# Towards Precision Modeling of Nuclear Schiff Moments and Tests of Fundamental Symmetry

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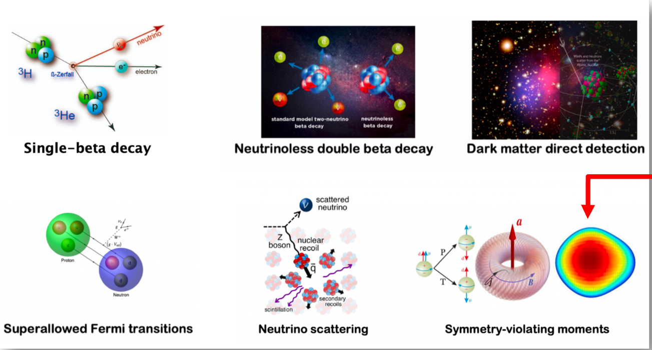
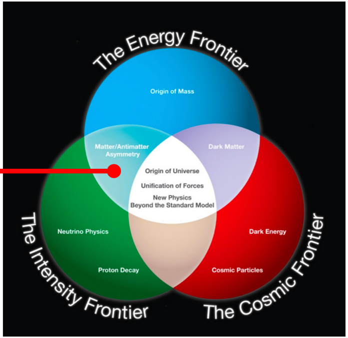
# Outline

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
3. Summary and outlook

# Probe new physics at nuclear energy scales

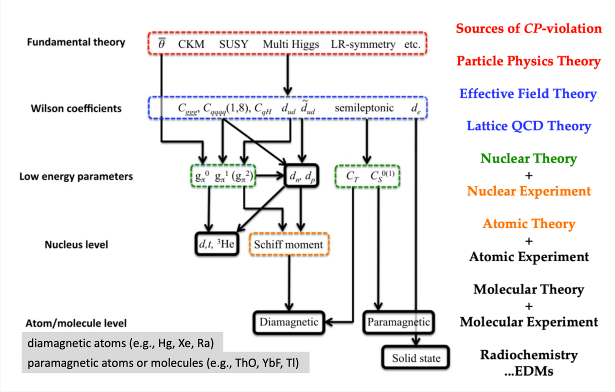





- Search for new physics (three frontiers): testing fundamental symmetries and interactions.
- Low-energy probes: requiring accurate nuclear matrix elements

- The sources of charge-parity violation (CPV) within the SM (the complex phase of the CKM matrix in weak interactions and the $\theta$ 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, Rev. Mod. Phys. 91, 015001 (2019)

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

# Search for atomic EDM: atoms in an external EM field

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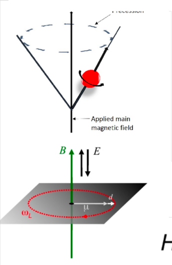
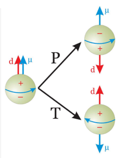
## An atom with nonzero spin and EDM

Larmor precession in external B and E fields

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



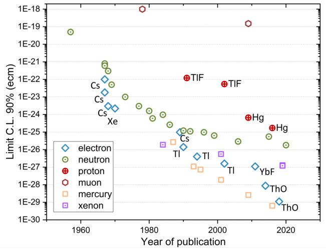

$$H_{EM} = -(\mu \cdot \mathbf{B} + \mathbf{d} \cdot \mathbf{E})$$

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 | $\lvert d_A \rvert [\times 10^{-26} e\text{cm}]$ | 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) |
| $^{225}$Ra | $< 1.4 \times 10^{3}$ | Bishof et al., PRC94, 025501 (2016) |




best

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

# Contributions to atomic EDMs



**Atomic EDMs**

**Electron EDMs**

- 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–odd electron–nucleon interaction**

- CP-violating **semileptonic interactions** between electrons and nucleons
- Include scalar–pseudoscalar ($k_{1,3}$), tensor–tensor ($k_2$) operators.

**nucleon EDMs**

- 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**.

**Nuclear Schiff moments**

- 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.

**Other nuclear moments**

- Magnetic quadrupole moments, etc.

# Atomic EDM arising from nuclear Schiff moment

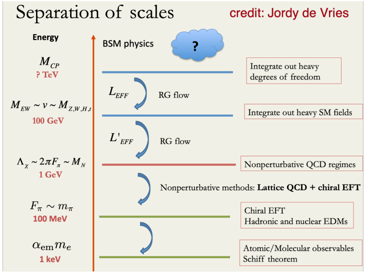
The atomic EDMs for the three popular atoms $^{129}$Xe, $^{199}$Hg, and $^{225}$Ra have been calculated with different atomic many-body theories, which differ from each other by less than 20%.

