

Beyond mean-field correlations on nuclear Schiff moments and P,T-odd nuclear forces

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1 Introduction

- CP violation and atomic EDMs
- Status of studies on nuclear Schiff moments

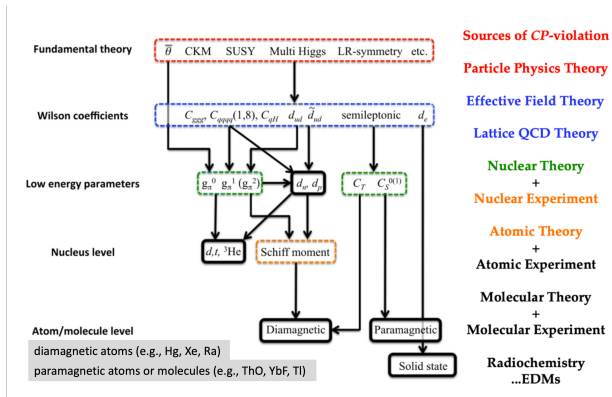
2 The multi-reference covariant density functional theory for ^{129}Xe , ^{199}Hg , and ^{225}Ra

- The framework of MR-CDFT
- Application to nuclear structural properties
- Application to nuclear Schiff moments
- Constraints on the P,T-odd nuclear forces

3 Summary

4 Appendix: preliminary results on ^{171}Yb

- The sources of **charge-parity violation (CPV)** within the SM (the complex phase of the CKM matrix in weak interactions and the θ term in QCD) **are not sufficient** to explain the observed **baryon asymmetry** of the universe.
- Hypothetical **new sources of CPV** beyond standard model (BSM), such as SUSY, multi-Higgs models, and LR-symmetry models.



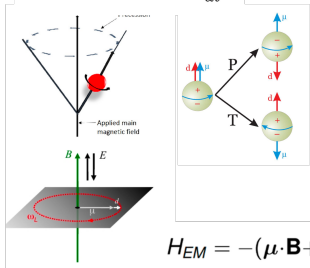
T. Chupp, et al., Rev. Mod. Phys. 91, 015001 (2019); credit to Jaideep Singh.

Observation of any sizable EDMs of elementary or composite particles would indicate new CP violation beyond the SM, potentially solving the **baryon asymmetry problem**.

An atom with nonzero spin and EDM

Larmor precession in external B and E fields

$$\vec{\tau} = \vec{\mu} \times \vec{B} \pm \vec{d} \times \vec{E} = \frac{d\vec{L}}{dt}$$



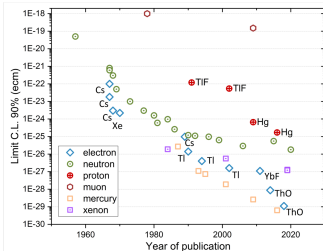
$$H_{EM} = -(\vec{\mu} \cdot \vec{B} + \vec{d} \cdot \vec{E})$$

Change in the frequency after flipping the direction of E

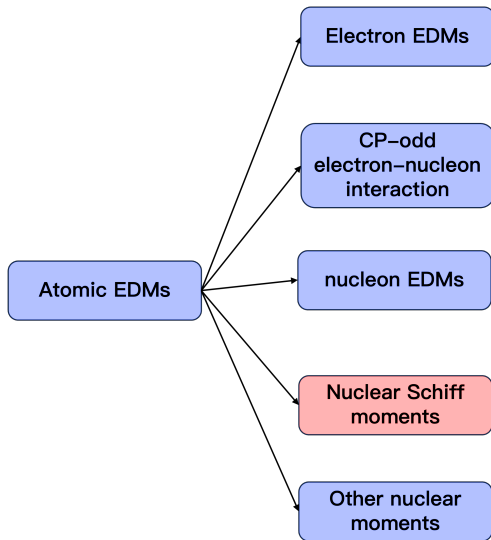
$$\omega_{\pm} = \frac{2(\mu B \pm dE)}{\hbar}$$

$$\omega_{+} - \omega_{-} = \frac{4dE}{\hbar}$$

Atoms	$ d_A [\times 10^{-26} \text{ ecm}]$	Exp. [References]
^{129}Xe	< 0.14	Sachdeva et al., PRL123, 143003 (2019)
^{171}Yb	< 1.5	Zheng et al., PRL129, 083001 (2022)
^{199}Hg	$< 7 \times 10^{-4}$	Graner et al., PRL116, 161601 (2016)
^{225}Ra	$< 5 \times 10^4$	Parker et al., PRL114, 233002 (2015)
^{223}Ra	$< 1.4 \times 10^3$	Bishof et al., PRC94, 025501 (2016)



	Standard Model	Experiment
^{199}Hg	10^{-33} e cm	$\leq 7.4 \cdot 10^{-30} \text{ e cm}$
electron	10^{-38} e cm	$\leq 9 \cdot 10^{-29} \text{ e cm}$
neutron	10^{-31} e cm	$\leq 1.9 \cdot 10^{-26} \text{ e cm}$
proton	10^{-31} e cm	$\leq 2.0 \cdot 10^{-25} \text{ e cm}$



- Paramagnetic atoms and molecules (e.g., ThO, YbF, Tl), where the unpaired electron(s) enhance the sensitivity.
- **Relativistic effect & heavy (Z^3) atoms** amplify this contribution.
- CP-violating **semileptonic interactions** between electrons and nucleons
- Include scalar–pseudoscalar ($k_{1,3}$), tensor–tensor (k_2) operators.
- Arises from **QCD θ -term** or BSM physics (e.g., quark chromo-EDMs, CP-violating four-quark operators).
- Induce a **nuclear EDM** or contribute to the **nuclear Schiff moment**.
- Arises from nucleon EDMs or **CP-violating nuclear forces**.
- Dominant contribution to the EDM of **diamagnetic atoms** (e.g., Xe, Yb, Hg, Ra), which have all the electrons paired.
- Magnetic quadrupole moments, etc.

- The measurements in **several diamagnetic atoms** are crucial for **disentangling the contributions from different effective operators**.
- The atomic EDMs have been calculated with different atomic many-body theories.

