Spectroscopy and theoretical uncertainties in medium-mass nuclei including 3N forces

Javier Menéndez

Institut für Kernphysik, TU Darmstadt
ExtreMe Matter Institute (EMMI)

with Kai Hebeler, Jason D. Holt, Achim Schwenk and Johannes Simonis

ICNT workshop: Physics of exotic nuclei: Theoretical advances and challenges

RIKEN, 10 June 2014

Outline

1. Valence-shell MBPT
2. Theoretical uncertainties
3. Masses, spectra, transitions

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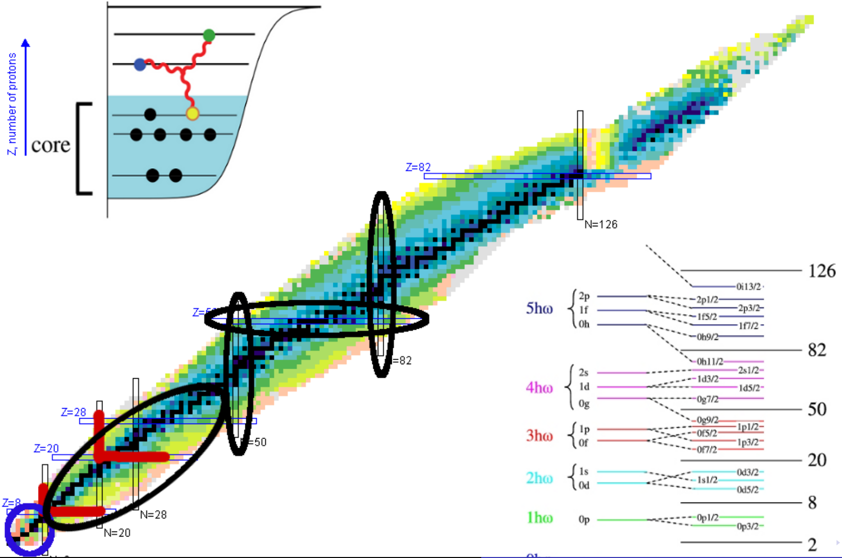
1 Valence-shell MBPT

2 Theoretical uncertainties

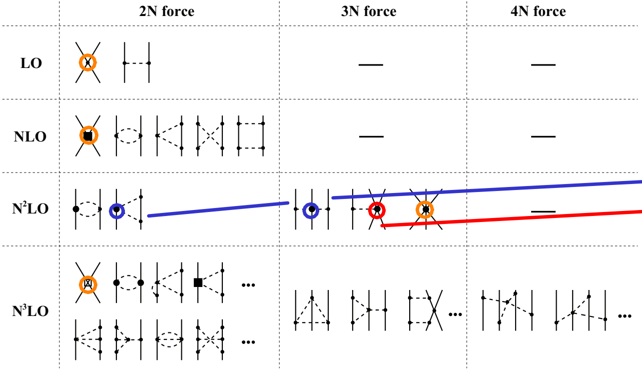
3 Masses, spectra, transitions

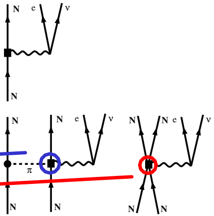
Medium-mass nuclei



Chiral EFT forces and currents

Chiral EFT: nuclear forces and electroweak currents



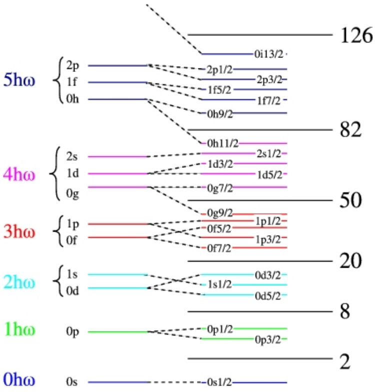


Weinberg, van Kolck, Kaplan, Savage, Epelbaum, Kaiser, Meißner...

Park et al.
PRC67 055206(2003)

Short-range couplings fit to experiment once

Medium-mass nuclei: shell model



Chose as basis states that of the 3D Harmonic Oscillator

To keep the problem feasible, the configuration space is separated into

- Outer orbits:
  orbits that are always empty
- Valence space: the space in which we explicitly solve the problem
- Inner core:
  orbits that are always filled

Solve in valence space: $H\left|\Psi\right\rangle = E\left|\Psi\right\rangle \rightarrow H_{eff}\left|\Psi\right\rangle_{eff} = E\left|\Psi\right\rangle_{eff}$

where H_{eff} is obtained in many-body perturbation theory (MBPT) includes the effect of inner core and outer orbits

Microscopic shell model

Take advantage of shell-model capabilities
at the same time using effective interactions rooted in chiral EFT

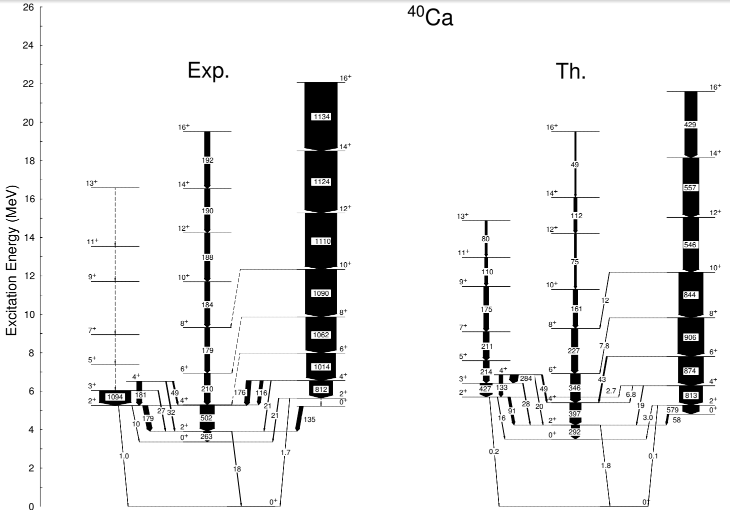
Core imposed in the calculation: not all nucleons solved explicitly