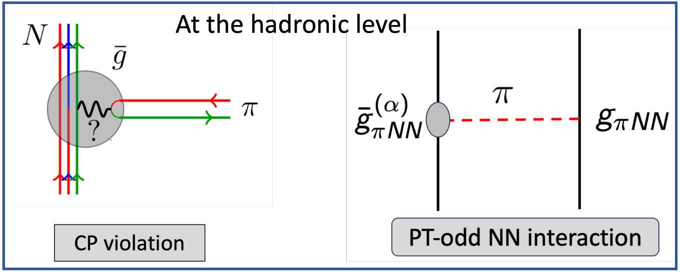
- The results of valence Dirac-Fock calculations: Dzuba:2002,Dzuba:2009

$$
\begin{aligned}
d_A(^{129}\mathrm{Xe}) &= +0.38 \times 10^{-17} S(e\ \mathrm{fm}^3)^{-1}(e\ \mathrm{cm}),\\
d_A(^{199}\mathrm{Hg}) &= -2.8 \times 10^{-17} S(e\ \mathrm{fm}^3)^{-1}(e\ \mathrm{cm}),\\
d_A(^{225}\mathrm{Ra}) &= -8.5 \times 10^{-17} S(e\ \mathrm{fm}^3)^{-1}(e\ \mathrm{cm}).
\end{aligned}
$$

- The results of relativistic coupled-cluster calculations: Latha:2009; Singh:2013; Singh:2015

$$
\begin{aligned}
d_A(^{129}\mathrm{Xe}) &= +0.34 \times 10^{-17} S(e\ \mathrm{fm}^3)^{-1}(e\ \mathrm{cm}),\\
d_A(^{199}\mathrm{Hg}) &= -2.46 \times 10^{-17} S(e\ \mathrm{fm}^3)^{-1}(e\ \mathrm{cm}),\\
d_A(^{225}\mathrm{Ra}) &= -6.79 \times 10^{-17} S(e\ \mathrm{fm}^3)^{-1}(e\ \mathrm{cm}).
\end{aligned}
$$




The standard $N\pi$ coupling vertex is

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

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

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

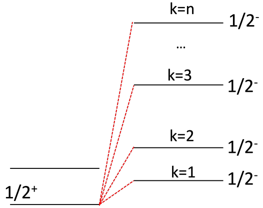
The Schiff moment can be written in terms of nuclear structure factors $a_\alpha$,

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

where (in units of $e$ fm$^3$)

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

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




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

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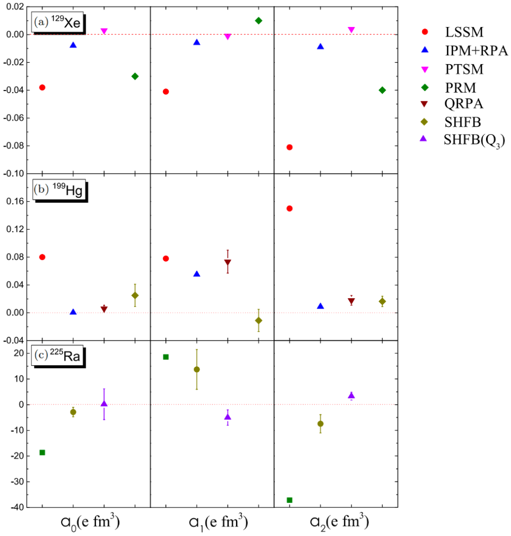
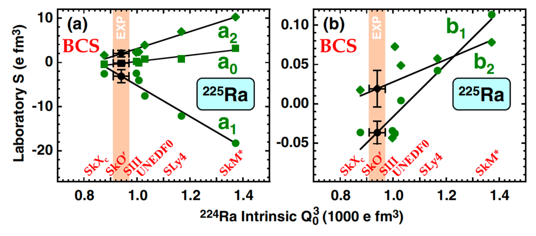



E.F. Zhou, JMY, IJMPE (2024)

Table 1. The coefficients $a_i$ ($e\,\mathrm{fm}^3$) 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] |

# A most recent study on nuclear Schiff moments




| | $a_0$ | $a_1$ | $a_2$ | $b_1$ | $b_2$ |
|---|---|---|---|---|---|
| $^{221}$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

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

- 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

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

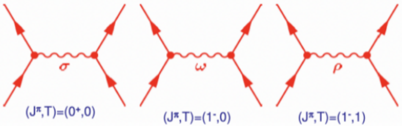
- **Correlation Reduces Uncertainty**: The strong correlation between the calculated intrinsic Schiff moment in 225Ra and the octupole moment in 224Ra helps significantly reduce systematic uncertainties associated with nuclear EDFs.
- **Sensitivity to Constraints**: Using different octupole moments to 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)

# The framework of MR-CDFT: relativistic EDF

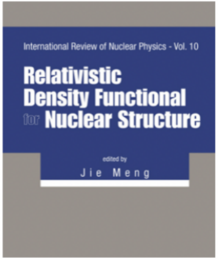


- The covariant density functional theory (CDFT)

★Meson-exchange models




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




★Point-coupling models

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


$G_\sigma(\rho)$ $\quad G_\omega(\rho)$ $\quad G_\rho(\rho)$

"No-sea" and "mean-field" approximations

Kohn-Sham DFT

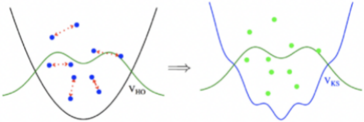
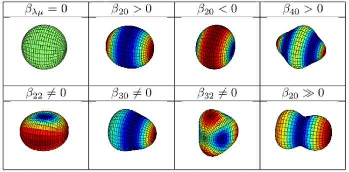