Different atomic theory calculations: differ by less than 20%

- The **valence Dirac-Fock+RPA/CI+MBPT** calculations: V. A. Dzuba et al., PRA80, 032120 (2009)

$$d_A(^{129}\text{Xe}) = +0.38 \times 10^{-17} S(e \text{ fm}^3)^{-1}(e \text{ cm}),$$

$$d_A(^{199}\text{Hg}) = -2.1 \times 10^{-17} S(e \text{ fm}^3)^{-1}(e \text{ cm}),$$

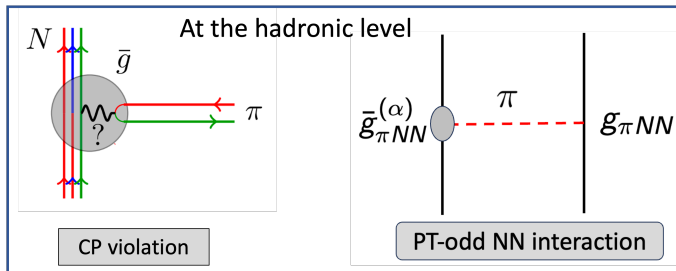
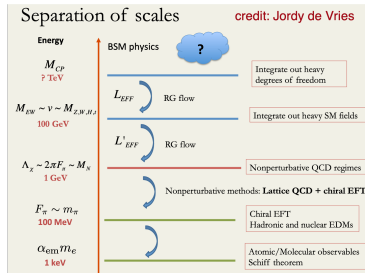
$$d_A(^{225}\text{Ra}) = -8.8 \times 10^{-17} S(e \text{ fm}^3)^{-1}(e \text{ cm}).$$

- The **relativistic coupled-cluster** calculations: Latha et al, PRL 115, 059902 (2015); B.K. Sahoo, B.P. Das, PRL120, 203001 (2018); Y. Singh and B. K. Sahoo, PRA 92, 022502 (2015)

$$d_A(^{129}\text{Xe}) = +0.34 \times 10^{-17} S(e \text{ fm}^3)^{-1}(e \text{ cm}),$$

$$d_A(^{199}\text{Hg}) = -1.77 \times 10^{-17} S(e \text{ fm}^3)^{-1}(e \text{ cm}),$$

$$d_A(^{225}\text{Ra}) = -6.79 \times 10^{-17} S(e \text{ fm}^3)^{-1}(e \text{ cm}).$$



The standard $N\pi$ coupling vertex is

$$\mathcal{L}^{(int)} = ig_{\pi NN} \bar{N} \gamma_5 N \vec{\tau} \cdot \vec{\pi}, \quad g_{\pi NN} = m_N g_A / f_\pi \simeq 12.9$$

The PT-odd $N\pi$ coupling vertex: iso-scalar, iso-vector and iso-tensor

$$\mathcal{L}_{PT}^{(int)} = \bar{g}_{\pi NN}^{(0)} \bar{N} N \vec{\tau} \cdot \vec{\pi} + \bar{g}_{\pi NN}^{(1)} \bar{N} N \pi_z + \bar{g}_{\pi NN}^{(2)} \bar{N} N (3\tau_z \pi_z - \vec{\tau} \cdot \vec{\pi})$$

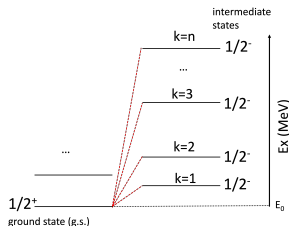
The Schiff moment can be written in terms of nuclear structure factors a_α ,

$$S = \sum_{k \neq 0} \frac{\langle \Psi_0^{(N)} | \hat{S}_z | \Psi_k^{(N)} \rangle \langle \Psi_k^{(N)} | \hat{V}_{PT} | \Psi_0^{(N)} \rangle}{E_0^N - E_k^N} + c.c. \equiv g_{\pi NN} \sum_{\alpha=0}^2 \bar{g}_{\pi NN}^{(\alpha)} a_\alpha,$$

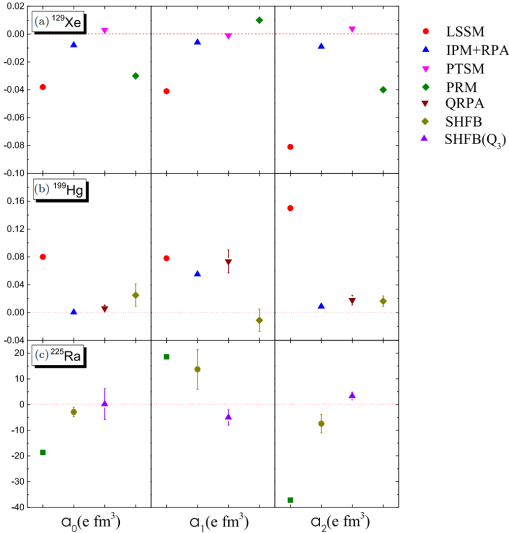
where (in units of $e \text{ fm}^3$)

$$\hat{S}_z = \frac{e}{10} \sum_p \left(\hat{r}_p^2 - \frac{5}{3} \langle r^2 \rangle_{\text{ch}} \right) \hat{z}_p,$$

$$a_\alpha = \frac{2}{g_{\pi NN}} \sum_{k \neq 0} \frac{M_S^{0k} M_{PT}^{k0(\alpha)}}{(E_0^N - E_k^N)}.$$



Accurate knowledge of nuclear Schiff moment is essential to connect experimental signatures (EDM) with the potential new physics (LECs of PT-odd nuclear forces).



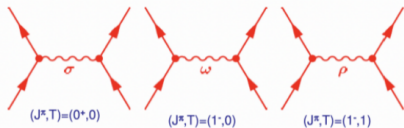
E.F. Zhou, JMY, IJMPPE (2024)

Table 1. The coefficients a_i (e fm^3) of nuclear Schiff moments from the calculations of different nuclear models.

