First principles calculations for neutrinoless $\beta\beta$ decay

Javier Menéndez

University of Barcelona

Snowmass Mini Workshop:
Nuclear theory of neutrinoless $\beta\beta$ decay
22nd July 2020

UNIVERSITAT DE BARCELONA

ICCUB

Calculating nuclear matrix elements

Nuclear matrix elements needed in low-energy new physics searches

$$\langle \text{Final} | \mathcal{L}_{\text{leptons}-\text{nucleons}} | \text{Initial} \rangle = \langle \text{Final} | \int dx\, j^{\mu}(x) J_{\mu}(x) | \text{Initial} \rangle$$

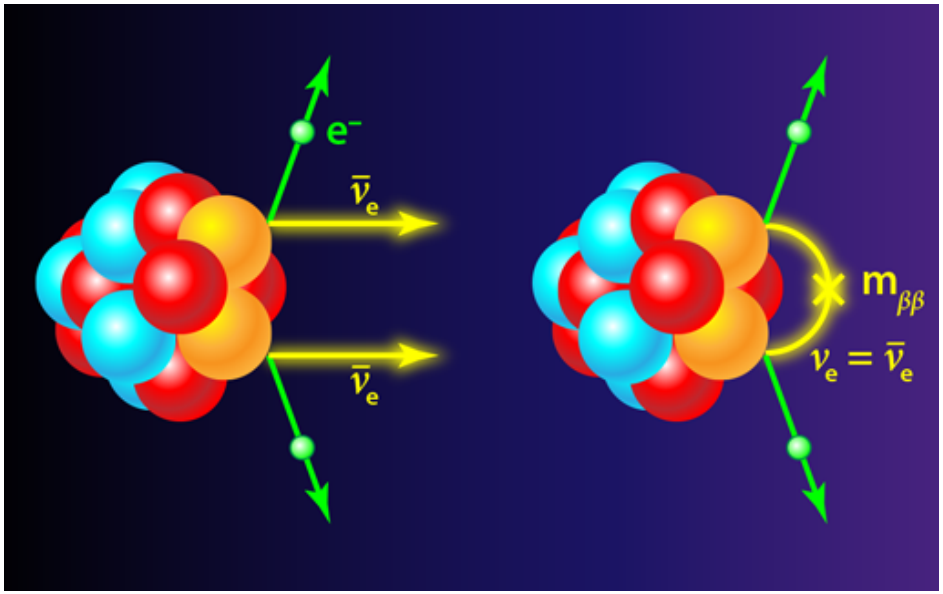
- Nuclear structure calculation of the initial and final states: Shell model, QRPA, IBM, Energy-density functional

  Ab initio many-body theory

  QMC, Coupled-cluster, IMSRG...

- Lepton-nucleus interaction: Hadronic current in nucleus: phenomenological,

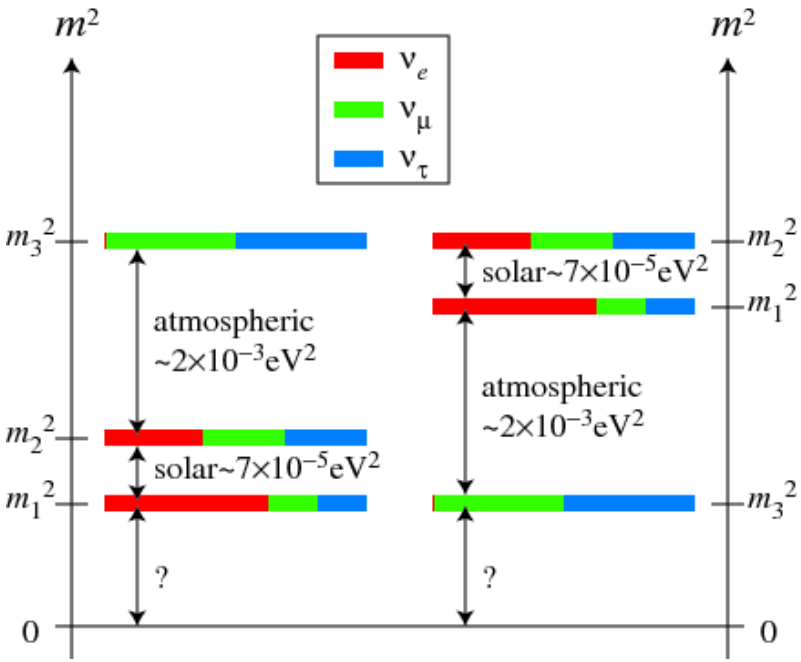
  Effective theory of QCD

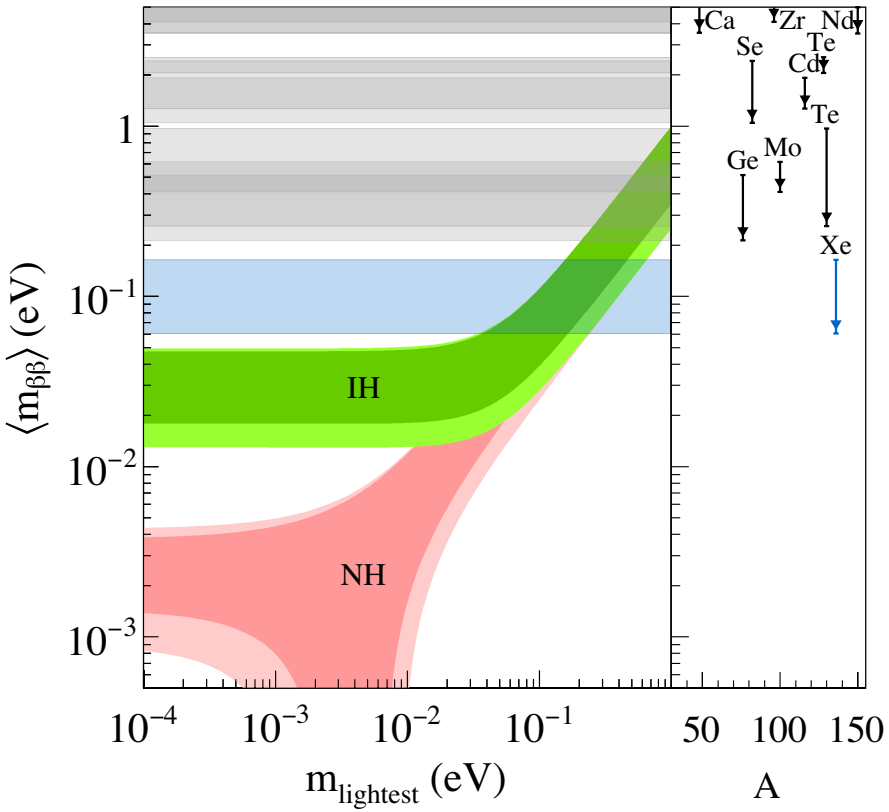


Next generation $0\nu\beta\beta$: inverted hierarchy

Decay rate sensitive to neutrino masses, hierarchy $m_{\beta\beta} = |\sum U_{ek}^2 m_k|$

$$T_{1/2}^{0\nu\beta\beta}\left(0^+ \to 0^+\right)^{-1} = G_{0\nu}\, g_A^4 \left|M^{0\nu\beta\beta}\right|^2 m_{\beta\beta}^2$$





KamLAND-Zen, PRL117 082503(2016)

Matrix elements assess if next generation experiments fully explore "inverted hierarchy"

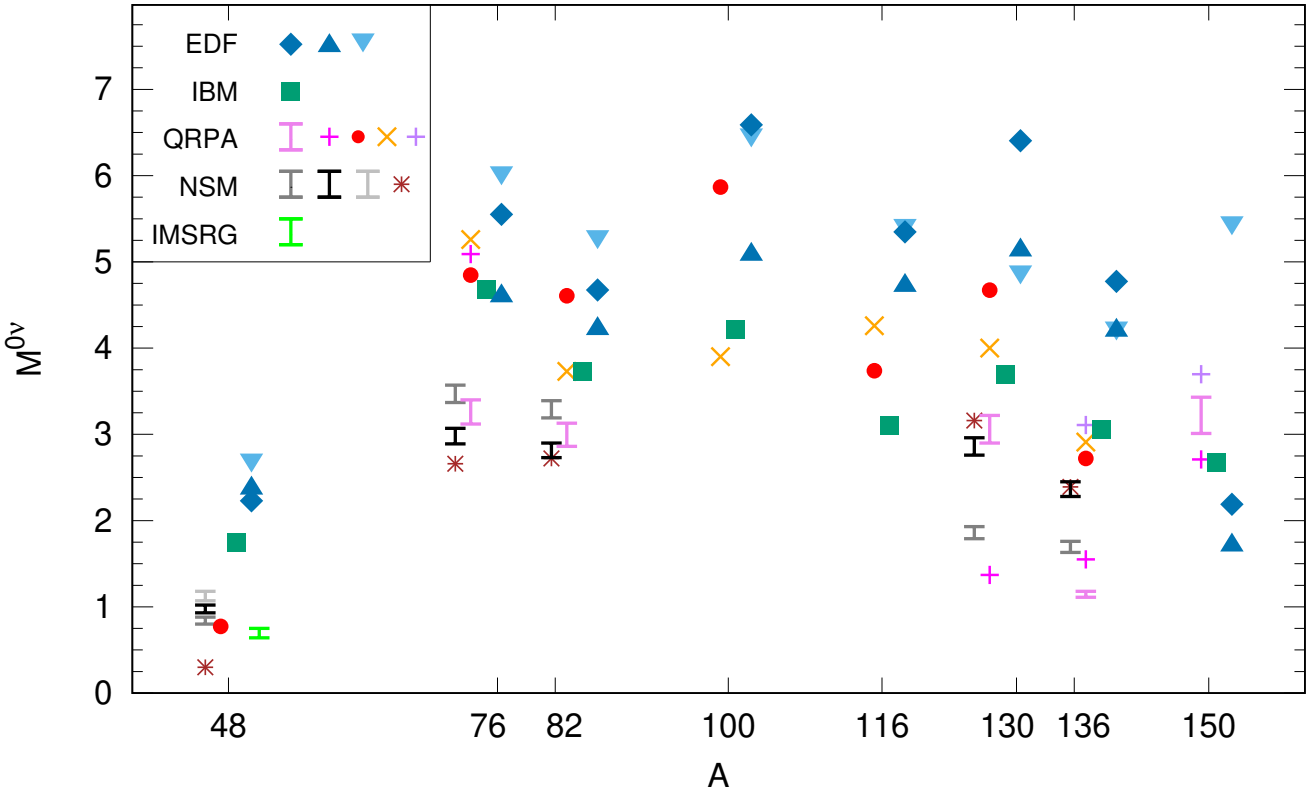
$0\nu\beta\beta$ decay nuclear matrix elements

