

Ab initio calculations for medium-mass nuclei and electromagnetic observables





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Low-Energy Electron Scattering for Nucleon and Exotic Nuclei @ Tohoku University (Oct. 31, 2024)

Collaborators



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EM observables can be used

- to investigate nuclear structure (shell structure, shape, ...)
- to test theories

To test our theories, we need:

- (precise) experimental data
- reasonable starting nuclear Hamiltonian(s)
- controllable many-body method(s)

higher-order contribution of EM operators (main focus of this talk)

 $egin{aligned} H|\Psi
angle &= E|\Psi
angle \ O_{
m EM}^{
m exp.} \sim \langle\Psi|\mathcal{O}_{
m EM}|\Psi
angle \end{aligned}$



Magnetic dipole moment:
$$\langle \mu \rangle = \sqrt{\frac{J}{(J+1)(2J+1)}} \langle J || \mu || J \rangle$$

Magnetic dipole operator:
$$\mu = \frac{e\hbar}{2m_p} \sum_i \left(g_i^l l_i + g_i^s \sigma_i\right)$$
 Point-nucleon approximation

Neighbors of doubly magic:
$$|J
anglepprox|{
m Core}:0^+
angle\otimes|j_p
angle,\;j_p=J$$

Schmidt limit

$$\langle \mu \rangle = \frac{e\hbar}{2m_p} \langle l_p j_p || g_i^l \boldsymbol{l}_i + g_i^s \boldsymbol{\sigma}_i || l_p j_p \rangle = j_p \left[g_l \mp (g_l - 2g_s) \frac{1}{2l_p + 1} \right], \ \left(j_p = l_p \pm \frac{1}{2} \right)$$

T. Schmidt 1937





Good agreement with data.

The deviation from the Schmidt value indicates how much the 0+ core is broken.



Ab initio IMSRG calculations

CP is included non-perturbatively!

A. Klose et al., Phys. Rev. C 99, 061301 (2019).



of ³⁶Ca. Compared to the USDA/B-EM1 calculations, the VS-IMSRG agrees with the dominance of the (620) partition for ³⁶Ca. However, the amount of the (522) partition that gives the core-polarization correction is a factor of 2 larger. The deviation is likely due to meson-exchange currents [39], which are not included in the present VS-IMSRG calculations, but are included indirectly through the effective *g* factors in the USDA/B-EM1 calculations.

A. R. Vernon et al., Nature 607, 260 (2022).



Nuclear ab initio calculation



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Nuclear many-body problem

- Green's function Monte Carlo
- No-core shell model
- Nuclear lattice effective field theory
- Self-consistent Green's function
- Coupled-cluster

...

- In-medium similarity renormalization group
- Many-body perturbation theory

Nuclear interaction from chiral EFT



Weinberg, van Kolck, Kaiser, Epelbaum, Glöckle, Meißner, Entem, Machleidt, ...

 $Q = p/\Lambda$ Lagrangian construction Two-nucleon force Three-nucleon force Four-nucleon force Chiral symmetry LO (Q⁰) Power counting NLO (Q²) Systematic expansion < | X N²LO (Q³) Unknown LECs Many-body interactions Ж. ... N³LO (Q⁴) Estimation of truncation error - |₄↓ | ★+ ★+ |++/1 |-★/1+ N⁴LO (Q⁵)

Figure is from E. Epelbaum, H. Krebs, and P. Reinert, Front. Phys. 8, 1 (2020).



Nuclear observables (EM properties, beta decay, ...) are measured through the interaction between a nucleus and external field.





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Nuclear observables (EM properties, beta decay, ...) are measured through the interaction between a nucleus and external field.



Chiral EFT allows us a systematic expansion for charge and current operators.

What about in heavier systems?

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Nuclear observables (EM properties, beta decay, ...) are measured through the interaction between a nucleus and external field.

Chiral EFT allows us a systematic expansion for charge and current operators.



$$r_{ch}^{2} = -\frac{6}{Z} \frac{1}{(4\pi)^{3/2}} \lim_{Q \to 0} \frac{d}{dQ^{2}} \int d\hat{Q} \tilde{\rho}(Q)$$

$$LO \ 2BC \ appear \ at \ Q^{1} \ order \ (N^{3}LO)$$

$$Q_{20} = -\frac{15}{8\pi} \lim_{Q \to 0} \frac{d^{2}}{dQ^{2}} \int d\hat{Q} Y_{20}(\hat{Q}) \tilde{\rho}(Q)$$

$$M_{10} = -i\frac{3}{8\pi} \lim_{Q \to 0} \frac{d}{dQ} \int d\hat{Q} \left\{ [\boldsymbol{Q} \times \nabla_{\boldsymbol{Q}}] Y_{10}(\hat{\boldsymbol{Q}}) \right\} \cdot \tilde{\boldsymbol{j}}(\boldsymbol{Q})$$

or
$$\boldsymbol{M} = -\frac{i}{2} \sqrt{\frac{3}{4\pi}} \lim_{Q \to 0} \nabla_{\boldsymbol{Q}} \times \tilde{\boldsymbol{j}}(\boldsymbol{Q})$$

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Magnetic dipole moments

Magnetic moment from IMSRG.