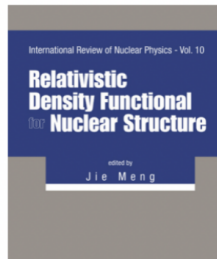
Isotopes	a_0	a_1	a_2	Nuclear models
^{153}Eu	-9.62	47.3	-25.53	PRM ¹⁴⁸
^{129}Xe	-0.038	-0.041	-0.081	LSSM ¹⁶⁰
^{129}Xe	-0.008	-0.006	-0.009	IPM + RPA ¹⁵¹
^{129}Xe	0.003	-0.001	0.004	PTSM ¹⁵⁹
^{129}Xe	-0.03	0.01	-0.04	PRM ¹⁶³
^{199}Hg	0.080	0.078	0.15	LSSM ¹⁶⁰
^{199}Hg	0.0004	0.055	0.009	IPM + RPA ^{151,169}
^{199}Hg	[0.002, 0.010]	[0.057, 0.090]	[0.011, 0.025]	SHFB + QRPA ¹⁵⁵
^{199}Hg	[0.009, 0.041]	[-0.027, +0.005]	[0.009, 0.024]	SHFB ¹⁵³
^{221}Rn	-0.04(10)	-1.7(3)	0.67(10)	SHFB(Q_3) ¹⁵⁴
^{223}Rn	-62	62	-100	PRM ¹⁵⁶
^{223}Rn	-0.08(8)	-2.4(4)	0.86(10)	SHFB(Q_3) ¹⁵⁴
^{223}Ra	-25	25	-50	PRM ¹⁵⁶
^{223}Fr	-31	31	-62	PRM ¹⁵⁶
^{223}Fr	-0.02	-0.02	-0.04	QOV ¹⁵⁷
^{223}Fr	0.07(20)	-0.8(7)	0.05(40)	SHFB(Q_3) ¹⁵⁴
^{225}Ra	-18.6	18.6	-37.2	PRM ¹⁵⁶
^{225}Ra	[-1.0, -4.7]	[6.0, 21.5]	[-3.9, -11.0]	SHFB ¹⁵²
^{225}Ra	0.2(6)	-5(3)	3.3(1.5)	SHFB(Q_3) ¹⁵⁴
^{227}Ac	-26	129	-69	PRM ¹⁴⁸
^{229}Pa	-1.2(3)	-0.9(9)	-0.3(5)	SHFB(Q_3) ¹⁵⁴
^{235}U	-7.8	38.7	-20.7	PRM ¹⁴⁸
^{237}Np	-15.6	77.4	-41.4	PRM ¹⁴⁸

- The covariant density functional theory (CDFT)

- ★ Meson-exchange models

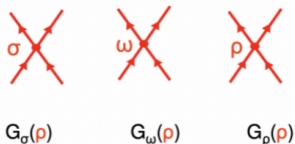


$$S(\mathbf{r}) = g_\sigma \sigma(\mathbf{r}) \quad V(\mathbf{r}) = g_\omega \omega(\mathbf{r}) + g_\rho \vec{\rho}(\mathbf{r}) + eA(\mathbf{r})$$



- ★ Point-coupling models

$$(\bar{\psi}\Gamma\psi)^2 \quad D(\bar{\psi}\psi)\Delta(\bar{\psi}\psi)$$



“No-sea” and “mean-field” approximations
Kohn-Sham DFT

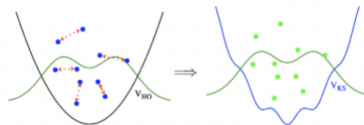
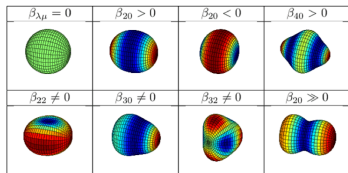


Figure from Drut PNP 2010

- Symmetry-breaking and restoration methods



With the courtesy of B.N. Lu

Mean-field solution (variation in a limited Hilbert space):

- ▶ Onset of different shapes
- ▶ Breaking of symmetries of Hamiltonian (rotation, parity, etc)
- ▶ Restoration of symmetry with projection operators

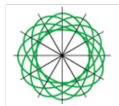
JMY, symmetry restoration methods,
arXiv:2204.12126v1 (2022)

“Deformed ”
mean-field



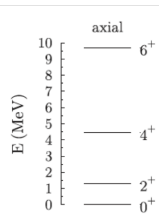
$$|\Phi(\mathbf{q})\rangle$$

Rotated
mean-field



$$\hat{R}(\Omega)|\Phi(\mathbf{q})\rangle$$

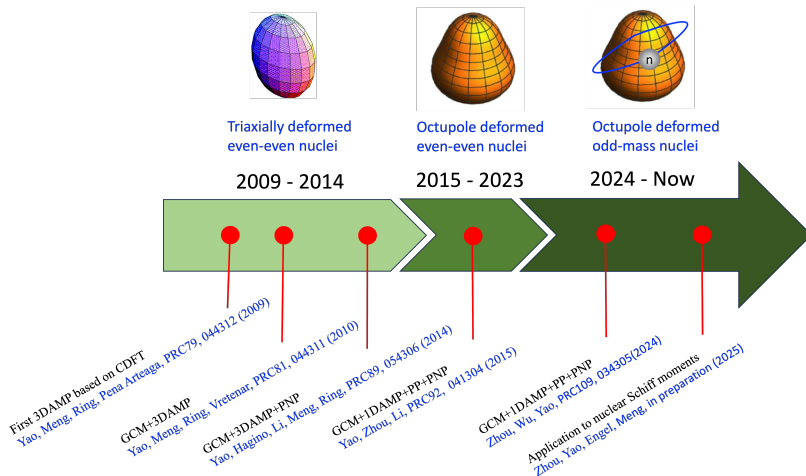
Nuclear low-lying states



$$|\Phi_{JM}(\mathbf{q})\rangle = \sum_K g_K^J \hat{P}_{MK}^J |\Phi(\mathbf{q})\rangle$$

$$\hat{P}_{MK}^J \equiv \frac{2J+1}{8\pi^2} \int_0^{2\pi} d\alpha \int_0^\pi \sin\beta d\beta \int_0^{2\pi} d\gamma D_{MK}^{J*}(\Omega) \hat{R}(\Omega)$$

