Modeling nuclear matrix elements for advancing new physics research in the era of high precision

Jiangming Yao (尧江明)

School of Physics and Astronomy, Sun Yat-sen University 中山大学物理与天文学院

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2 Lepton-number violation and nuclear matrix elements of $0
u\beta\beta$ decay

- Time-reversal symmetry violation and nuclear Schiff moment
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Searching for new physics at low-energy scales





- High-intensity/precision frontiers: searching for $0\nu\beta\beta$ decay, atomic EDM, dark matter, etc.
- Accurate nuclear matrix elements: crucial for testing fundamental symmetries and interactions with low-energy probes.

A hypothetical nuclear decay mode: $0\nu\beta\beta$ decay



• The two modes of $\beta^-\beta^-$ decay:

$$(A,Z) \rightarrow (A,Z+2) + 2e^- + (2\overline{\nu}_e)$$



Nuclear Chart: decay mode of the ground state nuclide(NUBASE2020)



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Theoretical studies of $0\nu\beta\beta$ decay and neutrino physics





If $0
u\beta\beta$ decay is driven by exchanging light massive Majorana neutrinos,

$$\langle m_{etaeta}
angle \equiv |\sum_{j=1}^{3} U_{ej}^2 m_j| = \left[rac{m_e^2}{g_A^4 G_{0
u} \, T_{1/2}^{0
u} \, |M^{0
u}|^2}
ight]^{1/2}$$

Accurate values of the NMEs $M^{0\nu}$ are crucial for designing and interpreting those experiments, as they link the observed decay rate to the neutrino mass scale.

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- Lifetime sensitivity of the ton-scale experiments: $T_{1/2}^{0\nu} > 10^{28}$ yr.
- Whether or not the ton-scale experiments are able to cover the entire parameter space for the IO case depends strongly on the employed NME.



The EFT provides a model-independent framework for describing 0 uetaeta decay.



The basic idea:

- Indentify the active dof at the nuclear energy scale: N, π, (e, ν)
- Write down all possible contributions to both nuclear force and transition operators according to a power counting rule, $(Q, m_{\pi})/\Lambda_{\chi}$.
- Carry out a quantum many-body calculation and compute the NME.



• Non-relativistic chiral 2N+3N interactions (Weinberg power counting and others)



K. Hebeler, Phys. Rep. 890, 1 (2020)

• Relativistic chiral 2N interaction (up to N²LO, different PC from the NR case)

J.-X. Lu et al., PRL128, 142002 (2022)

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The $0\nu\beta\beta$ decay operators in the chiral EFT

• At $E \sim 100$ MeV: LNV $0\nu\beta\beta$ -decay operators are expressed in terms of nucleons, pions, and leptons, arranged in the order $(Q, m_{\pi}/\Lambda_{\chi})^{\nu}$,

$$\nu = 2A + 2L - 2 + \sum_{i} (\frac{n_f}{2} + d - 2 + n_e)_i$$



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A novel ab initio framework for nuclei: IM-GCM



The Framework of IM-GCM



- In-medium similarity renormalization group (IMSRG): capture dynamic correlations associated with high-energy few-particle, few- hole excitations
- **Projected generator coordinate method (PGCM)**: include the collective (static) correlations associated with pairing and deformation.

Emergence of island of inversion around N = 20





E.F. Zhou et al., arXiv:2410.23113 (2024)

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The NME in the lightest candidate nucleus ⁴⁸Ca

• Multi-reference in-medium generator coordinate method (IM-GCM)

JMY et al., PRL124, 232501 (2020)

• Valence-space shell model+IMSRG (VS-IMSRG)

A. Belley et al., PRL126, 042502 (2021)

• Coupled-cluster with singlets, doublets, and partial triplets (CCSDT1).





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Contribution of the contact transition operator



- A contact transition operator which could either enhance or quench the $0\nu\beta\beta$ decay, is needed to be promoted to LO to ensure renormalizibility. V. Cirigliano et al., PRL120, 202001 (2018)
- We determine the unknown LEC g_{ν}^{NN} of the contact operator, consistent with the employed chiral interaction (EM1.8/2.0), based on the synthetic data for the process $2n \rightarrow 2p + 2e^-$. V. Cirigliano et al., PRL126, 172002 (2021)
- The contact term turns out to enhance the NME for ⁴⁸Ca by 43(7)%, thus reducing the half-life $T_{1/2}^{0\nu}$ significantly. R. Wirth, JMY, H. Hergert, PRL127, 242502 (2021)





