

Nuclear Schiff moment of Ac-227 calculated within the nuclear DFT framework

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EDMs2026: WE-Heraeus Workshop
École de Physique des Houches, France, March 2, 2026



Outline

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- ★ Schiff Theorem and Nuclear Schiff Moment

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- ★ Nuclear Laboratory Schiff Moment

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- ★ Nuclear Laboratory Schiff Moment
- ★ Nuclear Density Functional Theory

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- ★ Nuclear Laboratory Schiff Moment of ^{227}Ac

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- ★ Nuclear Laboratory Schiff Moment of ^{227}Ac
- ★ Summary and Outlook

EDM and Fundamental Symmetries

The non-zero expectation value of the operator

$$\hat{\mathbf{d}} = \sum_a e_a \mathbf{R}_a, \quad a = 1, \dots, Z$$

in a stationary state of an atom with a certain value \hat{J} of angular momentum requires simultaneous $\hat{\mathcal{P}}$ - and $\hat{\mathcal{T}}$ - violation.

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- ★ An atom can acquire an EDM from the nucleus.
- ★ A nucleus acquires an EDM from either nucleon EDM or $\hat{\mathcal{P}}, \hat{\mathcal{T}}$ -violating interaction between nucleons and pions.

Schiff Theorem

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Schiff Theorem

(Schiff theorem) In a homogeneous external electric field \mathbf{E}_0 , the nuclear EDM induces the rearrangement of electrons in such a way that they generate an electric field at the nucleus that opposes \mathbf{E}_0 .

L. I. Schiff, Phys. Rev. **132**, 2194 (1963)

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Electrostatic potential of a nucleus:

$$\varphi(\mathbf{R}) = \int \frac{e\rho(\mathbf{r})}{|\mathbf{R} - \mathbf{r}|} d^3r + \frac{1}{Z} (\mathbf{d} \cdot \nabla_{\mathbf{R}}) \int \frac{\rho(\mathbf{r})}{|\mathbf{R} - \mathbf{r}|} d^3r$$

$$\int d^3r \rho(\mathbf{r}) = Z; \quad \mathbf{d} = \int e\mathbf{r}\rho(\mathbf{r}) d^3r; \quad \mathbf{R} = \text{electron coordinate}$$

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Taylor expansion:
$$\frac{1}{|\mathbf{R} - \mathbf{r}|} = \frac{1}{R} - \mathbf{r} \cdot \nabla_R \frac{1}{R} + \frac{1}{2} (\mathbf{r} \cdot \nabla_R)^2 \frac{1}{R} - \dots$$

Nuclear Schiff Moment

Nuclear Schiff Moment

$$\begin{aligned}
 \varphi(\mathbf{R}) &= \int d^3r e\rho(\mathbf{r}) \left\{ \frac{1}{R} - (\mathbf{r} \cdot \nabla_R) \frac{1}{R} + \frac{1}{2} (\mathbf{r} \cdot \nabla_R)^2 \frac{1}{R} - \dots \right\} \\
 &+ \frac{1}{Z} (\mathbf{d} \cdot \nabla_R) \int d^3r \rho(\mathbf{r}) \left\{ \frac{1}{R} - (\mathbf{r} \cdot \nabla_R) \frac{1}{R} + \frac{1}{2} (\mathbf{r} \cdot \nabla_R)^2 \frac{1}{R} - \dots \right\} \\
 &= \frac{eZ}{R} - (\mathbf{d} \cdot \nabla_R) \frac{1}{R} + \frac{1}{2} \int d^3r e\rho(\mathbf{r}) (\mathbf{r} \cdot \nabla_R)^2 \frac{1}{R} - \frac{1}{6} \int d^3r e\rho(\mathbf{r}) (\mathbf{r} \cdot \nabla_R)^3 \frac{1}{R} + \dots \\
 &+ \frac{1}{Z} (\mathbf{d} \cdot \nabla_R) \frac{Z}{R} - \frac{1}{Z} (\mathbf{d} \cdot \nabla_R) \int d^3r \rho(\mathbf{r}) (\mathbf{r} \cdot \nabla_R) \frac{1}{R} + \frac{1}{Z} (\mathbf{d} \cdot \nabla_R) \int d^3r \frac{1}{2} \rho(\mathbf{r}) (\mathbf{r} \cdot \nabla_R)^2 \frac{1}{R} \\
 &- \dots \\
 &= \frac{eZ}{R} + \frac{1}{6} \Theta_{\alpha\beta} \nabla_{R;\alpha} \nabla_{R;\beta} \frac{1}{R} - Ze \frac{4\pi}{6} r_{\text{ch}}^2 \delta(\mathbf{R}) - \frac{1}{Ze} (\mathbf{d} \cdot \nabla_R)^2 \frac{1}{R} + \varphi^{(3)}(\mathbf{R}) \dots
 \end{aligned}$$

Nuclear Schiff Moment

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V. Spevak *et al.*,
PRC **56**, 1357
(1997)

Nuclear Schiff Moment

$$\Theta_{\alpha\beta} = \int d^3r e\rho(\mathbf{r}) \cdot 3T_{\alpha\beta}^{(2)} \quad (\text{Traceless quadrupole tensor})$$

$$T_{\alpha\beta}^{(2)} = r_{\alpha}r_{\beta} - \frac{1}{3}r^2\delta_{\alpha\beta}$$

$$\overline{r_{\text{ch}}^2} = \frac{1}{Z} \int d^3r \rho(\mathbf{r})r^2 \quad (\text{Mean-square charge radius})$$

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$$\begin{aligned} \varphi^{(3)}(\mathbf{R}) &= -\frac{1}{6} \int d^3r e\rho(\mathbf{r}) r_\alpha r_\beta r_\gamma \nabla_{R;\alpha} \nabla_{R;\beta} \nabla_{R;\gamma} \frac{1}{R} \\ &+ \frac{1}{2Z} (\mathbf{d} \cdot \nabla_R) \nabla_{R;\alpha} \nabla_{R;\beta} \frac{1}{R} \int d^3r \rho(\mathbf{r}) r_\alpha r_\beta \\ &= \varphi_{\text{octupole}}^{(3)}(\mathbf{R}) + \varphi_{\text{Schiff}}^{(3)}(\mathbf{R}) + \frac{1}{6Ze} (\mathbf{d} \cdot \nabla_R) \Theta_{\alpha\beta} \nabla_{R;\alpha} \nabla_{R;\beta} \frac{1}{R} \end{aligned}$$

Nuclear Schiff Moment

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$$\varphi_{\text{octupole}}^{(3)}(\mathbf{R}) = -\frac{1}{6} Q_{\alpha\beta\gamma} \nabla_{R;\alpha} \nabla_{R;\beta} \nabla_{R;\gamma} \frac{1}{R}; \quad Q_{\alpha\beta\gamma} = \int d^3r e\rho(\mathbf{r}) T_{\alpha\beta\gamma}^{(3)}$$
$$T_{\alpha\beta\gamma}^{(3)} = r_{\alpha} r_{\beta} r_{\gamma} - \frac{1}{5} r^2 (r_{\alpha} \delta_{\beta\gamma} + r_{\beta} \delta_{\alpha\gamma} + r_{\gamma} \delta_{\alpha\beta})$$

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Nuclear Schiff moment:

$$\mathbf{S} = \frac{1}{10} \left(\int d^3r e\rho(\mathbf{r}) r^2 \mathbf{r} - \frac{5}{3} \mathbf{d} \frac{1}{Z} \int d^3r \rho(\mathbf{r}) r^2 \right)$$

Nuclear Laboratory Schiff Moment

C. Maples, Nuclear
Data Sheets **22**, 275,
277-323 (1977)

Nuclear Laboratory Schiff Moment

$$S_{\text{lab}} \approx \sum_{i \neq 0} \frac{\langle \Psi_0 | \hat{S}_0 | \Psi_i \rangle \langle \Psi_i | \hat{V}_{\text{PT}} | \Psi_0 \rangle}{E_0 - E_i} + \text{c.c.}$$

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$$\hat{S}_0 = \frac{e}{10} \sqrt{\frac{4\pi}{3}} \sum_p \left(r_p^3 - \frac{5}{3} r_{\text{ch}}^2 r_p \right) Y_0^1(\Omega_p) \quad (\text{Schiff operator})$$

\hat{V}_{PT} = P,T-violating NN interaction

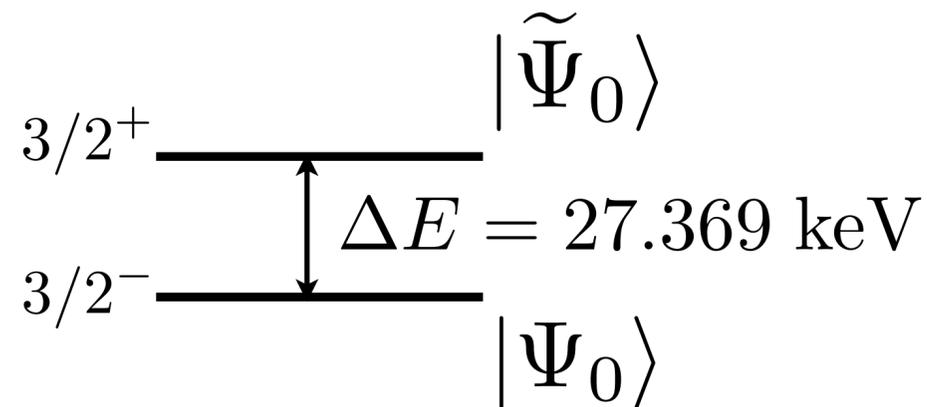
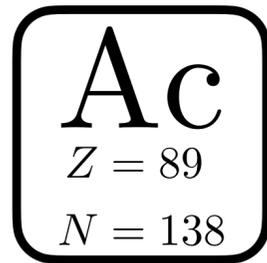
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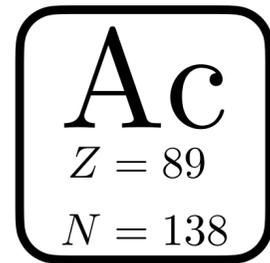
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$3/2^+ \quad |\tilde{\Psi}_0\rangle$
 $\Delta E = 27.369 \text{ keV}$
 $3/2^- \quad |\Psi_0\rangle$

$$\longrightarrow S_{\text{lab}} \approx -2\text{Re} \left\{ \frac{\langle \Psi_0 | \hat{S}_0 | \tilde{\Psi}_0 \rangle \langle \tilde{\Psi}_0 | \hat{V}_{\text{PT}} | \Psi_0 \rangle}{\Delta E} \right\}$$