Simplifies many-body calculations:

- Study wide range of nuclei:
  medium-mass, vicinity of closed shells
- Even-even, even-odd, odd-odd systems
- Masses, spectra, electromagnetic and weak responses
- Collective phenomena: deformation

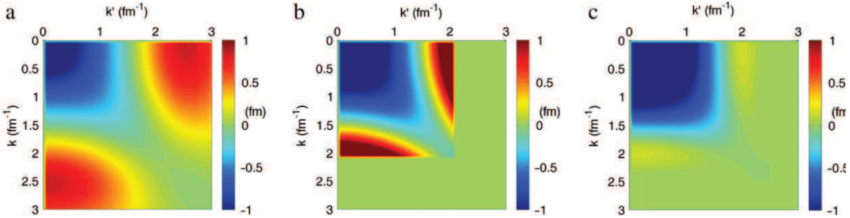
Hopefully, more controlled effective interaction for exotic systems,
complement and guide phenomenological interactions

Shell-model: detailed spectroscopy



RG evolution

Better convergence of chiral forces after RG transformation



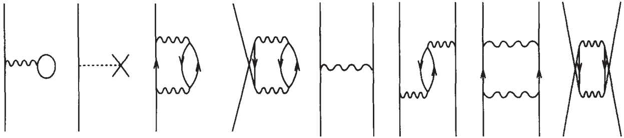
With the evolved NN Hamiltonian
fit 3N couplings c_D and c_E to ^{3}H binding energy and ^{4}He radius

Approximately take into account induced 3N forces,
but consistent 3N evolution to be performed

Many-body perturbation theory

Many-body perturbation theory: obtain effective shell-model interaction in the valence space

Single Particle Energies Two-Body Matrix Elements



NN and 3N interactions treated to third order in MBPT with intermediate states up to 15 (NN) and 5 (3N) major shells

Solve many-body problem with shell-model codes
ANTOINE (m-scheme) and NATHAN (J-coupled)
Diagonalize up to 10^{10} Slater determinants Caurier *et al.* RMP 77 (2005)

$$|\phi_\alpha\rangle = a^+_{i1} a^+_{i2} ... a^+_{iA} |0\rangle \qquad |\Psi\rangle_{eff} = \sum_\alpha c_\alpha |\phi_\alpha\rangle \qquad H_{eff} |\Psi\rangle_{eff} = E |\Psi\rangle_{eff}$$

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1. Valence-shell MBPT
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Uncertainties in MBPT valence-shell

Convergence in the MBPT expansion:
Estimate order-by-order convergence,
assess with non-perturbative methods

Convergence in intermediate-state excitations in MBPT

Convergence in size of valence space
Which orbitals can be treated perturbatively?

Treatment of 3N forces:
Normal-ordered 1b and 2b parts and residual 3N force

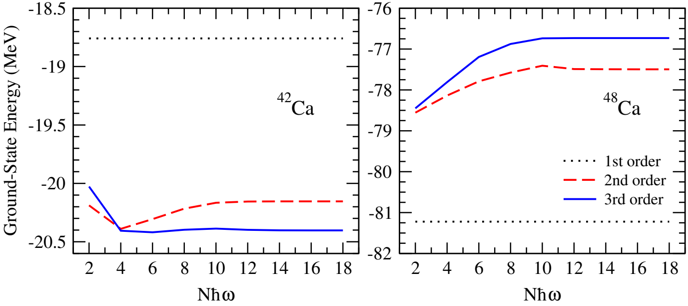
Center-of-mass contamination (beyond one major shell)

Sensitivity to initial Hamiltonian and low-energy couplings

Sensitivity due to the RG evolution

Convergence in many-body perturbation theory

Order-by-order convergence in many-body perturbation theory
(NN forces evolved to V_{lowk} interaction, empirical spe's)



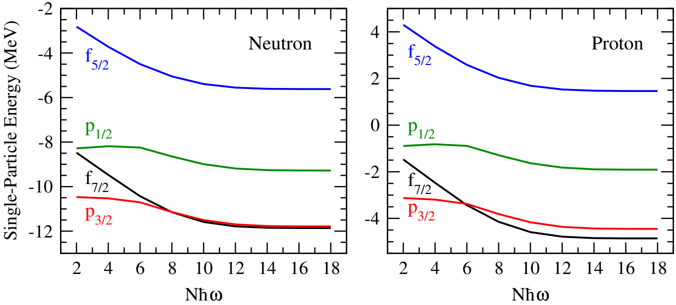
Associated uncertainty difficult to quantify, 3$^{\mathrm{rd}}$ order reasonable

Beyond third order very expensive: non-perturbative approaches

Convergence in term of intermediate states

Intermediate-state excitations convergence

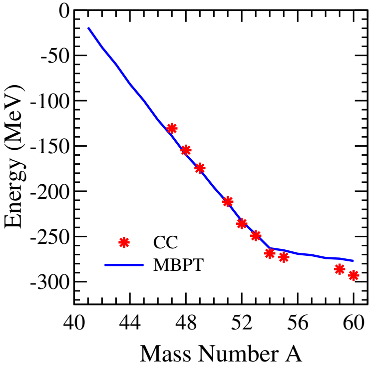
Single-particle energies, most sensitive ingredient in calculation, convergence in terms of intermediate states (NN forces only)