The true value of the NME can be written as

$$M^{0\nu} = M_k^{0\nu} + \epsilon_{\chi \rm EFT} + \epsilon_{\rm MBT} + \epsilon_{\rm OP} + \epsilon_{\rm EM},$$

where the posterior probability distribution (PPD) of an LEC sample to yield results for a set of calibration observables that match experimental data

$$PPD = \{ M_k^{0\nu}(\mathbf{c}) : \mathbf{c} \sim \mathcal{P}(\mathbf{c} | \text{calibration}) \}.$$

from which one finds the statistical error $\chi_{
m LEC}$,

- $\epsilon_{\chi \rm EFT}$: chiral expansion truncation on nuclear forces
- $\epsilon_{\rm MBT}$: approximation in many-body methods
- ϵ_{OP} : chiral expansion truncation on transition operators
- $\epsilon_{\rm EM}$: the error of the emulator

All the errors $\boldsymbol{\epsilon}$ are assumed to be normally distributed and mutually independent.

The error of EFT truncation on nuclear forces





- The NME converges with respect to the chiral expansion order χ of nuclear forces for candidate nuclei ⁴⁸Ca and ⁷⁶Ge.
- The EFT truncation error (evaluated using the BUQEYE method) is shrinking with the increase of χ expansion order ν .





- In the N2LO, we choose $\mu_{us} = m_{\pi}$ to eliminate all the terms depending on $\ln \frac{m_{\pi}^2}{\mu_{us}^2}$, and the LECs of the counterterms as $g_{\nu}^{\pi\pi} = -7.6 (36/5) \ln(\mu/m_{\rho})$, and $g_{\nu}^{\pi N} = 0$. V. Cirigliano, et al., PRC97, 065501 (2018)
- The NME for $^{76}{\rm Ge}$ converges with respect to the chiral expansion order ν of transition operators.

Quantification of the uncertainty in the NME of ⁷⁶Ge





- Our recommended value $M^{0\nu} = 2.60^{+1.28}_{-1.36}$.
- Together with the best half-life limit: $> 1.8 \times 10^{26}$ yr, it sets the upper limit $\langle m_{\beta\beta} \rangle = 187^{+205}_{-62}$ meV, and the sensitivity of the next-generation experiment $\langle m_{\beta\beta} \rangle = 22^{+24}_{-7}$ meV, covering almost the entire range of IO hierarchy.

A. Belley, JMY et al., PRL132, 182502 (2024)



- The charge-parity violation (CPV) (one of the three Sakharov's conditions) in the Standard Model are insufficient to account for the observed baryon asymmetry ($\eta \sim 10^{-9}$) of the universe.
- Hypothetical new sources of CPV, such as supersymmetry (SUSY), multi-Higgs models, and left-right (LR) symmetry, are expected to yield nonzero results in searches for atomic, hadronic, and leptonic electric dipole moments (EDMs).
- Searches for EDMs of diamagnetic atoms are helpful to determine the sources of CPV, constraining the LECs of PT-odd nuclear force.



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

$$egin{aligned} &\omega_{\pm}=rac{2\left(\mu B\pm dE
ight)}{\hbar}\ &\omega_{+}\!-\!\omega_{-}=rac{4dE}{\hbar} \end{aligned}$$

Atoms	$ d_A [imes 10^{-26}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	$< 7 imes 10^{-4}$	Graner et al., PRL116, 161601 (2016)
²²⁵ Ra	$< 5 imes 10^4$	Parker et al., PRL114, 233002 (2015)
²²⁵ Ra	$< 1.4 imes 10^3$	Bishof et al., PRC94, 025501 (2016)



Calculation of atomic EDM



• The atomic EDM d_A is mainly determined by nuclear Schiff moment

$$d_{A} \equiv \left\langle \Psi_{0}^{(at)} \middle| \hat{D}_{z} \middle| \Psi_{0}^{(at)} \right\rangle \simeq 2 \sum_{m \neq 0} \frac{\left\langle \Phi_{0}^{(at)} \middle| 4\pi e \sum_{i} \mathbf{S} \cdot \nabla \delta^{3}(R_{i}) \middle| \Phi_{m}^{(at)} \right\rangle \left\langle \Phi_{m}^{(at)} \middle| \hat{D}_{z} \middle| \Phi_{0}^{(at)} \right\rangle}{\mathcal{E}_{0}^{A} - \mathcal{E}_{m}^{A}},$$

where $|\Phi_0^{(at)}\rangle$ and $|\Phi_m^{(at)}\rangle$ denote the atomic ground state and excited states with $\mathcal{E}_0^A, \mathcal{E}_m^A$ being their energies.

