



Ab Initio Approach to Superallowed Fermi Transitions

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Superallowed Fermi Transitions

 $0^+ \rightarrow 0^+$ transitions: most stringent constraint on V_{ud} from corrected (parameterized) lifetime



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Nuclear structure theory

Isospin symmetry correction

dominates uncertainty in medium/heavy nuclei (and simple operator to calculate)

Progress of Ab Initio Theory Since 2010

2010: Limited capabilities for 3N forces; ¹⁶O heaviest



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Ab Initio Approach to Nuclear Structure

Aim of modern nuclear theory: develop unified *first-principles* picture of structure and reactions

(Approximately) solve nonrelativistic Schrödinger equation

 $H\psi_n = E_n\psi_n$



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Chiral Effective Field Theory

- Consistent treatment of 2N, 3N, 4N, ... forces
- Electroweak physics

Quantifiable uncertainties





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Valence-Space IMSRG

Explicitly construct unitary transformation from sequence of rotations

$$U = e^{\Omega} = e^{\eta_n} \dots e^{\eta_1} \quad \eta = \frac{1}{2} \arctan\left(\frac{2H_{\text{od}}}{\Delta}\right) - \text{h.c.}$$
$$\tilde{H} = e^{\Omega} H e^{-\Omega} = H + [\Omega, H] + \frac{1}{2} [\Omega, [\Omega, H]] + \cdots$$

All operators truncated at two-body level IMSRG(2) **IMSRG(3)** in progress

Step 1: Decouple core



Tsukiyama, Bogner, Schwenk, PRC 2012 Morris, Parzuchowski, Bogner, PRC 2015

Can we achieve accuracy of large-space methods?

Valence-Space IMSRG

Explicitly construct unitary transformation from sequence of rotations

$$U = e^{\Omega} = e^{\eta_n} \dots e^{\eta_1} \quad \eta = \frac{1}{2} \arctan\left(\frac{2H_{\text{od}}}{\Delta}\right) - \text{h.c.}$$
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All operators truncated at two-body level IMSRG(2) IMSRG(3) in progress

Tsukiyama, Bogner, Schwenk, PRC 2012 Morris, Parzuchowski, Bogner, PRC 2015



 $\underbrace{\tilde{\Psi}_n | P\tilde{H}P | \tilde{\Psi}_n \rangle \approx \langle \Psi_i | H | \Psi_i \rangle$

 $|\Phi_0\rangle = |^{16}O\rangle$

Valence-Space IMSRG

Explicitly construct unitary transformation from sequence of rotations

$$U = e^{\Omega} = e^{\eta_n} \dots e^{\eta_1} \quad \eta = \frac{1}{2} \arctan\left(\frac{2H_{\text{od}}}{\Delta}\right) - \text{h.c.}$$

$$\tilde{H} = e^{\Omega}He^{-\Omega} = H + [\Omega, H] + \frac{1}{2} \left[\Omega, [\Omega, H]\right] + \cdots$$

$$\tilde{\mathcal{O}} = e^{\Omega}\mathcal{O}e^{-\Omega} = \mathcal{O} + [\Omega, \mathcal{O}] + \frac{1}{2} \left[\Omega, [\Omega, \mathcal{O}]\right] + \cdots$$

$$\text{Step 1: Decouple core}$$

$$\text{Step 2: Decouple valence space}$$

$$\text{Step 3: Decouple additional operators}$$

$$\tilde{\Psi}_n | P\tilde{H}P | | \tilde{\Psi}_n \rangle \approx \langle \Psi_i | H | \Psi_i \rangle$$

$$\langle \tilde{\Psi}_n | P\tilde{M}_{0\nu}P | | \tilde{\Psi}_n \rangle \approx \langle \Psi_i | M_{0\nu} | \Psi_i \rangle$$

$$\text{Careful benchmarking essential}$$

$\langle P H P angle$	$\langle P H Q\rangle \to 0$
$\langle Q H P angle ightarrow 0$	$\langle Q H Q angle$

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Aim of modern nuclear theory: develop unified *first-principles* picture of structure and reactions

(Approximately) solve nonrelativistic Schrödinger equation



Extends ab initio to scope of traditional nuclear shell model

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(Approximately) solve nonrelativistic Schrödinger equation





Methods Exact up to Truncations

Single-particle basis $e_{\max} = 2n + l$

X Storage limits of 3N forces $e_1 + e_2 + e_3 \leq E_{3\max}$

Many-body operators: e.g., CCSD(T), IMSRG(2)

nitio Goes Global!

Long considered the domain of DFT or shell model

Ab initio calculations of ~700 nuclei from He to Fe!



Input Hamiltonians fit to A=2,3,4 – not biased towards known data

Apply to proton/neutron driplines separation energies?

