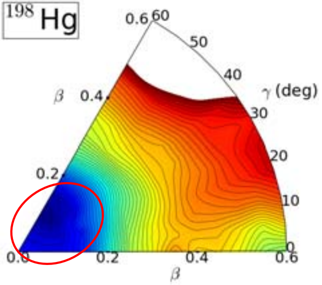

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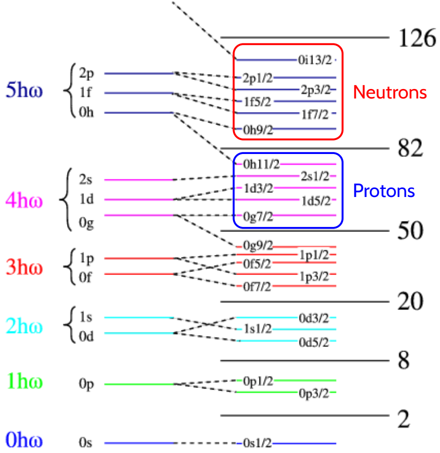
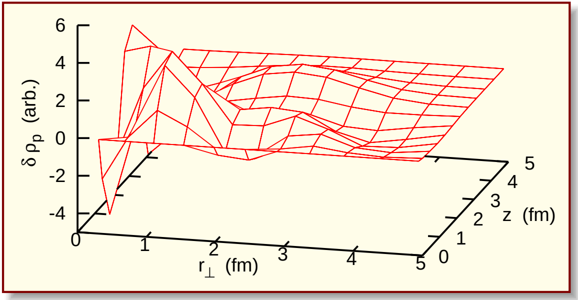
Shell-Model Representation



Full Self-Consistent DFT Calculation

Small and soft deformation a worst case scenario for mean-field.
We did it nonetheless[1].



Oscillating *PT*-odd density distribution indicates delicate Schiff moment.

[1]S. Ban, JE, J. Dobaczewski, A. Shukla, Phys. Rev. C **82**, 015501 (2010)

Results

$$\langle S \rangle_{\mathrm{Hg}} \equiv a_0\, g\bar{g}_0 + a_1\, g\bar{g}_1 + \ldots \qquad (\mathrm{e\ fm}^3)$$

	a_0	a_1
HFB SkM*	4.1	−2.7
HFB SLy4	1.3	−0.6
Typical QRPA	1.0	7.4
Shell Model[2]	8.0	7.8

Sign of a_1 not clear.

Yanase and Shimizu suggest HFB calculation examined the "wrong" $1/2^-$ state. We're re-examining the situation in an equivalent approach (Finite Amplitude Method, an implementation of QRPA).

New results soon.

[2] Yanase and Shimizu, PRC **102** 065502 (2020)

The Future

DFT: GCM: Mixing of many mean fields around the soft minimum.

No immediate plans to do this.

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DFT: GCM: Mixing of many mean fields around the soft minimum.

No immediate plans to do this.

Valence-Space IMSRG: Include V_{PT} as part of the Hamiltonian, so that the flow generator η and the transformed Hamiltonian will have negative-parity parts η^- and H^- :

$$\frac{d}{ds}H^-(s) = [\eta^0(s), H^-(s)] + [\eta^-(s), H^0(s)]$$

$$H^-(0) = V_{PT} .$$

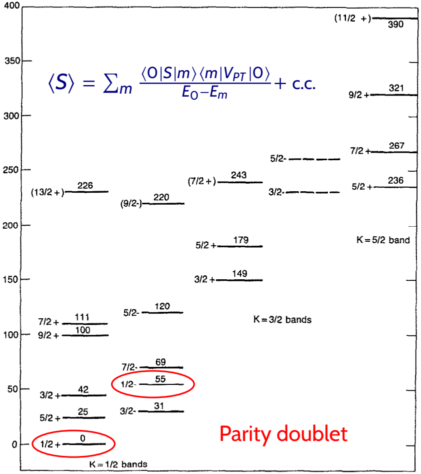
η^0 and H^0 are what you get without V_{PT}.

Diagonalize transformed Hamiltonian in shell-model space, and use transformed Schiff operator to compute $\langle S \rangle$.

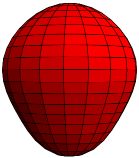
R. Stroberg doing this with me for ^{205}Tl first.

^{225}Ra and Other Light Actinides

Octupole Physics and DFT



Unlike in other nuclei, these two states are the whole story.