• The results of relativistic coupled-cluster calculations for atoms: $^{129}\rm Xe$ $_{\rm Singh:2013},$ $^{199}\rm Hg$ $_{\rm Latha:2009},$ and $^{225}\rm Ra$ $_{\rm Singh:2015}$ are as follows

$$\begin{split} &d_A(^{129}\text{Xe}) = +0.336 \times 10^{-17} S(e \text{ fm}^3)^{-1}(e \text{ cm}), \\ &d_A(^{199}\text{Hg}) = -2.46 \times 10^{-17} S(e \text{ fm}^3)^{-1}(e \text{ cm}), \\ &d_A(^{225}\text{Ra}) = -6.79 \times 10^{-17} S(e \text{ fm}^3)^{-1}(e \text{ cm}). \end{split}$$

Nuclear Schiff moment



Nuclear Schiff moment N. Auerbach et al., PRL76, 4316 (1996)

$$S = \sum_{k \neq 0} \frac{\langle \Psi_0^{(N)} | \hat{S}_0 | \Psi_k^{(N)} \rangle \langle \Psi_k^{(N)} | \hat{V}_{PT} | \Psi_0^{(N)} \rangle}{E_0^N - E_k^N} + c.c. \quad \hat{S}_0 = \frac{1}{10} \sum_{\rho=1}^Z e\left(\hat{r}_\rho^2 - \frac{5}{3}R_c^2\right) \hat{z}_\rho$$

In the non-relativistic approximation,

$$\hat{V}_{PT}(\mathbf{r}_{12}) ~=~ g_{\pi NN} \sum_{i=0}^2 ar{g}_i \mathcal{V}^{(ext{PT-odd})}_lpha(\mathbf{r}_{12})$$

$$g_{\pi NN} - - \overrightarrow{\pi} - - \overline{g}_i$$

$$\begin{split} \mathcal{V}_{0}^{(\mathrm{PT-odd})}(\mathbf{r}_{12}) &= -\frac{m_{\pi}^{2}}{8\pi m_{N}} (\vec{\tau}_{1} \cdot \vec{\tau}_{2}) (\boldsymbol{\sigma}_{12}^{-} \cdot \hat{\mathbf{r}}_{12}) \frac{e^{-x}}{x} (1 + \frac{1}{x}), \\ \mathcal{V}_{1}^{(\mathrm{PT-odd})}(\mathbf{r}_{12}) &= +\frac{m_{\pi}^{2}}{16\pi m_{N}} \bigg[(\tau_{1x} + \tau_{2x}) (\boldsymbol{\sigma}_{12}^{-} \cdot \mathbf{r}_{12}) \\ &+ (\tau_{1x} - \tau_{2x}) (\boldsymbol{\sigma}_{12}^{+} \cdot \hat{\mathbf{r}}_{12}) \bigg] \frac{e^{-x}}{x} (1 + \frac{1}{x}), \\ \mathcal{V}_{2}^{(\mathrm{PT-odd})}(\mathbf{r}_{12}) &= -\frac{m_{\pi}^{2}}{8\pi m_{N}} (3\tau_{1x}\tau_{2x} - \vec{\tau}_{1} \cdot \vec{\tau}_{2}) (\boldsymbol{\sigma}_{12}^{-} \cdot \hat{\mathbf{r}}_{12}) \frac{e^{-x}}{x} (1 + \frac{1}{x}). \end{split}$$

Here, $\mathbf{r}_{12} \equiv \mathbf{r}_{1} - \mathbf{r}_{2}, \ \hat{\mathbf{r}}_{12} \equiv \mathbf{r}_{12} / r_{12}, \ x \equiv m_{\pi} r_{12}, \ \boldsymbol{\sigma}_{12}^{\pm} \equiv \boldsymbol{\sigma}_{1} \pm \boldsymbol{\sigma}_{2}. \end{split}$

The Schiff moment can be rewritten as: $S = g_{\pi NN} (a_0 \bar{g}_0 + a_1 \bar{g}_1 + a_2 \bar{g}_2)$.

Nuclear Schiff moments by different nuclear models



 The Schiff moment in particle-rotor model V. V. Flambaum & H. Feldmeier, PRC 101, 015502 (2020)

$$S\simeq rac{J}{J+1}eta_2eta_3^2ZA^{2/3}rac{\mathrm{keV}}{|\Delta E|}{ imes}10^{-4}\eta[\mathrm{efm}^3]$$

where η is a linear combination of \bar{g}_i .

 The heavy nucleus (large Z, A) with large β₂, β₃ and nearly-degenerate parity doublets (same spin, opposite parities) has a larger Schiff moment.



From atomic EDMs to LECs of PT-odd interactions



Latest data on atomic EDMs

$$\begin{split} |d_A(^{129}\text{Xe})| &\leq 1.4 \times 10^{-27}(e\,\text{cm}), \\ |d_A(^{199}\text{Hg})| &\leq 7.4 \times 10^{-30}(e\,\text{cm}), \\ |d_A(^{225}\text{Ra})| &\leq 1.4 \times 10^{-23}(e\,\text{cm}) \end{split}$$

N. Sachdeva et al., Phys. Rev. Lett. **123** (2019) 143003.
B. Graner, Y. Chen, E. G. Lindahl and B. R. Heckel, Phys. Rev. Lett. **116** (2016) 161601
[Erratum-ibid. **119** (2017) 119901].
M. Bishof et al., Phys. Rev. C **94** (2016) 025501.

