Atomic EDMs and Nuclear Schiff Moments

J. Engel

May 19, 2023

Connection Between EDMs and T Violation

Consider non-degenerate ground state $|\mathrm{g.s.}:J,M\rangle$. Symmetry under rotations $R_y(\pi)$ for vector operator like $\vec{d} \equiv \sum_i e_i \vec{r}_i$ implies:

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

$R^{-1}R$ $R^{-1}R$

Connection Between EDMs and *T* Violation

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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

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

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

Connection Between EDMs and T Violation

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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.*

Screening of EDMs in Atoms

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.

Screening of EDMs in Atoms

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

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

K.E. + Coulomb

dipole perturbation

Screening of EDMs in Atoms

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

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

Screening of EDMs in Atoms

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!

Screening of EDMs in Atoms

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

$$\vec{d}' = \langle\tilde{0}|\sum_j e_j\vec{r}_j\,|\tilde{0}\rangle$$

$$= \langle 0|\left(1 - i\sum(1/e_k)\vec{d}_k\cdot\vec{p}_k\right)\left(\sum e_j\vec{r}_j\right)$$

Of course, the nucleus is not a point particle and electrons are not fully nonrelativistic, so the screening is not complete. But it reduces atomic EDMs by a few orders of magnitude.

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

$$= -\,\langle 0|\sum_k \vec{d}_k\,|0\rangle = -\sum_k \vec{d}_k$$

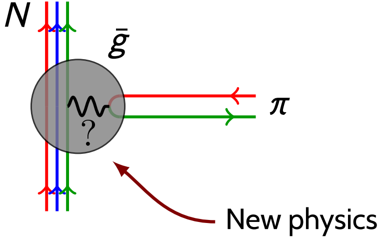
$$= -\,\vec{d}$$

So the net EDM is zero!

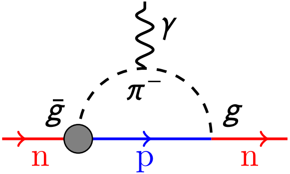
How Diamagnetic Atoms Get EDMs, Roughly

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.

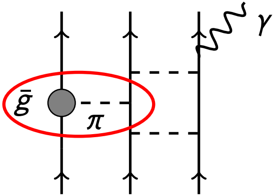
The source can work its way into nuclei through CP-violating πNN vertices (in chiral EFT)…



leading, e.g. to a neutron EDM…



How Diamagnetic Atoms Get EDMs, Roughly



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

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

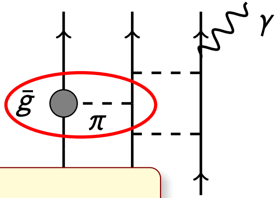
Atoms get EDMs from nuclei. Electronic shielding replaces nuclear dipole operator with "Schiff operator,"

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

making relevant nuclear quantity the Schiff moment:

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

How Diamagnetic Atoms Get EDMs, Roughly



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

$V_{PT} \propto \bar{g}$ … rms/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… clear dipole…

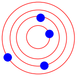
$$S \propto \sum_p \left(r_p^2 - \frac{5}{3} R_{\text{ch}}^2 \right) z_p + \ldots ,$$

making relevant nuclear quantity the Schiff moment:

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

Traditional Nuclear Models in One Slide

Starting point is always a mean field and potential



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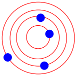

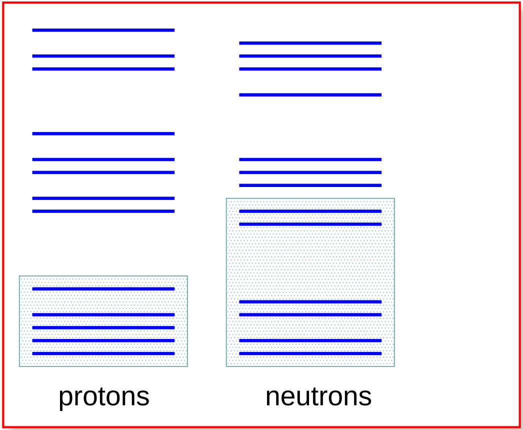

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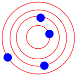