Deformed density

Two members of the parity doublet correspond to the same intrinsic mean-field state:

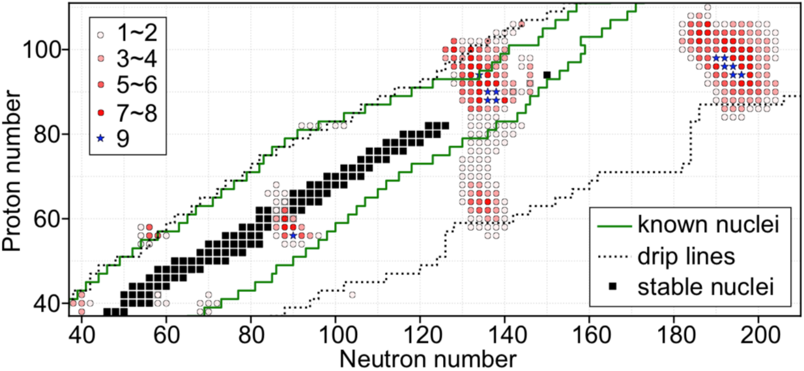
$$\left|\frac{1}{2}^{\pm}\right\rangle = \frac{1}{\sqrt{2}}\left(|\ \rangle \pm |\ \rangle\right)$$

and, to good approximation,

$$\langle S \rangle \approx \frac{2}{3} \frac{\overbrace{\langle\ | S_z |\ \rangle}^{\langle S \rangle_{\text{intr.}}}\langle\ | V_{PT} |\ \rangle}{E_+ - E_-}$$

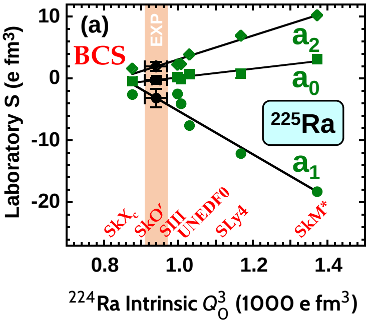
Octupole Systematics

More DFT



From Cao et al., Phys. Rev. C **102**, 024311 (2020)

Correlation of ^{225}Ra $\langle S \rangle$ with ^{224}Ra Octupole Moment



J. Dobaczewski et al., Phys. Rev. Lett. 121, 232501 (2018)

Looks good, but we're at the left end of the lines.

a_0	a_1
-0.4 – 0.8	-2 – -8

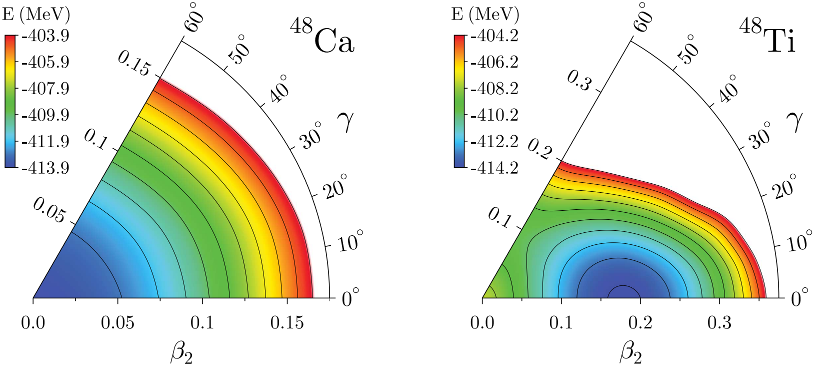
Range doesn't include systematic uncertainty.

IM-GCM

Application to Neutrinoless $\beta\beta$ Decay of ^{48}Ca

J.M. Yao et al., Phys. Rev. Lett. **124**, 232501 (2020).

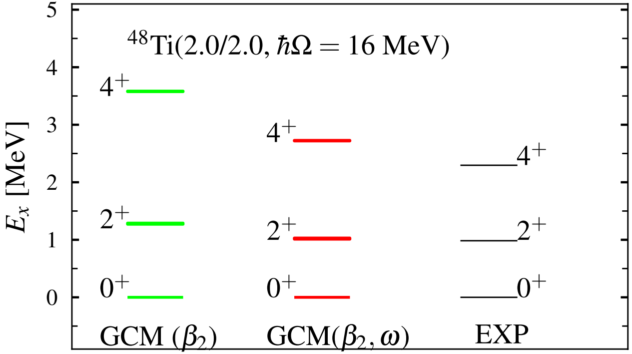
Potential Energy Surfaces



^{48}Ca is spherical and ^{48}Ti is weakly deformed.

Spectrum in ^{48}Ti

In 9 shells



E2's are realistic (large).

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Required Improvements to Methods

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  = more memory, processors
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That's about it!

How much smaller will the uncertainty be?

Not clear, but it will be more believable.

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That's all; thanks. 

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