Atomic calculation (RCC)

$$\begin{split} &d_A(^{129}\mathrm{Xe}) = 0.336\times 10^{-17}S(e\,\mathrm{fm^3})^{-1}(e\,\mathrm{cm}),\\ &d_A(^{199}\mathrm{Hg}) = -2.46\times 10^{-17}S(e\,\mathrm{fm^3})^{-1}(e\,\mathrm{cm}),\\ &d_A(^{225}\mathrm{Ra}) = -6.79\times 10^{-17}S(e\,\mathrm{fm^3})^{-1}(e\,\mathrm{cm}). \end{split}$$

Nuclear calculation (Skyrme EDF)

$$\begin{split} S(^{129}\text{Xe}) &= g_{\pi NN}(-0.008\bar{g}_0 - 0.006\bar{g}_1 - 0.009\bar{g}_2)(e\,\text{fm}^3),\\ S(^{199}\text{Hg}) &= g_{\pi NN}(+0.01\bar{g}_0 \pm 0.02\bar{g}_1 + 0.02\bar{g}_2)(e\,\text{fm}^3),\\ S(^{225}\text{Ra}) &= g_{\pi NN}(-1.5\bar{g}_0 + 6.0\bar{g}_1 - 4.0\bar{g}_2)(e\,\text{fm}^3), \end{split}$$

J. Engel et al., Prog. Part. Nucl. Phys. 71 (2013) 21

Constraints on the LECs of PT-odd NN interaction

 $\begin{array}{l} \text{for the case } a_1(^{199}\text{Hg}) = 0.02\\ & \bar{g}_0 \in [-0.78, 0.80] \times 10^{-8},\\ & \bar{g}_1 \in [-0.14, 0.14] \times 10^{-8},\\ & \bar{g}_2 \in [-0.48, 0.45] \times 10^{-8} \end{array}$ $\begin{array}{l} \text{for the case } a_1(^{199}\text{Hg}) = -0.02,\\ & \bar{g}_0 \in [-24, 23] \times 10^{-8},\\ & \bar{g}_1 \in [-5.5, 5.6] \times 10^{-8},\\ & \bar{g}_2 \in [-17, 17] \times 10^{-8}. \end{array}$

E. F. Zhou & JMY, IJMPE32, 2340011(2023)

Energy surfaces and density profile of ²²⁵Ra

- Extension of mutil-reference covariant density functional theory (MR-CDFT) to low-lying states of odd-mass nuclei with quadrupole-octupole deformations. E.F.
 Zhou, X.Y. Wu, JMY, PRC 109, 034305 (2024)
- Application to the nucleus ²²⁵Ra of candidate atom, showing strong octupole correlation.



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MR-CDFT for the spectrum of ²²⁵Ra





Schiff moment of ²²⁵Ra: impact of particle-number projection Schiff moment of ²²⁵Ra: impact of particle-number projection



J. Dobaczewski et al., PRL121, 232501 (2018)

- At the mean-field level, the values of *a_i* by the relaitivistic EDF PC-PK1 are consistent with those by the Skyrme EDFs.
- The restoration of particle numbers has 10% -20% impact on the structure factors *a_i*.



Summary and outlook



- Accurate nuclear matrix elements (NMEs) are crucial for designing and interpreting the experiments of high-precision measurements for new physics at low-energy scales, including the searches for $0\nu\beta\beta$ decay and atomic EDM.
- The existence of large uncertainty in the NMEs of phenomenological nuclear models mainly arisen from systematical uncertainty impacts the interpretation of the measurements.
- We developed a novel nuclear ab initio framework which allows us to determine the values of NMEs and their uncertainties using the operators derived consistently within the chiral EFT. We have successfully applied our method to compute the NMEs of $0\nu\beta\beta$ decay in light candidate nuclei. Its application to nuclear Schiff moment is more challenging, but it is on the way.
- Outlook: extension of ab initio methods for nuclear Schiff moments; reduction of uncertainties in the NMEs.



Collaborators

SYSU

C.R. Ding, C. F. Jiao, X. Zhang, E.F. Zhou

- MSU: H. Hergert, R. Wirth
- UNC: J. Engel, A. M. Romero

- TRIUMF: A. Belly, J. Holt
- TU Darmstadt: T. Miyagi
- Notre-Dame U: R. Stroberg
- UAM: B. Bally, T.Rodriguez

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