Large difference in nuclear matrix element calculations: factor $\sim 2-3$

$$\langle 0_f^+ | \sum_{n,m} \tau_n^- \tau_m^- \sum_x H^x(r)\, \Omega^x \, | 0_i^+ \rangle$$

Ω^x = Fermi ($\mathbb{1}$), GT ($\sigma_n \sigma_m$),Tensor

$H(r)$ = neutrino potential



EDF: large NMEs

QRPA: wider range

NSM: small NMEs

IMSRG ab initio
^{48}Ca NME: quite small

Additional uncertainty:
"g_A quenching"?

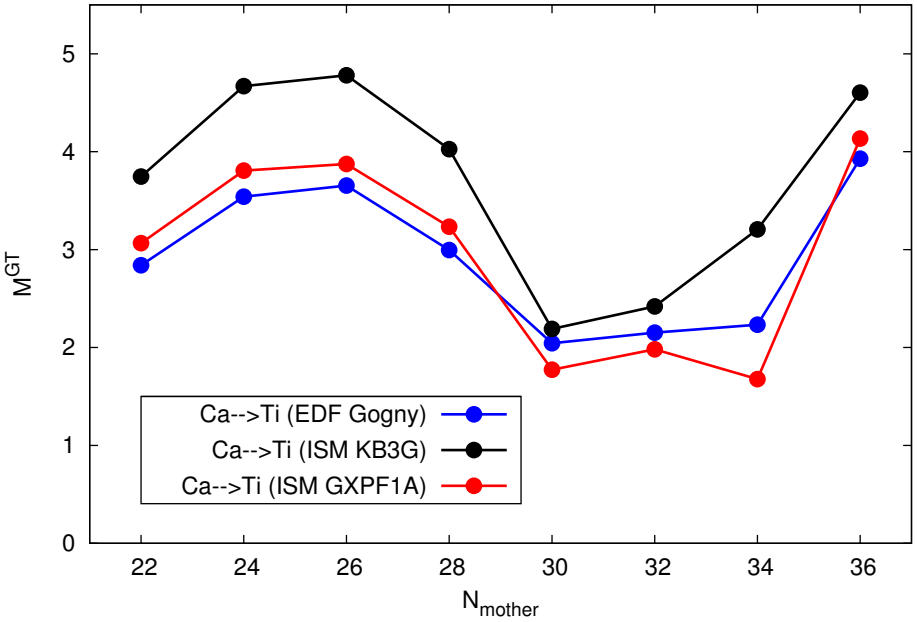
Engel, JM, Rep. Prog. Phys. 80 046301 (2017)

M. Agostini, G. Benato, J. Detwiler, JM, F. Vissani, in preparation

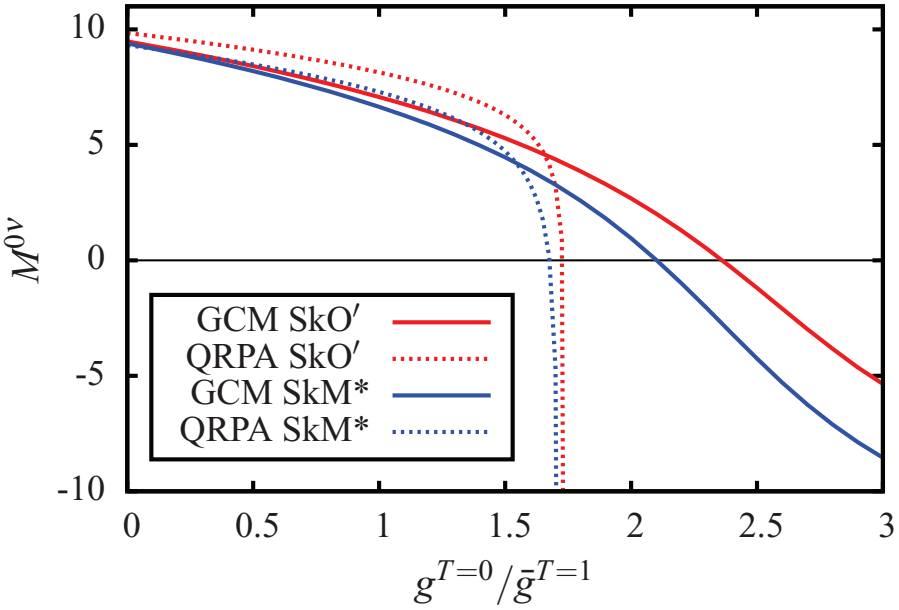
Correlations: proton-neutron pairing

$0\nu\beta\beta$ NMEs agree without nuclear correlations (very simplistic nuclei)

NMEs too large if proton-neutron pairing correlations are neglected



JM et al. PRC90 024311(2014)



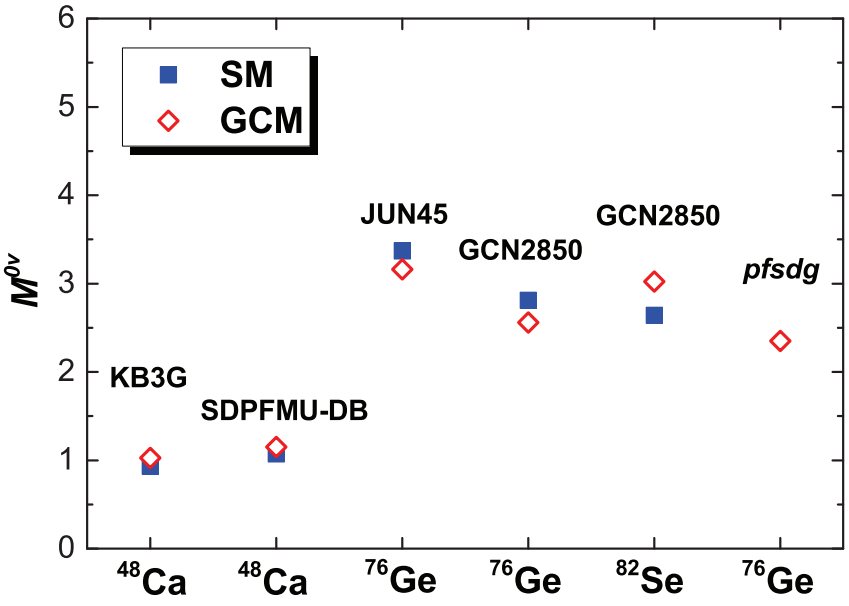
Hinohara, Engel PRC90 031301 (2014)

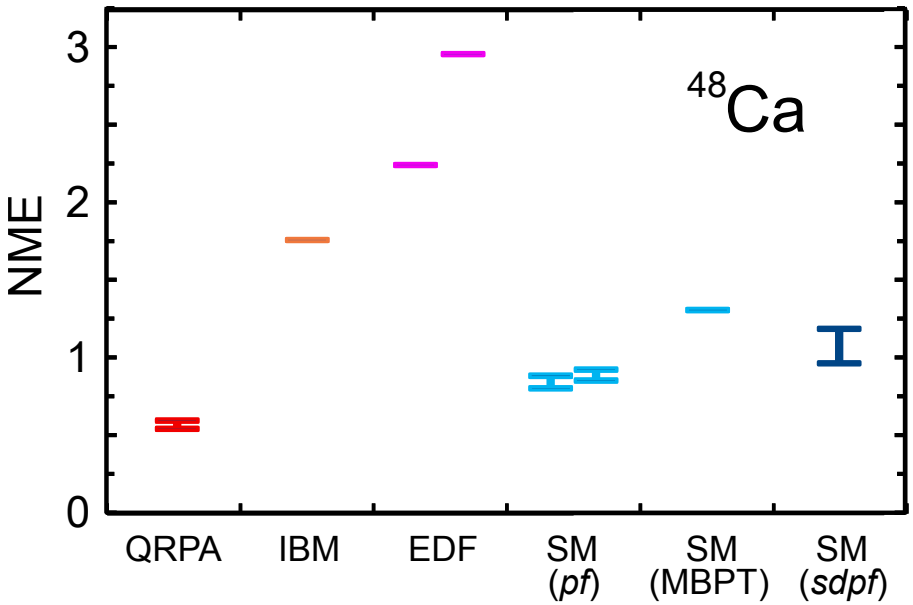
Related to approximate $SU(4)$ symmetry of the $\sum H(r)\boldsymbol{\sigma}_i\boldsymbol{\sigma}_j\tau_i\tau_j$ operator

Correlations: large configuration space

^{48}Ca extended configuration space from *pf* to *sdpf*, 4 to 7 orbitals dimension 10^5 to 10^9
^{48}Ca 0_2^+ state lowered by 1.3 MeV
nuclear matrix elements enhanced only moderately 30%

Iwata et al. PRL116 112502 (2016)