Figure from Drut PPNP 2010

- Symmetry-breaking and restoration methods



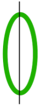

With the courtesy of B.N. Lu

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

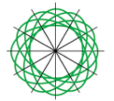
- Onset of different shapes
- Breaking of symmetries of Hamiltonian (rotation, parity, etc)
- Restoration of symmetry with projection operators

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

“Deformed ” mean-field

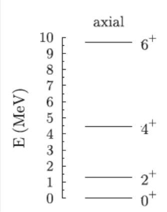


Rotated mean-field



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

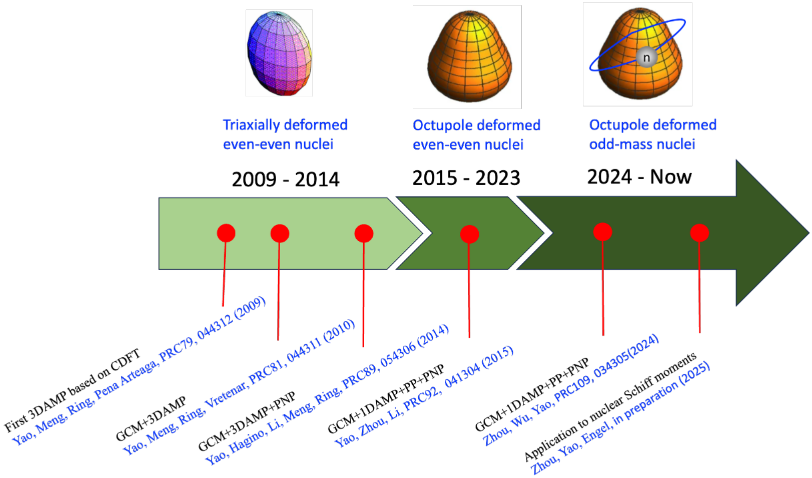
Nuclear low-lying states




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

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

Development of the MR-CDFT for nuclear structure and moments



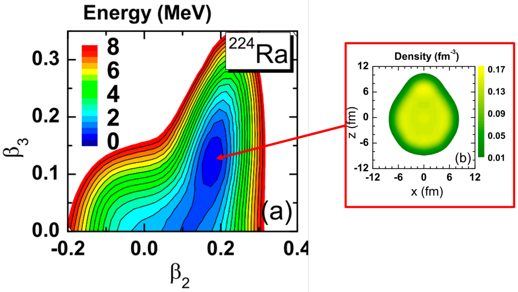
# For odd-mass nuclei with quadrupole-octupole correlations

- Wave function for nuclear low-lying states

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

Mean-field wave functions from constraint REDF (RMF+BCS) calculaitons

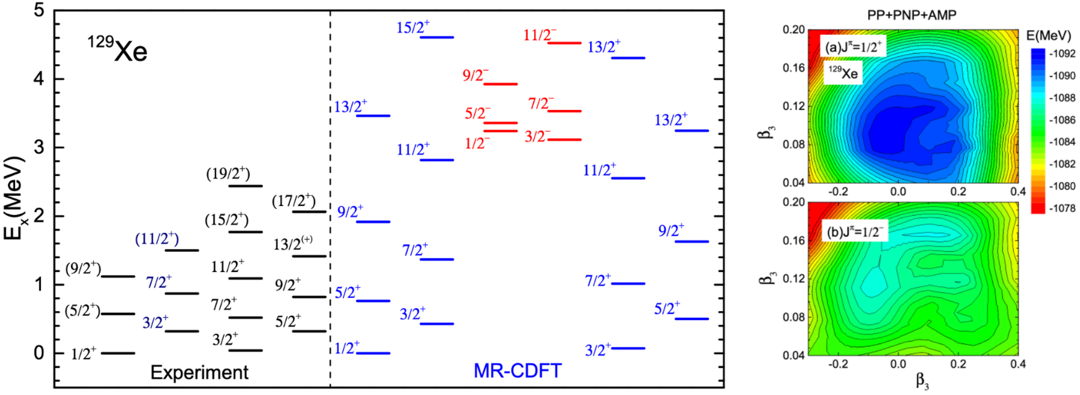
$$E[\Phi] = \langle\Phi(\mathbf{q})|\,\hat{H} - \sum_{\tau=n,p}\lambda_{\tau}\hat{N}_{\tau}\,|\Phi(\mathbf{q})\rangle$$
$$+\frac{1}{2}\sum_{\lambda=1,2,3} C_{\lambda}\left(\langle\Phi(\mathbf{q})|\,\hat{Q}_{\lambda 0}\,|\Phi(\mathbf{q})\rangle - q_{\lambda 0}\right)^{2}$$