Development of the MR-CDFT for nuclear spectroscopy



- Wave function for nuclear low-lying states

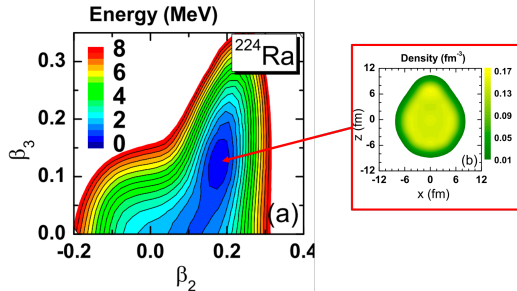
$$|JMK\pi, \alpha\rangle = \sum_{\mathbf{q}} f_{\alpha}^{JK\pi}(\mathbf{q}) |NZJK\pi; \mathbf{q}\rangle, \quad |NZJK\pi; \mathbf{q}\rangle = \hat{P}_{MK}^J \hat{P}^N \hat{P}^Z \hat{P}^{\pi} |\Phi_k^{(\text{OA})}\rangle$$

Mean-field wave configurations:

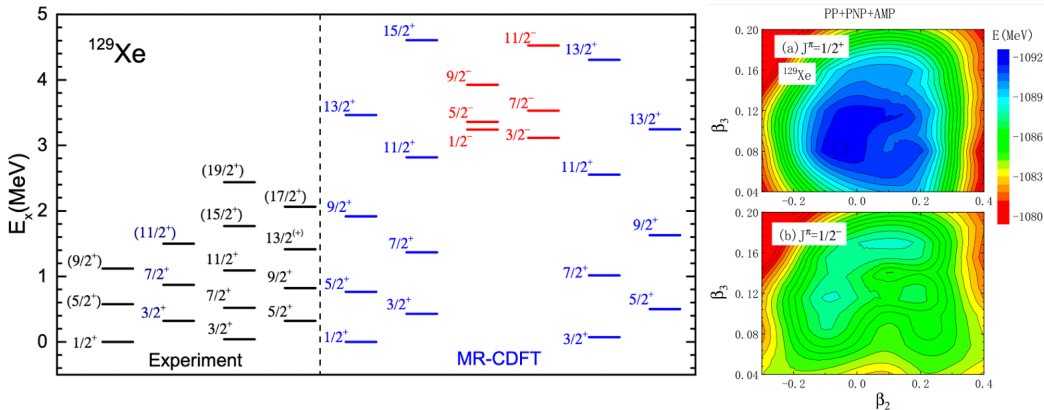
$$E[\Phi] = \langle \Phi(\mathbf{q}) | \hat{H} - \sum_{\tau=n,p} \lambda_{\tau} \hat{N}_{\tau} | \Phi(\mathbf{q}) \rangle + \frac{1}{2} \sum_{\lambda=1,2,3} C_{\lambda} \left(\langle \Phi(\mathbf{q}) | \hat{Q}_{\lambda 0} | \Phi(\mathbf{q}) \rangle - q_{\lambda 0} \right)^2$$

For odd-mass nuclei,

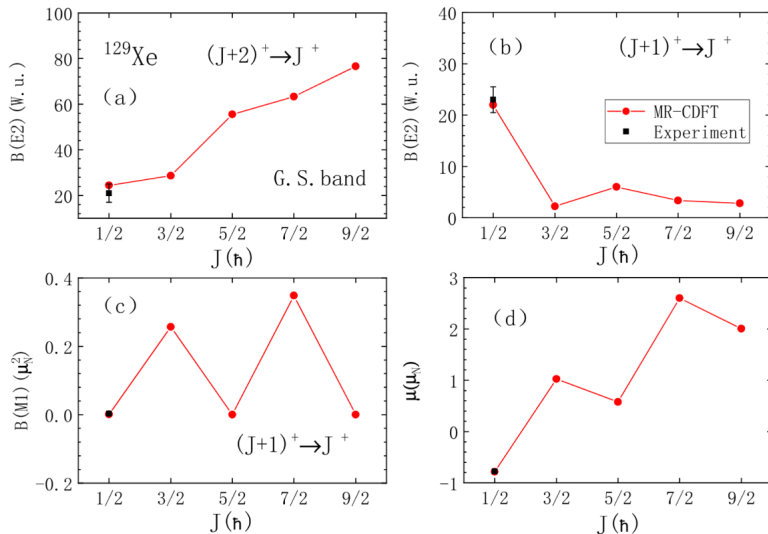
$$|\Phi_{\kappa}^{(\text{OA})}(\mathbf{q})\rangle = \alpha_{\kappa}^{\dagger} |\Phi_{(\kappa)}(\beta_2, \beta_3)\rangle.$$

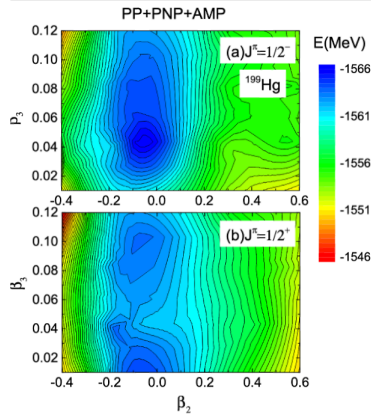
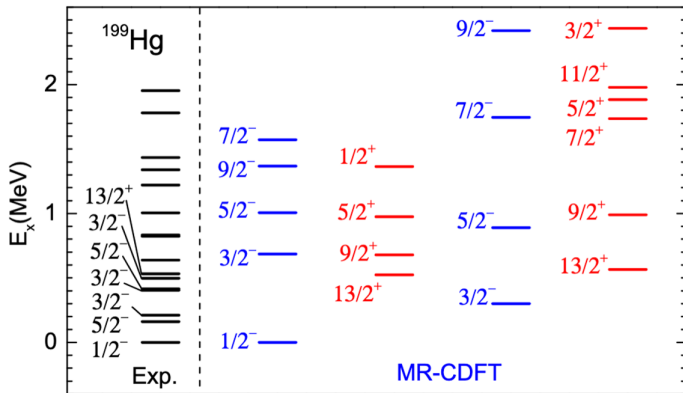


JMY, E.F. Zhou, Z.P. Li, PRC92, 041304(R) (2015)