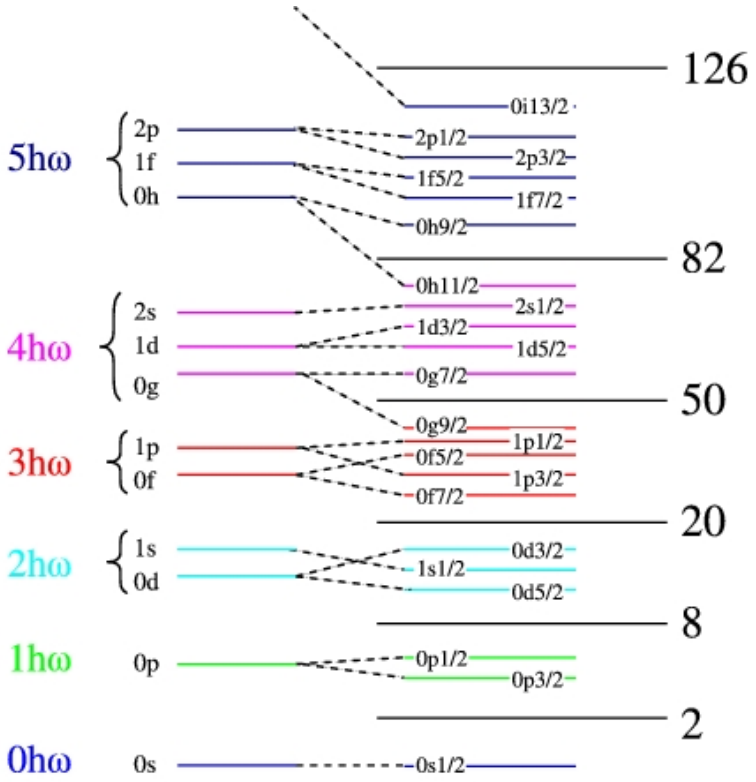
Also small effect of large space with perturbative calculation

Coraggio et al. PRC 101 044315 (2020)

Likewise, very mild effect found in ^{76}Ge GCM calculations

Jiao et al. PRC96 054310 (2017)

Nuclear shell model



Nuclear shell model configuration space
only keep essential degrees of freedom

- High-energy orbits: always empty
- Configuration space:
  where many-body problem is solved
- Inert core: always filled

$$H\,|\Psi\rangle = E\,|\Psi\rangle \;\rightarrow H_{eff}\,|\Psi\rangle_{eff} = E\,|\Psi\rangle_{eff}$$

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

Shell model codes (1 major oscillator shell)
$\sim 10^{10}$ Slater dets. Caurier et al. RMP77 (2005)
$\gtrsim 10^{24}$ Slater dets. with Monte Carlo SM
Otsuka, Shimizu, Tsunoda

Dimension $\sim$

$$\binom{(p+1)(p+2)_\nu}{N}\binom{(p+1)(p+2)_\pi}{Z}$$

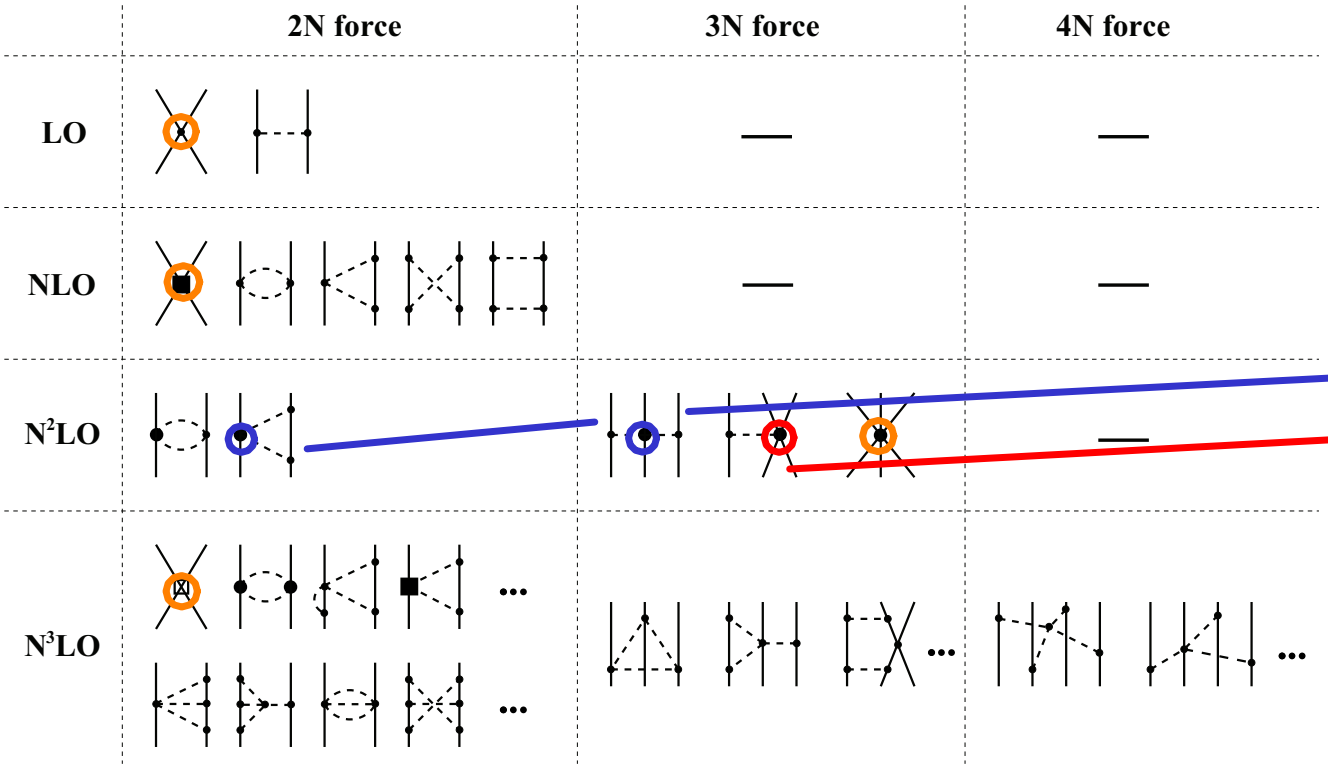
H_{eff} obtained phenomenologically or with ab initio method: eg VS-IMSRG

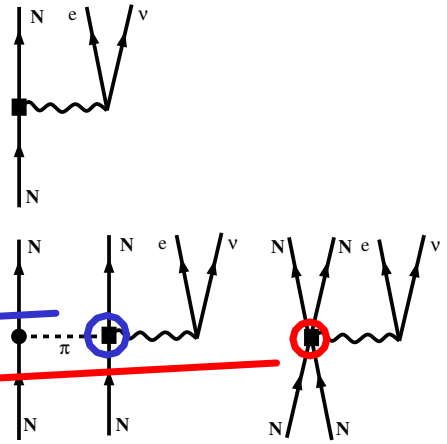
Chiral effective field theory

Chiral EFT: low energy approach to QCD, nuclear structure energies

Approximate chiral symmetry: pion exchanges, contact interactions

Systematic expansion: nuclear forces and electroweak currents





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

Park, Klos, Krebs, Baroni...

Short-range couplings fitted to experiment once

Ab initio nuclear calculations

Oxygen dripline using chiral NN+3N forces correctly reproduced
ab-initio calculations treating explicitly all nucleons
excellent agreement between different approaches

No-core shell model
(Importance-truncated)

In-medium SRG

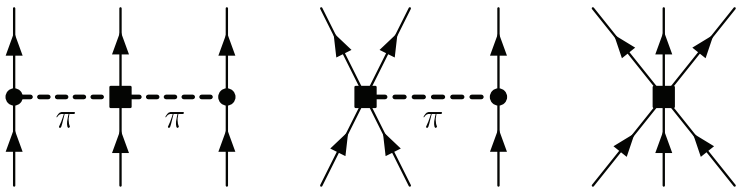
Hergert et al. PRL110 242501(2013)

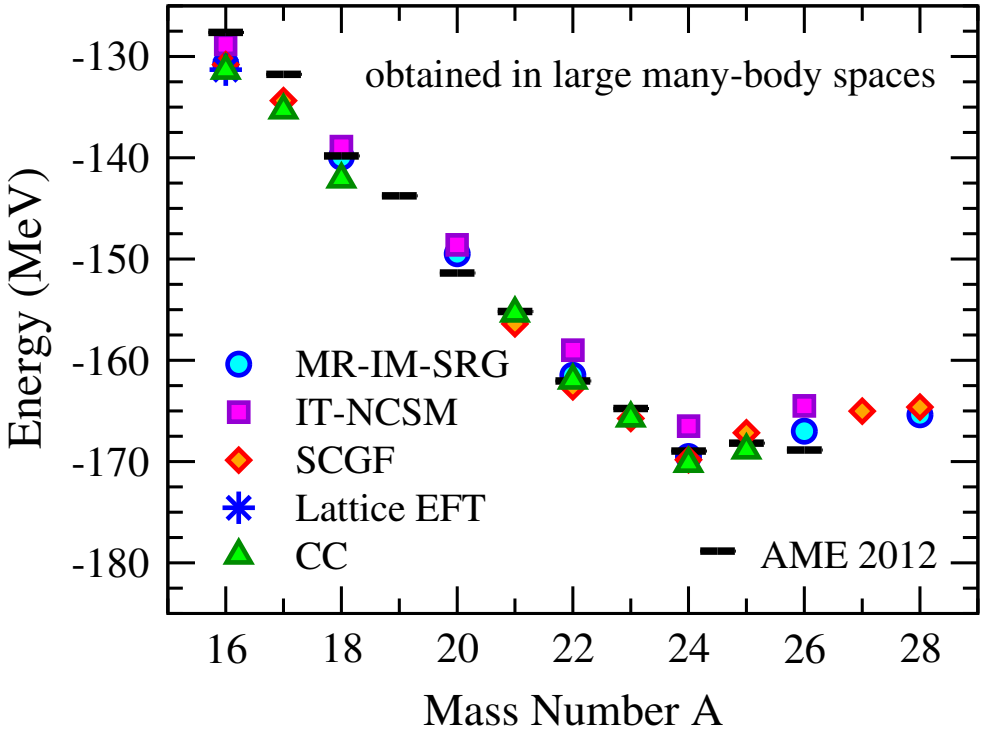
Self-consistent Green's function

Cipollone et al. PRL111 062501(2013)