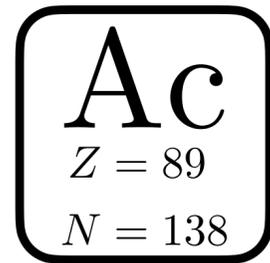
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$$\hat{Q}_0^3 = e \sum_p r_p^3 Y_0^3(\Omega_p) \quad (\text{Octupole operator})$$

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Rigid Deformation Approximation

J. Dobaczewski *et al.*, PRL **121**, 232501 (2018) and
the supplemental material

Rigid Deformation Approximation

Reduced matrix elements:

J. Dobaczewski *et al.*, PRL **121**, 232501 (2018) and
the supplemental material

$$\langle \Psi^{J_1, +} || \hat{X}^\lambda || \Psi^{J_2, -} \rangle_{\text{rigid}} = \sqrt{2J_2 + 1} \langle J_2 K \lambda 0 | J_1 K \rangle \langle \Phi_1 | \hat{X}_0^\lambda | \Phi_2 \rangle$$

intrinsic expectation value

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intrinsic expectation value

Laboratory matrix elements:

$$\begin{aligned} \langle \Psi_{M_1}^{J_1,+} | \hat{X}_\mu^\lambda | \Psi_{M_2}^{J_2,-} \rangle_{\text{rigid}} &= \frac{1}{\sqrt{2J_1 + 1}} \langle J_2 M_2 \lambda \mu | J_1 M_1 \rangle \\ &\times \langle \Psi^{J_1,+} || \hat{X}^\lambda || \Psi^{J_2,-} \rangle_{\text{rigid}} \end{aligned}$$

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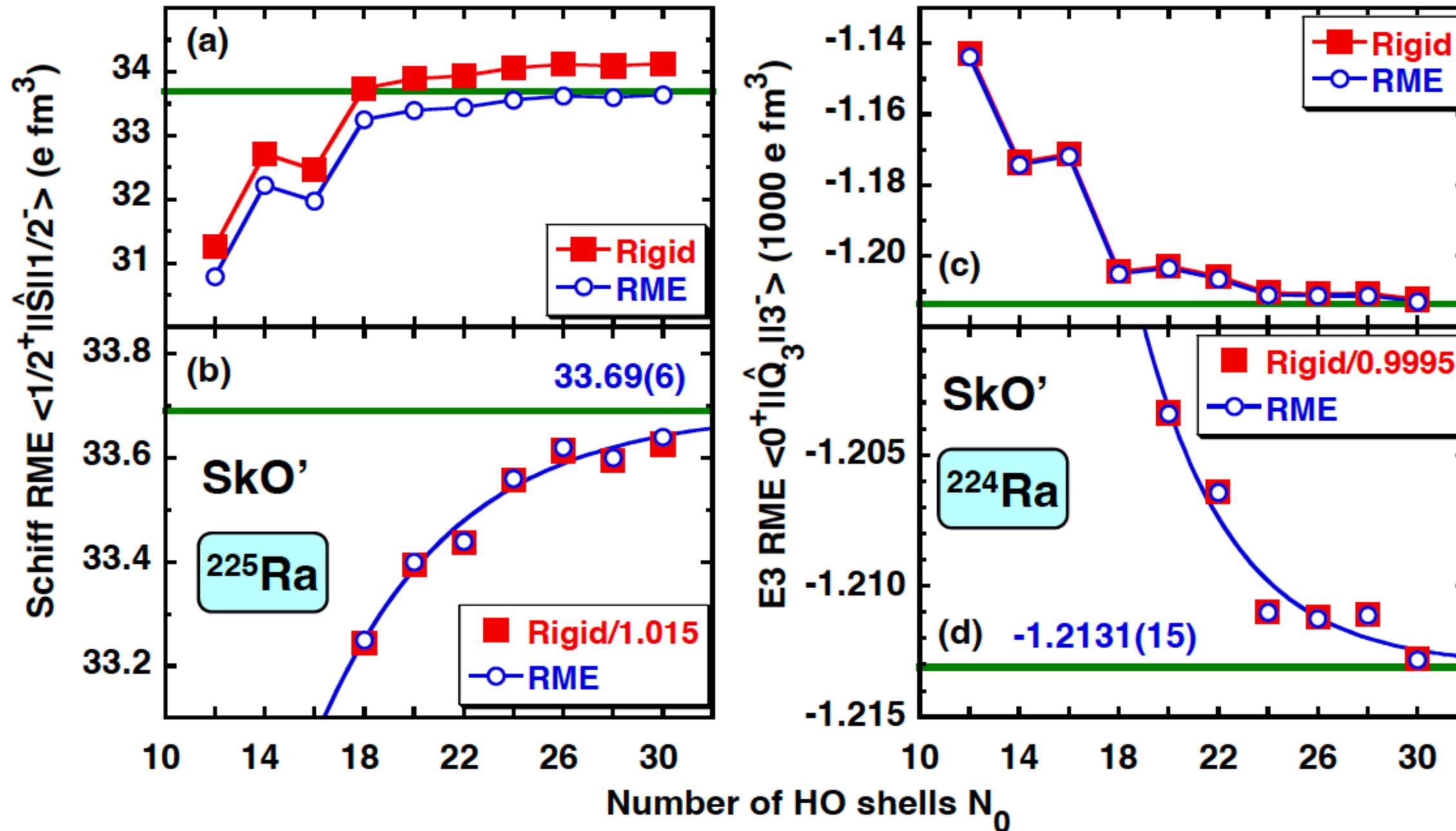
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$$J_1 = J_2 = M_1 = M_2 = K$$

$$\langle JK10 | JK \rangle = \frac{K}{\sqrt{J(J+1)}} \quad \longrightarrow \quad \langle \Psi_0 | \hat{S}_0 | \tilde{\Psi}_0 \rangle_{\text{rigid}} = \frac{J}{J+1} S_{\text{int}}$$

$$\langle JK00 | JK \rangle = 1 \quad \longrightarrow \quad \langle \tilde{\Psi}_0 | \hat{V}_{\text{PT}} | \Psi_0 \rangle_{\text{rigid}} = \langle \hat{V}_{\text{PT}} \rangle_{\text{int}}$$

Accuracy of Rigid Deformation Approximation



J. Dobaczewski *et al.*, PRL **121**, 232501 (2018) and the supplemental material

P, T-violating interaction

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$$\hat{V}_{\text{PT}}(\mathbf{r}_1 - \mathbf{r}_2) = -\frac{gm_\pi^2}{8\pi m_N} \left\{ (\boldsymbol{\sigma}_1 - \boldsymbol{\sigma}_2) \cdot (\mathbf{r}_1 - \mathbf{r}_2) \left[\bar{g}_0 \vec{\tau}_1 \cdot \vec{\tau}_2 - \frac{\bar{g}_1}{2} (\tau_{1z} + \tau_{2z}) + \bar{g}_2 (3\tau_{1z}\tau_{2z} - \vec{\tau}_1 \cdot \vec{\tau}_2) \right] - \frac{\bar{g}_1}{2} (\boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2) \cdot (\mathbf{r}_1 - \mathbf{r}_2) (\tau_{1z} - \tau_{2z}) \right\} \frac{\exp(-m_\pi |\mathbf{r}_1 - \mathbf{r}_2|)}{m_\pi |\mathbf{r}_1 - \mathbf{r}_2|^2} \left[1 + \frac{1}{m_\pi |\mathbf{r}_1 - \mathbf{r}_2|} \right] + \frac{1}{2m_N^3} [\bar{c}_1 + \bar{c}_2 \vec{\tau}_1 \cdot \vec{\tau}_2] (\boldsymbol{\sigma}_1 - \boldsymbol{\sigma}_2) \cdot \nabla \delta^3(\mathbf{r}_1 - \mathbf{r}_2),$$

C. M. Maekawa, E. Mereghetti, J. de Vries, and U. van Kolck,
Nucl. Phys. **A872**, 117 (2011)

W. C. Haxton and E. M. Henley, Phys. Rev. Lett. **51**, 1937 (1983)

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Nuclear Laboratory Schiff Moment

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Rigid deformation approximation:

$$\langle \Psi_0 | \hat{S}_0 | \tilde{\Psi}_0 \rangle_{\text{rigid}} = \frac{J}{J+1} S_{\text{int}}$$

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S_{int} and $\langle \hat{V}_{\text{PT}} \rangle_{\text{int}}$ are calculated within nuclear DFT.

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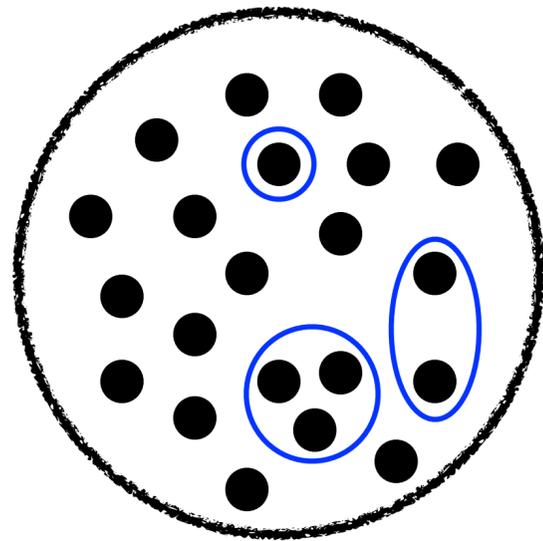
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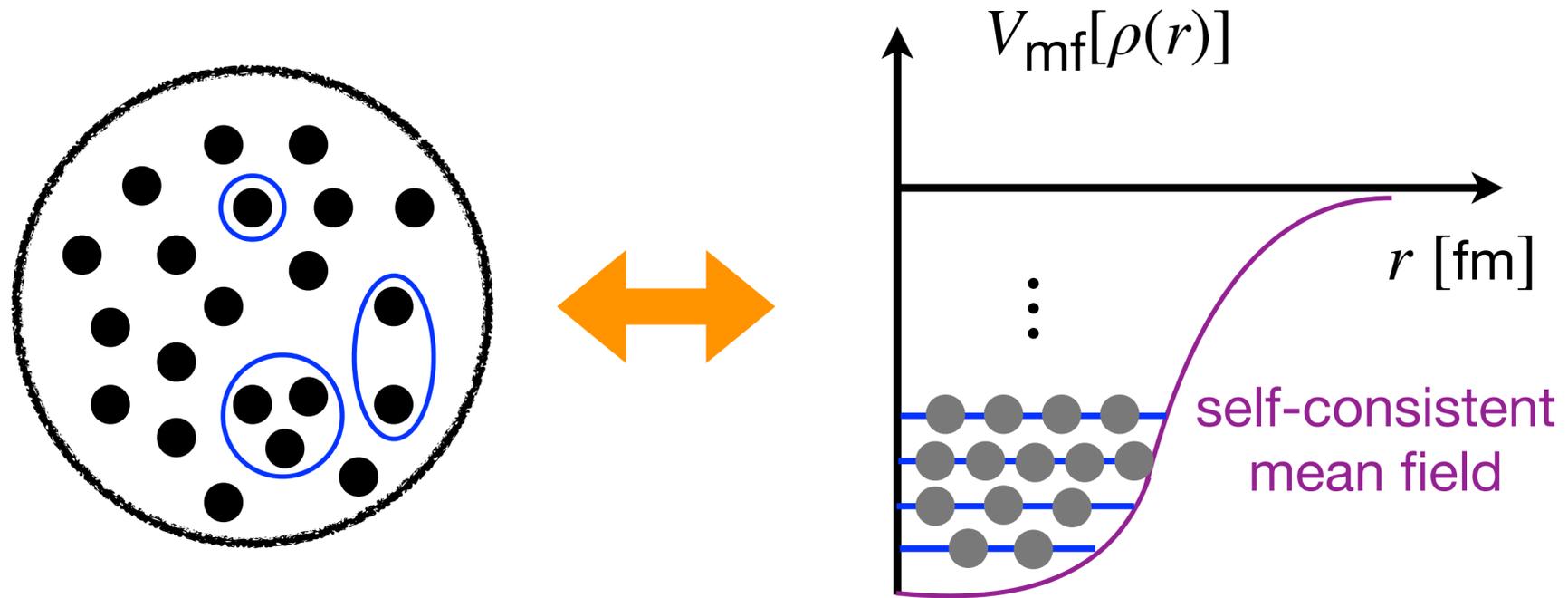
$$a_i = -\frac{2J}{J+1} \frac{S_{\text{int}} v_i}{\Delta E} \quad \text{and} \quad b_i = -\frac{2J}{J+1} \frac{S_{\text{int}} w_i}{\Delta E}$$