Intermediate-state excitations seem to be under control

Benchmark to coupled-cluster

Benchmark against coupled-cluster calculations,
same V_{lowk} NN interaction, $\hbar\omega = 12$ MeV



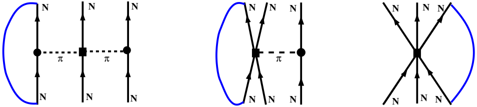
Single-particle energies from coupled-cluster PA-EOM-CCSD energies in ^{41}Ca

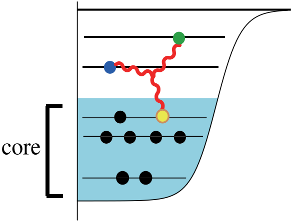
Agreement better than 5% in *pf*-shell nuclei: in heavier systems beyond-*pf* orbitals start to be relevant in coupled-cluster calculations

Normal-ordered 3N Forces

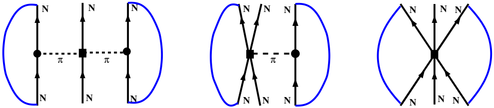
Treatment of 3N forces:

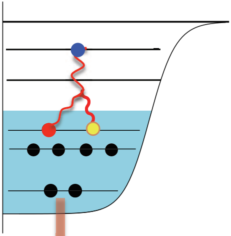
normal-ordered 2B: 2 valence, 1 core particle
⇒ Two-body Matrix Elements





normal-ordered 1B: 1 valence, 2 core particles
⇒ Single particle energies

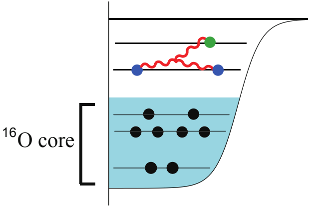


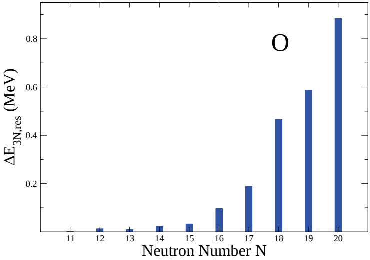


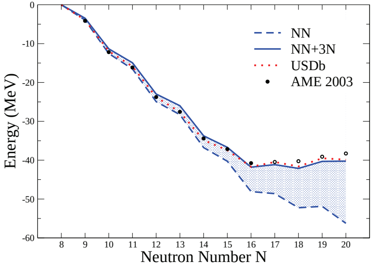
Residual 3N Forces

In the most neutron-rich isotopes,
3N forces between 3 valence neutrons
(suppressed by $N_{valence}/N_{core}$)

Evaluated perturbatively: $\langle\Psi|V^{3N}|\Psi\rangle$





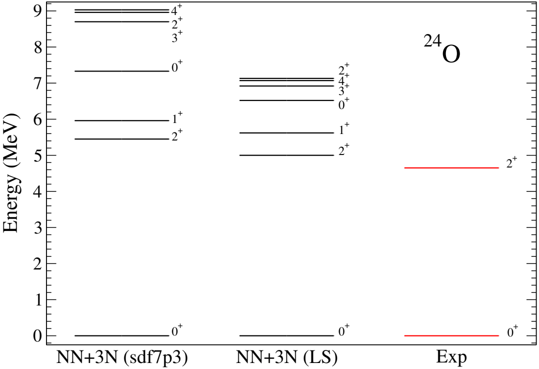


Residual 3N small and repulsive Caesar, Simonis et al. PRC88 034313 (2013)

Center-of-mass contamination

Extended valence spaces (larger than major oscillator shell) may suffer from center-of-mass contamination

Non-vanishing $\langle H_{CM} \rangle$, non-vanishing cross-shell matrix elements



Perform non-perturbative Okubo-Lee-Suzuki transformation to major oscillator shell

Build *sd* interaction reproduce ^{18}O spectra: free from center-of-mass excitations

Excitation spectra can be affected up to 1MeV

Towards theoretical uncertainties

Estimate theoretical uncertainties
allows meaningful comparison to experiment
and better predictions of properties of non-accessible isotopes

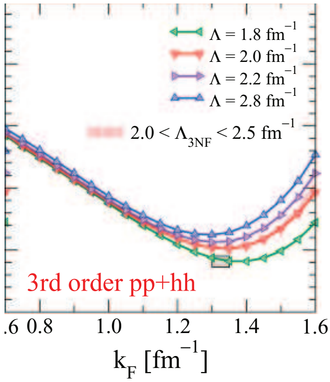
- Theoretical uncertainties associated to nuclear force:

  Explore sensitivity of results with respect to cutoff of RG evolution of unevolved chiral Hamiltonian

  Impose correct nuclear matter saturation

  Outlook: consider different unevolved chiral Hamiltonians

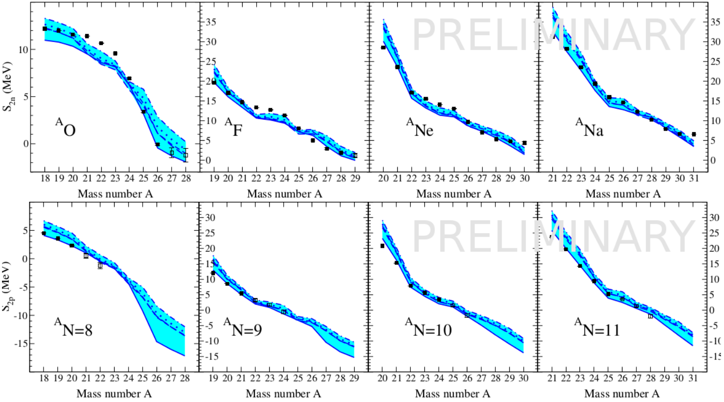
- Theoretical uncertainties associated to the many-body approach