1.8/2.0 (EM) interaction (see talk by P. Arthuis)

Single-particle analytical limits do not always explain the experimental data.

A better agreements with IMSRG, but not perfect.

Suppression from many-body correlation



Magnetic dipole moments

Magnetic moment from IMSRG.

1.8/2.0 (EM) interaction (see talk by P. Arthuis)

Single-particle analytical limits do not always explain the experimental data.

A better agreements with IMSRG, but not perfect.

2BC globally improves the magnetic moments.

Enhancement from 2BC



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 $Fy(\Delta r)$

170

172

^AYb

174

176

Recent precise mass and laser spectroscopy measurements —> new physics M. Door et al., arXiv:2403.07792 $\nu^{A} - \nu^{A'} = K\mu_{A,A'} + F\delta\langle r^{2}\rangle_{A,A'} + G^{(2)}[\delta\langle r^{2}\rangle^{2}]_{A,A'} + G^{(4)}\delta\langle r^{4}\rangle_{A,A'} + \dots + (\text{new physics})$ 14 Expt. relative to $\delta(r^4)^{176, 174} = 7 \text{ fm}^4$ 12 Combination with the MCSM technique was essential. $\delta(r^4)^{A,A-2} [fm^4]$ N. Shimizu et al., Phys. Rev. C 103, 014312 (2021). See talk by T. Otsuka Precise atomic and nuclear theories are needed. 1.8/2.0 (EM), VS1 Ab initio 1.8/2.0 (EM), VS2 Expt. (α_{PTB} , fiducial) $\Delta N^2 LO_{GO}$, VS1 -O- Expt. (α_{PTR} , core holes) Extracted delta<r^4> 14 Expt. relative to $\delta(r^4)^{176, 174} = 7 \text{ fm}^4$ 12 Hamiltonian uncertainty sizable $\delta(r^4)^{A,A-2} \, [fm^4]$ Valence-space uncertainty small Small many-body uncertainty was estimated SV-mir Expt. (α_{PTB} , fiducial) Expt. (α_{PTB} , core holes)

Flat trend over the isotopes



In M. Door et al., arXiv:2403.07792, only the R_p^4 was computed.

4th moment of charge density: $R_{\rm ch}^4 = \frac{60}{F_{\rm ch}(0)} \lim_{q \to 0} \frac{d}{da^2} \frac{d}{da^2} F_{\rm ch}(q).$

Charge form factor:
$$F_{ch}(q) = e \sum_{i=1}^{A} \left\{ G_{i}^{E}(q^{2}) \left[1 - \frac{q^{2}}{8m^{2}} \right] j_{0}(x_{i}) - \frac{q^{2}}{2m^{2}} \left[G_{i}^{M}(q^{2}) - \frac{1}{2} G_{i}^{E}(q^{2}) \right] (\ell_{i} \cdot \sigma_{i}) \frac{j_{1}(x_{i})}{x_{i}} \right\},$$

 $x_{i} = q |\mathbf{r}_{i} - \mathbf{R}_{cm}|$ G^E and G^M are Sachs form factors
 $\mathbf{R}_{ch}^{4} = R_{n}^{4} + \frac{10}{2} \left(r_{n}^{2} R_{n}^{2} + \frac{N}{Z} r_{n}^{2} R_{n}^{2} \right) + \frac{5}{2m^{2}} \left(R_{n}^{2} + r_{n}^{2} + \frac{N}{Z} r_{n}^{2} \right) + r_{n}^{4} + \frac{N}{Z} r_{n}^{4} + R_{SO}^{4}$

$$\mathsf{R}_{ch}^4: \ \ R_{ch}^4 = R_p^4 + \frac{10}{3} \left(r_p^2 R_p^2 + \frac{N}{Z} r_n^2 R_n^2 \right) + \frac{5}{2m^2} \left(R_p^2 + r_p^2 + \frac{N}{Z} r_n^2 \right) + r_p^4 + \frac{N}{Z} r_n^4 + R_{SO}^4 r_n^2 + \frac{N}{Z} r_n^2 r_n^2 + \frac{N}{Z} r_n^2 r_n^2 r_n^2 + \frac{N}{Z} r_n^2 r_n$$

See also:

H. Kurasawa and T. Suzuki, Prog. Theor. Exp. Phys., 113D01 (2019). H. Kurasawa and T. Suzuki, Prog. Theor. Exp. Phys., 013D02 (2020). T. Suzuki, R. Danjo, T. Suda, Prog. Theor. Exp. Phys., 093D02 (2024).