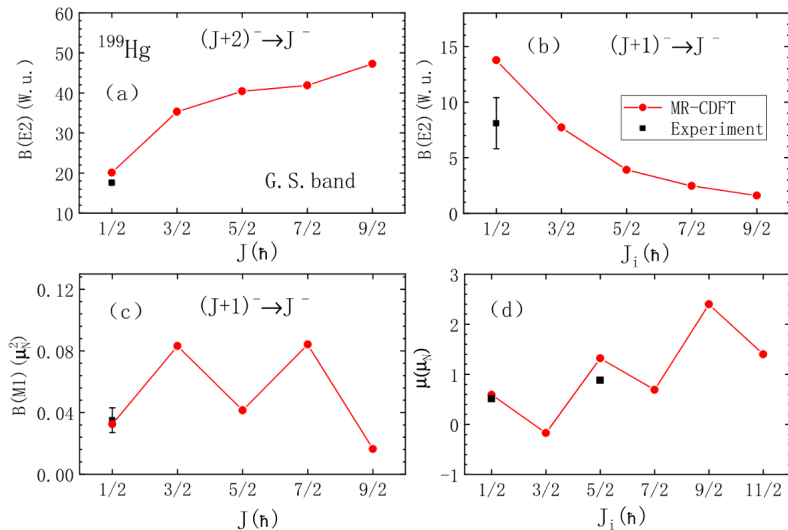


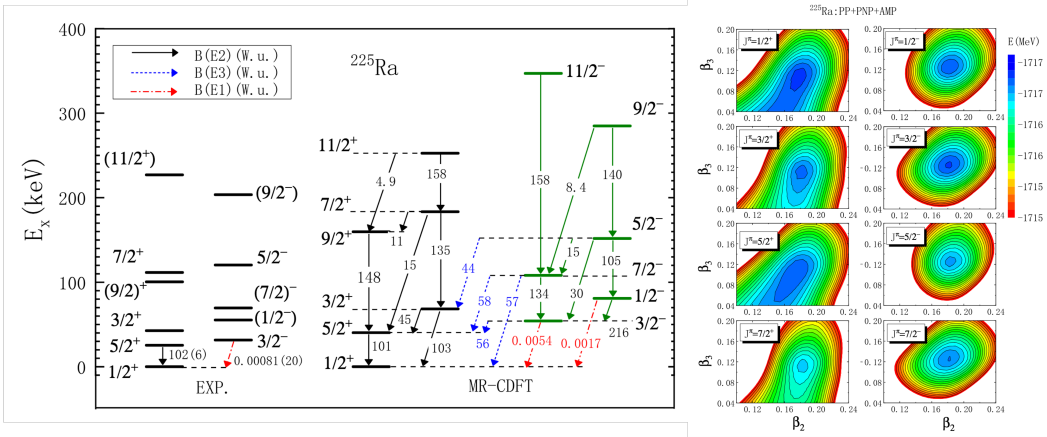
- The ground state dominated by the weakly deformed configuration with $(\beta_{20}, \beta_{30}) = (-0.08, 0.08)$.
- The excitation energy of the $1/2_1^-$ is predicted around 3.2 MeV.



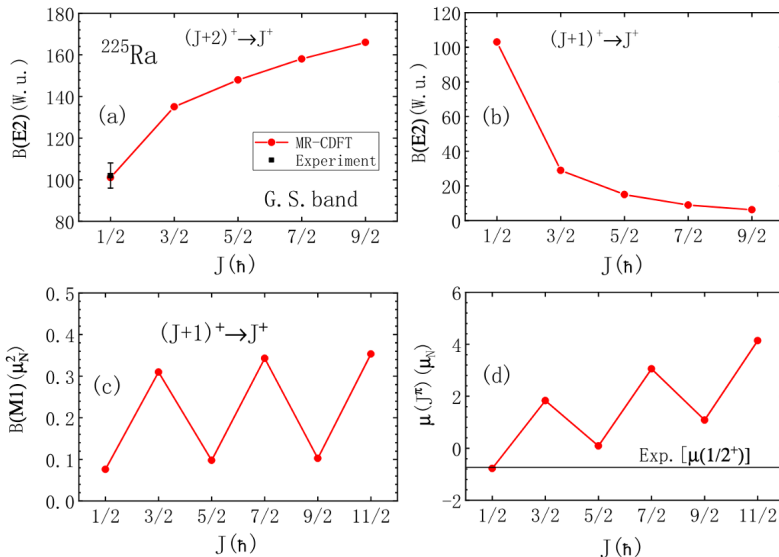


- The ground state dominated by the weakly deformed configuration with $(\beta_{20}, \beta_{30}) = (-0.05, 0.04)$.
- The first excited state $1/2^+$ is predicted around 1.6 MeV.





- The ground state $1/2_1^+$ is strongly octupole deformed.
- The first $1/2^-$ state is predicted around 0.069 MeV, compared to data 0.055 MeV.