Nuclear Density Functional Theory (A primer)

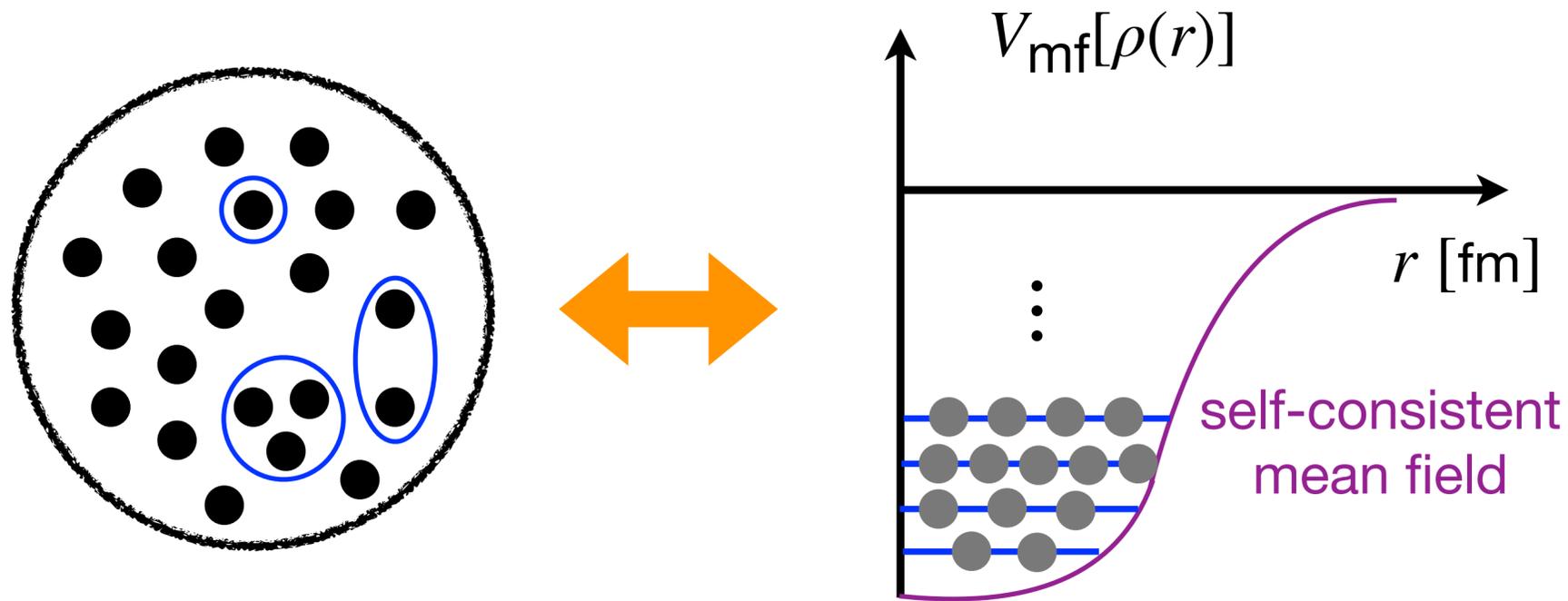
Nuclear Density Functional Theory (A primer)



Nuclear Density Functional Theory (A primer)



Nuclear Density Functional Theory (A primer)



Energy density functional (EDF): $\mathcal{E} = \int d^3r \mathcal{H}(\mathbf{r})$

$$\mathcal{H}(\mathbf{r}) = \frac{\hbar^2}{2m} \tau(\mathbf{r}) - \frac{1}{2} C \rho^2(\mathbf{r}), \quad \rho(\mathbf{r}) = \sum_i^A \phi_i(\mathbf{r}) \phi_i^*(\mathbf{r}),$$

$$\tau(\mathbf{r}) = \sum_{i=1}^A (\nabla \phi_i(\mathbf{r})) \cdot (\nabla \phi_i^*(\mathbf{r}))$$

Nuclear Density Functional Theory (A primer)

Variational principle:

$$\frac{\delta \mathcal{E}}{\delta \phi_i^*(\mathbf{r})} = 0$$

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Kohn-Sham equation:

$$\left[-\frac{\hbar^2}{2m} \nabla^2 - C\rho(\mathbf{r}) \right] \phi_i(\mathbf{r}) = \epsilon_i \phi_i(\mathbf{r})$$

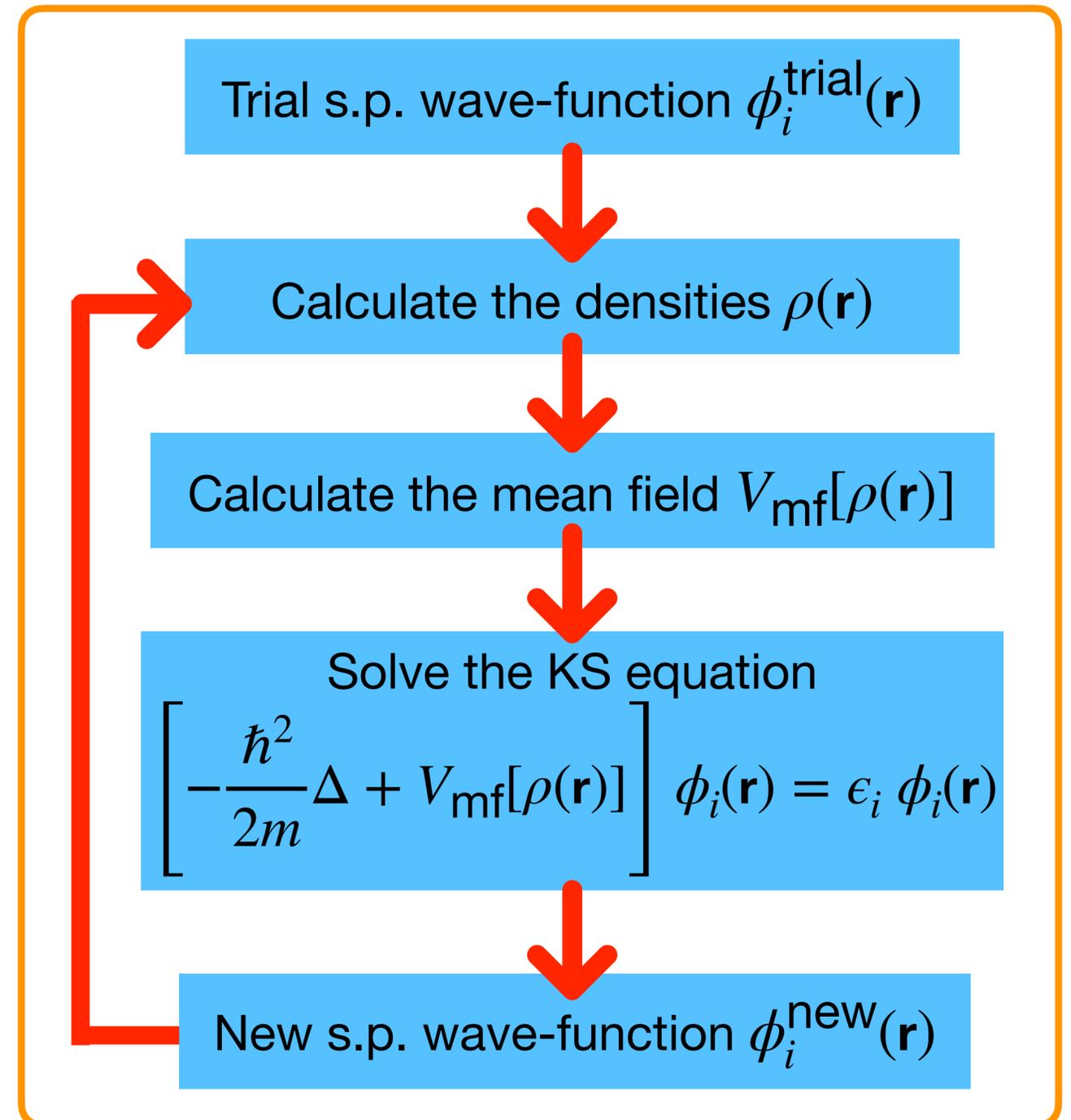
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Nuclear Density Functional Theory (This work)