Hebeler et al. PRC 83 031301 (2011)

Theoretical uncertainties in *sd* nuclei

Sensitivity to resolution-scale dependence of RG-evolved Hamiltonian

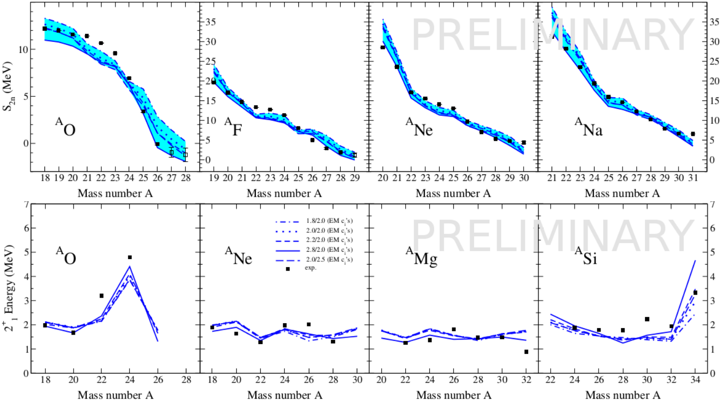


Experimental trends very well reproduced in S_{2n}'s and S_{2p}'s

Uncertainties in S_{2n}'s $\sim 1-3$MeV, in spectra much smaller $\sim$ 500keV

Theoretical uncertainties in *sd* nuclei

Sensitivity to resolution-scale dependence of RG-evolved Hamiltonian



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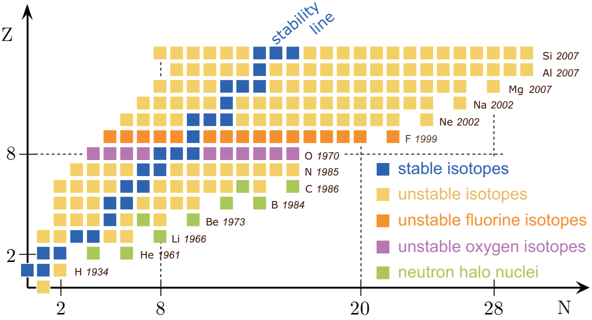
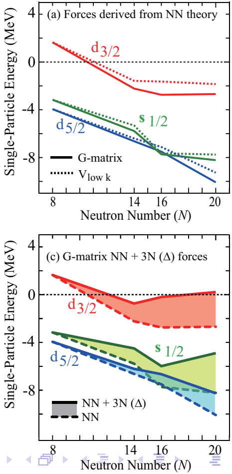
Oxygen dripline anomaly and 3N forces

O isotopes: 'anomaly' in the dripline at ^{24}O, doubly magic nucleus
Chiral NN+3N forces provided repulsion needed to predict dripline



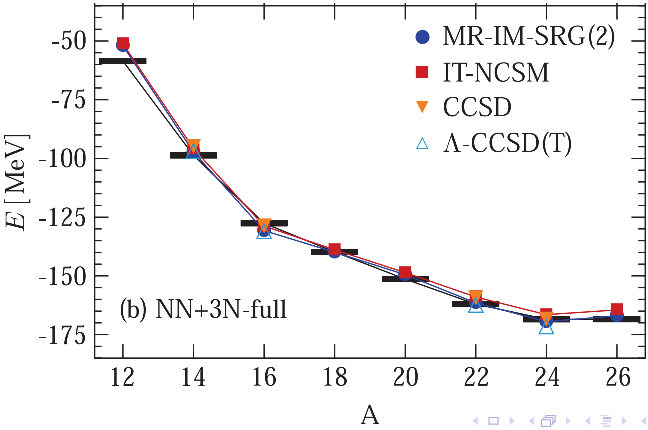


Based on many-body perturbation theory

Otsuka et al. PRL105 032501 (2010)

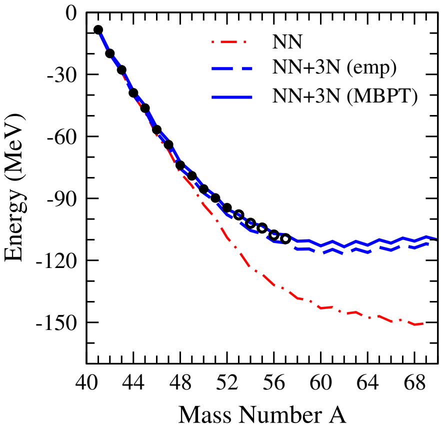
Ab-initio oxygen dripline

Oxygen dripline in ab-initio approaches:
No-core shell model (truncated), In-medium SRG,
Coupled-cluster, Self-consistent Green's function



Ca masses

Ca isotopes: explore nuclear shell evolution $N = 20, 28, 32?, 34?$



Ca measured from ^{40}Ca core

$\hbar\omega = 11.48$ MeV

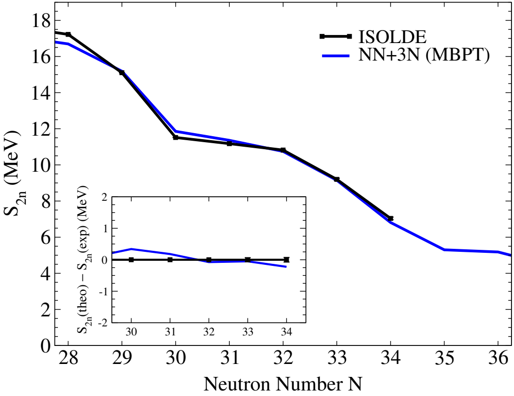
pf $g_{9/2}$ valence space

3N forces repulsive contribution, chiral NN-only forces too attractive

Sensitivity to single particle energies
MBPT (calculated from NN+3N forces)
Empirical (from GXPF1 interaction)
Estimate of associated uncertainty