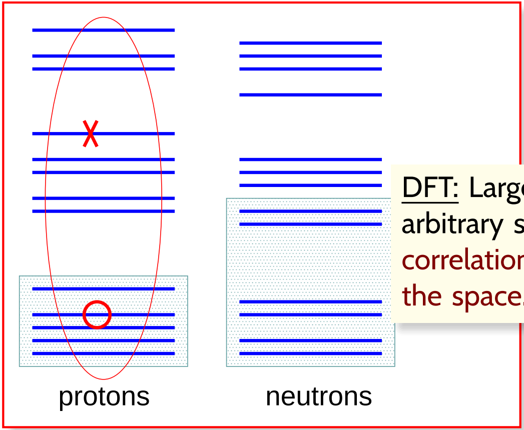

DFT: Large single-particle spaces in arbitrary single mean field; simple correlations and excitations within the space.

Traditional Nuclear Models in One Slide

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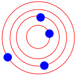

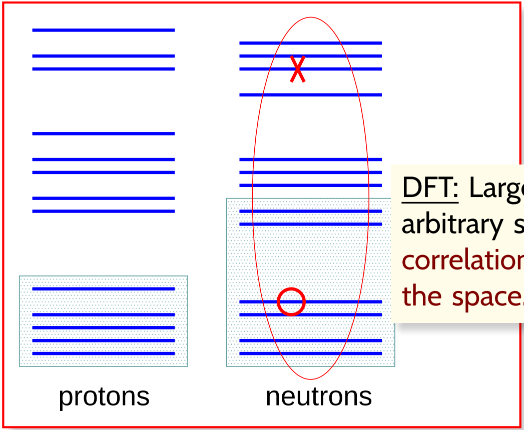

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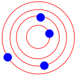

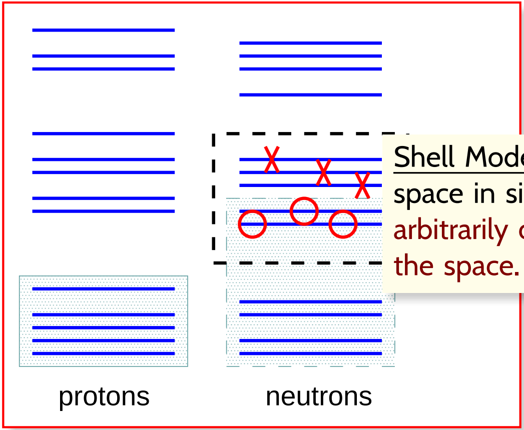

Shell Model: Small single-particle space in simple spherical mean field; arbitrarily complex correlations within the space.

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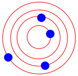
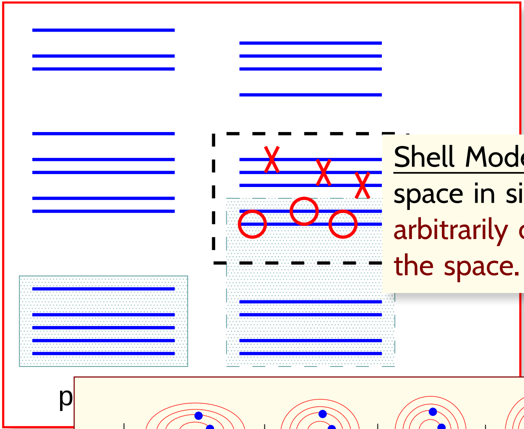
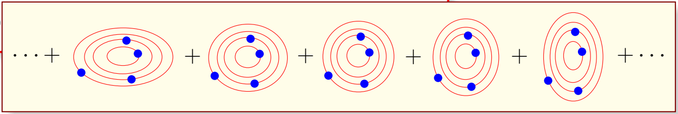




<u>Shell Model:</u> Small single-particle space in simple spherical mean field; arbitrarily complex correlations within the space.



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

Traditional Nuclear Models in One Slide

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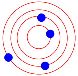
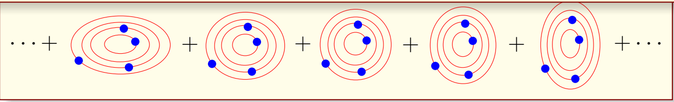


All such models require phenomenological Hamiltonian/operators, with coefficients fit to energies/transitions in heavy nuclei.