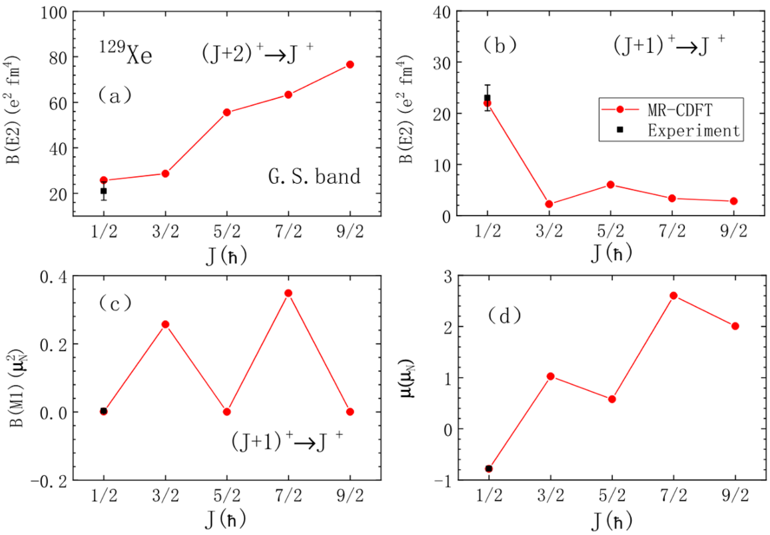

For odd-mass nuclei,

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

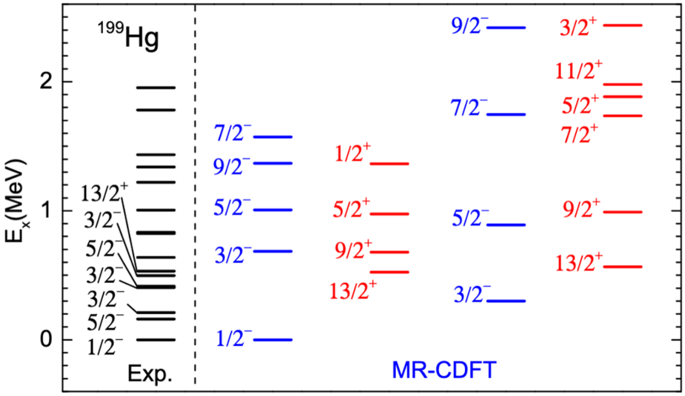
# Structural properties of $^{129}$Xe

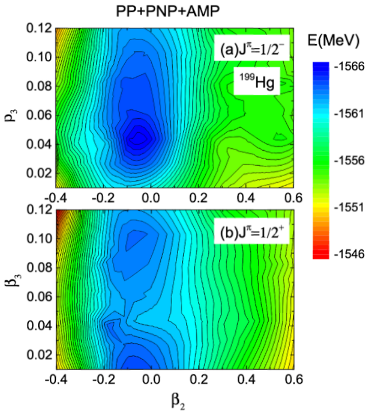



- The ground state $1/2^+_1$ is weakly octupole deformed.
- The excited excitation energy of the $1/2^-_1$ is predicted around 3.2 MeV.

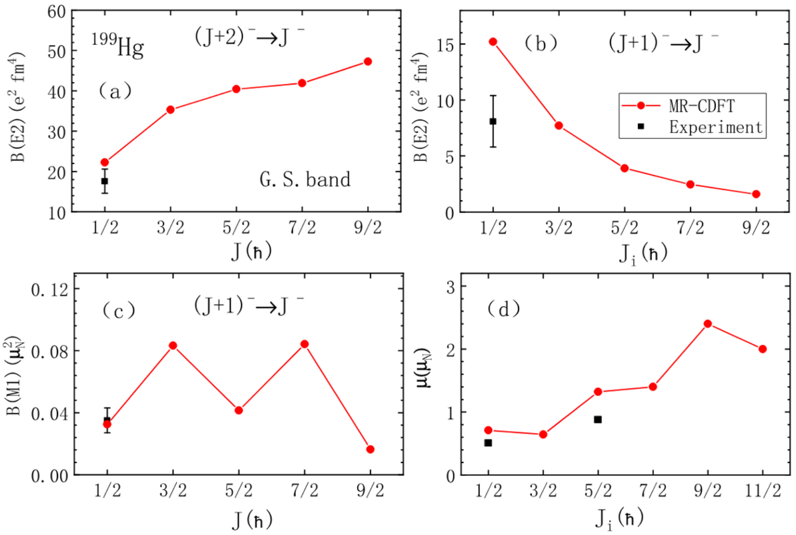


B(E2) (e² fm⁴)
100
80
60
40
20
¹²⁹Xe
(J+2)⁺→J⁺
(a)
G. S. band
1/2
3/2
5/2
7/2
9/2
J(ħ)
40
30
20
10
0
(b)
(J+1)⁺→J⁺
MR-CDFT
Experiment
B(M1) (μ²_N)
0.4
0.2
0.0
-0.2
(c)
(J+1)⁺→J⁺
μ(μ_N)
3
2
1
0
-1
(d)




- The ground state $1/2_1^-$ is weakly octupole deformed.
- The first excited state $1/2^+$ is predicted around 1.4 MeV.