4th moment of charge density

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The Rch4 operator looks like the 4-body operator —> $R_{ch}^4 = \frac{60}{F_{ch}(0)} \lim_{q \to 0} \frac{d}{dq^2} \frac{d}{dq^2} F_{ch}(q)$.

Gaussian process:

Derivative is also a Gaussian process





4th moment of charge density





The correlation is strong for Rch2 and Rn2, while it is weak for Rskin

Uncertainty quantification is not completed yet.

Summary



Magnetic dipole moments

♦ For most of doubly-closed shell nuclei +/- 1 systems, the 2BC improves the agreements.

4th moment of charge density of ²⁰⁸Pb

Strong correlation with ms charge and neutron radii

Future works:

- 2BC effect with finite momentum transfer Q
- ◆ Exploring how we can leverage the correlation of R_{ch}⁴ and the other observables.
- Uncertainty quantification

Backup slides



Normal ordering wrt a single Slater determinant

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Initial Hamiltonian is expressed with respect to nucleon vacuum

$$H = \sum_{pq} t_{pq} a_p^{\dagger} a_q + \frac{1}{4} \sum_{pqrs} V_{pqrs} a_p^{\dagger} a_q^{\dagger} a_s a_r + \frac{1}{36} V_{pqrstu} a_p^{\dagger} a_q^{\dagger} a_r^{\dagger} a_u a_t a_s$$

Hamiltonian normal ordered with respect to a single Slater determinant

$$H = E_0 + \sum_{pq} f_{pq} \{a_p^{\dagger} a_q\} + \frac{1}{4} \sum_{pqrs} \Gamma_{pqrs} \{a_p^{\dagger} a_q^{\dagger} a_s a_r\} + \frac{1}{36} W_{pqrstu} \{a_p^{\dagger} a_q^{\dagger} a_r^{\dagger} a_u a_t a_s\}$$

$$E_{0} = \sum_{pq} t_{pq} \rho_{pq} + \frac{1}{2} \sum_{pqrs} V_{pqrs} \rho_{pr} \rho_{qs} + \frac{1}{6} \sum_{pqrstu} V_{pqrstu} \rho_{ps} \rho_{qt} \rho_{ru}, \quad \Gamma_{pqrs} = V_{pqrs} + \sum_{tu} V_{pqtrsu} \rho_{tu}$$

$$f_{pq} = t_{pq} + \sum_{rs} V_{prqs} \rho_{rs} + \frac{1}{2} \sum_{rstu} V_{prsqtu} \rho_{rt} \rho_{su}, \qquad \qquad W_{pqrstu} = V_{pqrstu}$$

• Normal ordered two-body (NO2B) approximation: $\frac{1}{4} \sum_{pqrs} \Gamma_{pqrs} \{a_p^{\dagger} a_q^{\dagger} a_s a_r\}$

Model-space convergence



NN+3N Hamiltonian (harmonic oscillator basis)

Parameters:

hw

- emax=max(2n+I)*
- ◆ E_{3max}=max(e₁+e₂+e₃).

As e_{max} and E_{3max} increases, the observable should not depend on all the parameters.

*Equivalent to (number of major shells)+1



E_{3max} convergence in heavy nuclei





[S. Binder et al., Phys. Rev. C 87, 021303 (2013).]

TM, S. R. Stroberg, P. Navrátil, K. Hebeler, and J. D. Holt, Phys. Rev. C 105, 014302 (2022).



Radii





Convergence of ²⁰⁹Bi





$$\begin{split} E(L_{\text{eff}}) &= E_{\infty} + A_{\infty} \exp(-2k_{\infty}L_{\text{eff}}) \\ L_{\text{eff}} &= \sqrt{\frac{\sum_{nl} n_{nl}^{\text{occ}} a_{nl}^2}{\sum_{nl} n_{nl}^{\text{occ}} \kappa_{nl}^2}}, \ \kappa_{nl}^2 \approx \frac{a_{nl}^2}{2b^2(N_l + 7/2)} \\ b^2 &= \frac{\hbar}{m\omega} \\ N_l &= \begin{cases} e_{\max} & e_{\max} + l \equiv 0 \pmod{2} \\ e_{\max} - 1 & e_{\max} + l \equiv 1 \pmod{2} \\ n_{nl}^{\text{occ}} : \text{occupation number of an orbit specified by } n \text{ and } l \\ a_{nl} : (n+1)\text{-th zero of the spherical Bessel function} \end{split}$$