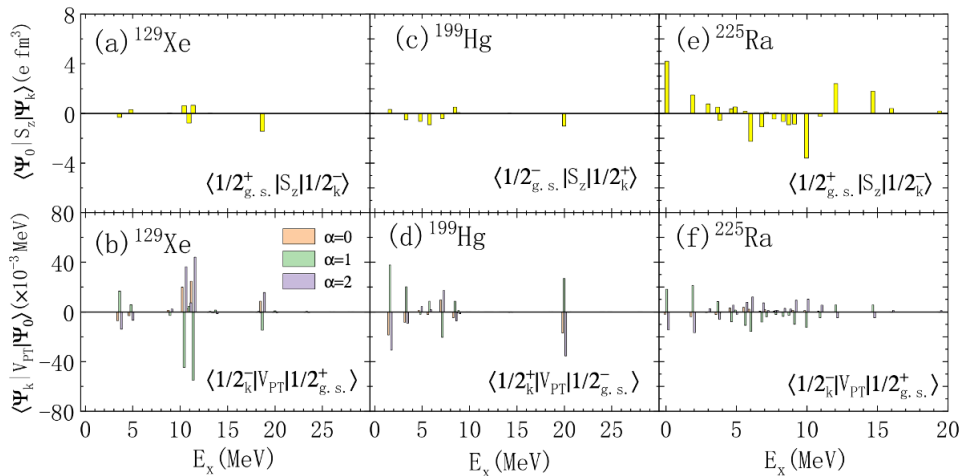


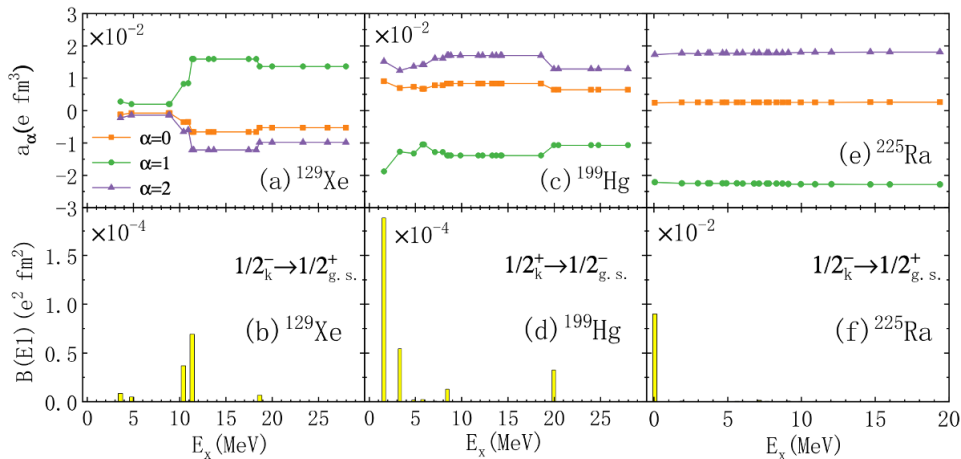
We compute the two-body matrix element of the PT-violating NN interaction in the relativistic framework directly,

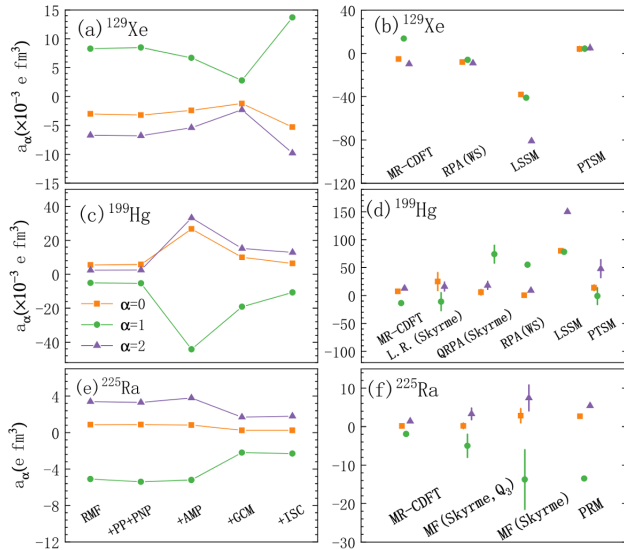
$$\begin{aligned}\langle jI | V_{PT} | ik \rangle &= \sum_{\alpha=0}^2 \langle jI | V_{PT}^{(\alpha)} | ik \rangle \\ &= (4\pi)^2 i g_{\pi NN} \sum_{\alpha=0}^2 \bar{g}_{\pi NN}^{(\alpha)} \sum_{LM} \int \frac{q^2 dq}{(2\pi)^3} \frac{1}{q^2 + m_{\pi}^2} \langle jI | V_{PT}^{(\alpha)}(q) | ik \rangle \\ &\quad + \text{exch. terms}\end{aligned}$$

where

$$\begin{aligned}\langle jI | V_{PT}^{(0)}(q) | ik \rangle &= \langle j | \gamma^0 \gamma_5 \vec{\tau} j_L(qr_1) Y_{LM}(\hat{\mathbf{r}}_1) | i \rangle \langle I | \gamma^0 \vec{\tau} j_L(qr_2) Y_{LM}^*(\hat{\mathbf{r}}_2) | k \rangle \\ \langle jI | V_{PT}^{(1)}(q) | ik \rangle &= \langle j | \gamma^0 \gamma_5 \tau_z j_L(qr_1) Y_{LM}(\hat{\mathbf{r}}_1) | i \rangle \langle I | \gamma^0 j_L(qr_2) Y_{LM}^*(\hat{\mathbf{r}}_2) | k \rangle \\ \langle jI | V_{PT}^{(2)}(q) | ik \rangle &= 3 \langle j | \gamma^0 \gamma_5 \tau_z j_L(qr_1) Y_{LM}(\hat{\mathbf{r}}_1) | i \rangle \langle I | \gamma^0 \tau_z j_L(qr_2) Y_{LM}^*(\hat{\mathbf{r}}_2) | k \rangle \\ &\quad - \langle j | \gamma^0 \gamma_5 \vec{\tau} j_L(qr_1) Y_{LM}(\hat{\mathbf{r}}_1) | i \rangle \langle I | \gamma^0 \vec{\tau} j_L(qr_2) Y_{LM}^*(\hat{\mathbf{r}}_2) | k \rangle\end{aligned}$$





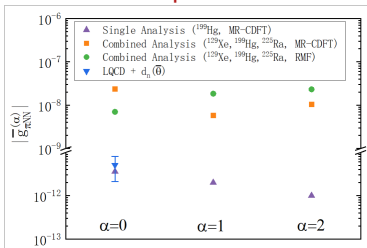


- The inclusion of parity and particle-number projection (PP+PNP) does not change significantly a_α for the three nuclei.
- The additional **angular-momentum projection (AMP)** modifies the values (a_0, a_1, a_2) of ^{129}Xe and ^{199}Hg by (25%, 21%, 21%) and (368%, 734%, 1228%), respectively.
- For the well-deformed ^{225}Ra , the effect of AMP is minor. However, the **shape-mixing effect** reduces the a_α by (71%, 58%, 55%), respectively.

Table: The final values for the nuclear structure factors a_α ($e \text{ fm}^3$) by the MR-CDFT calculation with the extrapolation of $N_{\text{sh}} \rightarrow \infty$.