$^{199}$Hg
$(J+2)^- \rightarrow J^-$
(a)
G. S. band
B(E2) ($e^2$ fm$^4$)
J (ħ)
(b)
$(J+1)^- \rightarrow J^-$
MR-CDFT
Experiment
B(E2) ($e^2$ fm$^4$)
$J_i$ (ħ)
(c)
$(J+1)^- \rightarrow J^-$
B(M1) ($\mu_N^2$)
J (ħ)
(d)
$\mu(\mu_N)$
$J_i$ (ħ)

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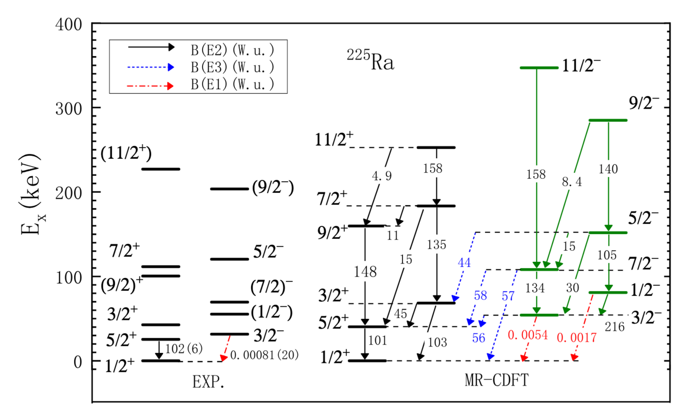
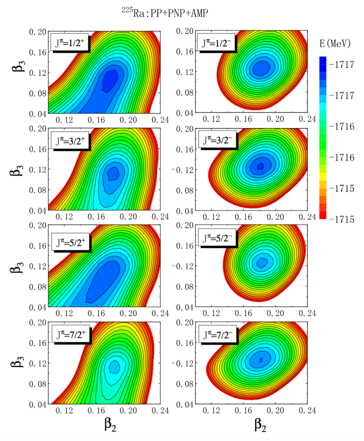
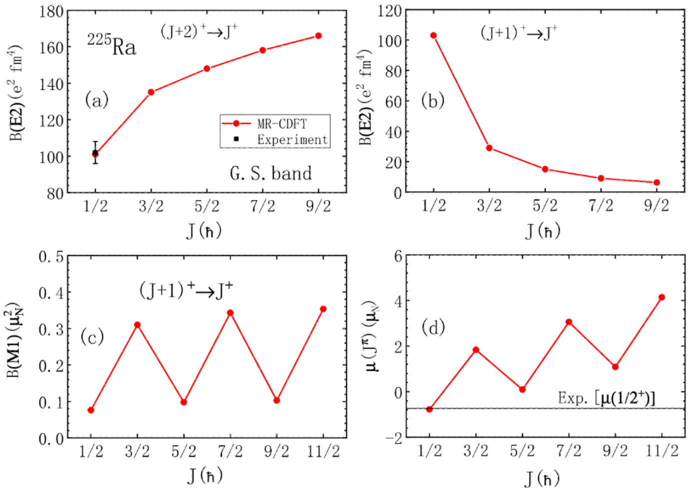



- The ground state $1/2_1^+$ is strongly octupole deformed.
- The first $1/2^-$ state is predicted around 0.080 MeV, compared to data 0.055 MeV.



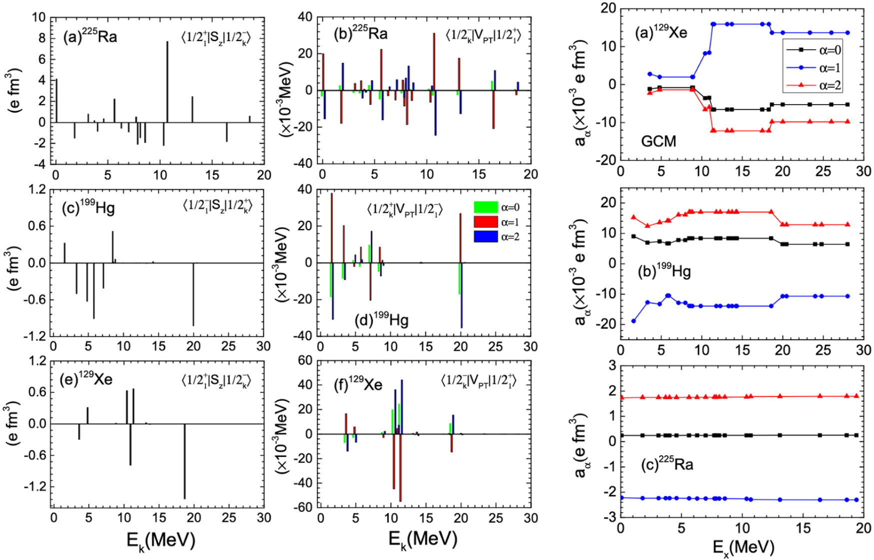
225Ra
(J+2)+→J+
(a)
MR-CDFT
Experiment
G. S. band
B(E2) (e2 fm4)
J (ħ)
(J+1)+→J+
(b)
B(E2) (e2 fm4)
J (ħ)
(J+1)+→J+
(c)
B(M1) (μN2)
J (ħ)
(d)
Exp. [μ(1/2+)]
μ(Jπ) (μN)
J (ħ)