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



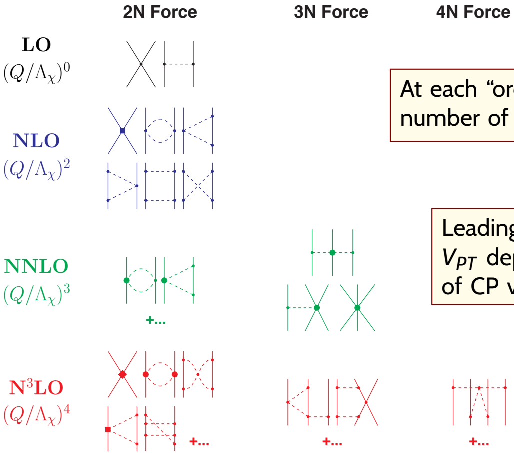
Generator-Coordinate Method (GCM): extension of DFT that mixes many mean-field states with different collective properties.

Ab Initio Nuclear Structure

Starts with ~~chiral effective field theory~~ useless junk

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

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

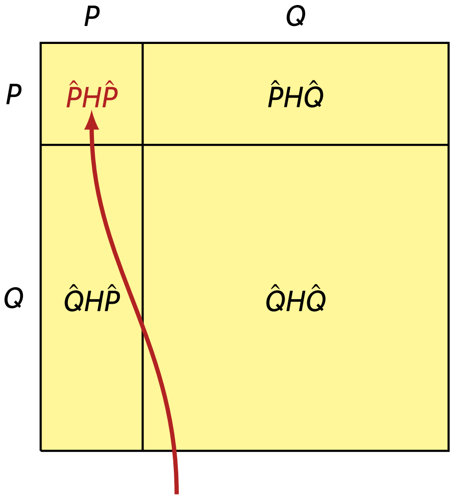


At each "order," only a finite number of operators exist.

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

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.

Ab Initio Many-Body Methods

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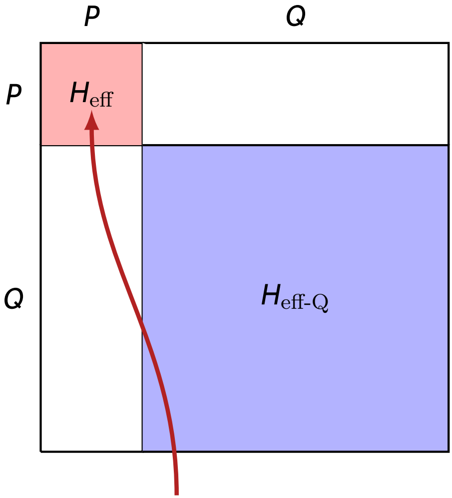

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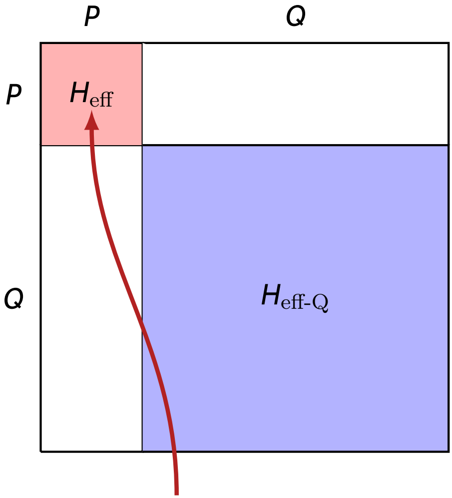

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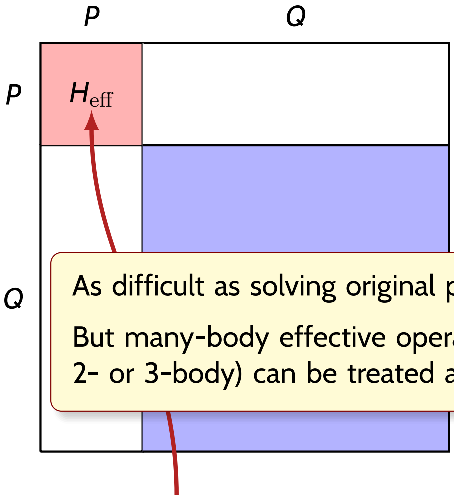
Task: Find unitary transformation to make *H* block-diagonal in *P* and *Q*, with H_{eff} in *P* reproducing most important eigenvalues.