Coupled-clusters

Jansen et al. PRL113 142502(2014)





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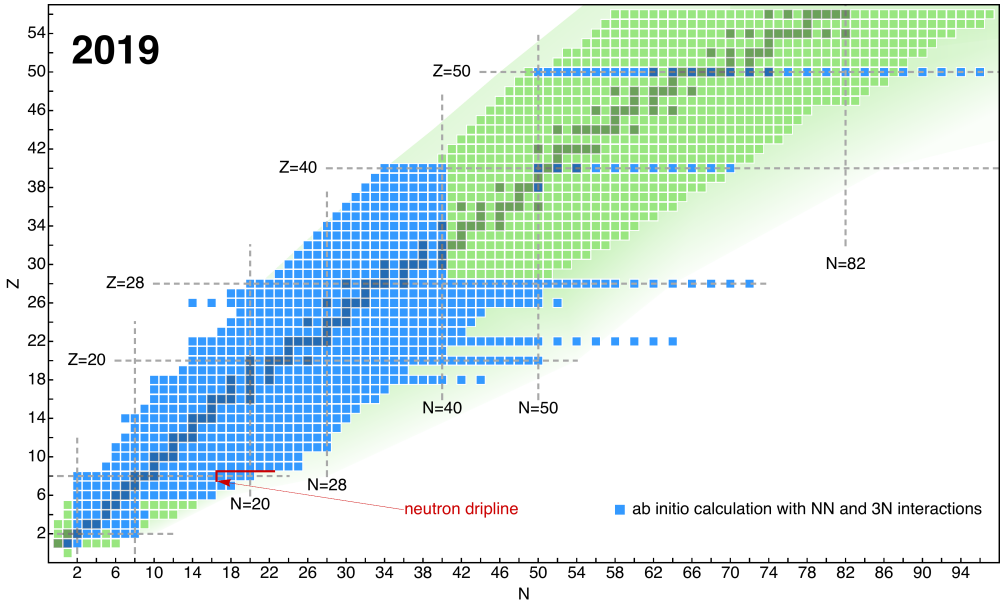
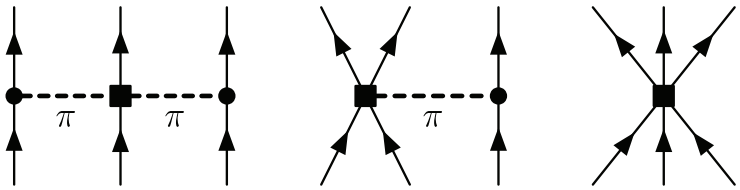


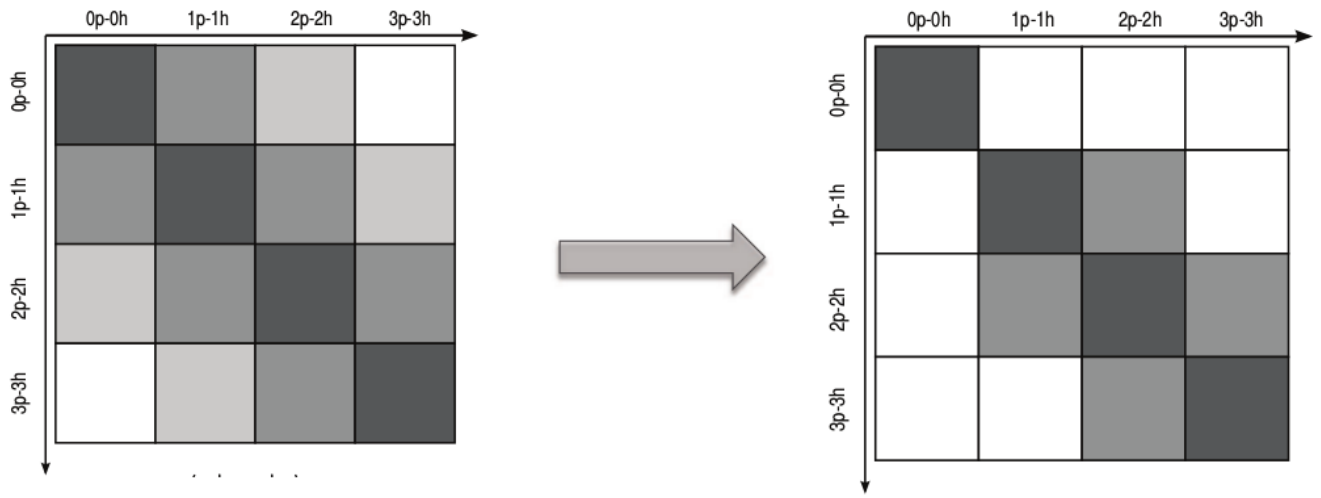
credit: H. Hergert



In-Medium Similarity Renormalization Group

The in-medium similarity renormalization group (IMSRG) method uses a similarity (unitary) transformation to decouple reference state from particle-hole excitations

Bogner, Schwenk, Hergert, Stroberg...



$\langle i|H|j\rangle$ $\qquad$ $\langle \mathrm{n}p\mathrm{n}h|H(\infty)|\Phi_{\mathrm{core}}\rangle = 0$

The original Hamiltonian is "evolved" by unitary transformations typically fixed by a given generator η

$$H = T + V \rightarrow H(s) = U(s)HU^{\dagger}(s)$$

$$\frac{dH}{ds} = [\eta(s), H(s)] \quad \text{with } \eta(s) = [G(s), H(s)]$$

Valence-space IMSRG: first principles shell model

Use in-medium similarity renormalization group to obtain H_{eff}
decouple A particles in valence space from core and high-energy orbitals

In addition to H_{eff}, VS-IMSRG provides the energy of the core

Stroberg et al. Ann. Rev. Nucl. Part. Sci. 69, 307 (2019)

IMSRG: unitary transformation:

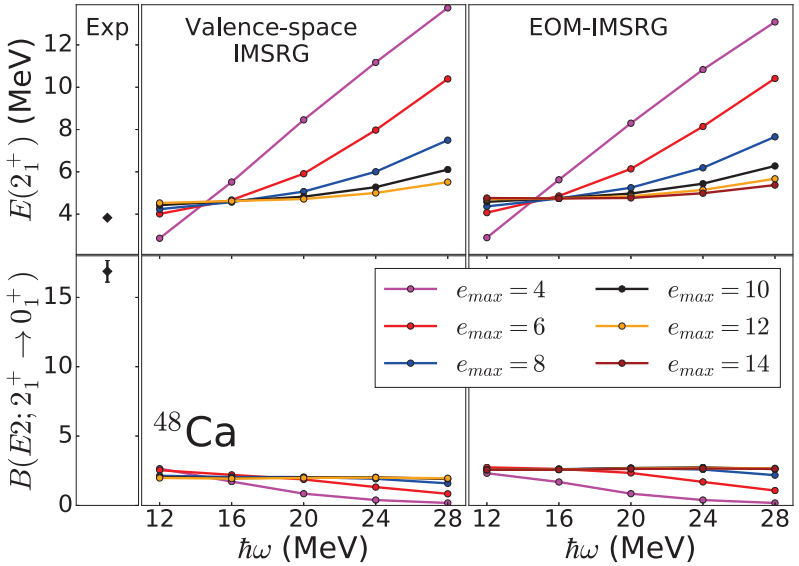
$$H_{\text{eff}} = U^{\dagger} H U$$

demands consistent transformation for transition operators:

$$O_{\text{eff}} = U^{\dagger} O U$$

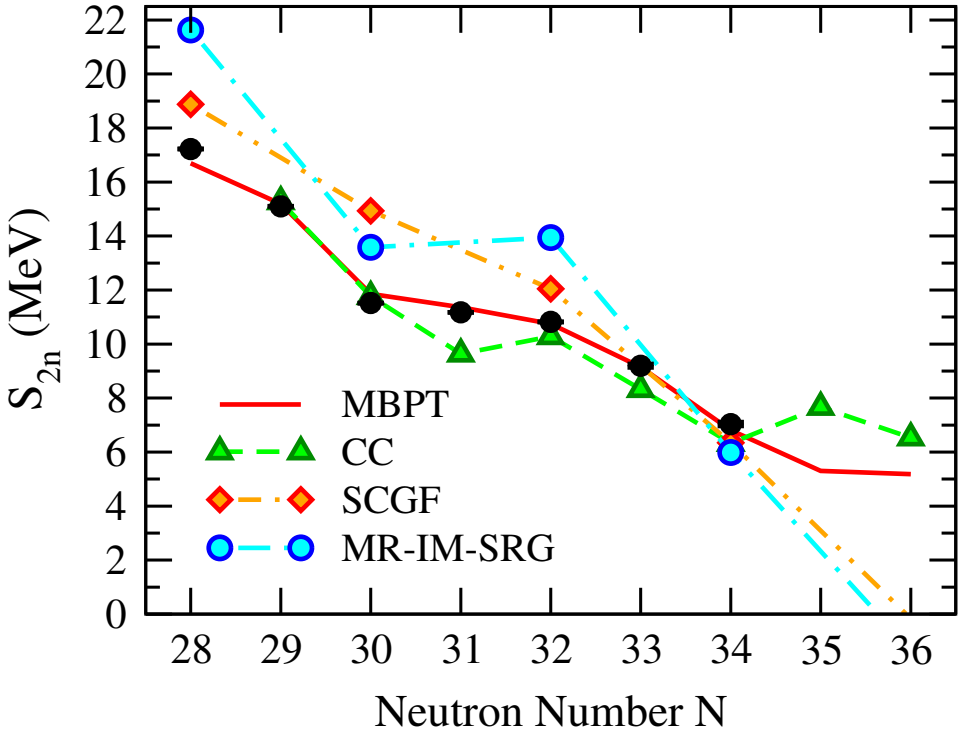
Magnus formulation for IMSRG

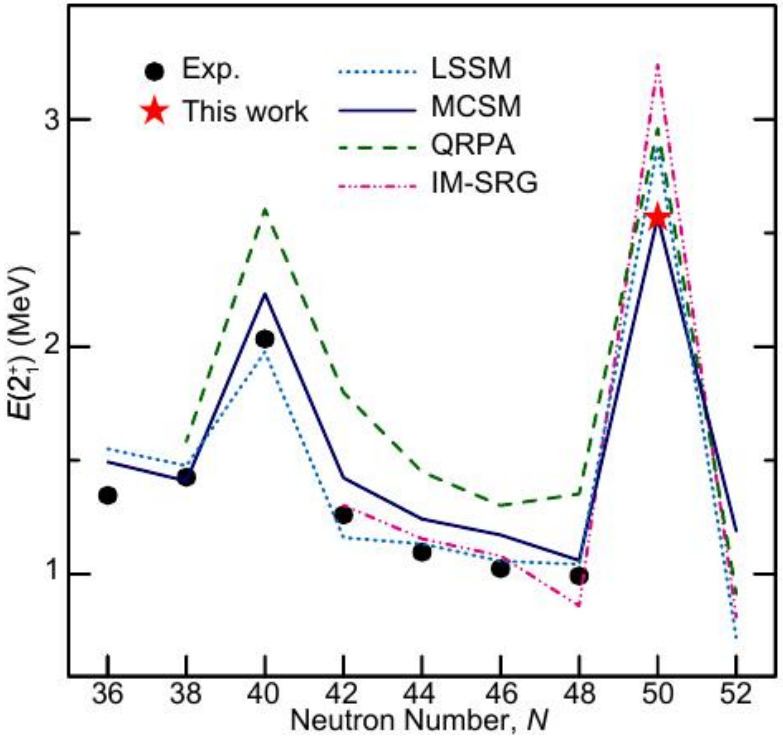
Parzuchowski et al. PRC96 034324 (2017)



Doubly-magic calcium and nickel isotopes

Calculations with NN+3N forces predict shell closures at ^{52}Ca, ^{54}Ca, ^{78}Ni





$^{51-54}$Ca masses [TRIUMF/ISOLDE]

^{54}Ca 2_1^+ state excitation energy [RIBF]

Hebeler, Holt, JM, Schwenk ARNPS 65 457(2015)

^{78}Ni 2_1^+ state excitation energy [RIBF]

ARTICLE

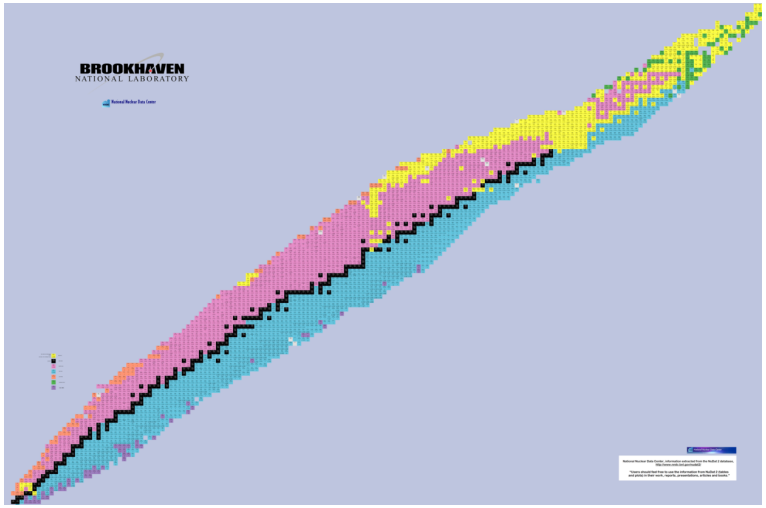
https://doi.org/10.1038/s41586-019-1155-x

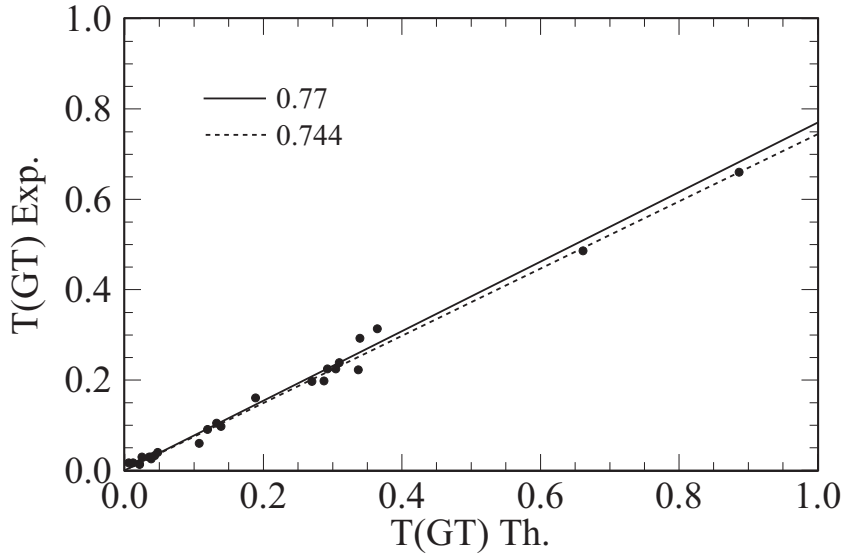
^{78}Ni revealed as a doubly magic stronghold against nuclear deformation

R. Taniuchi[1,2], C. Santamaria[2,3], P. Doornenbal[2*], A. Obertelli[2,3,4], K. Yoneda[2], G. Authelet[3], H. Baba[2], D. Calvet[3], F. Château[3], A. Corsi[3], A. Delbart[3], J.-M. Gheller[3], A. Gillibert[3], J. D. Holt[5], T. Isobe[2], V. Lapoux[3], M. Matsushita[6], J. Menéndez[6], S. Momiyama[1,2], T. Motobayashi[2], M. Niikura[1], F. Nowacki[7], K. Ogata[8,9], H. Otsu[2], T. Otsuka[1,2,6], C. Péron[3], S. Péru[10], A. Peyaud[3], E. C. Pollacco[3], A. Poves[11], J.-Y. Roussé[3], H. Sakurai[1,2], A. Schwenk[4,12,13], Y. Shiga[2,14], J. Simonis[4,12,15], S. R. Stroberg[2,16], S. Takeuchi[2], Y. Tsunoda[6], T. Uesaka[2], H. Wang[2], F. Browne[17], L. X. Chung[18], Z. Dombradi[19], S. Franchoo[20], F. Giacoppo[21], A. Gottardo[20], K. Hadyńska-Klęk[21], Z. Korkulu[19], S. Koyama[1,2], Y. Kubota[2,6], J. Lee[22], M. Lettmann[4], C. Louchart[4], R. Lozeva[7,23], K. Matsui[1,2], T. Miyazaki[1,2], S. Nishimura[2], L. Olivier[20], S. Ota[6], Z. Patel[24], E. Şahin[21], C. Shand[24], P.-A. Söderström[2], I. Stefan[20], D. Steppenbeck[6], T. Sumikama[25], D. Suzuki[20], Z. Vajta[19], V. Werner[4], J. Wu[2,26] & Z. Y. Xu[22]

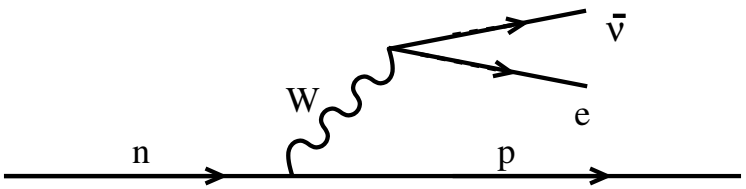
β decay: "quenching"

β decays (e^- capture) main decay model along nuclear chart
In general well described by nuclear structure theory: shell model...