Nuclei	a_0	a_1	a_2	$d[10^{-26} e \text{ fm}]$	$S[10^{-10} e \text{ fm}^3]$
^{129}Xe	-0.0052	+0.0134	-0.0097	< 0.14 <small>Sachdeva:2019PRL</small>	< 3.7
^{199}Hg	+0.0075	-0.0136	+0.0169	$< 7.4 \times 10^{-4}$ <small>Graner:2016PRL</small>	$< 3.5 \times 10^{-3}$
^{225}Ra	+0.15	-1.9	+1.3	$< 1.4 \times 10^3$ <small>Bishop:2016PRC</small>	$< 1.59 \times 10^3$

The ratios $a_\alpha(^{225}\text{Ra})/a_\alpha(^{199}\text{Hg})$ are 20, 140, and 77, respectively, significantly smaller than the previous estimation based on different nuclear models for different nuclei.



- The constraints are derived through a Monte Carlo analysis with 10^9 random samples at the 95% confidence level.
- Incorporating BMF correlations and intermediate-state contributions to the Schiff moments can change the constraints on $|\bar{g}_{\pi NN}^{(\alpha)}|$ by a factor of 2–4.

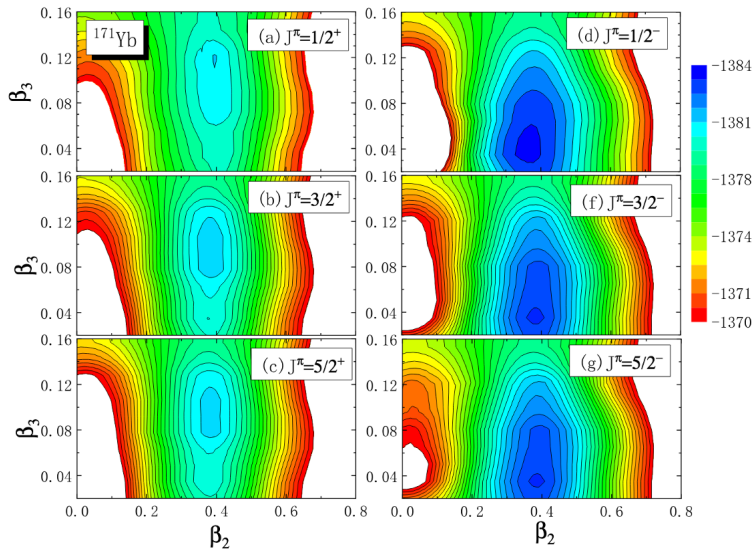
- **Nuclear Schiff Moments (NSMs):** Essential for interpreting experiments that search for CP- (or T-) violating EDMs in certain atoms and molecules.
- **Existing calculations of NSMs:** discrepancies among different nuclear models are significant, even with different signs.
- **This work:** We have presented the **first beyond relativistic mean-field study** of NSMs in ^{129}Xe , ^{199}Hg and ^{225}Ra using the MR-CDFT. **This study can in principle be applied to nuclear Schiff moments of any interesting odd-mass nuclei.**
- **Our findings:** A strong correlation between the contributions of nuclear intermediate states to the **Schiff moment and the $E1$ transition** from these states and the ground state, suggesting that measurements of these transitions can help **constrain nuclear model predictions of NSMs**. Beyond-mean-field effects, together with intermediate-state contributions, can either enhance or suppress the structure factors by **50% to 400%**, and modify the allowed ranges of the LECs of P,T-odd nuclear forces by a factor up to 4.

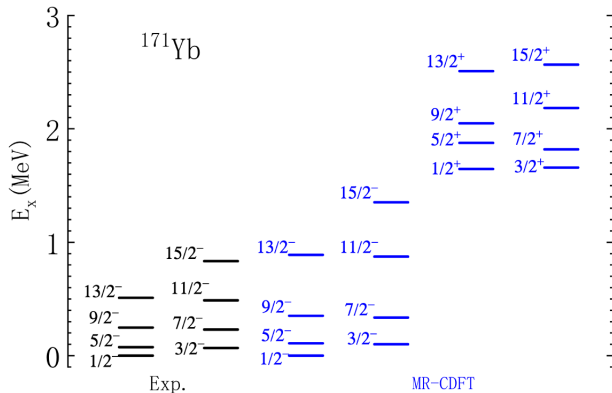
Collaborators

- **SYSU**: C.R. Ding, Q.Y. Luo, C.C. Wang, **E. F. Zhou**
- **MSU**: H. Hergert
- **UNC**: J. Engel
- **PKU**: J. Meng

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Thank you for your attention!





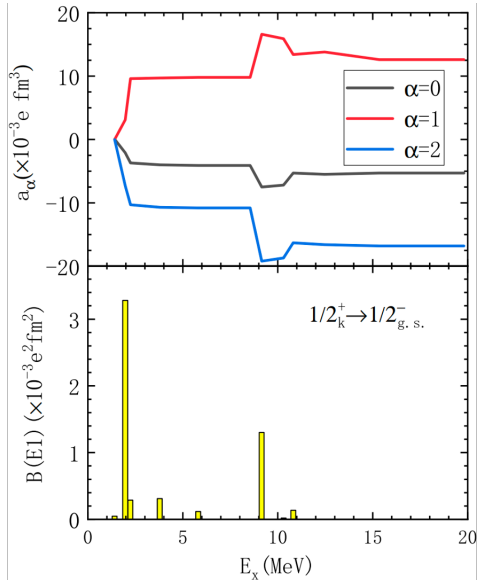
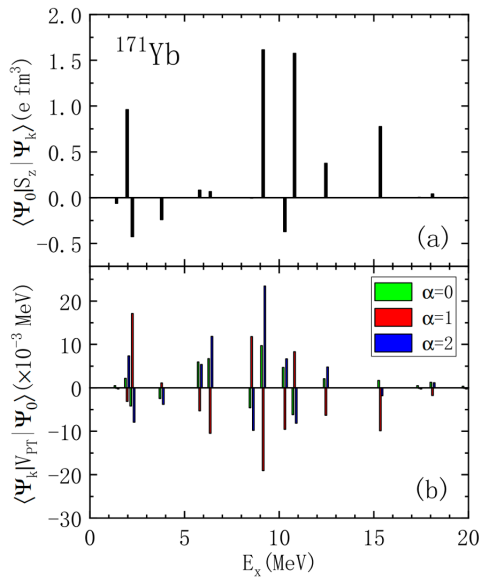
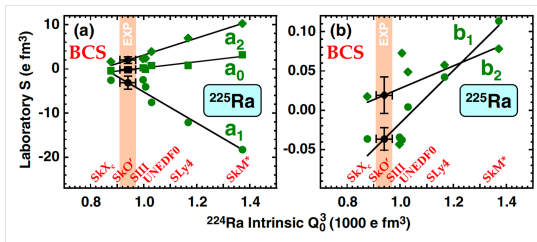


Table: The structure factors a_α (e fm^3) in the nuclear Schiff moments of ^{171}Yb from the CDFT calculation at various levels of approximation.