% TRIUMF Dripline Predictions to Medium Mass Region

Predictions of proton and neutron driplines from first principles



Known drip lines predicted within uncertainties (artifacts at shell closures)

Ab initio guide for neutron-rich driplines

Progress of Ab Initio Theory Since 2010

2010: Limited capabilities for 3N forces; ¹⁶O heaviest



Tremendous progress in ab initio reach, largely due to polynomially scaling methods!

Calculate essentially all properties all of nuclei... up to N, Z ~ 50 54 2022 50 Z=50 Key Limitation 46 42 **3NF matrix element storage** Z=40 38 $e_1 + e_2 + e_3 \le E_{3\max}$ 34 N=82 30 Ν Z=28 26 22 Z=20 **2010** 18 2013 N=50 14 2016 10 2019 2022

N

Ab Initio Calculations of Heavy Nuclei

Limited by typical memory/node: $e_1 + e_2 + e_3 \leq E_{3max}$





Convergence of N=82 Gap

Size of N=70 gap well converged at E_{3max}=28 for neutron-rich Sn, In, Cd!



Convergence in Heavy Nuclei: ²⁰⁸Pb

Previous limit, no hope of convergence in ²⁰⁸Pb g.s. energy...



Convergence in Heavy Nuclei: ²⁰⁸Pb

Previous limit, no hope of convergence in ²⁰⁸Pb g.s. energy

Improved $E_{3\max} = 18 \rightarrow 28$ clear convergence



First converged ab initio calculation of ²⁰⁸Pb!

Recalibrating Ab Initio Progress

Rapid progress in ab initio reach, due to valence-space approach... up to...



Major Questions in Nuclear Structure





Nuclear skins/halos/clusters

Limits of existence + formation/evolution of magic numbers



²H ³H ⁴He ⁴He ³H ⁴He ³H ⁴He ³H ⁴He ³H ³H ⁴He ⁴He ³H ⁴He ³H ⁴He ⁵H ⁵H



Heavy Nuclei + r-process

Continuum and nuclear reactions

Infinite matter/Neutron stars

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Searches for BSM Physics



Neutrinoless double beta decay



Dark matter direct detection



Superallowed Fermi transitions







Neutrino scattering

Symmetry-violating moments

Atomic theory

∂TRIUMF

Searches for BSM Physics



Neutrinoless double beta decay



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Neutrino scattering

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Atomic theory



Two-Body Currents for Gamow-Teller Transitions and g_A Quenching



LETTERS https://doi.org/10.1038/s41567-019-0450-7

nature physics

Discrepancy between experimental and theoretical β-decay rates resolved from first principles

P. Gysbers^{1,2}, G. Hagen^{3,4*}, J. D. Holt¹, G. R. Jansen^{3,5}, T. D. Morris^{3,4,6}, P. Navrátil¹, T. Papenbrock^{3,4}, S. Quaglioni⁷, A. Schwenk^{8,9,10}, S. R. Stroberg^{1,11,12} and K. A. Wendt⁷

Beta-Decay "Puzzle": Quenching of g_A

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Long-standing problem in weak decays: experimental values systematically smaller than theory $M_{\rm GT} = g_A \langle f | \mathcal{O}_{\rm GT} | i \rangle \ \mathcal{O}_{\rm GT} = \mathcal{O}_{\sigma\tau}^{\rm 1b} + \mathcal{O}_{2BC}^{\rm 2b}$ Using $g_A^{\mathrm{eff}} pprox 0.77 imes g_A^{\mathrm{free}}$ agrees with data π T(GT) 1.0 Missing Wavefunction correlationsEFFECTIVE FREE-NUCLEON 8.0 Renormalized VS operator? EXPERIMENT 0.6 Naglected two-body currents? 0.4 Model-space truncations? ۲ 0.2 Large M_{GT} **Explore in ab initio framework** in sd-shel 0.0 .2 0.6 0.8 0.8 0.4 THEORY Brown, Wildenthal (1985)

TRIUMF Large-Scale Efforts for Ab Initio GT Transitions

Calculate large GT matrix elements

$$M_{\rm GT} = g_A \left\langle f | \mathcal{O}_{\rm GT} | i \right\rangle$$
$$\mathcal{O}_{\rm GT} = \mathcal{O}_{\sigma\tau}^{\rm 1b} + \mathcal{O}_{2BC}^{\rm 2b}$$

- Light, medium, and heavy regions
- Benchmark different ab initio methods
- Range of NN+3N forces
- Consistent inclusion of 2BC

NUCLEAR PHYSICS

Beta decay gets the ab initio treatment

One of the fundamental radioactive decay modes of nuclei is β decay. Now, nuclear theorists have used first-principles simulations to explain nuclear β decay properties across a range of light- to medium-mass isotopes, up to ¹⁰⁰Sn.



