

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

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

To test our theories, we need:

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

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

 $H|\Psi\rangle = E|\Psi\rangle$ $O_{\rm EM}^{\rm exp.} \sim \langle \Psi | {\cal O}_{\rm EM} | \Psi \rangle$

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

Magnetic dipole operator: $\bm{\mu} = \frac{1}{2m_n}\sum_{i,j} (g_i \bm{\iota}_i + g_i \bm{\sigma}_i)$ Point-nucleon approximation

Neighbors of doubly magic:
$$
|J\rangle \approx |\text{Core}:0^+\rangle \otimes |j_p\rangle
$$
, $j_p = J$

Schmidt limit

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

T. Schmidt 1937

Good agreement with data.

 \rightarrow 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 ${}^{36}Ca$. Compared to the USDA/B-EM1 calculations, the VS-IMSRG agrees with the dominance of the (620) partition for ${}^{36}Ca$. 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

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, …

- Lagrangian construction
	- **← Chiral symmetry**
	- **← Power counting**
- Systematic expansion
	- **← Unknown LECs**
	- ✦ Many-body interactions
	- **← Estimation of truncation error**

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 Q¹ order (N³LO)

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

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

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

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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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 AYb

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Recent precise mass and laser spectroscopy measurements —> new physics M. Door et al., arXiv:2403.07792 $\nu^{A} - \nu^{A'} = K \mu_{A,A'} + F \delta \langle r^{2} \rangle_{A,A'} + G^{(2)} [\delta \langle r^{2} \rangle^{2}]_{A,A'} + G^{(4)} \delta \langle r^{4} \rangle_{A,A'} + \cdots +$ (new physics) 14 Expt. relative to $\delta \langle r^4 \rangle^{176, 174} = 7$ fm⁴ 12 Combination with the MCSM technique was essential. $\delta(r^4)^{A,A-2}$ [fm⁴]
o ∞ b ∞ N. Shimizu et al., Phys. Rev. C 103, 014312 (2021). See talk by T. OtsukaPrecise atomic and nuclear theories are needed. 1.8/2.0 (EM), VS1 Ab initio 1.8/2.0 (EM), VS2 Expt. (α_{PTB}) fiducial) Δ N²LO_{GO}, VS1 $\overline{\mathbf{O}}$ Expt. (α_{PTB} , core holes) \triangle Extracted delta $\leq r^4$ 14 Expt. relative to $\delta \langle r^4 \rangle^{176,174} = 7$ fm⁴ 12 ✤ Hamiltonian uncertainty sizable $\delta(r^4)^{A.A-2}$ [fm⁴] 10 **❖ Valence-space uncertainty small ★ Small many-body uncertainty was estimated** SV-mir Expt. (α _{PTB}, fiducial) $-Q-$ Expt. (α_{PTB} , core holes) $Fy(\Delta r)$ ✤ Flat trend over the isotopes 170 172 174 176

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

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

Change form factor:

\n
$$
F_{\text{ch}}(q) = e \sum_{i=1}^{A} \left\{ G_i^E(q^2) \left[1 - \frac{q^2}{8m^2} \right] j_0(x_i) - \frac{q^2}{2m^2} \left[G_i^M(q^2) - \frac{1}{2} G_i^E(q^2) \right] (\ell_i \cdot \sigma_i) \frac{j_1(x_i)}{x_i} \right\},
$$
\n
$$
x_i = q | \mathbf{r}_i - \mathbf{R}_{\text{cm}} | \qquad \text{G}^E \text{ and } \text{G}^M \text{ are Sachs form factors}
$$
\n
$$
R_{\text{ch}}^4: \quad R_{\text{ch}}^4 = R_p^4 + \frac{10}{3} \left(r_p^2 R_p^2 + \frac{N}{Z} r_n^2 R_n^2 \right) + \frac{5}{2m^2} \left(R_p^2 + r_p^2 + \frac{N}{Z} r_n^2 \right) + r_p^4 + \frac{N}{Z} r_n^4 + R_{\text{SO}}^4
$$

See also:

H. Kurasawa and T. Suzuki, Prog. Theor. Exp. Phys., 013D02 (2020). ₁₇ H. Kurasawa and T. Suzuki, Prog. Theor. Exp. Phys., 113D01 (2019). 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 $_{19}$

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:

- \rightarrow 2BC effect with finite momentum transfer Q
- \triangle 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

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

✦ Hamiltonian normal ordered with respect to a single Slater determinant

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

$$
E_0 = \sum_{pq} t_{pq} \rho_{pq} + \frac{1}{2} \sum_{pqrs} V_{pqrs} \rho_{pr} \rho_{qs} + \frac{1}{6} \sum_{pqrstu} V_{pqrstu} \rho_{ps} \rho_{qt} \rho_{ru}, \quad \Gamma_{pqrs} = V_{pqrs} + \sum_{tu} V_{pqtrsu} \rho_{tu}
$$

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

A Normal ordered two-body (NO2B) approximation: $\frac{1}{4}\sum \Gamma_{pqrs}\{a^\dagger_p a^\dagger_q a_s a_r\}$ pq $pqrs$

Model-space convergence

NN+3N Hamiltonian (harmonic oscillator basis)

Parameters:

✦ hw

- \triangle emax=max(2n+l)*
- \triangle E_{3max}=max(e₁+e₂+e₃).

As emax and E3max increases, the observable should not depend on all the parameters.