		$a_0(10^{-3})$	$a_1(10^{-3})$	$a_2(10^{-3})$
$^{171}\text{Yb}(\text{PC-PK1})$	RMF	-1.4	4.3	-9.2
	AMP+PP+PNP	-4.8	10.2	-25.1
	PGCM(1)	0.12	-0.38	-0.54
	PGCM(all)	-5.3	12.6	-16.8

- The **valence Dirac-Fock+RPA/CI+MBPT** calculations: V. A. Dzuba et al., PRA80, 032120 (2009)

$$d_A(^{171}\text{Yb}) = -2.1 \times 10^{-17} S(\text{e fm}^3)^{-1} (\text{e cm})$$



	a_0	a_1	a_2	b_1	b_2
^{221}Rn	$-0.04(10)$	$-1.7(3)$	$0.67(10)$	$-0.015(5)$	$-0.007(4)$
^{223}Rn	$-0.08(8)$	$-2.4(4)$	$0.86(10)$	$-0.031(9)$	$-0.008(8)$
^{223}Fr	$0.07(20)$	$-0.8(7)$	$0.05(40)$	$0.018(8)$	$-0.016(10)$
^{225}Ra	$0.2(6)$	$-5(3)$	$3.3(1.5)$	$-0.01(3)$	$0.03(2)$
^{229}Pa	$-1.2(3)$	$-0.9(9)$	$-0.3(5)$	$0.036(8)$	$0.032(18)$

- The nuclear Schiff moment

$$\begin{aligned}
 S &= \sum_{k \neq 0} \frac{\langle \Psi_0^{(N)} | \hat{S}_z | \Psi_k^{(N)} \rangle \langle \Psi_k^{(N)} | \hat{V}_{PT} | \Psi_0^{(N)} \rangle}{E_0^N - E_k^N} + c.c. \\
 &= a_0 g \bar{g}_0 + a_1 g \bar{g}_1 + a_2 g \bar{g}_2 + b_1 \bar{c}_1 + b_2 \bar{c}_2.
 \end{aligned}$$

- Single-state approximation

$$S \approx -2 \frac{\langle \Psi_0 | \hat{S}_0 | \bar{\Psi}_0 \rangle \langle \bar{\Psi}_0 | \hat{V}_{PT} | \Psi_0 \rangle}{\Delta E},$$

- Rigid rotor approximation

$$\begin{aligned}
 \langle \Psi_0 | \hat{S}_0 | \bar{\Psi}_0 \rangle_{\text{rigid}} &= \frac{J}{J+1} S_0, \\
 \langle \bar{\Psi}_0 | \hat{V}_{PT} | \Psi_0 \rangle_{\text{rigid}} &= \langle \hat{V}_{PT} \rangle,
 \end{aligned}$$

- Correlation Reduces Uncertainty:** The strong correlation between the calculated intrinsic Schiff moment in ^{225}Ra and the octupole moment in ^{224}Ra helps significantly reduce systematic uncertainties associated with nuclear EDFs.
- Sensitivity to Constraints:** Using different octupole moments to constrain model coefficients can result in notably different values, indicating sensitivity to the choice of experimental input. [J. Dobaczewski, J. Engel, M. Kortelainen, and P. Becker, PRL121, 232501 \(2018\)](#)

- Within the SM, the CP Violation from the topological θ term of QCD Lagrangian

$$\mathcal{L}_\theta = \frac{\bar{\theta} g_s^2}{32\pi^2} G_{\mu\nu}^a \tilde{G}^{\mu\nu a}$$

where $G_{\mu\nu}^a$ is the gluon field strength tensor, $\tilde{G}^{\mu\nu a} = \epsilon^{\mu\nu\alpha\beta} G_{\alpha\beta}^a / 2$ is its dual, and $\bar{\theta}$ is the CP-violating parameter QCD.

- This term introduces an asymmetry in the quark electric charge distribution inside the neutron, and thus induces a nonzero neutron EDM (d_n) through quark-gluon interactions, which would break time-reversal (T) symmetry.
- The strong CP problem arises because experimental constraints (from neutron EDM searches) suggest $\bar{\theta} < 10^{-10}$, which is unnaturally small, leading to the hypothesis of axions as a possible solution.

- The neutron EDM induced by the theta term of QCD is estimated as:

$$d_n = \frac{e}{m_p} \frac{g_{\pi NN} \bar{g}_{\pi NN}^{(0)}}{4\pi^2} \ln(m_\rho/m_\pi) \approx 10^{-16} \bar{\theta} \text{ e} \cdot \text{cm}$$

- The neutron EDM induced by the CKM C. Y. Seng, Phys. Rev. C 91, 025502 (2015)

$$d_n = (1 - 6) \times 10^{-32} \text{ e} \cdot \text{cm}$$

- Current experimental upper limit:

$$|d_n| < 1.8 \times 10^{-26} \text{ e} \cdot \text{cm} = 1.8 \times 10^{-13} \text{ e} \cdot \text{fm}$$

This means $\bar{\theta} \lesssim 10^{-10}$, unexpectedly small if CP violation were naturally large in QCD.

- The LEC $\bar{g}_{\pi NN}^{(0)}$ originated from the θ term

$$\bar{g}_{\pi NN}^{(0)} \simeq -0.027\theta$$