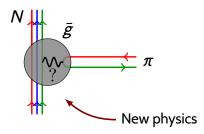


Because SM CP violation is so weak, an additional undiscovered source is required to explain why there is so much more matter than antimatter.

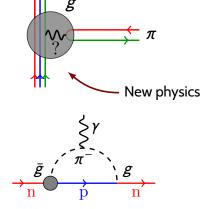
The source can work its way into nuclei through CP-violating πNN vertices (in chiral EFT)...



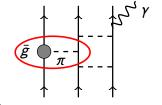
Because SM CP violation is so weak, an additional undiscovered source is required to explain why there is so much more matter than antimatter.

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

leading, e.g. to a neutron EDM...

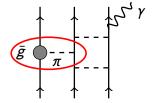


...and to a nuclear EDM from the nucleon EDM or a T-violating NN interaction:



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

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



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

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

$$S \propto \sum_{p} \left(r_p^2 - \frac{5}{3}R_{ch}^2\right) z_p + \dots,$$

making relevant nuclear quantity the Schiff moment:

$$\langle S \rangle = \sum_{m} \frac{\langle O | S | m \rangle \langle m | V_{PT} | O \rangle}{E_{O} - E_{m}} + c.c.$$

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

npute dend on the on EDM).

 $V_{PT} \propto 1$

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).

Atom:

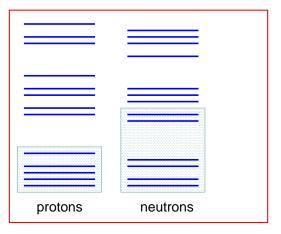
It's up to QCD/EFT to compute the dependence of the \bar{g} vertices on fundamental sources of $\it CP$ violation.

See talks by Vincenzo, Jordy, Michael.

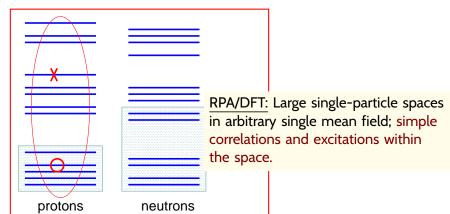
making relevant nuclear quantity the Schiff moment:

$$\langle S \rangle = \sum_{m} \frac{\langle O | S | m \rangle \langle m | V_{PT} | O \rangle}{E_{O} - E_{m}} + c.c.$$

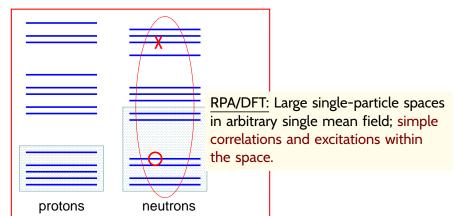




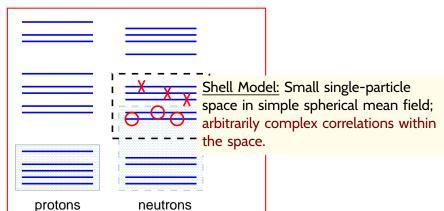






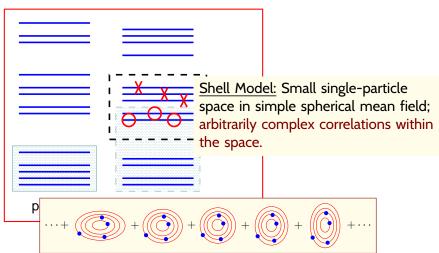






Nuclear Models in One Slide Starting point is always a mean field

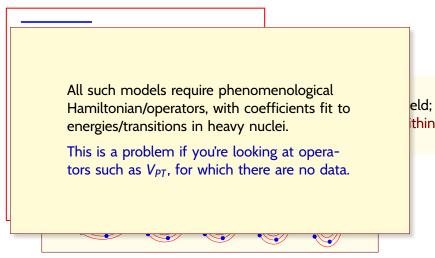




Generator-Coordinate Method (GCM): extension of DFT that mixes many mean-field states with different collective properties.



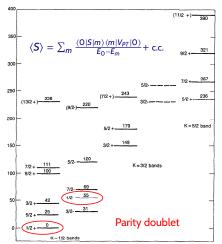
Starting point is always a mean field



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

²²⁵Ra and Other Light Actinides

Octupole Physics and DFT



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



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

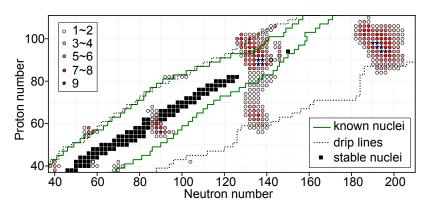
$$|\frac{1}{2}^{\pm}\rangle = \frac{1}{\sqrt{2}} (|\bigcirc\rangle \pm |\bigcirc\rangle)$$

and, to good approximation,

$$\langle S \rangle \approx \frac{2}{3} \frac{\langle S \rangle_{\text{intr.}}}{\langle E_{+} - E_{-}}$$

Octupole Systematics

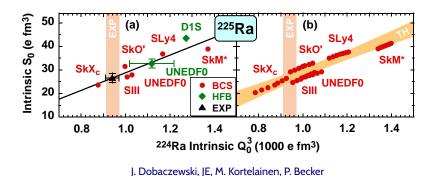
More DFT



From Cao et al., arXiv:2004.01319

See talk by W. Nazarewicz?