*Equivalent to (number of major shells)+1

E3max convergence in heavy nuclei

NO2B approximation error \sim a few % [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

$$
E(L_{\text{eff}}) = E_{\infty} + A_{\infty} \exp(-2k_{\infty}L_{\text{eff}})
$$

\n
$$
L_{\text{eff}} = \sqrt{\frac{\sum_{nl} n_{nl}^{\text{occ}} a_{nl}^2}{\sum_{nl} n_{nl}^{\text{occ}} \kappa_{nl}^2}}, \ \kappa_{nl}^2 \approx \frac{a_{nl}^2}{2b^2(N_l + 7/2)}
$$

\n
$$
b^2 = \frac{\hbar}{m\omega}
$$

\n
$$
N_l = \begin{cases} e_{\text{max}} & e_{\text{max}} + l \equiv 0 \pmod{2} \\ e_{\text{max}} - 1 & e_{\text{max}} + l \equiv 1 \pmod{2} \\ n_{nl}^{\text{occ}} : \text{occupation number of an orbit specified by } n \text{ and } l \\ a_{nl} : (n + 1)\text{-th zero of the spherical Bessel function} \end{cases}
$$

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: $\langle J||\mu||J\rangle$

$$
\text{The simplest limit:} \hspace{.2cm} |JM\rangle = [|j_1\ldots j_{A-1}:0^+\rangle \otimes |j_p m_p\rangle]\delta_{j_pJ}\delta_{m_pM}
$$

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

$$
J||\mu||J\rangle \approx \delta_{Jj_p} \sum_{q \in \text{core}} \langle p0 : j_p || \mu_{pq} || p0 : j_p \rangle
$$

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

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:

$$
\langle \mu \rangle \sim \sum_{q \in \text{core}} \langle pq|\bar{\mu}|pq \rangle
$$

$$
\langle pq|\bar{\mu}|pq \rangle = \delta_{Jj_p} \sqrt{\frac{1}{2J+1}} C_{J0J}^{J1J} \sum_{I} \frac{2I+1}{2j_q+1} (-1)^{j_p+j_q+I+1} \left\{ \begin{array}{ll} j_p & I & j_q \\ I & j_p & 1 \end{array} \right\}
$$

$$
\times \frac{\sqrt{2I+1}}{C_{J+m_q0J+m_q}^{I1I}} \left[C_{Jm_qJ+m_q}^{j_pj_qI} \right]^2 \frac{1}{1+\delta_{n_pn_q}\delta_{l_pl_q}\delta_{j_pj_q}\delta_{t_{z,p}t_{z,q}}} \langle pq|\mu|pq \rangle
$$

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.

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.

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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!

$$
- \bullet \quad s_{1/2} d_{3/2} f_{7/2} p_{3/2} (\beta = 3) \quad - \bullet \quad \text{pf}
$$
\n
$$
- \bullet \quad s_{1/2} d_{3/2} f_{7/2} p_{3/2} (\beta = 4)
$$
\n
$$
0.3 \rightarrow \quad \text{p}
$$

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Mass dependence of 2B contribution

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

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

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) $\langle J||\mu||J\rangle \sim \sum \int f(j_p, j_q, I) \langle pq : I||\mu||pq : I\rangle$ $q \in \text{core}$ I

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).

Adv Sale Links

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

$$
\begin{aligned} \text{Change form factor:} \quad & F_{\text{ch}}(q) = e \sum_{i=1}^{A} \left\{ G_{i}^{E}(q^{2}) \left[1 - \frac{q^{2}}{8m^{2}} \right] j_{0}(x_{i}) - \frac{q^{2}}{2m^{2}} \left[G_{i}^{M}(q^{2}) - \frac{1}{2} G_{i}^{E}(q^{2}) \right] (\boldsymbol{\ell}_{i} \cdot \boldsymbol{\sigma}_{i}) \frac{j_{1}(x_{i})}{x_{i}} \right\}, \\ & x_{i} = q | \boldsymbol{r}_{i} - \boldsymbol{R}_{\text{cm}} | \qquad \qquad \mathsf{G}^{\text{E}} \text{ and } \mathsf{G}^{\text{M}} \text{ are Sachs form factors} \\ \text{Re}^{\text{4}} \text{Re}^{\text{4}} & = R_{p}^{4} + \frac{10}{3} \left(r_{p}^{2} R_{p}^{2} + \frac{N}{Z} r_{n}^{2} R_{n}^{2} \right) + \frac{5}{2m^{2}} \left(R_{p}^{2} + r_{p}^{2} + \frac{N}{Z} r_{n}^{2} \right) + r_{p}^{4} + \frac{N}{Z} r_{n}^{4} + R_{\text{SO}}^{4} \\ & \xrightarrow{R_{\text{ch}}^{2} = \frac{1}{2} \sum_{i=1}^{A} \left(\frac{1 + \tau_{i}}{2} \right) | \boldsymbol{r}_{i} - \boldsymbol{R}_{\text{cm}} |^{2}, \qquad R_{\text{SO}}^{4} = \frac{2}{m^{2} Z} \sum_{i=1}^{A} \left[\left(\frac{1 + \tau_{i}}{2} \right) \left(\mu_{p} - \frac{1}{2} \right) + \left(\frac{1 - \tau_{i}}{2} \right) \mu_{n} \right] \left(\boldsymbol{\ell}_{i} \cdot \boldsymbol{\sigma}_{i} \right) | \boldsymbol{r}_{i} - \boldsymbol{R}_{\text{cm}} |^{2} } \\ & \xrightarrow{R_{\text{H}}^{4} = \frac{1}{2} \sum_{i=1}^{A} \left(\frac{1 + \tau_{i}}{2} \right) | \boldsymbol{r}_{i} - \boldsymbol{R}_{\text{cm}} |^{2}, \qquad R_{\text{SO}}^{4} = \frac{2}{m^{2} Z} \sum_{i=1}^{A} \left[\left(\frac
$$

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