Must must apply same unitary transformation to transition operator.

Ab Initio Many-Body Methods

Partition of Full Hilbert Space



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 ... nvalues.

... ly same unitary ... to transition operator.

As difficult as solving original problem.

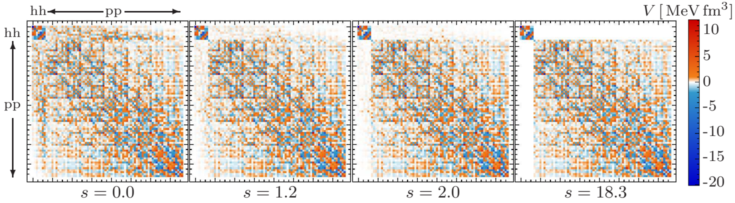
But many-body effective operators (beyond 2- or 3-body) can be treated approximately.

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

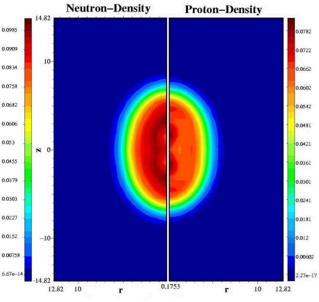
$$\frac{d}{ds}H(s) = [\eta(s), H(s)]\,, \qquad \eta(s) = [H_d(s), H_{od}(s)]\,, \qquad H(\infty) = H_{\text{eff}}$$

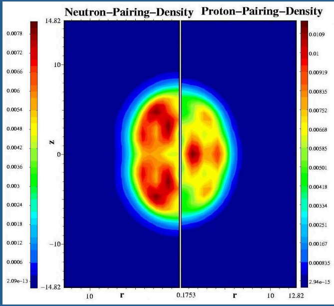
Trick is to keep all 1- and 2-body terms in *H* at each step *after normal ordering* with respect to states in reference space.

Reference space can be states contained in valence shell, 1p-1h excitations of mean-field state, a single GCM state, etc.

Skyrme DFT

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



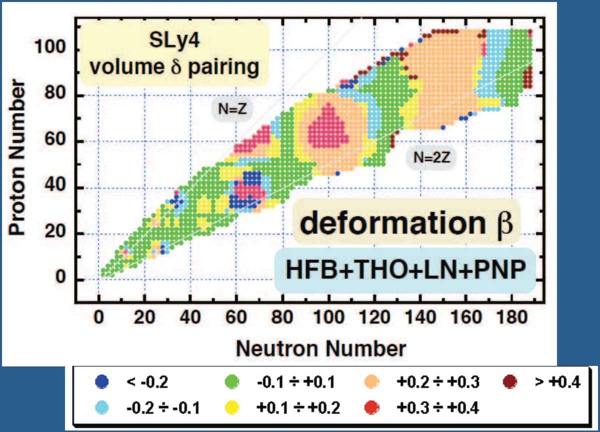


HFB: $\beta_2^{(p)}$=0.43 exp: $\beta_2^{(p)}$=0.42(5) , J.K. Hwang et al., Phys. Rev. C (2006)

Applied Everywhere

Nuclear ground state deformations (2-D HFB)

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



DFT Technique

With grad student D. Stilwell and J. Dobaczewski

Simply add solve mean-field equations for

$$\begin{aligned} H &= H_{\mathrm{Skyrme}} + V_{PT} \\ &= H_{\mathrm{Skyrme}} + \lambda F_{PT} \,, \end{aligned}$$

where $\lambda = \bar{g}g$ for some small $\bar{g}$ of your choice. Then compute

$$a \equiv \frac{\langle S \rangle}{\lambda} \,.$$

When $\langle S \rangle_{\mathrm{exp.}}$ is measured, you can compute $\bar{g}_{\mathrm{exp.}}$ from

$$\langle S \rangle_{\mathrm{exp.}} = \bar{g}_{\mathrm{exp.}} \, g \, a \,.$$

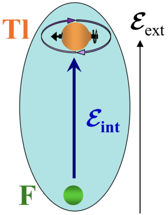
Or you can bound $\bar{g}_{\mathrm{exp.}}$ if there is only a limit on $\langle S \rangle_{\mathrm{exp.}}$.