Total energy: $\mathcal{E} = \mathcal{E}^{\text{kin.}} + \mathcal{E}^{\text{Skyrme}} + \mathcal{E}^{\text{Coul.}} + \mathcal{E}^{\text{mult.}} + \mathcal{E}^{\text{cran.}}$

$$\mathcal{E}^{\text{kin.}} = \frac{\hbar^2}{2m} \left(1 - \frac{1}{A} \right) \int d^3r [\tau_p(\mathbf{r}) + \tau_n(\mathbf{r})]$$

$$\mathcal{E}^{\text{mult.}} = \sum_{\lambda\mu} C_{\lambda\mu} \left[\langle \hat{Q}_{\lambda\mu} \rangle - \bar{Q}_{\lambda\mu} \right]^2$$

$$\mathcal{E}^{\text{cran.}} = -\omega_y \langle \hat{J}_y \rangle$$

$$\begin{aligned} \mathcal{E}^{\text{Skyrme}} &= \int d^3r \sum_{t=0,1} \left\{ C_t^\rho \rho_t^2(\mathbf{r}) + C_t^s s_t^2(\mathbf{r}) + C_t^{\Delta\rho} \rho_t(\mathbf{r}) \nabla^2 \rho_t(\mathbf{r}) + C_t^\tau \rho_t(\mathbf{r}) \tau_t(\mathbf{r}) + \right. \\ &+ C_t^J \overleftrightarrow{J}_t^2(\mathbf{r}) + C_t^{\Delta s} \mathbf{s}_t(\mathbf{r}) \cdot \nabla^2 \mathbf{s}_t(\mathbf{r}) + C_t^T \mathbf{s}_t(\mathbf{r}) \cdot \mathbf{T}_t(\mathbf{r}) + C_t^j j_t^2(\mathbf{r}) + \\ &+ \left. C_t^{\nabla J} \rho_t(\mathbf{r}) \nabla \cdot \mathbf{J}_t(\mathbf{r}) + C_t^{\nabla j} \mathbf{s}_t(\mathbf{r}) \cdot [\nabla \times \mathbf{j}_t(\mathbf{r})] \right\} \\ &= \sum_{t=0,1} \int d^3r \left\{ \mathcal{H}_t^{\text{even}}(\mathbf{r}) + \mathcal{H}_t^{\text{odd}}(\mathbf{r}) \right\}, \end{aligned}$$

Nuclear Density Functional Theory (This work)

$$\mathcal{H}_t^{\text{even}}(\mathbf{r}) = C_t^\rho \rho_t^2(\mathbf{r}) + C_t^{\Delta\rho} \rho_t(\mathbf{r}) \nabla^2 \rho_t(\mathbf{r}) + C_t^\tau \rho_t(\mathbf{r}) \tau_t(\mathbf{r}) + C_t^J \overleftrightarrow{\mathbf{J}}_t^2(\mathbf{r}) + C_t^{\nabla J} \rho_t(\mathbf{r}) \nabla \cdot \mathbf{J}_t(\mathbf{r}),$$

$$\mathcal{H}_t^{\text{odd}}(\mathbf{r}) = C_t^s s_t^2(\mathbf{r}) + C_t^{\Delta s} \mathbf{s}_t(\mathbf{r}) \cdot \nabla^2 \mathbf{s}_t(\mathbf{r}) + C_t^T \mathbf{s}_t(\mathbf{r}) \cdot \mathbf{T}_t(\mathbf{r}) + C_t^j j_t^2(\mathbf{r}) + C_t^{\nabla j} \mathbf{s}_t(\mathbf{r}) \cdot [\nabla \times \mathbf{j}_t(\mathbf{r})].$$

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★ 7 parametrizations of Skyrme energy density functional (EDF) have been used.

Nuclear Density Functional Theory (This work)

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- ★ Hartree-Fock-Bogoliubov (HFB) equations are solved.

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$$\begin{pmatrix} \hat{h}' - \lambda & \Delta \\ -\Delta^* & -\hat{h}'^* + \lambda \end{pmatrix} \begin{pmatrix} \chi_k^{\text{upper}} \\ \chi_k^{\text{lower}} \end{pmatrix} = \begin{pmatrix} \chi_k^{\text{upper}} \\ \chi_k^{\text{lower}} \end{pmatrix} E_k$$

Nuclear Density Functional Theory (This work)

$$\mathcal{H}_t^{\text{even}}(\mathbf{r}) = C_t^\rho \rho_t^2(\mathbf{r}) + C_t^{\Delta\rho} \rho_t(\mathbf{r}) \nabla^2 \rho_t(\mathbf{r}) + C_t^\tau \rho_t(\mathbf{r}) \tau_t(\mathbf{r}) + C_t^J \overleftrightarrow{\mathbf{J}}_t^2(\mathbf{r}) + C_t^{\nabla J} \rho_t(\mathbf{r}) \nabla \cdot \mathbf{J}_t(\mathbf{r}),$$

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Single-particle Routhian operators:

$$\hat{h}'_n = -\frac{\hbar^2}{2m} \nabla^2 + (\Gamma_0^{\text{even}} + \Gamma_0^{\text{odd}} + \Gamma_1^{\text{even}} + \Gamma_1^{\text{odd}}) + \hat{U}^{\text{mult.}} - \omega_y \hat{J}_y$$

$$\hat{h}'_p = -\frac{\hbar^2}{2m} \nabla^2 + (\Gamma_0^{\text{even}} + \Gamma_0^{\text{odd}} - \Gamma_1^{\text{even}} - \Gamma_1^{\text{odd}}) + U^{\text{Coul.}} + \hat{U}^{\text{mult.}} - \omega_y \hat{J}_y$$

Nuclear Density Functional Theory (This work)

J. Dobaczewski and J. Dudek, CPC 102, 166 (1997)

M. Athanasakis-Kaklamanakis, *et al.*,
Nature 648, 562-568 (2025)

Nuclear Density Functional Theory (This work)

Multipole constraints:

J. Dobaczewski and J. Dudek, CPC 102, 166 (1997)

$$\hat{U}^{\text{mult.}} = 2 \sum_{\lambda\mu} C_{\lambda\mu} \left[\langle \hat{Q}_{\lambda\mu} \rangle - \bar{Q}_{\lambda\mu} \right] \hat{Q}_{\lambda\mu}$$

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Anti-symmetric pairing potential Δ depends on the standard form factor of zero-range density-dependent pairing force:

$$f(\mathbf{r}) = V_0 + \cancel{V_1} \rho^\alpha(\mathbf{r})$$

$V_{0,p}$ was adjusted to reproduce the experimental pairing gap of ^{227}Ac isotope.

16

How do we calculate the ground state of an odd nucleus?

P. Ring and P. Schuck, *The Nuclear Many-Body Problem*
J. Dobaczewski *et al.*, CPC 180, 2361 (2009)

How do we calculate the ground state of an odd nucleus?

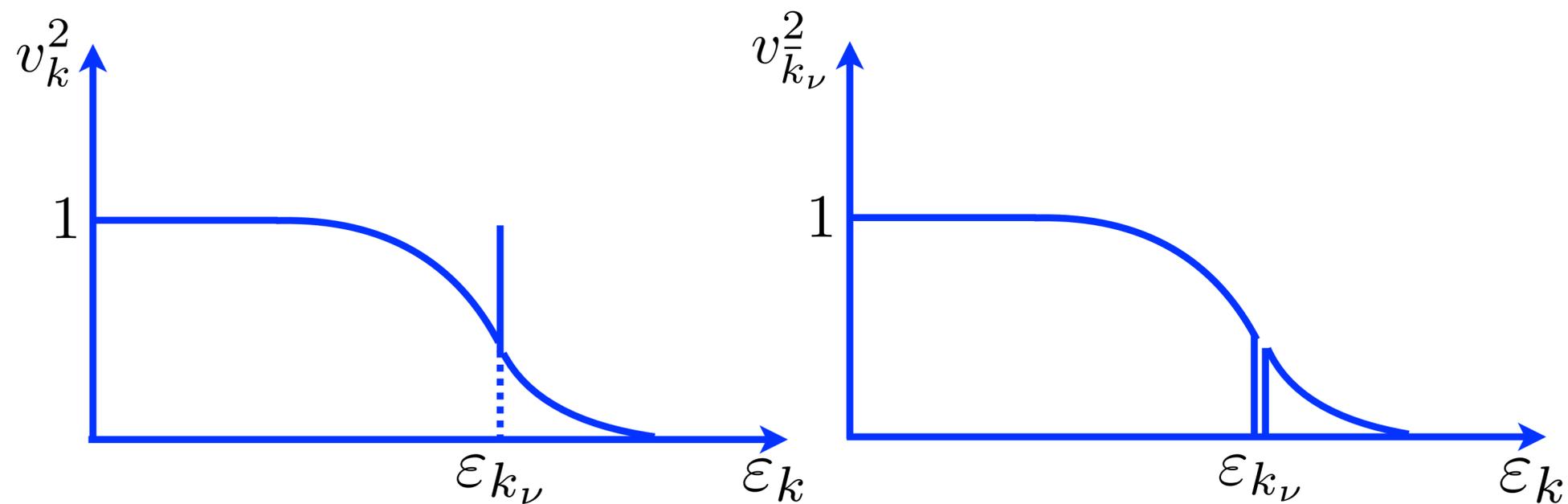
$$|\Psi\rangle_{\text{HFB}}^{\text{even}} = \prod_{\mu>0} \left(u_{\mu} + v_{\mu} \hat{a}_{\bar{\mu}}^{\dagger} \hat{a}_{\mu}^{\dagger} \right) |0\rangle$$

$$|\Psi\rangle_{\text{HFB}}^{\text{odd}} = \hat{\beta}_{\nu}^{\dagger} |\Psi\rangle_{\text{HFB}}^{\text{even}} = \hat{a}_{\nu}^{\dagger} \prod_{\nu \neq \mu > 0} \left(u_{\mu} + v_{\mu} \hat{a}_{\bar{\mu}}^{\dagger} \hat{a}_{\mu}^{\dagger} \right) |0\rangle$$

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T. Duguet, P. Bonche, P. -H. Helen and J. Meyer, Phys. Rev. C **65**, 014310 (2001)

T. Duguet, P. Bonche, P. -H. Helen and J. Meyer, Phys. Rev. C **65**, 014311 (2001)

J. Dobaczewski *et al.*, Comp. Phys. Commun. **180**, 2361 (2009)

H. Wibowo *et al.*, [J. Phys. G: Nucl. Part. Phys. 52, 6 \(2025\)](#)

Two-step procedure to determine the ground state of an odd nucleus:

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★ **Falsevacuum**: an even HFB vacuum with an average odd number of particles

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Two-step procedure to determine the ground state of an odd nucleus:

★ **Falsevacuum**: an even HFB vacuum with an average odd number of particles

★ **Tagging mechanism**: $\max \left\{ \langle \phi_\ell | \chi_k^{\text{upper}} \rangle, \langle \phi_\ell | \chi_k^{\text{lower}} \rangle \right\}$

Quasiparticle blocked state was tagged by $\pi[532]3/2^-$.

Calculations were performed using HFODD code.