GT Transitions in Light Nuclei + ¹⁰⁰Sn

NCSM in light nuclei, **CC** calculations of GT transition in ¹⁰⁰Sn from different forces



Large quenching from correlations in ¹⁰⁰Sn

Addition of 2BC further quenches; reduces spread in results

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Solution to g_A-Quenching Problem

VS-IMSRG calculations throughout sd and pf shells



Ab initio calculations across the chart explain data with unquenched g_A Refine results: improvements in forces and many-body methods

Complete GT Picture: Light to 100Sn

Ab initio calculations throughout sd and pf shells



Ab initio calculations across the chart explain data with unquenched g_A Including p-shell: q=0.99(21)



Ab Initio Approach to ISB and Superallowed $0^+ \rightarrow 0^+$



Editors' Suggestion

Testing isospin symmetry breaking in *ab initio* nuclear theory

M. S. Martin, S. R. Stroberg, J. D. Holt, and K. G. Leach Phys. Rev. C **104**, 014324 – Published 30 July 2021

Explore ab initio isospin symmetry breaking

Webaric mass multiplet equation (IMME) relates energies between members of multiplets

 $E(T_z) = a + bT_z + cT_z^2$

≈ TRIUMF



Compare ab initio with experimental determination of IMME coefficients to gauge success Calculate all nuclei relevant for superallowed transitions; 2 NN+3N forces

Ab initio IMME: bare vs IMSRG

Isobaric mass multiplet equation (IMME) relates energies between members of multiplets

$$E(T_z) = a + bT_z + cT_z^2$$



Bands: normal ordering reference dependence

Overall little effect/improvement when applying IMSRG transformation for both b, c

Ab initio IMME: bare vs IMSRG

Isobaric mass multiplet equation (IMME) relates energies between members of multiplets $E(T_z) = a + bT_z + cT_z^2$

Compare VS-IMSRG b, c coefficients to HF and results from a uniform charged sphere



Systematics already largely captured (better) by mean field or charged sphere Ambiguous results... turn to superallowed Fermi transitions

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Compton amplitude in the NCSM

- Nuclear matrix elements for γW -box
 - 1) Express currents in momentum space
 - 2) Multipole expansion of current operators
 - 3) Connect currents to effective one-body operators



Lanczos continued fractions

$$T_{3}(q_{0},Q^{2}) = -4\pi i \frac{q_{0}}{q} \sqrt{M_{i}M_{f}} \sum_{J=1}^{\infty} (2J+1)$$

$$\times \left\langle A\lambda_{f}J_{f}M_{f} \right| \left[T_{J0}^{mag}(q) \frac{G(M_{f}+q_{0}+i\epsilon)}{G(M_{f}+q_{0}+i\epsilon)} T_{J0}^{5,el}(q) + T_{J0}^{el}(q) \frac{G(M_{f}+q_{0}+i\epsilon)}{G(M_{f}-q_{0}+i\epsilon)} T_{J0}^{5,mag}(q) + T_{J0}^{5,mag}(q) \frac{G(M_{i}-q_{0}+i\epsilon)}{G(M_{i}-q_{0}+i\epsilon)} T_{J0}^{el}(q) + T_{J0}^{5,el}(q) \frac{G(M_{i}-q_{0}+i\epsilon)}{G(M_{i}-q_{0}+i\epsilon)} T_{J0}^{mag}(q) \right] \left| A\lambda_{i}J_{i}M_{i} \right\rangle$$

Courtesy, M. Gennari

$G(M_i - q_0 + i\epsilon)$ terms: T = 0 EM current



Courtesy, M. Gennari

Preliminary

$G(M_i - q_0 + i\epsilon)$ terms: T = 1 EM current



Courtesy, M. Gennari

Preliminary

Preliminary

$G(M_f + q_0 + i\epsilon)$ terms: T = 0 EM current

50 ${^{10}C|T_{J=2}^{mag, 5}G_{nuc}(E_i + q_0)T_{J=2, T=0}^{el}|^{10}B}$ $({}^{10}C|T_{J=1}^{el, 5}G_{nuc}(E_i + q_0)T_{J=1, T=0}^{mag}|{}^{10}B)$ 40 (MeV) 30 20 10 0 100 200 300 100 200 0 300 0 q (MeV) q (MeV) -1e-04 -5e-05 0e+00 5e-05 1e-04 -5e-05 0e+00 5e-05 1e-04 Courtesy, M. Gennari