New Nuclei for Us

- ^{205}Tl for CENTREX experiment on TlF molecule

Quantum Sci. Technol. **6**, 044007 (2021)

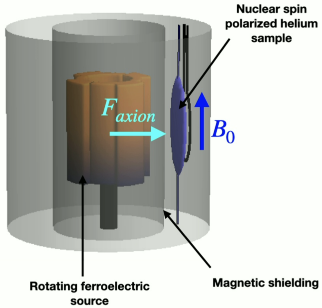
^{205}Tl is spherical.



- ^{235}U for "Ferroaxionic effect"

A. Arvanitaki, JE, A.A. Geraci, A. Madden, K. Van Tilburg, in prep.

^{235}U is almost pear shaped.



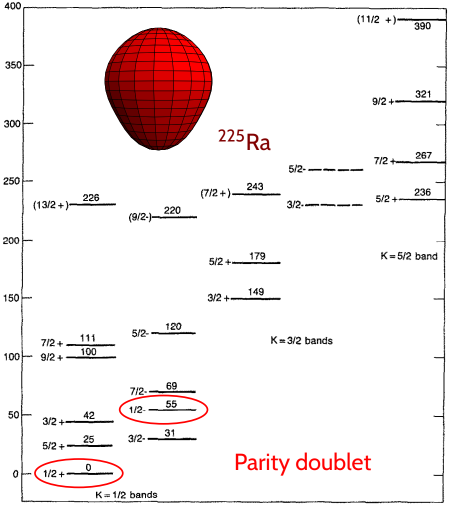
^{205}Tl

Preliminary calculation with one Skyrme interaction

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

	a_0	a_1	a_2
SkM*	0.04	−0.09	0.1
SLy4	0.03	−0.07	0.1
⋮	⋮	⋮	⋮

A Little on Pear-Shaped Nuclei



Because V_{PT} is so weak:

$$\langle S \rangle = \sum_{i \neq 0} \frac{\langle 0|S|i\rangle \langle i|V_{PT}|0\rangle}{E_0 - E_i} + c.c.$$

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

Mixing of the two states in the parity doublet by V_{PT} is the whole story here.

In ^{225}Ra:

$$a_0 \approx 0.2 \quad a_1 \approx -5 \quad a_2 \approx 3.3,$$

almost two orders of magnitude bigger than in ^{205}Tl.

^{235}U

This nucleus is symmetric but barely stable against "pear-ness". The result is a low-lying "octupole vibration"

We use our DFT method with symmetric ground state to treat ^{235}U.

Preliminary result

	a_0	a_1	a_2
SkM*	−0.1	−1.1	0.8
SLy4	⋮	⋮	⋮
⋮	⋮	⋮	⋮

A few times smaller than in ^{225}Ra.

Underway: Ab Initio Shell-Model Calculation

For nuclei that are not too deformed

New!

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^- :

$$H(s) = H_+(s) + \lambda H_-(s) + \mathcal{O}(\lambda^2) \qquad \eta = \eta_+(s) + \lambda \eta_-(s)$$

with

$$H_+(0) = T + V_\chi \qquad H_-(0) = F_{PT}$$

Grouping by powers of λ:

$$\frac{dH_+(s)}{ds} = [\eta_+(s), H_+(s)] + \mathcal{O}(\lambda^2)$$

$$\frac{d}{ds}H^-(s) = [\eta^+(s), H^-(s)] + [\eta^-(s), H^+(s)] + \mathcal{O}(\lambda^2)$$

η_+ and H_+ are what you get without V_{PT}.

You then evolve the Schiff operator, which develops a positive parity part.

Ragnar Stroberg doing this with and UNC postdoc David Kekejian and me.

To Conclude…

Thanks for listening!