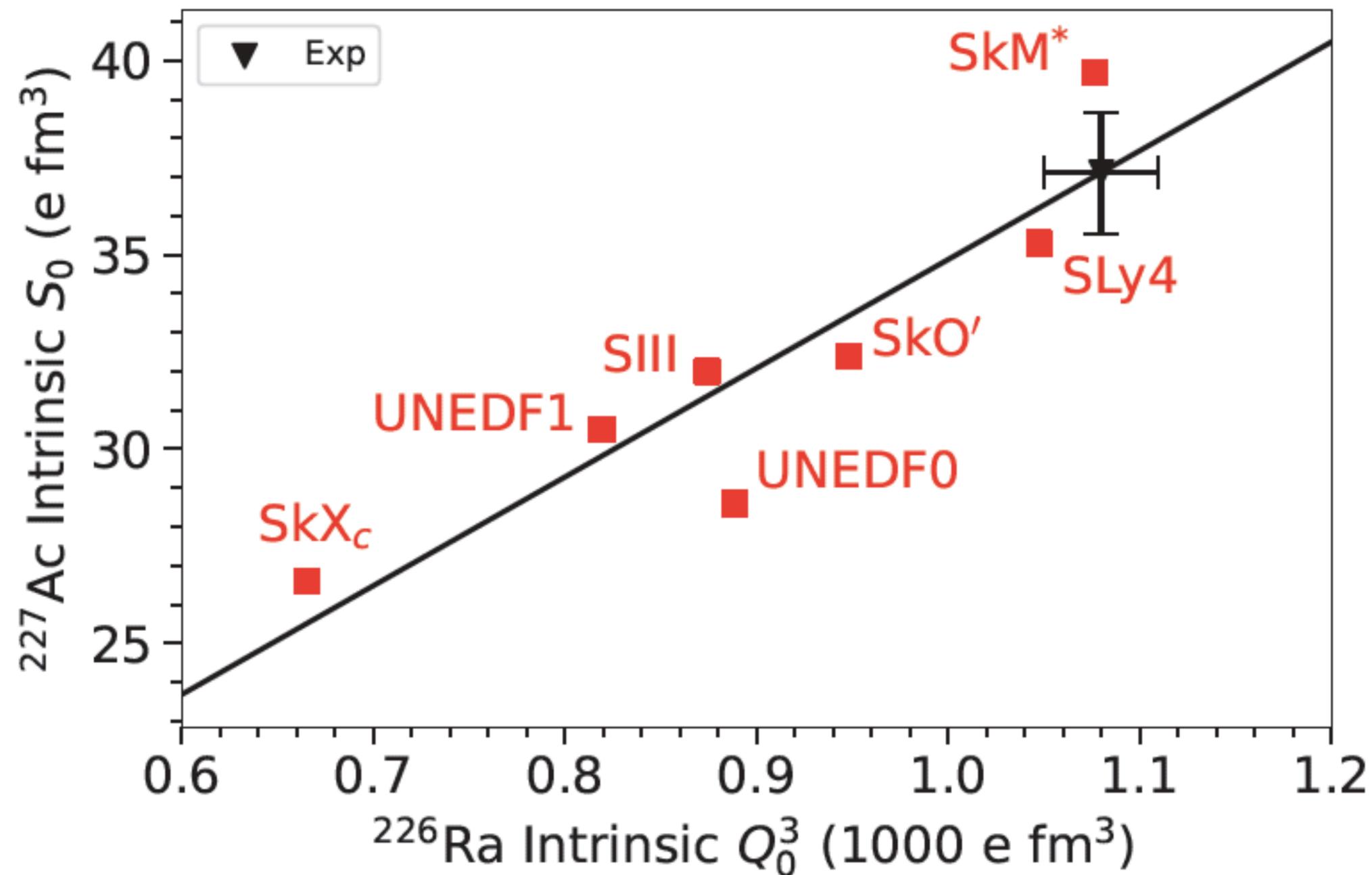
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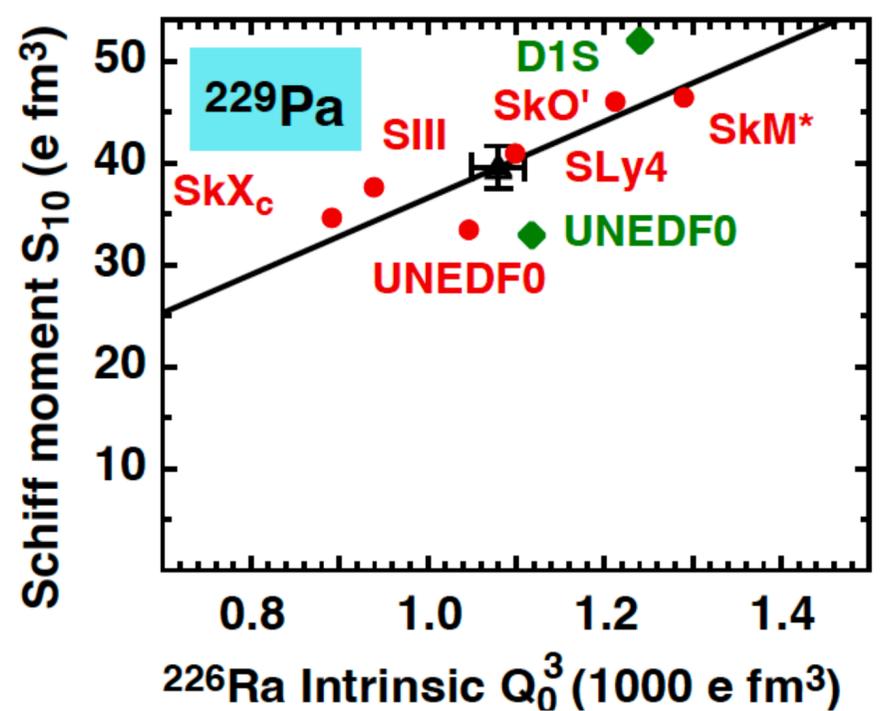
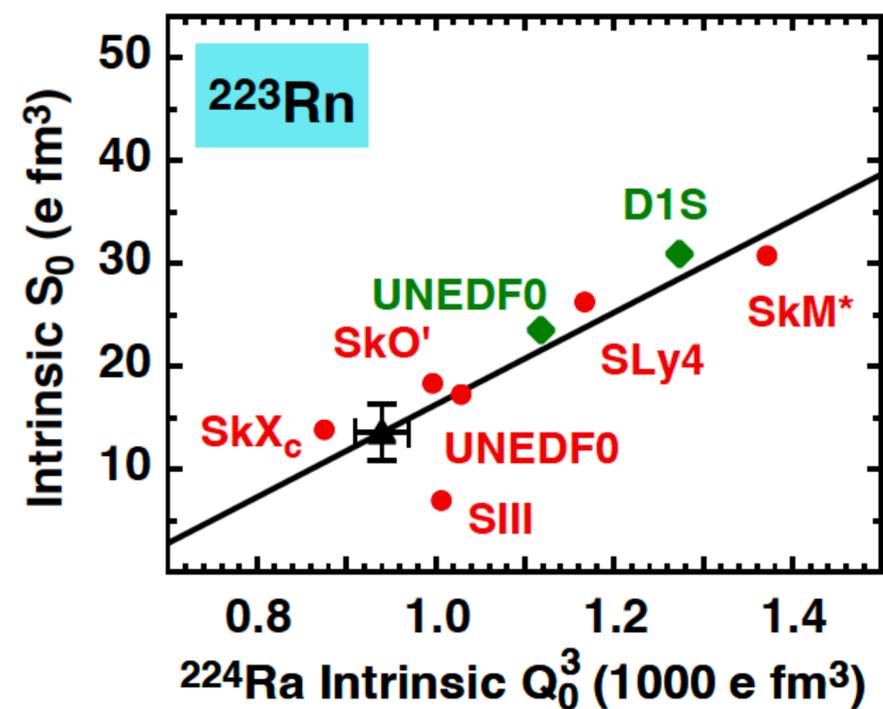
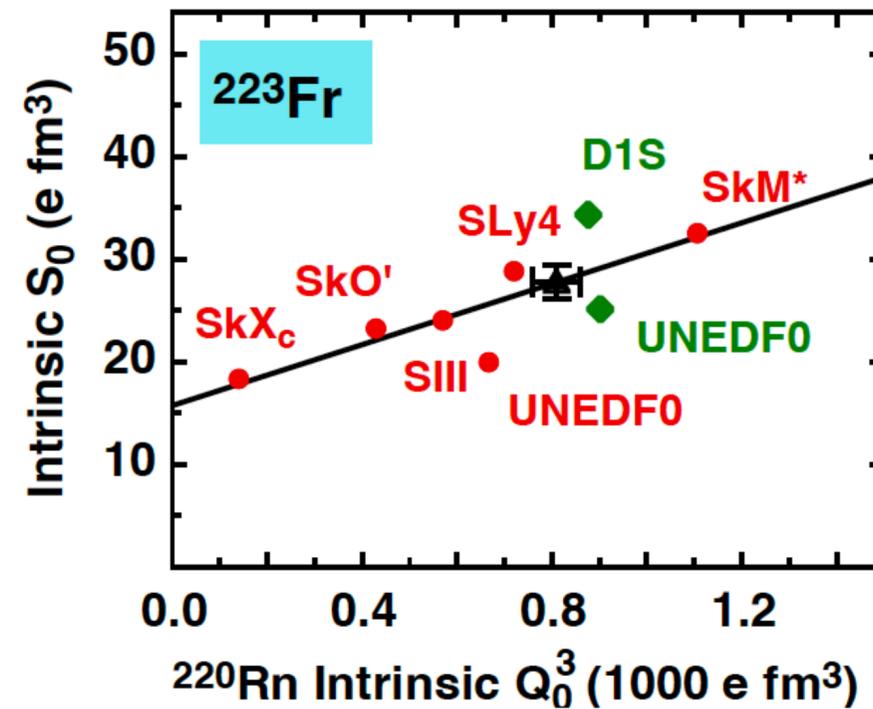
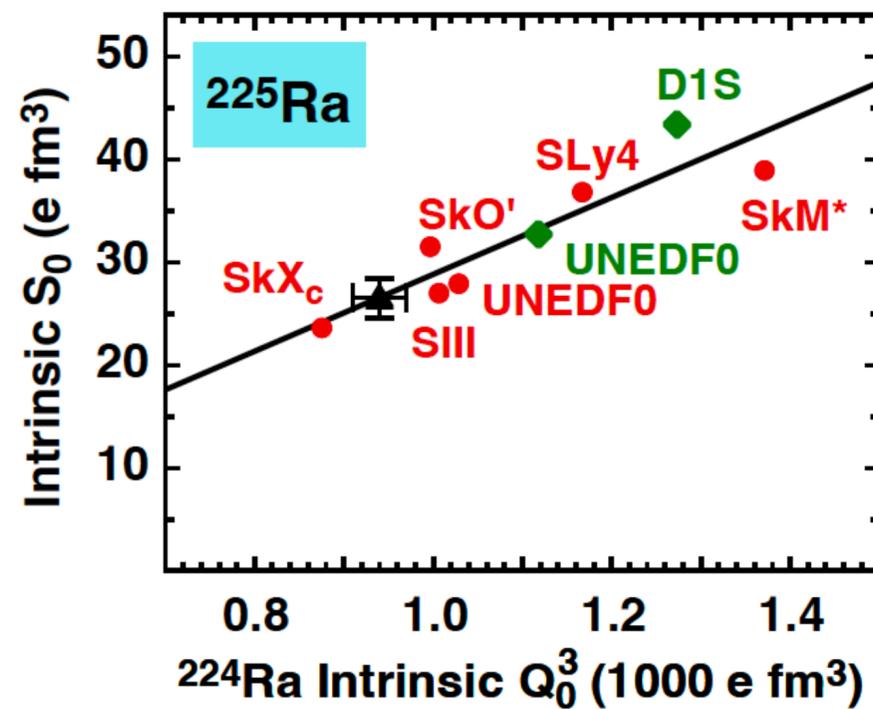
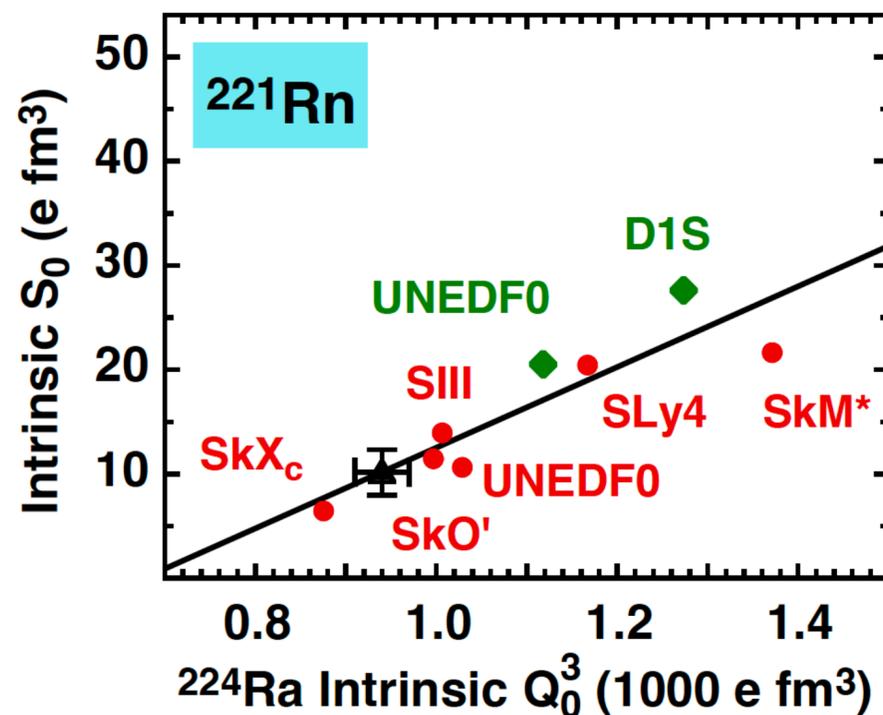
H. Wibowo *et al.*, [J. Phys. G: Nucl. Part. Phys. 52, 6 \(2025\)](#)