Correlation of 225 Ra $\langle S \rangle_{intr.}$ with 224 Ra Octupole Defm.

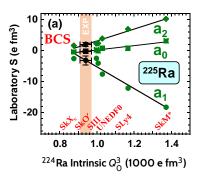


Correlation with octupole moment of ²²⁵Ra even better.

That moment will be determined at ANL.

Observables also correlated in other octupole-deformed actinides.

Implications of Correlation for Lab Schiff Moment



Looks good, but situation is more complicated when we include octupole moments in other nuclei. The resulting a_i for ²²⁵Ra:

isoscalar	isovector	isotensor
-0.4 - 0.8	-2 – -8	2 – 5

Range doesn't include systematic uncertainty.

The problem is that we don't have information about $\langle V_{PT} \rangle$.

The problem is that we don't have information about $\langle V_{PT} \rangle$.

Can we find measurements that will constrain its matrix element?

In one-body approximation $V_{PT} \approx \vec{\sigma} \cdot \vec{\nabla} \rho$. The closest simple one body operator is $\vec{\sigma} \cdot \vec{r}$.

Can we measure $\langle 1/2^-|\vec{\sigma}\cdot\vec{r}\,|1/2^+\rangle$ or something like it, in some octupole-deformed nucleus?

The problem is that we don't have information about $\langle V_{PT} \rangle$.

Can we find measurements that will constrain its matrix element?

In one-body approximation $V_{PT} \approx \vec{\sigma} \cdot \vec{\nabla} \rho$. The closest simple one body operator is $\vec{\sigma} \cdot \vec{r}$.

Can we measure $\langle 1/2^-|\vec{\sigma}\cdot\vec{r}|1/2^+\rangle$ or something like it, in some octupole-deformed nucleus?

What about charge-changing transition strength to isobar analog of |1/2⁻⟩ in ²²⁵Fr? Axial-charge β decays in other nuclei?
V_{PT} is similar to two-body current operator in axial-charge channel.

The problem is that we don't have information about $\langle V_{PT} \rangle$.

Can we find measurements that will constrain its matrix element?

In one-body approximation $V_{PT} \approx \vec{\sigma} \cdot \vec{\nabla} \rho$. The closest simple one body operator is $\vec{\sigma} \cdot \vec{r}$.

Can we measure $\langle 1/2^-|\vec{\sigma}\cdot\vec{r}|1/2^+\rangle$ or something like it, in some octupole-deformed nucleus?

What about charge-changing transition strength to isobar analog of |1/2⁻⟩ in ²²⁵Fr? Axial-charge β decays in other nuclei? V_{PT} is similar to two-body current operator in axial-charge channel.

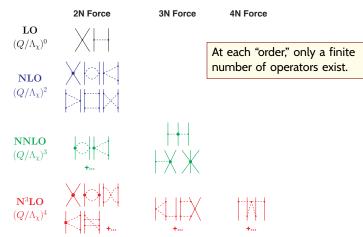
The other option is an ab-initio calculation with controlled errors!

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.

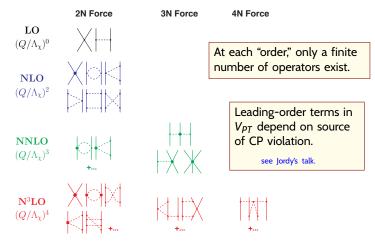


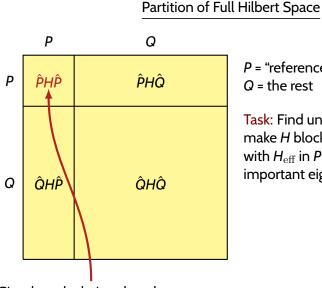
Ab Initio Nuclear Structure

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.