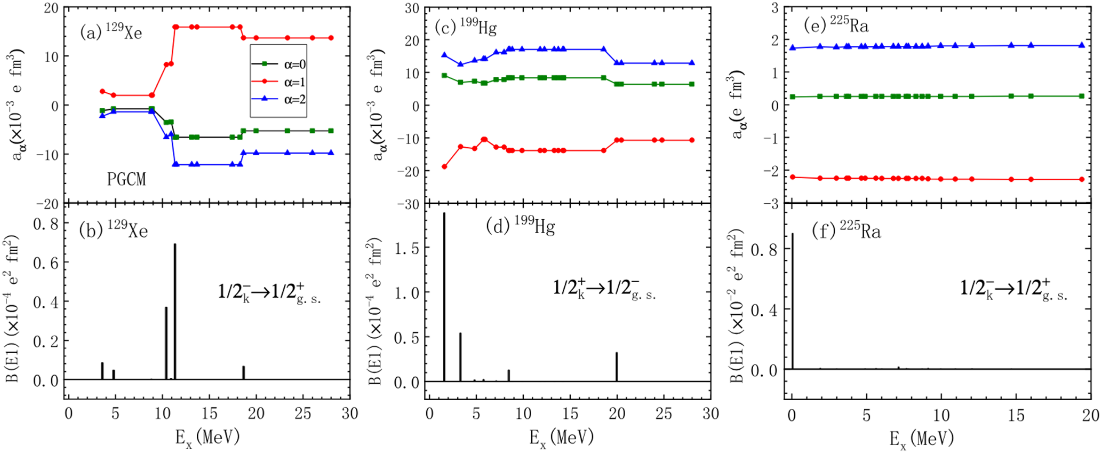
The two-body matrix element of the PT-violating $NN$ interaction in the relativistic framework,

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

where

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

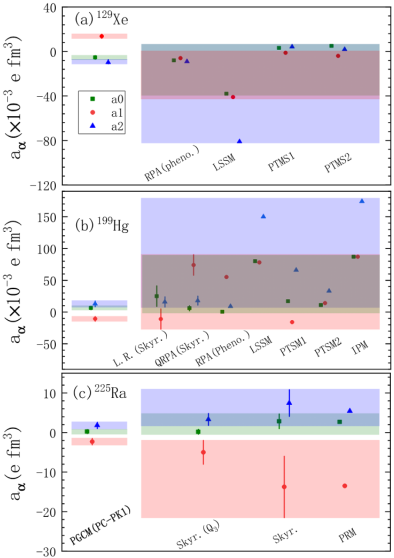

(a)$^{225}$Ra
⟨1/2$_1^+$|S$_z$|1/2$_k^-$⟩
(e fm$^3$)
(b)$^{225}$Ra
⟨1/2$_k^-$|V$_{PT}$|1/2$_1^+$⟩
(×10$^{-3}$MeV)
(c)$^{199}$Hg
⟨1/2$_1^-$|S$_z$|1/2$_k^+$⟩
(d)$^{199}$Hg
⟨1/2$_k^+$|V$_{PT}$|1/2$_1^-$⟩
α=0
α=1
α=2
(e)$^{129}$Xe
⟨1/2$_1^+$|S$_z$|1/2$_k^-$⟩
(f)$^{129}$Xe
⟨1/2$_k^-$|V$_{PT}$|1/2$_1^+$⟩
E$_k$(MeV)
(a)$^{129}$Xe
GCM
a$_α$(×10$^{-3}$ e fm$^3$)
(b)$^{199}$Hg
(c)$^{225}$Ra
a$_α$(e fm$^3$)
E$_x$(MeV)


(a) $^{129}$Xe
PGCM
$\alpha$=0
$\alpha$=1
$\alpha$=2
$a_\alpha(\times10^{-3}$ e fm$^3)$
(b) $^{129}$Xe
$1/2^-_k \to 1/2^+_{g.s.}$
B(E1) ($\times10^{-4}$ e$^2$ fm$^2$)
(c) $^{199}$Hg
$a_\alpha(\times10^{-3}$ e fm$^3)$
(d) $^{199}$Hg
$1/2^+_k \to 1/2^-_{g.s.}$
B(E1) ($\times10^{-4}$ e$^2$ fm$^2$)
(e) $^{225}$Ra
$a_\alpha$(e fm$^3$)
(f) $^{225}$Ra
$1/2^-_k \to 1/2^+_{g.s.}$
B(E1) ($\times10^{-2}$ e$^2$ fm$^2$)
$E_x$ (MeV)

# Comparison with other models

TABLE I. The structure factors $a_i$ (e fm$^3$) in the nuclear Schiff moments of $^{129}$Xe, $^{199}$Hg, and $^{255}$Ra from the CDFT calculation with the PC-PK1 parameter set at various levels of approximation.