Correlation between Octupole and Schiff Moments



M. Athanasakis-Kaklamanakis, *et al.*,
Nature 648, 562-568 (2025)

J. Dobaczewski, *et al.*,
arXiv:2511.04632v2 (2025)



Estimated Intrinsic Schiff Moment

M. Athanasakis-Kaklamanakis, *et al.*,
Nature 648, 562-568 (2025)

H. Wollersheim *et al.*, Nucl. Phys. A **556**, 261 (1993)

J. Dobaczewski *et al.*, PRL **121**, 232501 (2018) and
the supplemental material

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Intrinsic Schiff moment:

$$S_0(\text{est}) = a + bQ_0^3(\text{exp})$$

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Estimated Intrinsic Schiff Moment

Intrinsic Schiff moment: $S_0(\text{est}) = a + bQ_0^3(\text{exp})$

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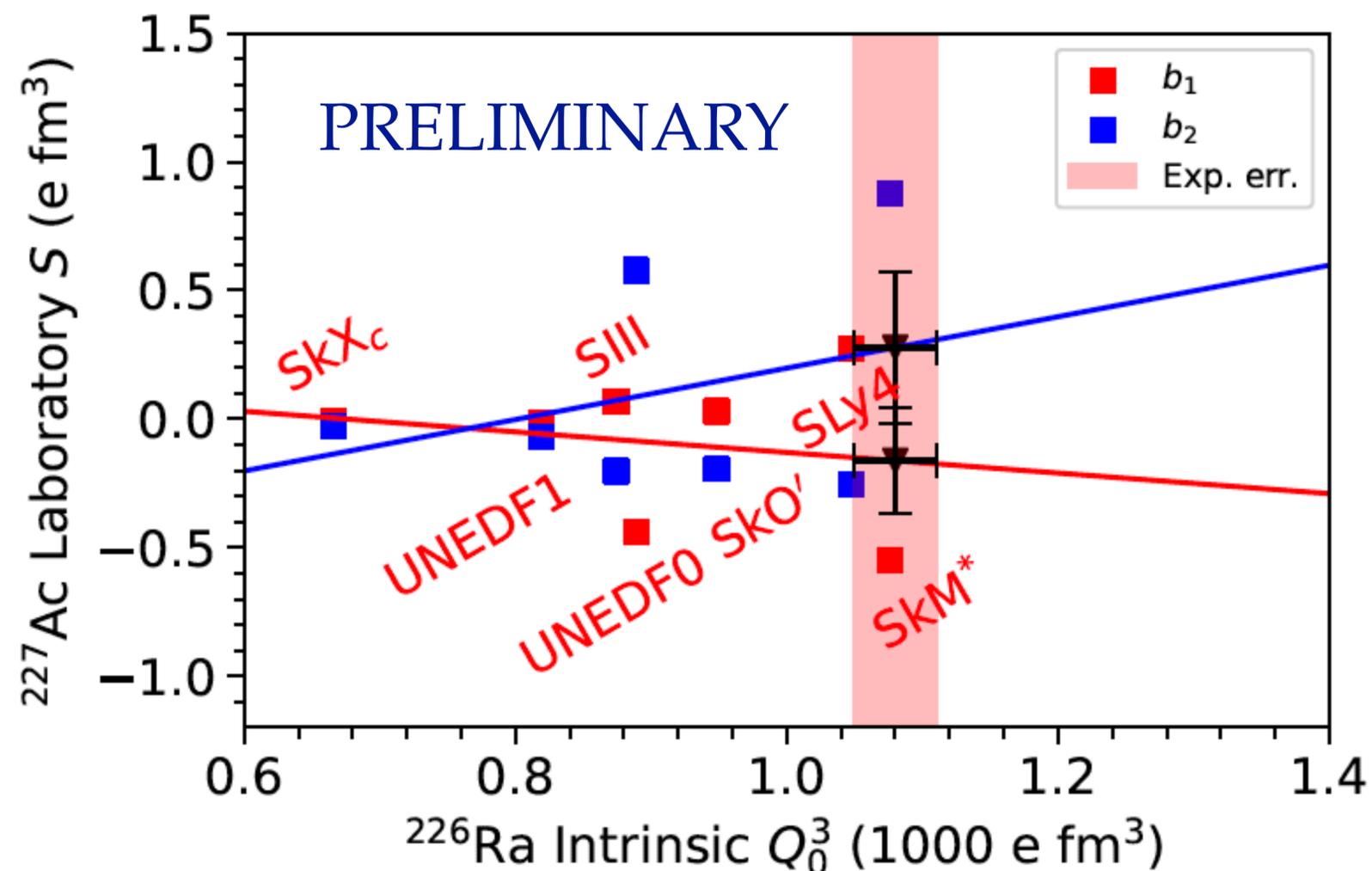
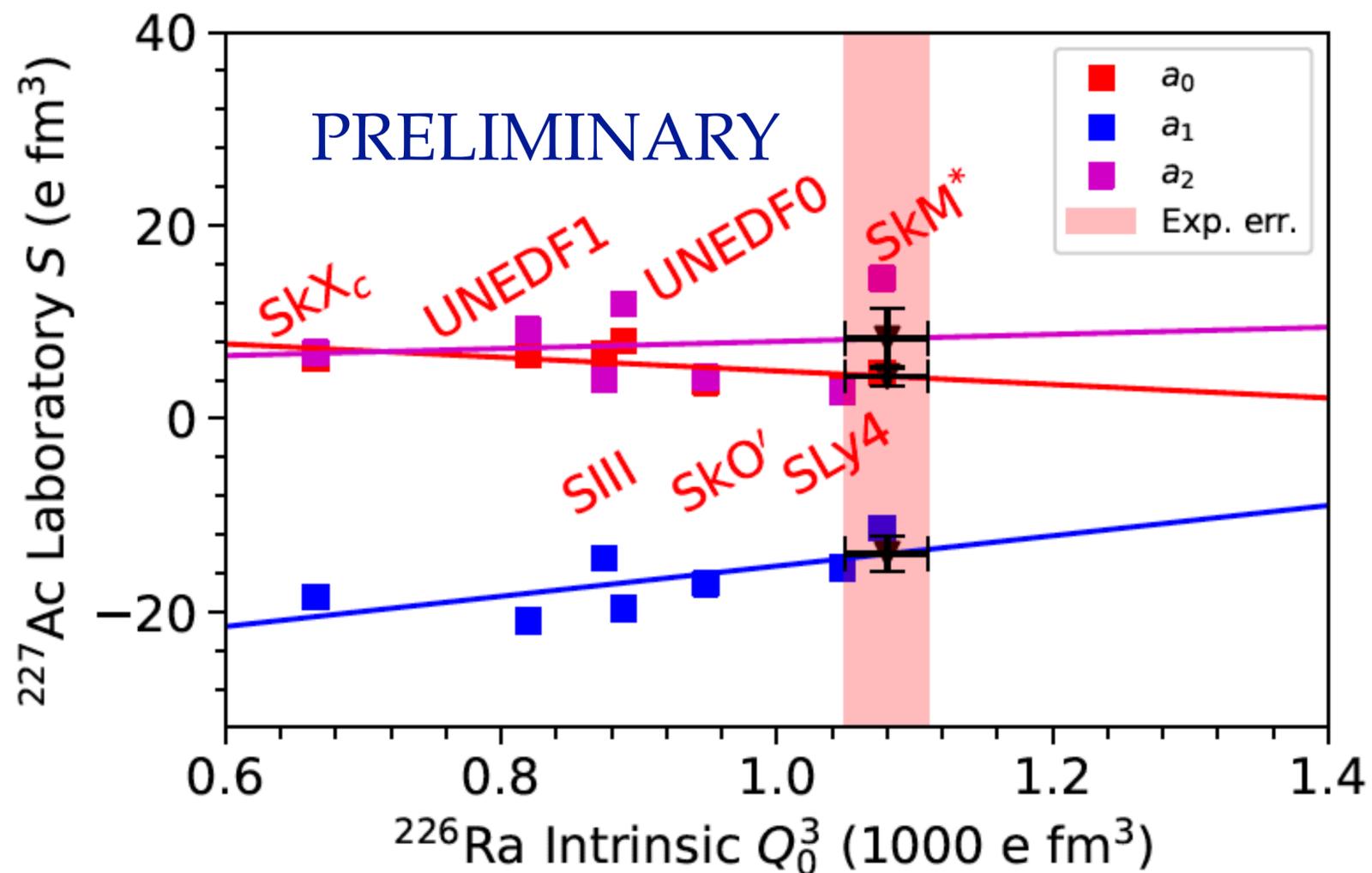
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$$S_0(^{227}\text{Ac}) = 37.1(1.6) \text{ e fm}^3 \quad \text{M. Athanasakis-Kaklamanakis, et al., Nature 648, 562-568 (2025)}$$