Ca two-neutron separation energies

Precise ^{51,52}Ca / ^{53,54}Ca masses at TRIUMF/ISOLDE



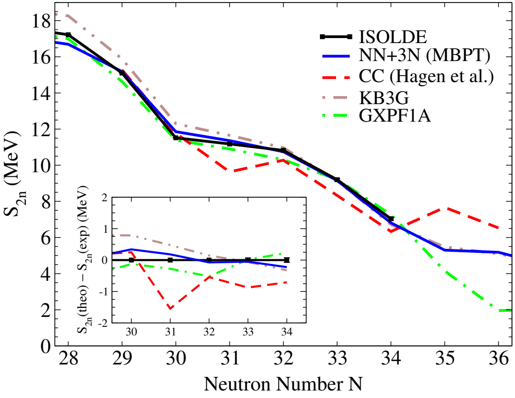
Excellent agreement with theoretical prediction

S_{2n} evolution:
^{52}Ca–^{54}Ca decrease similar to ^{48}Ca–^{50}Ca unambiguously establishes $N = 32$ shell closure

Gallant et al. PRL 109 032506 (2012)
Wienholtz et al. Nature 498 346 (2013)

Two-neutron separation energies

Compare to other theoretical calculations



Phenomenology
good agreement to experiment
masses/gaps as input

Coupled-Cluster calculations
good agreement to experiment
with phenomenological 3N forces

Gorkov Green's Function
Vittorio Somà talk yesterday

Gallant et al. PRL 109 032506 (2012)
Wienholtz et al. Nature 498 346 (2013)

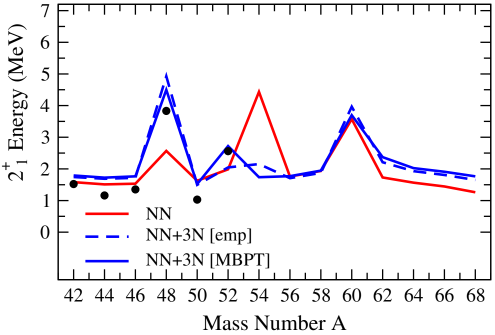
Shell closures and 2_1^+ energies

2_1^+ energies characterize shell closures

Correct closure at $N = 28$ when 3N forces are included

Holt et al. JPG39 085111(2012)

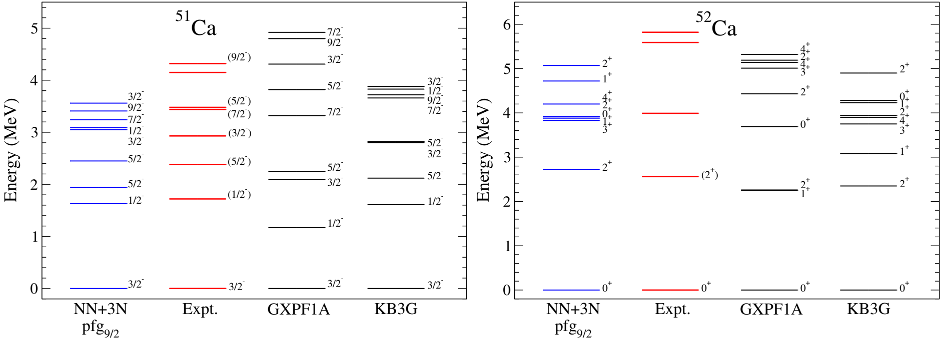
Holt, JM, Schwenk, JPG40 075105 (2013)



- 3N forces enhance closure at $N = 32$
- 3N forces predict 2_1^+ in ^{54}Ca at 1.7-2.2 MeV
  Expt: 2.04 MeV (RIKEN), suggest $N = 34$ shell closure
  Steppenbeck et al. Nature 502 207(2013)

Excitation spectra

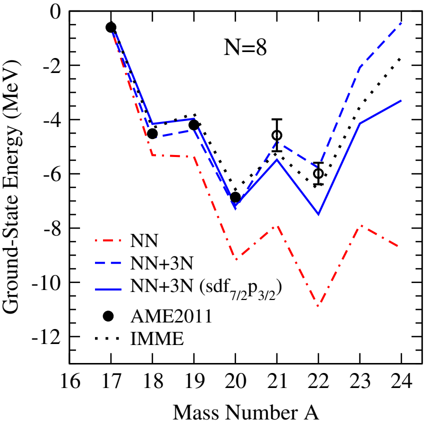
Spectra for neutron-rich calcium isotopes



Good agreement with experiment when available, comparable to phenomenological interactions

Predictions in very neutron-rich nuclei, test in upcoming experiments

Proton-rich nuclei



Holt, JM, Schwenk PRL110 022502 (2013)

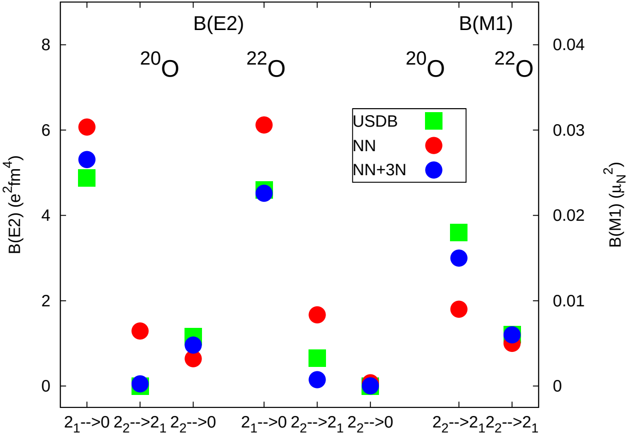
Compare NN+3N theory to
isobaric mass-multiplet formula (IMME)
$E(A,T,T_z) = E(A,T,-T_z) + 2b(A,T)T_z$