Martinez-Pinedo et al. PRC53 2602(1996)



$$\langle F| \sum_i [g_A\, \boldsymbol{\sigma}_i \tau_i^-]^{\rm eff} |I\rangle\,, \quad [\boldsymbol{\sigma}_i \tau]^{\rm eff} \approx 0.7 \boldsymbol{\sigma}_i \tau$$

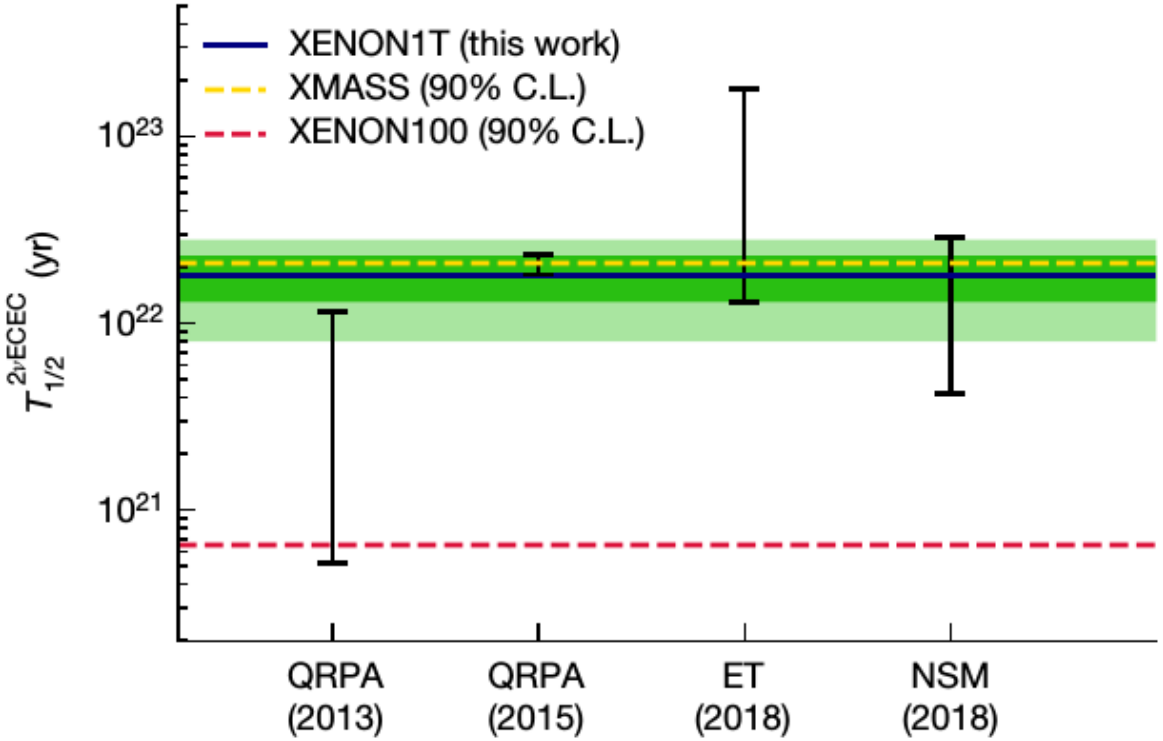
Gamow-Teller transitions:
theory needs $\boldsymbol{\sigma}_i \tau$ "quenching"

Deficient many-body approach,
or transition operator?

Two-neutrino ECEC of ^{124}Xe

Predicted 2νECEC half-life:
shell model error bar largely dominated by "quenching" uncertainty

$$\frac{1}{T^{2\nu\beta\beta}} = G_{2\nu}\, g_A^4\, (M^{2\nu\beta\beta})^2, \qquad M^{2\nu\beta\beta} = \sum_k \frac{\langle 0_f^+ | \sum_n \sigma_n \tau_n^- | 1_k^+ \rangle \langle 1_k^+ | \sum_m \sigma_m \tau_m^- | 0_i^+ \rangle}{E_k - (M_i + M_f)/2}$$



Suhonen
JPG 40 075102 (2013)

Pirinen, Suhonen
PRC 91, 054309 (2015)

Coello Pérez, JM, Schwenk
PLB 797 134885 (2019)

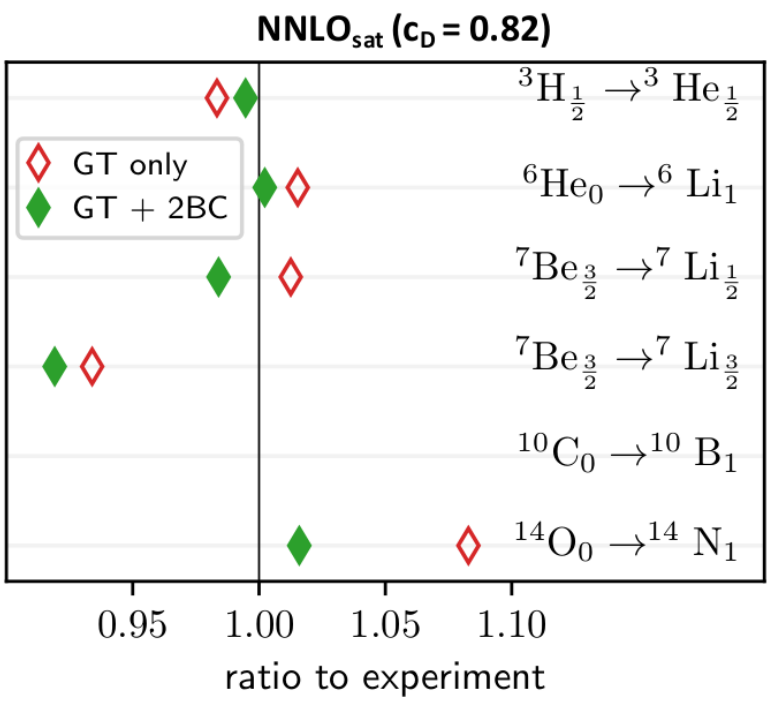
XENON1T
Nature 568 532 (2019)

Shell model, QRPA and Effective theory (ET) predictions
good agreement with XENON1T measurement of 2νECEC!

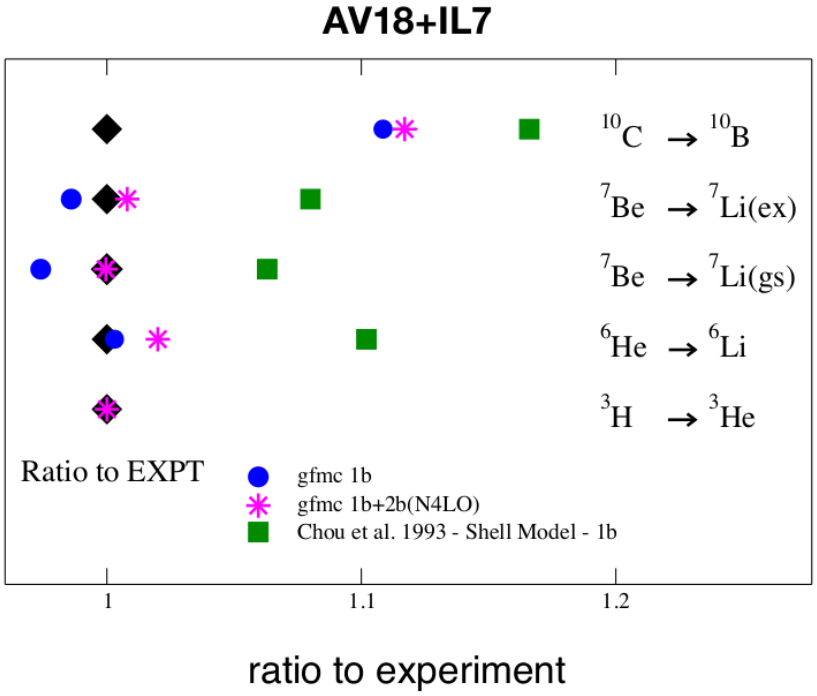
β decay in very light nuclei: GFMC vs NCSM

Quantum Monte Carlo, No Core Shell Model β decays in $A \leq 14$

Pastore et al. PRC97 022501 (2018), Gysbers et al. Nature Phys. 15 428 (2019)



No-core shell model



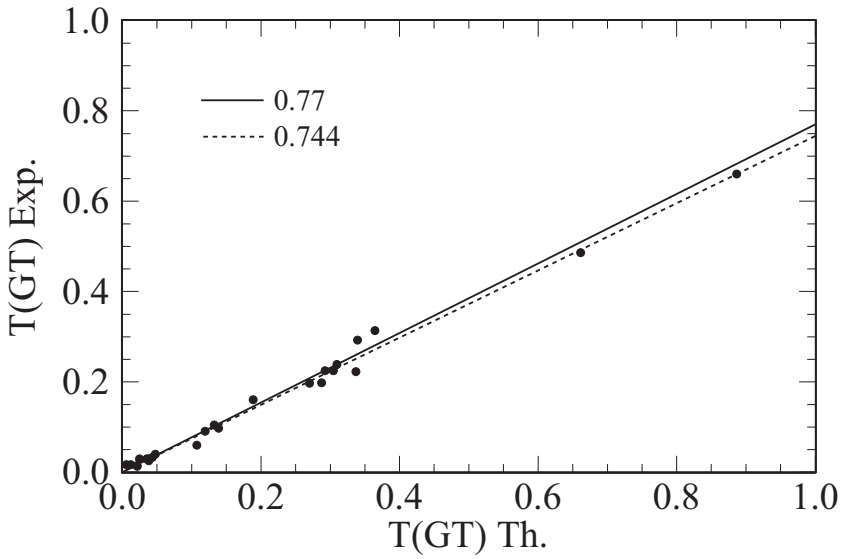
Quantum Monte Carlo

Very good agreement to experiment, except ^{10}C (structure)

Impact of 2b currents small (few %), disagreement on sign

Gamow-Teller β decay medium nuclei with VS-IMSRG

β decays (e^- capture) challenge for nuclear theory



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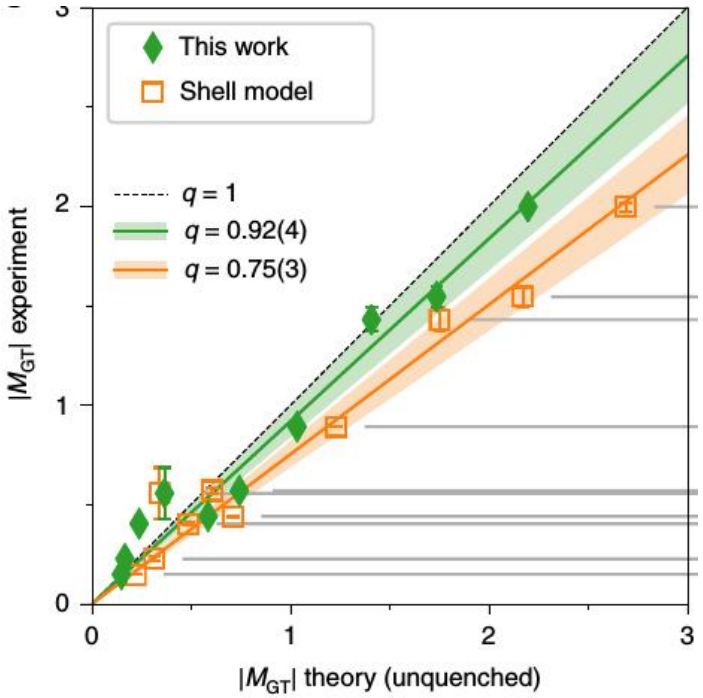