$G(M_f + q_0 + i\epsilon)$ terms: T = 1 EM current

Courtesy, M. Gennari

Preliminary

$G(M_f + q_0 + i\epsilon)$ terms: T = 1 EM current

Courtesy, M. Gennari

Preliminary

Comment on many-body convergence

Preliminary

Next step: implement in VS-IMSRG for all superallowed nuclei

Courtesy, M. Gennari

Superallowed Fermi Transitions

 $0^+ \rightarrow 0^+$ transitions: most stringent constraint on V_{ud} from corrected (parameterized) lifetime

Superallowed Fermi Transitions

Ab initio calculations of all cases with 1.8/2.0 (EM) interaction

Standard approach (T/H): Split contribution

$$\delta_C = \delta_{C1} + \delta_{C2}$$

Configuration mixing wavefunction mismatch

Ab initio approach: calculate directly

$$|M_F|^2 = |M_F^0|^2 (1 - \delta_C)$$
$$\delta_C = 1 - \frac{|M_F|^2}{2}$$

 $M_F = \langle \Psi_F || \tau || \Psi_i \rangle$

Superallowed Fermi Transitions

Ab initio calculations of all cases with 1.8/2.0 (EM) interaction

Standard approach (T/H): Split contribution

 $\delta_C = \delta_{C1} + \delta_{C2}$

Configuration mixing

wavefunction mismatch

Ab initio approach: calculate directly

$$M_F|^2 = |M_F^0|^2 (1 - \delta_C)$$
$$\delta_{\alpha} = 1 \qquad |M_F|^2$$

$$M_F = \langle \Psi_F || \tau || \Psi_i \rangle$$

Leach, Holt, arXiv:1809.10793

Results comparable to T-H and DFT

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Convergence Issues

Can we provide rigorous uncertainty estimates?

Significant effect from 1b to 1b+2b

Significant reference-state dependence in some cases; unclear convergence with e_{max} Large effect from CC with continuum indicates generally difficult for ab inito

Natural Orbitals (perturbatively improved) basis:

Add *perturbations* caused by interactions between particles to the HF-basis system

$$|\Psi\rangle = |\Phi\rangle + \sum_{n=1}^{\infty} \left(\frac{H_I}{H_0 - E^{(0)}}\right)^n |\Phi\rangle$$

$$E = E^{(0)} + \sum_{n=1}^{\infty} \left\langle \Phi | H_I \left(\frac{H_I}{H_0 - E^{(0)}} \right)^n | \Phi \right\rangle$$

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Dramatic improvement in energies and radii

Can it help with superallowed convergence?

IMSRG

max

Natural Orbitals (perturbatively improved) basis:

Add *perturbations* caused by interactions between particles to the HF-basis system

$$\begin{split} |\Psi\rangle &= |\Phi\rangle + \sum_{n=1}^{\infty} \left(\frac{H_I}{H_0 - E^{(0)}}\right)^n |\Phi\rangle \\ E &= E^{(0)} + \sum_{n=1}^{\infty} \left\langle \Phi | H_I \left(\frac{H_I}{H_0 - E^{(0)}}\right)^n |\Phi\rangle \end{split} \qquad n \end{split}$$

∂TRIUMF

Dramatic improvement in energies and radii

Can it help with superallowed convergence?

Natural Orbitals (perturbatively improved) basis:

Medium mass:

consistent results for NAT orbitals chosen potentially small reference-state dependence still unclear e_{max} convergence

Cr46→V46

Natural Orbitals (perturbatively improved) basis:

Medium mass:

consistent results for NAT orbitals chosen potentially small reference-state dependence still unclear e_{max} convergence

Lighter systems "quirks" in convergence...

Work still in progress...

Nuclear Structure/Astrophysics

Development of forces and currents Ab initio to ²⁰⁸Pb: neutron skin, r-process Dripline predictions to medium-masses Evolution of magic numbers:

masses, radii, spectra, EM transitions Multi-shell theory:

Islands of inversion, forbidden decays Nuclear EOS/Neutron star properties Atomic systems

McGill UNIVERSITY *T. Miyagi, B. S. Hu, L. Jokiniemi*

A. Belley, I. Ginnett, C. G. Payne M. Bruneault, J. Padua S. Leutheusser

E. Love

K. Evidence, D. Kush

G. Tenkila, H. Patel, V. Chand

B. Wong, X. Cao

S. R. Stroberg N. Vassh

Present and Future for Ab Initio Theory

Fundamental Symmetries/BSM Physics

EW operators: GT quenching, muon capture 0vββ **decay matrix elements + DGT/ECEC/Dg WIMP-Nucleus scattering for dark matter detection Coherent elastic neutrino-nucleus scattering Superallowed Fermi transitions** Symmetry-violating moments: EDM, anapole...

Work in progress

Higher-order many-body physics: IMSRG(3) Monte Carlo shell model diagonalization Extension to superheavy nuclei