Estimated Laboratory Schiff Moment



$$a_0 = 4.4(10) e \cdot \text{fm}^3$$

$$a_1 = -14.0(18) e \cdot \text{fm}^3$$

$$a_2 = 8.3(31) e \cdot \text{fm}^3$$

$$b_1 = -0.2(2) e \cdot \text{fm}^3$$

$$b_2 = 0.3(3) e \cdot \text{fm}^3$$

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arXiv:2511.04632v2 (2025)

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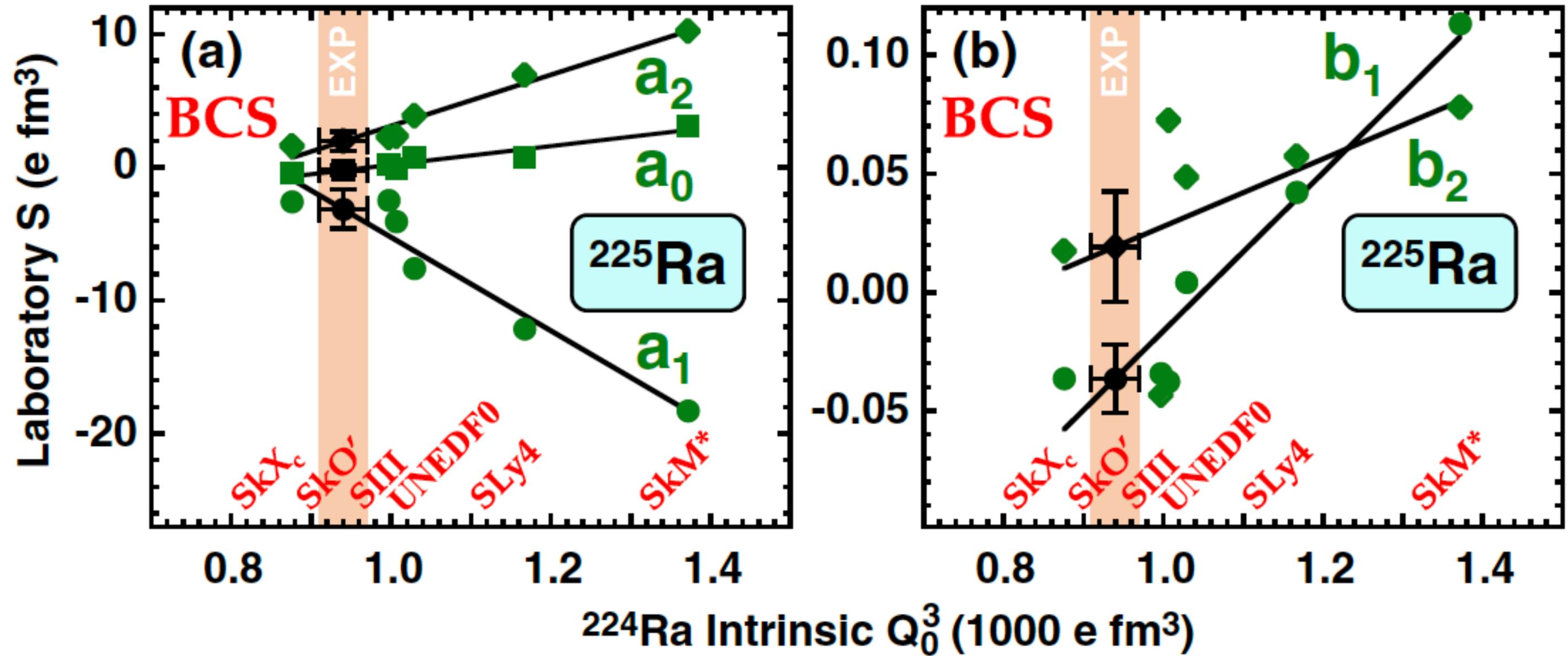


TABLE I. Coefficients a_0 , a_1 , a_2 , b_1 , and b_2 (in e fm³) [from Eq. (5)], determined by regression analysis. For ²²¹Rn and ²²³Rn we show values propagated to the experimental octupole moment of ²²⁰Rn, whereas for ²²³Fr, ²²⁵Ra, and ²²⁹Pa we show averages of those propagated to ²²⁴Ra and ²²⁶Ra. Details are in the Supplemental Material [34]. Values determined with a precision better than 25% are in boldface and those compatible with zero are in italics.

	a_0	a_1	a_2	b_1	b_2
²²¹ Rn	<i>-0.04(10)</i>	-1.7(3)	0.67(10)	<i>-0.015(5)</i>	<i>-0.007(4)</i>
²²³ Rn	<i>-0.08(8)</i>	-2.4(4)	0.86(10)	<i>-0.031(9)</i>	<i>-0.008(8)</i>
²²³ Fr	<i>0.07(20)</i>	<i>-0.8(7)</i>	<i>0.05(40)</i>	<i>0.018(8)</i>	<i>-0.016(10)</i>
²²⁵ Ra	<i>0.2(6)</i>	<i>-5(3)</i>	<i>3.3(1.5)</i>	<i>-0.01(3)</i>	<i>0.03(2)</i>
²²⁹ Pa	-1.2(3)	<i>-0.9(9)</i>	<i>-0.3(5)</i>	0.036(8)	<i>0.032(18)</i>
²²⁷ Ac	<i>4.4(10)</i>	<i>-14.0(18)</i>	<i>8.3(31)</i>	<i>-0.2(2)</i>	<i>0.3(3)</i>

Summary and Outlook

 Summary

 Outlook

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$$\mathbf{S}^n = \frac{1}{6} \sum_{i=1}^A (r_i^2 - \langle r^2 \rangle_{\text{ch}}) \mathbf{d}_i$$

$$S_{\text{lab}} = a_0 g \bar{g}_0 + a_1 g \bar{g}_1 + a_2 g \bar{g}_2 \\ + b_1 \bar{c}_1 + b_2 \bar{c}_2 + a_p d_p + a_n d_n$$

Acknowledgements

We acknowledge the support from a **Leverhulme Trust Research Project Grant**. This work was partially supported by the **STFC Grant** Nos. ST/P003885/1, ST/V001035/1 and ST/Y000285/1, and by the **Polish National Science Centre** under Contract No. 2018/31/B/ST2/02220. We acknowledge the **CSC-IT Center for Science Ltd., Finland** and the **IFT Computer Center of the University of Warsaw, Poland**, for allocating computational resources. This project was partly undertaken on the **Viking Cluster**, which is a high performance compute facility provided by the **University of York**. We are grateful for computational support from the **University of York High Performance Computing service, Viking and the Research Computing team**.

Back Up Slides

EDM and Fundamental Symmetries

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★ The necessity of parity symmetry breaking

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$$\langle \hat{\mathbf{d}} \rangle \equiv \langle jm | \hat{\mathbf{d}} | jm \rangle$$

$$\hat{\pi}^{-1} = \hat{\pi}^\dagger = \hat{\pi}$$

$$\hat{\pi} |jm\rangle \equiv \hat{\pi} |n\ell jm\rangle = (-1)^\ell |n\ell jm\rangle, \quad \ell = 0, 1, 2, \dots, n$$

$$\langle \hat{\mathbf{d}} \rangle = \langle jm | \hat{\pi}^\dagger \hat{\pi} \hat{\mathbf{d}} \hat{\pi}^\dagger \hat{\pi} | jm \rangle = (-1)^{2\ell} \langle jm | (-\hat{\mathbf{d}}) | jm \rangle = -\langle \hat{\mathbf{d}} \rangle$$

$$\langle \hat{\mathbf{d}} \rangle = 0.$$

★ The necessity of time-reversal symmetry breaking

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$$|\tilde{\alpha}\rangle = \hat{\Theta}|\alpha\rangle \quad \text{and} \quad |\tilde{\beta}\rangle = \hat{\Theta}|\beta\rangle$$

$$\langle\tilde{\beta}|\tilde{\alpha}\rangle = \langle\beta|\alpha\rangle^* = \langle\alpha|\beta\rangle$$

$$\langle\beta|\hat{A}|\alpha\rangle = \langle\tilde{\alpha}|\hat{\Theta}\hat{A}^\dagger\hat{\Theta}^{-1}|\tilde{\beta}\rangle = \langle\tilde{\alpha}|\hat{\Theta}\hat{A}\hat{\Theta}^{-1}|\tilde{\beta}\rangle$$

$$\langle\alpha', jm'|\hat{V}_q|\alpha, jm\rangle = \frac{\langle\alpha', jm|\hat{\mathbf{J}} \cdot \hat{\mathbf{V}}|\alpha, jm\rangle}{\hbar^2 j(j+1)} \langle jm'|\hat{J}_q|jm\rangle$$

$$\langle jm|\hat{\mathbf{d}}|jm\rangle = c\langle jm|\hat{\mathbf{J}}|jm\rangle, \quad c \text{ is a real constant and } m\text{-independent.}$$

$$\langle jm'|\hat{\mathbf{d}} \cdot \hat{\mathbf{J}}|jm\rangle = \frac{\langle jm00|jm'\rangle}{\sqrt{2j+1}} \langle j||\hat{\mathbf{d}} \cdot \hat{\mathbf{J}}||j\rangle = \delta_{mm'} \frac{\langle j||\hat{\mathbf{d}} \cdot \hat{\mathbf{J}}||j\rangle}{\sqrt{2j+1}}$$

$$\langle jm|\hat{\mathbf{d}}|jm\rangle = \langle j\tilde{m}|\hat{\Theta}\hat{\mathbf{d}}\hat{\Theta}^{-1}|j\tilde{m}\rangle = +\langle j\tilde{m}|\hat{\mathbf{d}}|j\tilde{m}\rangle = (-1)^{2(j-m)}\langle j(-m)|\hat{\mathbf{d}}|j(-m)\rangle$$

$$\langle jm|\hat{\mathbf{J}}|jm\rangle = \langle j\tilde{m}|\hat{\Theta}\hat{\mathbf{J}}\hat{\Theta}^{-1}|j\tilde{m}\rangle = -\langle j\tilde{m}|\hat{\mathbf{J}}|j\tilde{m}\rangle = -(-1)^{2(j-m)}\langle j(-m)|\hat{\mathbf{J}}|j(-m)\rangle$$

$$\langle j(-m)|\hat{\mathbf{d}}|j(-m)\rangle = -c\langle j(-m)|\hat{\mathbf{J}}|j(-m)\rangle$$

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$$\langle jm|\hat{\mathbf{d}}|jm\rangle = -c\langle jm|\hat{\mathbf{J}}|jm\rangle$$

$$\langle jm|\hat{\mathbf{d}}|jm\rangle = 0$$

★ Therefore, the non-zero $\langle\hat{\mathbf{d}}\rangle$ requires parity and time-reversal symmetry to be broken simultaneously.