Isospin-symmetry breaking terms
predicted by chiral EFT
Coulomb included in calculations

Proton dripline not certain
predicted at ^{20}Mg or ^{22}Si:
S_{2p}= -0.12 (Theory) / +0.01 (IMME)

Excitation spectra predicted:
test in RIB facilities

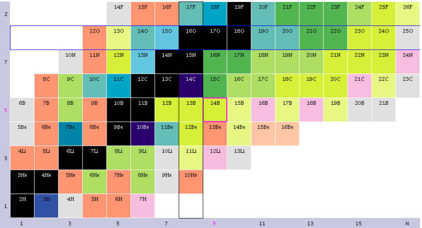
Oxygen electromagnetic transitions



Electromagnetic transitions (decay lifetimes)

B(E2) transitions in 2_2^+ states, ^{20}O and ^{22}O

Carbon electromagnetic transitions



Electromagnetic transitions can be calculated in p-shell

No need of effective charges

Still require consistent evolution of transition operator

Second 2_2^+ state decay sensitive to 3N forces

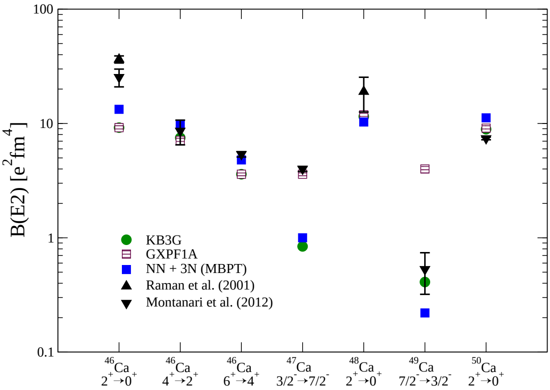
Decay not seen experimentally: 3N forces favored

Forssen et al.

JPG 40 055105 (2013)

$\frac{B(\mathrm{E2}; J_i \to J_f)}{B(\mathrm{E2}; 2_1^+ \to 0_1^+)}$	CDB2k	chiral NN	chiral $NN+NNN$
$2_1^+ \to 0_1^+$	1	1	1
$2_2^+ \to 0_1^+$	2.2	0.75	0.11
$2_2^+ \to 2_1^+$	2.0	1.7	0.65
$3_1^+ \to 2_1^+$	0.36	0.31	0.02
$4_1^+ \to 2_1^+$	0.89	0.69	0.80

Calcium B(E2) transition strengths



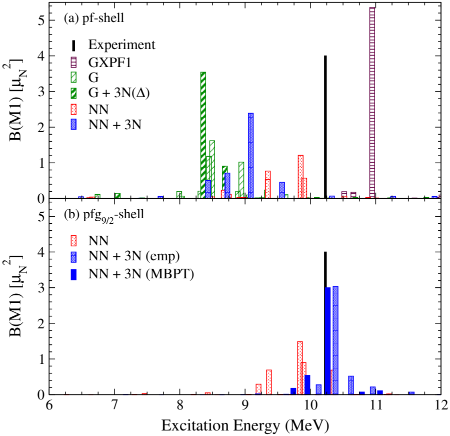
B(E2)s in reasonable agreement with experiment, spread two over orders of magnitude

Similar quality as phenomenological interactions, in particular very close to KB3G

^{46}Ca: *sd* degrees of freedom?

Phenomenological effective charges

B(M1) Transition in ^{48}Ca



B(M1) strength in ^{48}Ca too fragmented in *pf* space

Phenomenological calculations reproduce experimental concentration

In the extended $pfg_{9/2}$ space NN forces also fragmented strength

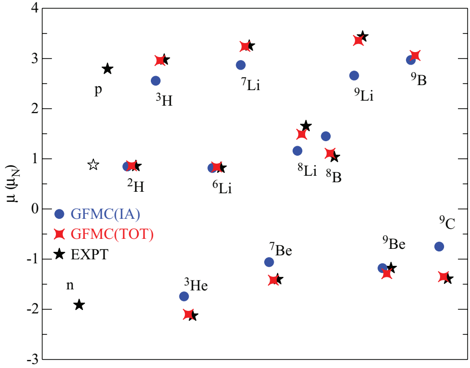
NN+3N calculation in $pfg_{9/2}$ very good agreement with experiment
Phenomenological effective g-factors

Currents and operators

Good agreement with ground-states, spectroscopy and electromagnetic transitions but with effective charges and g-factors

Origin of the need of this phenomenological input?

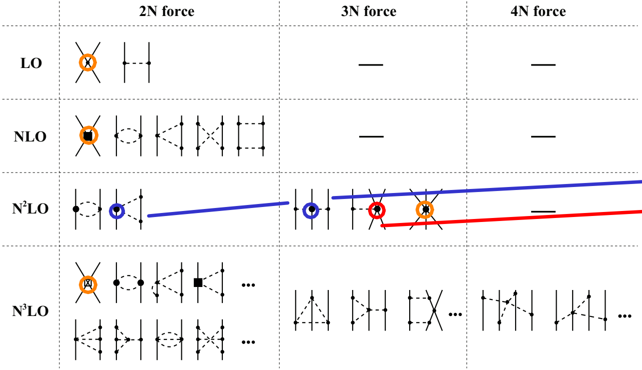
- Shell-model calculation in limited valence space: Appropriate effective operators to be obtained perturbatively or non-perturbatively
- Transition operators non-evolved
- Operators are not complete: Need of two-body currents well known from light nuclei



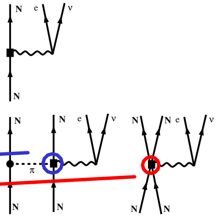
Pastore et al. PRC87 035503 (2013)

Chiral 2b currents

Chiral EFT: nuclear forces and electroweak currents



Weinberg, van Kolck, Kaplan, Savage, Epelbaum, Kaiser, Meißner...