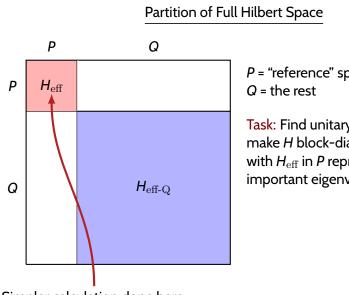




P = "reference" space Q = the rest

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

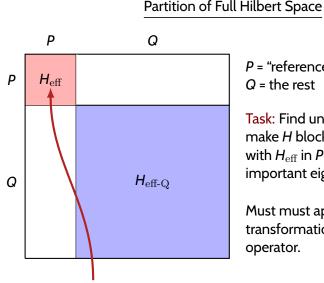
Simpler calculation done here.



P = "reference" space

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

Simpler calculation done here.

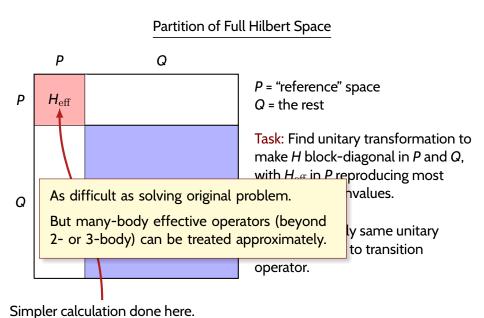


P = "reference" space Q =the rest

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

Must must apply same unitary transformation to transition operator.

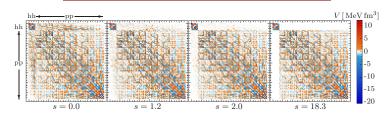
Simpler calculation done here.



In-Medium Similarity Renormalization Group

One way to determine the transformation

Flow equation for effective Hamiltonian. Gradually decouples reference space.



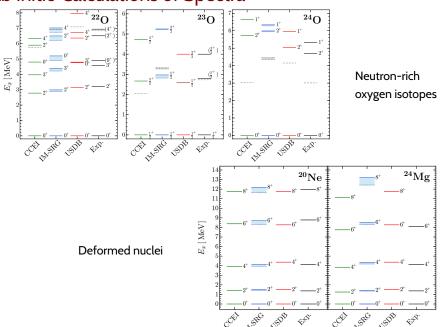
from H. Hergert

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

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.

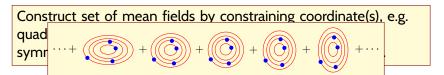
Ab Initio Calculations of Spectra



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 $\langle Q_0 \rangle$.

Background: Generator Coordinate Method

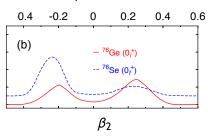


Background: Generator Coordinate Method

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 $\langle Q_0 \rangle$.

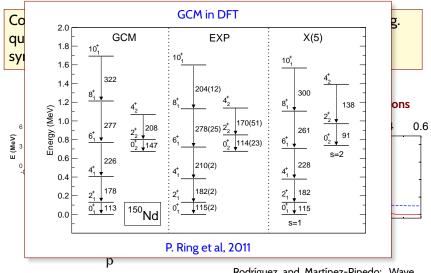
Li et al.: Potential energy surface for ¹³⁰Xe

Collective squared wave functions



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

Background: Generator Coordinate Method



Li et al.: Potential energy surface for ¹³⁰Xe

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

J.M. Yao, B. Bally, JE, R. Wirth, T.R. Rodríguez, H. Hergert

Uses GCM reference state to capture collective multi-particle multi-hole correlations, include the rest through IMSRG.

J.M. Yao, B. Bally, JE, R. Wirth, T.R. Rodríguez, H. Hergert

Uses GCM reference state to capture collective multi-particle multi-hole correlations, include the rest through IMSRG.

Procedure for Schiff moment, which involves two states:

 Use bare Hamiltonian to construct approximate GCM states for ground state and its partner, and create the statistical ensemble:

$$\rho = \alpha \left| 1/2^+ \right\rangle \left\langle 1/2^+ \right| + b \left| 1/2^- \right\rangle \left\langle 1/2^- \right|$$

J.M. Yao, B. Bally, JE, R. Wirth, T.R. Rodríguez, H. Hergert

Uses GCM reference state to capture collective multi-particle multi-hole correlations, include the rest through IMSRG.

Procedure for Schiff moment, which involves two states:

 Use bare Hamiltonian to construct approximate GCM states for ground state and its partner, and create the statistical ensemble:

$$\rho = \alpha \left| 1/2^+ \right\rangle \left\langle 1/2^+ \right| + b \left| 1/2^- \right\rangle \left\langle 1/2^- \right|$$

2. Use flow equation to construct Hamiltonian \bar{H} so that $\text{Tr}(\rho \bar{H})$ is minimized, apply resulting transformation to V_{PT} and \bar{S} to get \bar{V}_{PT} and \bar{S} .

J.M. Yao, B. Bally, JE, R. Wirth, T.R. Rodríguez, H. Hergert

Uses GCM reference state to capture collective multi-particle multi-hole correlations, include the rest through IMSRG.