Gysbers et al. Nature Phys. 15 428 (2019)

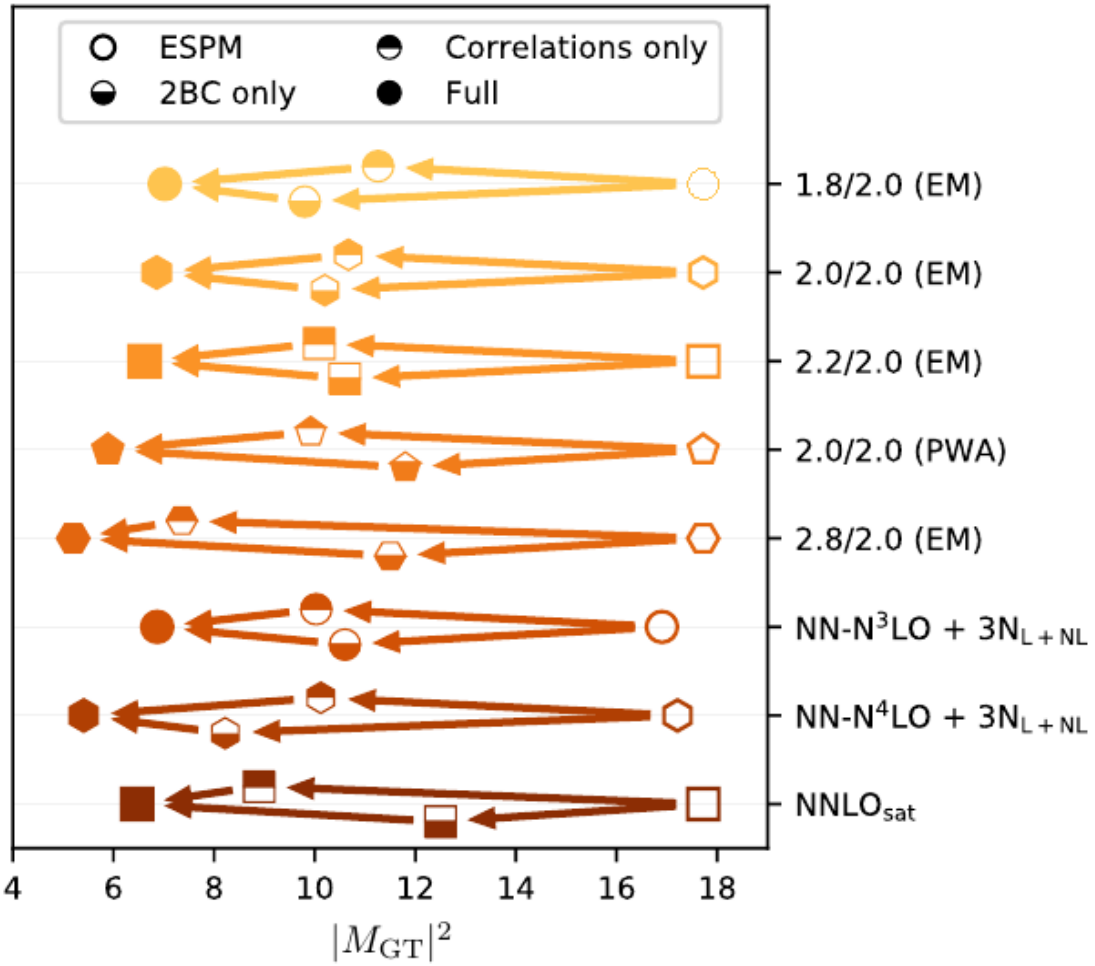
$$\langle F| \sum_i [g_A\, \boldsymbol{\sigma}_i \tau_i^-]^{\rm eff} |I\rangle\,, \quad [\boldsymbol{\sigma}_i \tau]^{\rm eff} \approx 0.7 \boldsymbol{\sigma}_i \tau$$

Phenomenological models need $\boldsymbol{\sigma}_i \tau$ "quenching"

Ab initio calculations including meson-exchange currents do not need any "quenching"

Origin of β decay "quenching"

Which are main effects missing in conventional β-decay calculations?
Test case: GT decay of ^{100}Sn



Relatively similar and complementary impact of

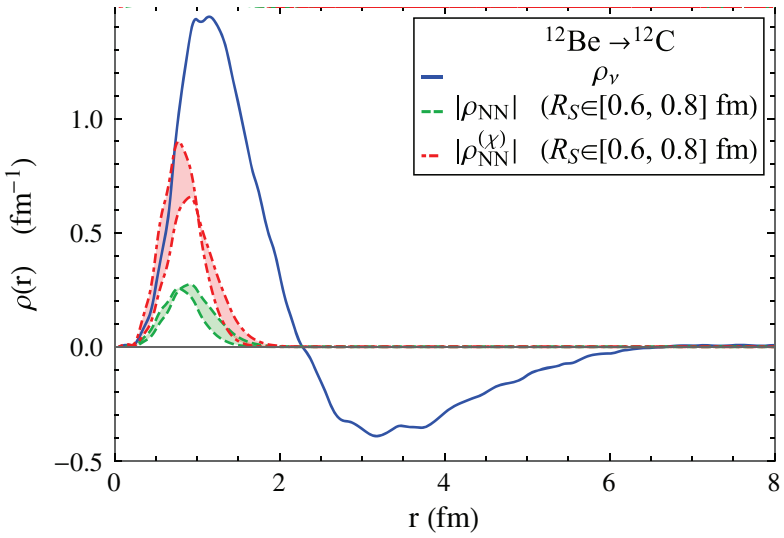
- nuclear correlations
- meson-exchange currents

Gysbers et al.
Nature Phys. 15 428 (2019)

Experiment: $|M_{GT}|^2 = 4.4^{+0.9}_{-0.7}$ Lubos et al. PRL122 222502 (2019)

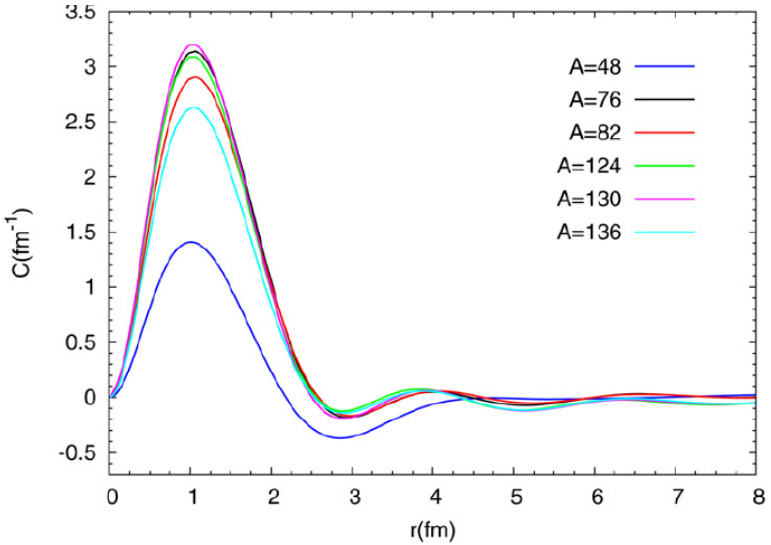
First principles NMEs in ^{12}Be: radial cancellation

Quantum Monte Carlo calculations for very light ^{12}Be leads to very small NMEs $M^{0\nu} \approx 0.4 - 0.5$



Pastore et al. PRC97 014606 (2018)

Cirigliano et al. PRL120 202001(2018)



JM et al. NPA818 139 (2009)

Cancellation between short- and long-range contributions to NME, not observed in shell model or QRPA calculations of heavier nuclei

Implications for short-range contribution to $0\nu\beta\beta$ NME **E. Mereghetti's talk**

First principles IMSRG NME for ^{48}Ca

Complete nuclear correlations included in ab initio calculations
IMSRG (in-medium similarity renormalization group) for ^{48}Ca NME