Park et al.
PRC67 055206(2003)

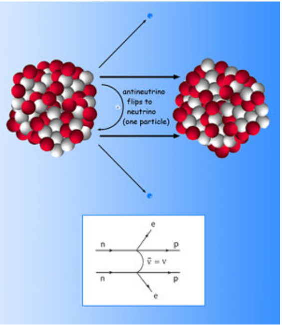
Short-range couplings fit to experiment once

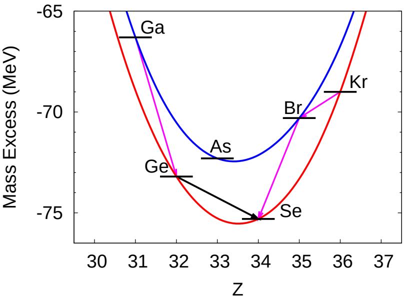
2b currents beyond light nuclei

2b currents: β and electromagnetic decays in light nuclei
How important are they in heavier systems?

Study neutrinoless double-beta decay ($0\nu\beta\beta$):
lepton-number violation, Majorana nature of neutrinos

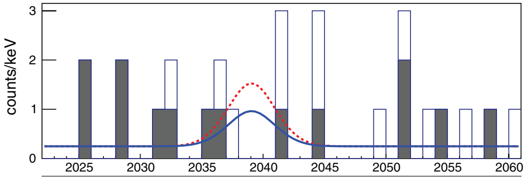
Second order process only observable with forbidden/hindered β-decay





$^{48}Ca \rightarrow {}^{48}Ti$
$^{76}Ge \rightarrow {}^{76}Se$
$^{82}Se \rightarrow {}^{82}Kr$
$^{96}Zr \rightarrow {}^{96}Mo$
$^{100}Mo \rightarrow {}^{100}Ru$
$^{110}Pd \rightarrow {}^{110}Cd$
$^{116}Cd \rightarrow {}^{116}Sn$
$^{124}Sn \rightarrow {}^{124}Te$
$^{130}Te \rightarrow {}^{130}Xe$
$^{136}Xe \rightarrow {}^{136}Ba$
$^{150}Nd \rightarrow {}^{150}Sm$

Nuclear Matrix Elements (NMEs)



GERDA Collaboration, PRL111 122503(2013)

$0\nu\beta\beta$ decay not observed

Long-standing ^{76}Ge claim rejected

Strong experimental efforts:
EXO, KamLAND-ZEN, GERDA, MAJORANA, SNO+...

$$\left(T_{1/2}^{0\nu\beta\beta}\left(0^+ \rightarrow 0^+\right)\right)^{-1} = G_{01}\left|M^{0\nu\beta\beta}\right|^2 \left(\frac{m_{\beta\beta}}{m_e}\right)^2, \quad m_{\beta\beta} = \left|\sum_k U_{ek}^2 m_k\right|$$

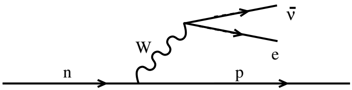
$M^{0\nu\beta\beta}$s identify best isotopes for experiment
and connect lifetime with absolute neutrino masses and hierarchy

Nuclear Matrix Element:

- Many-body method to describe initial and final nuclear states
- Transition operator from chiral EFT

$M^{0\nu\beta\beta}$ uncertainty: quenching

Major $M^{0\nu\beta\beta}$ uncertainty, g_A: $M^{0\nu\beta\beta} \propto g_A^2 \Rightarrow \left(T_{1/2}^{0\nu\beta\beta}\right)^{-1} \propto g_A^4$



$$\mathbf{J}_{n,1B} = g_A\, \sigma_n \tau_n^- \,,$$
$$g_A^{\mathrm{eff}} = q g_A, \quad q \approx 0.75.$$

Theory needs to “quench“ Gamow-Teller operator to reproduce GT lifetimes and strength functions, two-neutrino $\beta\beta$ decay

Wildenthal et al. PRC28 1343(1983)
Martínez-Pinedo et al. PRC53 2602(1996)
Caurier, Nowacki, Poves PLB711 62(2012)
Bender et al. PRC65 054322(2002)

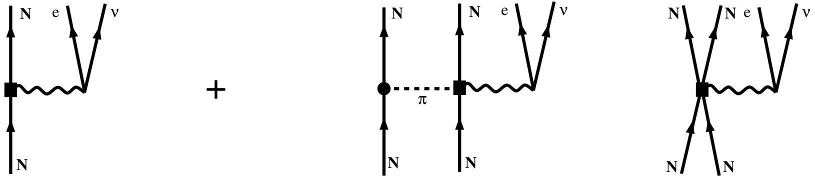
$M^{0\nu\beta\beta}$ severely reduced if quenching

This puzzle has been the target of many theoretical efforts:
Arima, Rho, Towner, Bertsch and Hamamoto, Wildenthal and Brown...