| | | $a_0(10^{-3})$ | $a_1(10^{-3})$ | $a_2(10^{-3})$ |
|---|---|---|---|---|
| $^{129}$Xe | MF | −3.0 | 8.3 | −6.7 |
| | PP+PNP | −3.4 | 8.5 | −6.8 |
| | AMP+PP+PNP | −2.4 | 6.7 | −5.4 |
| | PGCM(1) | −1.2 | 2.8 | −2.3 |
| | PGCM(all) | −5.3 | 13.7 | −9.8 |
| $^{199}$Hg | MF | 5.5 | −5.1 | 2.4 |
| | PP+PNP | 5.8 | −5.4 | 2.6 |
| | AMP+PP+PNP | 26.7 | −44.2 | 33.2 |
| | PGCM(1) | 10.0 | −19.1 | 15.2 |
| | PGCM(all) | 6.4 | −10.7 | 12.9 |
| | | $a_0$ | $a_1$ | $a_2$ |
| $^{225}$Ra | MF | 0.86 | −5.1 | 3.4 |
| | PP+PNP | 0.88 | −5.4 | 3.6 |
| | AMP+PP+PNP | 0.80 | −5.2 | 3.8 |
| | PGCM(1) | 0.24 | −2.2 | 1.7 |
| | PGCM(all) | 0.25 | −2.3 | 1.8 |



- **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 carried out a MR-CDFT study—the first to employ the projected generator coordinate method (PGCM)—to investigate NSMs in several key nuclei ($^{129}$Xe, $^{199}$Hg, $^{225}$Ra).
- Our results reveal substantial contributions from high-lying intermediate states and shape-mixing effects to NSMs.
- The measurements of $E1$ transitions between ground state and intermediate states at HIAF are helpful to constrrain NSMs.

## Outlook

- Towards ab initio modeling of the NSMs starting from chiral nuclear Hamiltonians.

**Collaborators**

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- UNC: J. Engel

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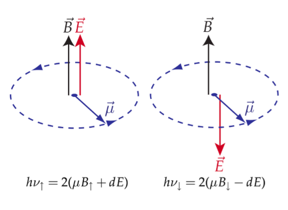
# Thank you for your attention!

In reality, the shielding with the presence of external EM is not complete because of the following effects: Liu et al., PRC 76, 035503 (2007)

- The atomic nucleus has a finite size (true, electron penetration effect).
- The atomic electrons are relativistic (espectialy true for heavy atoms).
- There exist nonelectrostatic interactions between the constituents (The $e$-$e$ and $e$-$N$ electromagnetic interactions contain current-current components).

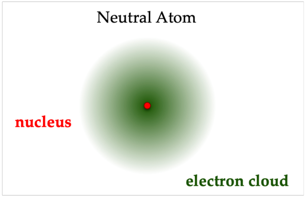
Atoms acquire nonzero EDMs $d_A$ from nuclei. If $d_A \neq 0$, its interaction with the external electric field $E_{\rm lab}$ would lead to a shift in the Larmor precession frequency that depends linearly on $E_{\rm lab}$.

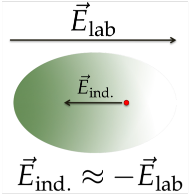


Schiff pointed out that L. I. Schiff, Phys. Rev. 132, 2194 (1963)

- In an atom consisting of a point-like nucleus and nonrelativistic electrons that interact only electrostatically, the effect of any nonzero (electronic, nuclear) electric dipole moment (EDM) is completely screened by the atomic electrons, irrespective of the external potential $E_{\rm lab}$.

$$\boxed{\langle \mathbf{d}_N \cdot (\mathbf{E}_{\rm lab} + \mathbf{E}_{\rm ind.}) \rangle = 0}$$



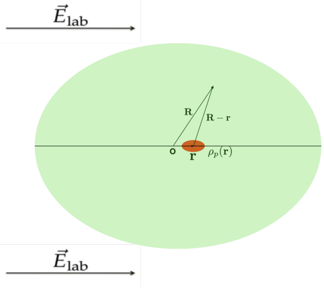

In reality, the shielding is not complete because of the finite size of atomic nucleus and other effects. Thus, atoms can acquire nonzero EDMs $d_A$ from nuclei.

## How the atomic EDM $d_A$ arises from atomic nuclei?

- The electrostatic potential arisen from a nucleus in the external electric field is given by, O. P. Sushkov et al., Zh. Eksp. Teor. Fiz. 87, 1521 (1984); N. Auerbach et al., PRL76, 4316 (1996)

$$\varphi(R) = \int \frac{e\rho(\mathbf{r})}{|\mathbf{R}-\mathbf{r}|} d^3 r + \frac{1}{Z}(\mathbf{d}_N \cdot \nabla_R) \int \frac{\rho(\mathbf{r})}{|\mathbf{R}-\mathbf{r}|} d^3 r = -4\pi \mathbf{S} \cdot \nabla_R \delta^3(R) + \cdots$$

The second term is for the screening effect.




$$\begin{aligned} \mathbf{d}_N &= \int d^3 r \mathbf{r} \rho(\mathbf{r}), \quad Z = \int d^3 r \rho(\mathbf{r}), \\ \mathbf{S} &= \frac{1}{10}\left[\int e\rho(\mathbf{r})\ r^2\ \mathbf{r}\ d^3 r - \frac{5}{3Z}\mathbf{d} \int \rho(\mathbf{r})\ r^2\ d^3 r\right] \end{aligned}$$

where $\mathbf{d}_N$ is the **nuclear EDM**, and $Z$ is the proton number, $\rho(\mathbf{r})$ is the **proton density**, $\mathbf{S}$ the **Schiff moment**.