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Magnetic moments of In isotopes



VS-IMSRG(2), 1.8/2.0 (EM), emax=14, E3max=24, hw = 16 MeV



2B contribution with the simplest limit



Expectation value: $\langle J||\mu||J
angle$

The simplest limit:
$$|JM\rangle = [|j_1 \dots j_{A-1} : 0^+\rangle \otimes |j_p m_p\rangle] \delta_{j_p J} \delta_{m_p M}$$

The expectation value depends a particle in the core and last unpaired particle.

$$\begin{split} J||\mu||J\rangle &\approx \delta_{Jj_p} \sum_{q \in \text{core}} \langle p0: j_p ||\mu_{pq}||p0: j_p \rangle \\ &= \delta_{Jj_p} \sum_{q \in \text{core}} \sum_{I} \frac{2I+1}{(2j_p+1)(2j_q+1)} \langle ((pq)I, q: j_p ||\mu_{pq}||(pq)I, q: j_p \rangle \\ &= \delta_{Jj_p} \sum_{q \in \text{core}} \sum_{I} \frac{2I+1}{2j_q+1} (-1)^{j_p+j_q+I+1} \left\{ \begin{array}{cc} j_p & I & j_q \\ I & j_p & 1 \end{array} \right\} \langle pq: I||\mu||pq: I \rangle \end{split}$$

2B contribution with the simplest limit



The simplest limit:
$$|JM\rangle = [|j_1 \dots j_{A-1} : 0^+\rangle \otimes |j_p m_p\rangle] \delta_{j_p J} \delta_{m_p M}$$

A simpler expression:

$$\begin{split} \langle \mu \rangle &\sim \sum_{q \in \text{core}} \langle pq | \bar{\mu} | pq \rangle \\ \langle pq | \bar{\mu} | pq \rangle &= \delta_{Jj_p} \sqrt{\frac{1}{2J+1}} \mathcal{C}_{J0J}^{J1J} \sum_{I} \frac{2I+1}{2j_q+1} (-1)^{j_p+j_q+I+1} \left\{ \begin{array}{c} j_p & I & j_q \\ I & j_p & 1 \end{array} \right\} \\ &\times \frac{\sqrt{2I+1}}{\mathcal{C}_{J+m_q0J+m_q}^{I1I}} \left[\mathcal{C}_{Jm_qJ+m_q}^{j_p j_q I} \right]^2 \frac{1}{1+\delta_{n_p n_q} \delta_{l_p l_q} \delta_{j_p j_q} \delta_{t_{z,p} t_{z,q}}} \langle pq | \mu | pq \rangle \end{split}$$

Test of input M1 operator matrix elements

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NCSM vs Faddeev

NCSM requires the M1 operator, which can also be used in IMSRG calculations.

Faddeev results are obtained from the normalization of the magnetic form factor.

M1 matrix elements are correctly implemented!

R. Seutin et al., arXiv: 2308.00136.





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Nuclear observables (EM properties, beta decay, ...) are measured through the interaction between a nucleus and external field.

Chiral EFT allows us a systematic expansion for charge and current operators.



Is ⁴⁰Ca magic?

2BC makes agreement worse.

Activating the ⁴⁰Ca core explains the magnetic moments better

The radii are not explained. Further investigations are needed!



$$- s_{1/2}d_{3/2}f_{7/2}p_{3/2}(\beta = 3) - pf$$

$$- s_{1/2}d_{3/2}f_{7/2}p_{3/2}(\beta = 4)$$



VS-IMSRG(2), 1.8/2.0 (EM) TM et al., Phys. Rev. Lett. 132, 232503 (2024).



Mass dependence of 2B contribution



The size of 2BC contribution is larger in heavier systems.



Mass dependence of 2B contribution

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The size of 2BC contribution is larger in heavier systems.

The simplest configuration limit is 0⁺ core + 1 particle (or hole) $\langle J||\mu||J\rangle \sim \sum_{q\in \text{core}} \sum_{I} f(j_p, j_q, I) \langle pq: I||\mu||pq: I\rangle$





The peak position moves to larger R for heavier systems.

TM et al., Phys. Rev. Lett. 132, 232503 (2024).

4th moment of charge density

See also: H. Kurasawa and T. Suzuki, Prog. Theor. Exp. Phys., 113D01 (2019). H. Kurasawa and T. Suzuki, Prog. Theor. Exp. Phys., 013D02 (2020). T. Suzuki, R. Danjo, T. Suda, Prog. Theor. Exp. Phys., 093D02 (2024).

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