Revisit in the framework of chiral EFT currents, including 2b currents

2b currents: GT quenching

Include 1b and 2b currents from chiral EFT



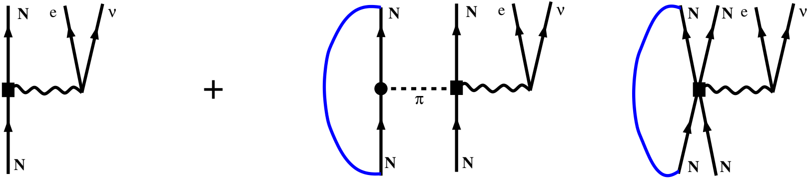
The normal-ordered two-body currents modify GT operator

$$\mathbf{J}^{\mathrm{eff}}_{n,2b} \simeq -\frac{g_A \rho}{f_\pi^2} \tau_n^- \sigma_n \left[\frac{2}{3} c_3 \frac{\mathbf{p}^2}{4m_\pi^2 + \mathbf{p}^2} + I(\rho, P) \left(\frac{1}{3} (2c_4 - c_3) + \frac{1}{6m_N} \right) \right],$$

long-range p dependent long-range p independent

2b currents: GT quenching

Include 1b and 2b currents from chiral EFT



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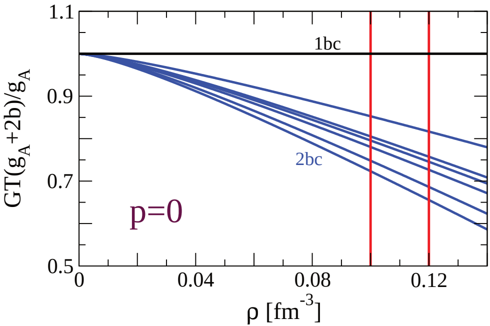
long-range p dependent   long-range p independent

Contribution of 2b currents

2b currents at $p = 0$: GT, $2\nu\beta\beta$ decays

$$\mathbf{J}^{\text{eff}}_{n,2b} \simeq -\frac{g_A \rho}{f_\pi^2} \tau_n^- \sigma_n \left[I(\rho, P) \left(\frac{1}{3}(2c_4 - c_3) + \frac{1}{6m_N} \right) \right],$$



$\rho = 0.10 \ldots 0.12\ \text{fm}^{-3}$

Couplings c_3, c_4 from NN potentials

Entem et al. PRC68 041001(2003)

Epelbaum et al. NPA747 362(2005)

Rentmeester et al. PRC67 044001(2003)

$\delta c_3 = -\delta c_4 \approx 1\ \text{GeV}^{-1}$

JM, Gazit, Schwenk PRL107 062501 (2011)

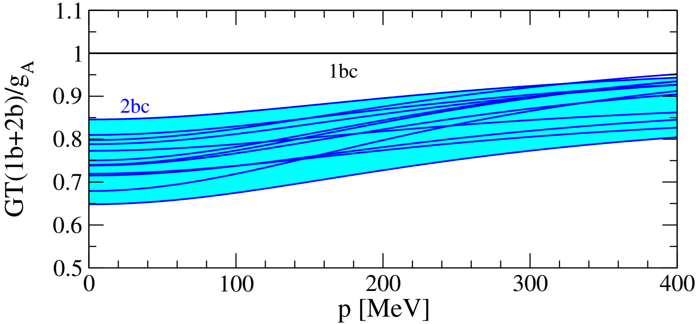
2b currents predict g_A quenching $q = 0.85 \ldots 0.66$

Similarly there is an isoscalar contribution to g-factors

Transferred-momentum dependence

The $\sigma\tau^-$ term depends on transferred momentum p:

$$-\frac{g_A\rho}{f_\pi^2}\tau_n^-\sigma_n\frac{2}{3}\,c_3\,\frac{\mathbf{p}^2}{4m_\pi^2+\mathbf{p}^2}$$

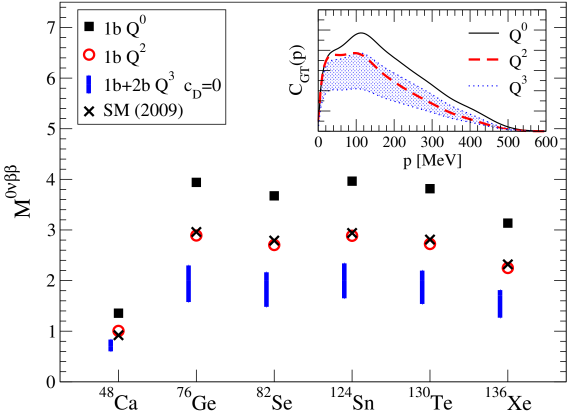


JM, Gazit, Schwenk PRL107 062501 (2011)

Quenching reduced at $p > 0$, relevant for $0\nu\beta\beta$ decay where $p \sim m_\pi$

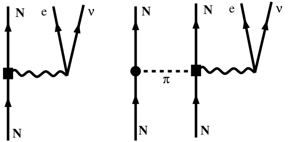
Similarly, electromagnetic sector can be probed with e^- scattering

Nuclear matrix elements for $0\nu\beta\beta$ decay



JM, Gazit, Schwenk PRL107 062501 (2011)

Order Q^0+Q^2 similar to phenomenological currents
JM, Poves, Caurier, Nowacki
NPA818 139 (2009)



Order Q^3 2b currents reduce NMEs $\sim$ 15% – 40%

Momentum-transfer dependence predicted

Similarly, vector currents will impact electromagnetic transitions

Summary

Shell Model calculation based on chiral effective field theory including NN+3N forces and many-body perturbation theory

- Shell structure: very good agreement with neutron-rich Ca S_{2n}'s (TRIUMF, ISOLDE) establish close shell at $N = 32$ and ^{54}Ca 2_1^+ (RIKEN) suggessting shell closure at $N = 34$
- Towards theoretical uncertainty quantification of calculations in medium-mass nuclei: uncertainties associated to the Hamiltonian and to the many-body method
- Excitation spectra, electromagnetic and weak transitions: good agreement to experiment but unclear role of effective charges, g-factors, g_A coupling
  Include chiral 2b currents predicted in chiral EFT