# Atomic EDM and nuclear Schiff moment

The CP-violating electrostatic interaction $\hat{H}_{CP}^{(eN)}$ between electrons and nuclear Schiff moment $\mathbf{S}$ in the atom is given by

$$\hat{H}_{CP}^{(eN)} = -4\pi e \sum_i \hat{\mathbf{S}} \cdot \boldsymbol{\nabla} \delta^3(R_i)$$

where $i$ runs over all electrons. The above term mixes atomic states of opposite parity and induces a nonzero EDM $d_A$ in the atomic ground state

$$d_A \equiv \left\langle \bar{\Psi}_0^{(at)} \right| \hat{D}_z \left| \bar{\Psi}_0^{(at)} \right\rangle \simeq \sum_{m\neq 0} \frac{\left\langle \Phi_0^{(at)} \right| \hat{H}_{CP}^{(eN)} \left| \Phi_m^{(at)} \right\rangle \left\langle \Phi_m^{(at)} \right| \hat{D}_z \left| \Phi_0^{(at)} \right\rangle}{\mathcal{E}_0^A - \mathcal{E}_m^A} + c.c.,$$

- $\bar{\Psi}_0^{(at)}$: wave function of atomic state with parity mixing.
- $\Phi_m^{(at)}$: parity-conserving wave functions of atomic states.
- $\mathcal{E}_m^A$: energies of atomic ststes, and $\hat{D}_z$ is the electric dipole operator.

In the adiabatic Born–Oppenheimer (ABO) approximation,

$$\begin{aligned}\left\langle \Phi_0^{(at)} \right| \hat{H}_{CP}^{(eN)} \left| \Phi_m^{(at)} \right\rangle &= -4\pi \sum_i \left\langle \Phi_0^{(at)} \right| e\hat{\mathbf{S}} \cdot \boldsymbol{\nabla}\delta^3(R_i) \left| \Phi_m^{(at)} \right\rangle \\ &\simeq -4\pi \sum_i \left\langle \bar{\Psi}_0^{(N)} \right| \hat{\mathbf{S}} \left| \bar{\Psi}_0^{(N)} \right\rangle \cdot \left\langle \Phi_0^{(e)} \right| e\boldsymbol{\nabla}\delta^3(R_i) \left| \Phi_m^{(e)} \right\rangle .\end{aligned}$$

where $\left|\Psi_0^{(N)}\right\rangle$ is the wave function of nuclear ground state, $\left|\Phi_m^{(e)}\right\rangle$ is the wave function of electrons in the $m$-th state. Thus, the atomic EDM can be written as

$$d_A \equiv \left\langle \Psi_0^{(at)} \right| \hat{D}_z \left| \Psi_0^{(at)} \right\rangle \simeq \mathbf{S} \cdot \mathbf{d}^{(e)},$$

where $e\nabla\delta^3(R_i)$ term is the gradient of the electron density,

$$\mathbf{d}^{(e)} \equiv -8\pi \sum_{m\neq 0} \frac{\left\langle \Phi_0^{(e)} \right| \sum_i e\nabla\delta^3(R_i) \left| \Phi_m^{(e)} \right\rangle \left\langle \Phi_m^{(e)} \right| \hat{D}_z \left| \Phi_0^{(e)} \right\rangle}{\mathcal{E}_0^A - \mathcal{E}_m^A},$$

# Atomic EDM and nuclear Schiff moment

The rotational symmetry only allows for the $z$-component of $S$, which is nonzero if there is PT-odd $NN$ interaction, and computed usually in the perturbation theory,

$$\begin{aligned} S &\equiv \left\langle \bar{\Psi}_0^{(N)} \right| \hat{S}_z \left| \bar{\Psi}_0^{(N)} \right\rangle \simeq \left\langle \Psi_0^{(N)} \right| \hat{S}_z \left| \delta\Psi_0^{(N)} \right\rangle + c.c. \\ &= \sum_{k\neq 0} \frac{\langle \Psi_0^{(N)} | \hat{S}_z | \Psi_k^{(N)} \rangle \langle \Psi_k^{(N)} | \hat{V}_{PT} | \Psi_0^{(N)} \rangle}{E_0^N - E_k^N} + c.c. \equiv 2 \sum_{k\neq 0} \frac{M_S^{0k} M_{PT}^{k0}}{E_0^N - E_k^N}. \end{aligned}$$

- $\bar{\Psi}_0^{(N)}$: parity-broken wave function of nuclear ground state.
- $\Psi_k^{(N)}$: parity-conserving wave functions of nuclear states.
- $\hat{V}_{PT}$: PT-odd two-body $NN$ interaction

$$\hat{V}_{PT} = \sum_{j<l, i<k} \langle jl | V_{PT} | ik \rangle a_j^\dagger a_l^\dagger a_k a_i .$$

# The theta term of QCD

- Within the SM, the CP Violation from the topological $\theta$ term of QCD Lagrangian

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

where $G^a_{\mu\nu}$ is the gluon field strength tensor, $\tilde{G}^{\mu\nu a} = \epsilon^{\mu\nu\alpha\beta} G^a_{\alpha\beta}/2$ 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 ime-reversal (T) symmetry.
- The strong CP problema rises 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 and strong CP problem

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

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

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

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

- Current experimental upper limit:

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

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

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

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