Procedure for Schiff moment, which involves two states:

 Use bare Hamiltonian to construct approximate GCM states for ground state and its partner, and create the statistical ensemble:

$$\rho = \alpha \left| 1/2^+ \right\rangle \left\langle 1/2^+ \right| + b \left| 1/2^- \right\rangle \left\langle 1/2^- \right|$$

- 2. Use flow equation to construct Hamiltonian \bar{H} so that $\text{Tr}(\rho \bar{H})$ is minimized, apply resulting transformation to V_{PT} and S to get \bar{V}_{PT} and \bar{S} .
- 3. Neither $|1/2^+\rangle$ or $|1/2^-\rangle$ is an exact eigenvector of \bar{H} , even without truncation of flow equations, so do a second set of GCM calculations with \bar{H} .

J.M. Yao, B. Bally, JE, R. Wirth, T.R. Rodríguez, H. Hergert

Uses GCM reference state to capture collective multi-particle multi-hole correlations, include the rest through IMSRG.

Procedure for Schiff moment, which involves two states:

 Use bare Hamiltonian to construct approximate GCM states for ground state and its partner, and create the statistical ensemble:

$$\rho = \alpha \left| 1/2^+ \right\rangle \left\langle 1/2^+ \right| + b \left| 1/2^- \right\rangle \left\langle 1/2^- \right|$$

- 2. Use flow equation to construct Hamiltonian \bar{H} so that $\text{Tr}(\rho \bar{H})$ is minimized, apply resulting transformation to V_{PT} and \bar{S} to get \bar{V}_{PT} and \bar{S} .
- 3. Neither $|1/2^+\rangle$ or $|1/2^-\rangle$ is an exact eigenvector of \bar{H} , even without truncation of flow equations, so do a second set of GCM calculations with \bar{H} .
- **4**. Compute Schiff moment with \bar{V}_{PT} and \bar{S} .

J.M. Yao, B. Bally, JE, R. Wirth, T.R. Rodríguez, H. Hergert

Uses GCM reference state to capture collective multi-particle multi-hole correlations, include the rest through IMSRG.

Procedure for Schiff moment, which involves two states:

We have already done this for the $\beta\beta$ decay of ⁴⁸Ca to ⁴⁸Ti (also involving two states).

Now doing it for the decay of ⁷⁶Ge.

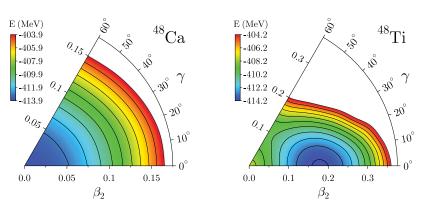
is minimized, apply resulting transformation to V_{PT} and S to get \bar{V}_{PT} and \bar{S} .

- 3. Neither $|1/2^+\rangle$ or $|1/2^-\rangle$ is an exact eigenvector of H, even without truncation of flow equations, so do a second set of GCM calculations with \bar{H} .
- **4**. Compute Schiff moment with \bar{V}_{PT} and \bar{S} .

In-Medium GCM for Decay of ⁴⁸Ca

GCM Reference States for IMSRG

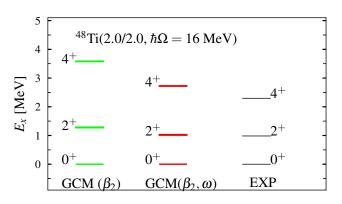
Potential Energy Surfaces



⁴⁸Ca is spherical and ⁴⁸Ti is weakly deformed.

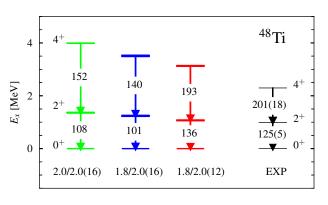
Spectrum in ⁴⁸Ti





Spectrum in ⁴⁸Ti

In 9 shells



 β_2 only

We get large E2's.

Required Improvements to Methods

More nucleons will require larger spaces = more memory, processors = supercomputer use (maybe).

Required Improvements to Methods

- ▶ More nucleons will require larger spaces = more memory, processors = supercomputer use (maybe).
- Chiral interactions will need to be tested in really heavy nuclei.

Required Improvements to Methods

- More nucleons will require larger spaces = more memory, processors = supercomputer use (maybe).
- Chiral interactions will need to be tested in really heavy nuclei.

That's about it!

How much smaller will the uncertainty be?

Not clear, but it will be more believable.

Required Improvements to Methods

▶ More nucleons will require larger spaces = more memory,

That's all; thanks. 📫

How much smaller will the uncertainty be?

Not clear, but it will be more believable.