Schiff Theorem

$$\hat{H}_{\text{atom}} = \hat{H}_{\text{el.}} + \hat{H}_{\text{nucl.}} - \sum_a e\varphi(\mathbf{R}_a)$$

$$\varphi(\mathbf{R}) = \int d^3x \frac{e\rho(\mathbf{r})}{|\mathbf{R} - \mathbf{r}|}$$

$$\hat{H}_{\text{ext.}} = e \sum_a \mathbf{R}_a \cdot \mathbf{E}_0 - \hat{\mathbf{d}} \cdot \mathbf{E}_0$$

$$\hat{\mathcal{H}} = \hat{H}_{\text{atom}} + \hat{H}_{\text{ext.}} = \hat{H}_{\text{atom}} + e \sum_a \mathbf{R}_a \cdot \mathbf{E}_0 - \hat{\mathbf{d}} \cdot \mathbf{E}_0$$

$$\hat{\mathcal{H}}' = e^{i\hat{U}} \hat{\mathcal{H}} e^{-i\hat{U}} \approx \hat{\mathcal{H}} + i[\hat{U}, \hat{\mathcal{H}}]$$

$$\hat{U} = \frac{\langle \hat{\mathbf{d}} \rangle}{Ze} \cdot \sum_a \hat{\mathbf{P}}_a$$

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$$i[\hat{U}, \hat{\mathcal{H}}] = \frac{1}{Z} \langle \hat{\mathbf{d}} \rangle \cdot [\mathbf{E}_e + Z\mathbf{E}_0]$$

$$\mathbf{E}_e \equiv - \sum_a \nabla_a \varphi(\mathbf{R}_a) \equiv \text{Electric field on nucleus generated by electrons.}$$

$$\langle \Psi | [\hat{U}, \hat{\mathcal{H}}] | \Psi \rangle = \langle \Psi | \hat{U} \hat{\mathcal{H}} | \Psi \rangle - \langle \Psi | \hat{\mathcal{H}} \hat{U} | \Psi \rangle \propto (E - E) = 0$$

$$Z\mathbf{E}_0 + \langle \mathbf{E}_e \rangle = 0 \rightarrow \langle \mathbf{E}_e \rangle = -Z\mathbf{E}_0 \quad (\text{Schiff theorem})$$

$$\hat{\mathcal{H}}' = \hat{H}_{\text{atom}} + \hat{H}_{\text{ext.}} + i[\hat{U}, \hat{\mathcal{H}}]$$

$$= \hat{H}_{\text{atom}} + \hat{H}_{\text{ext.}} - (\hat{\mathbf{d}} - \langle \hat{\mathbf{d}} \rangle) \cdot \mathbf{E}_0 + e \sum_a \mathbf{R}_a \cdot \mathbf{E}_0 + \sum_a e \varphi'(\mathbf{R}_a)$$

$$\varphi'(\mathbf{R}_a) = \varphi(\mathbf{R}_a) + \frac{1}{Ze} \langle \hat{\mathbf{d}} \rangle \cdot \nabla_a \varphi(\mathbf{R}_a)$$

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Linear Regression Analysis

$$\chi^2 = \sum_i [S_0(i) - a - bQ_0^3(i)]^2$$

$$\bar{b} = \frac{\langle S_0 Q_0^3 \rangle - \langle S_0 \rangle \langle Q_0^3 \rangle}{\langle [Q_0^3(i)]^2 \rangle - \langle Q_0^3 \rangle^2}$$

$$\bar{a} = \langle S_0 \rangle - \bar{b} \langle Q_0^3 \rangle$$

$$\langle S_0 \rangle = \frac{1}{N_d} \sum_i S_0(i), \quad \langle Q_0^3 \rangle = \frac{1}{N_d} \sum_i Q_0^3(i),$$

$$\langle S_0 Q_0^3 \rangle = \frac{1}{N_d} \sum_i S_0(i) Q_0^3(i), \quad \langle [Q_0^3(i)]^2 \rangle = \frac{1}{N_d} \sum_i [Q_0^3(i)]^2$$

$$s = \frac{\chi_0^2}{N_d - N_p} \quad \mathcal{C} = s\mathcal{M}^{-1} \quad \mathcal{M}_{ij} = \frac{1}{2} \frac{\partial}{\partial p_i} \frac{\partial}{\partial p_j} \chi^2 \Big|_{\mathbf{p}=\bar{\mathbf{p}}}$$

$$\mathcal{C}_{aa} = \frac{s}{N_d} \frac{\langle [Q_0^3]^2 \rangle}{\langle [Q_0^3]^2 \rangle - \langle Q_0^3 \rangle^2},$$

$$\mathcal{C}_{ab} = \mathcal{C}_{ba} = -\frac{s}{N_d} \frac{\langle Q_0^3 \rangle}{\langle [Q_0^3]^2 \rangle - \langle Q_0^3 \rangle^2}$$

$$\mathcal{C}_{bb} = \frac{s}{N_d} \frac{1}{\langle [Q_0^3]^2 \rangle - \langle Q_0^3 \rangle^2}.$$

Different definitions of octupole moment

$$Q_0^3 = e \sqrt{\frac{16\pi}{7}} \sum_p r_p^3 Y_0^3(\Omega_p) \quad (\text{definition 1})$$

$$\hat{Q}_0^3 = e \sum_p r_p^3 Y_0^3(\Omega_p) \quad (\text{definition 2})$$

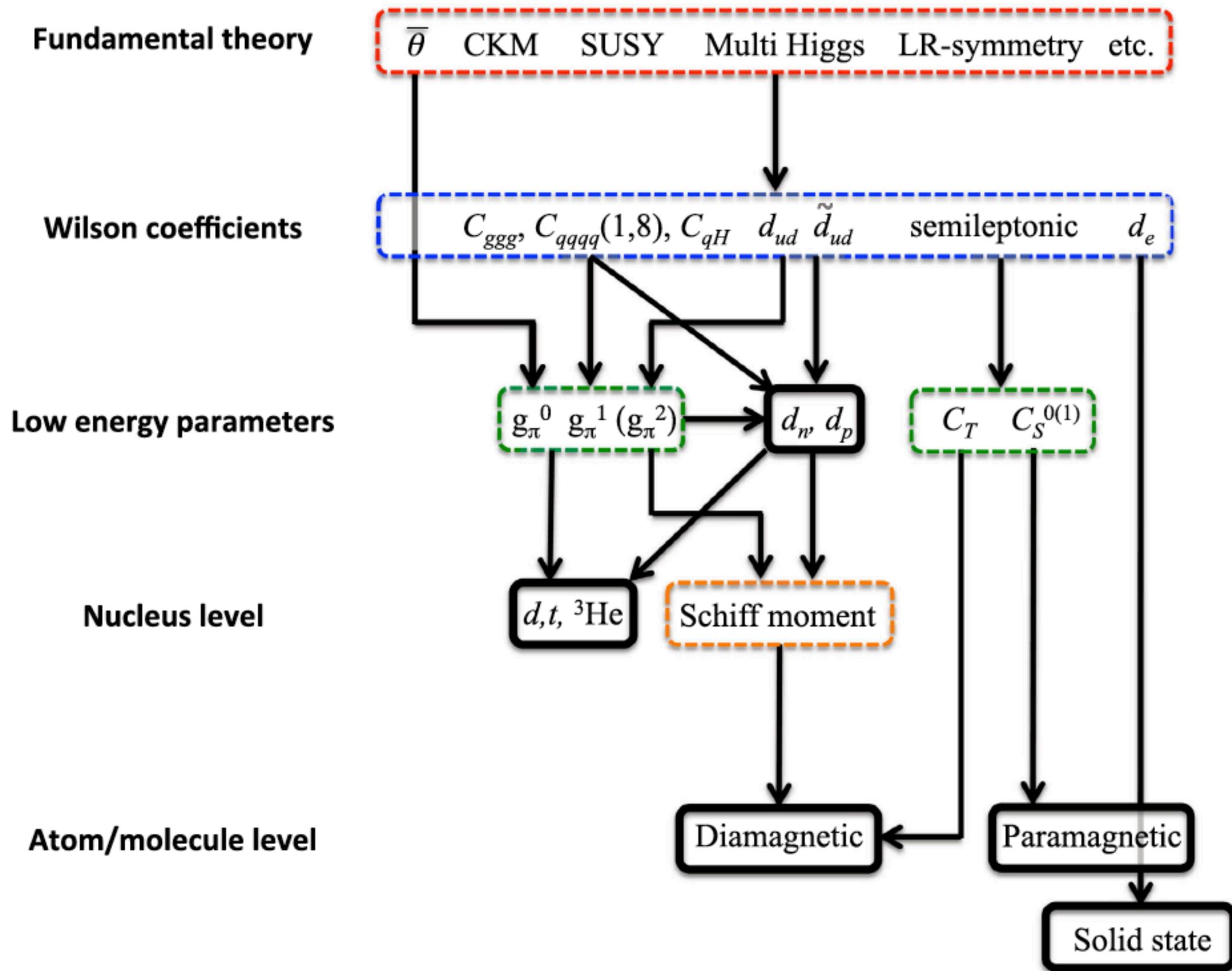
$$Q_0^3(\text{exp}) = 810(50) \text{ e fm}^3 \quad ({}^{220}\text{Rn})$$

$$= 940(30) \text{ e fm}^3 \quad ({}^{224}\text{Ra})$$

$$= 1080(30) \text{ e fm}^3 \quad ({}^{226}\text{Ra})$$

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