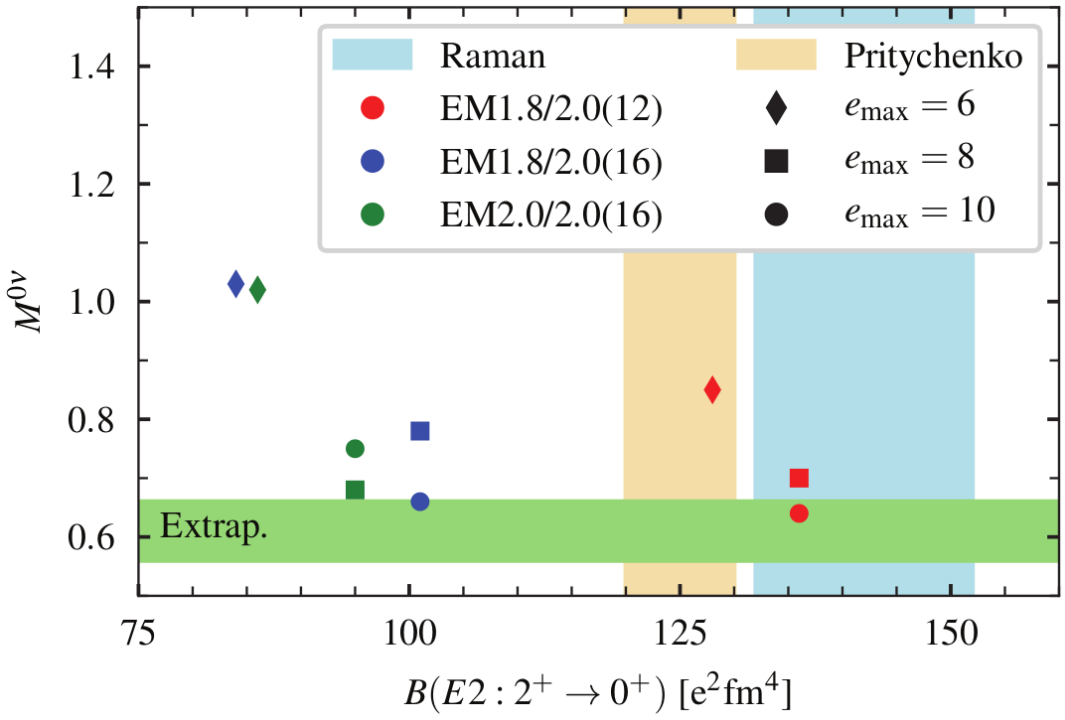
Correlations systematically built on collective reference state
Generator coordinate method: deformation, isoscalar pairing

Benchmark against first principles NME in ^{6}He
Basili et al. PRC102 014302 (2020)

Best calculation reproduces electromagnetic transitions in ^{48}Ti

NME $\sim$ 0.4/30% smaller than nuclear shell model

Yao et al.
PRL 124 232501 (2020)



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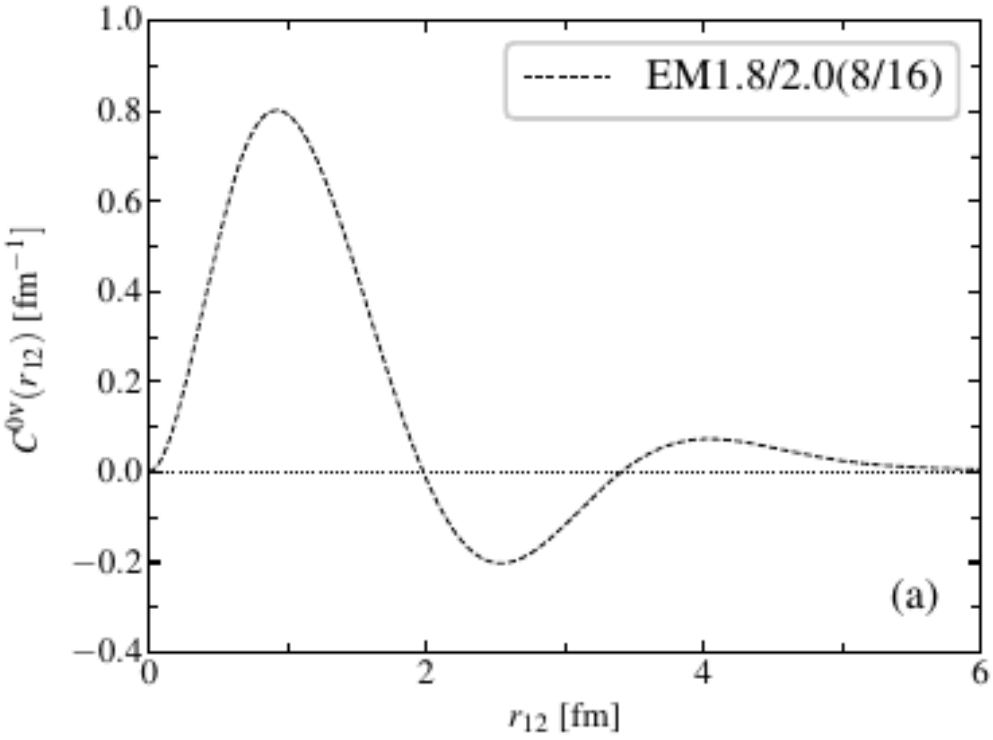


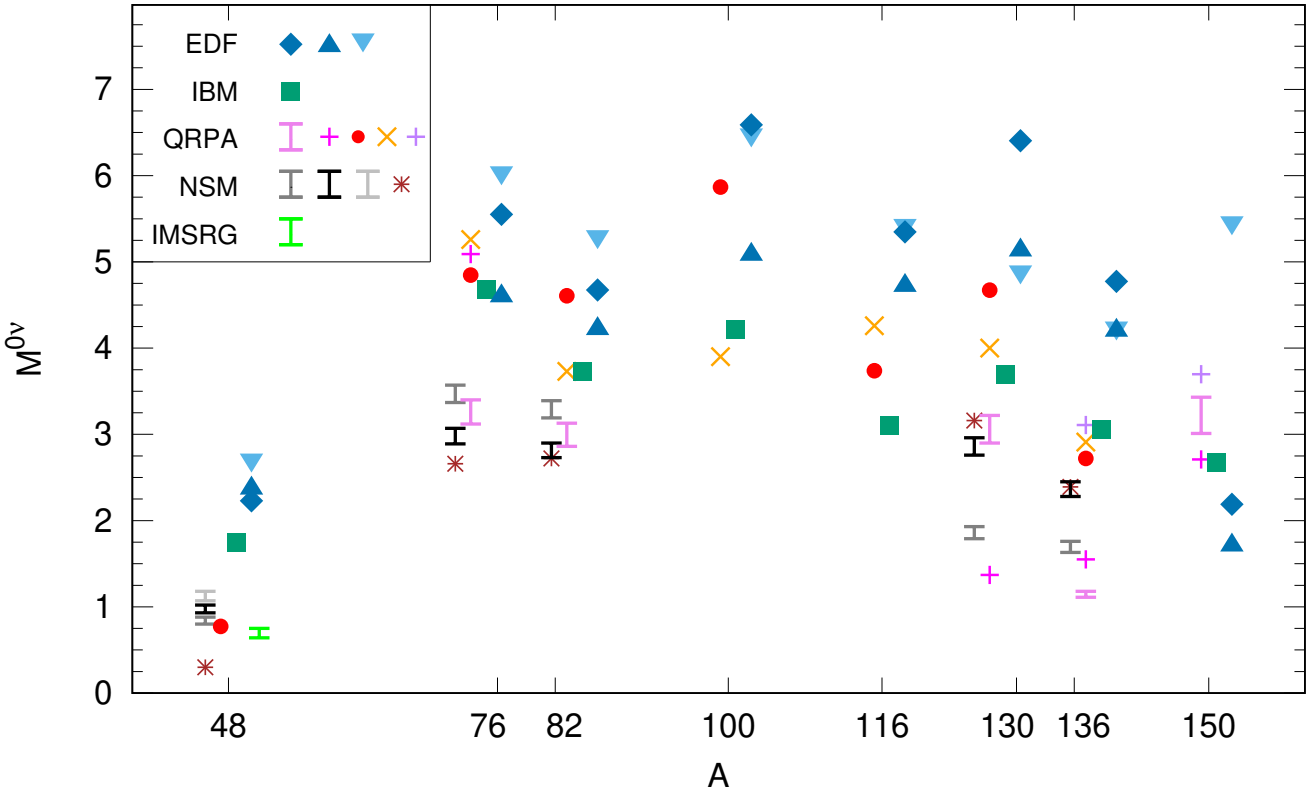
$0\nu\beta\beta$ decay nuclear matrix elements

Large difference in nuclear matrix element calculations: factor $\sim 2-3$

$$\langle 0_f^+ | \sum_{n,m} \tau_n^- \tau_m^- \sum_x H^x(r)\, \Omega^x \, | 0_i^+ \rangle$$

Ω^x = Fermi ($\mathbb{1}$), GT ($\sigma_n \sigma_m$),Tensor

$H(r)$ = neutrino potential



EDF: large NMEs

QRPA: wider range

NSM: small NMEs

IMSRG ab initio
^{48}Ca NME: quite small

Additional uncertainty:
"g_A quenching"?

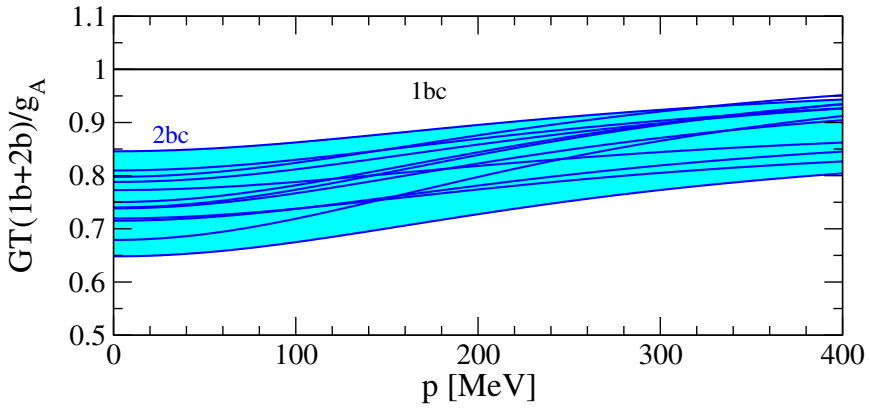
Engel, JM, Rep. Prog. Phys. 80 046301 (2017)

M. Agostini, G. Benato, J. Detwiler, JM, F. Vissani, in preparation

2b currents in $\beta\beta$ decay

In $0\nu\beta\beta$ decay, two weak currents lead to four-body operator when including the product of two 2b currents: computational challenge

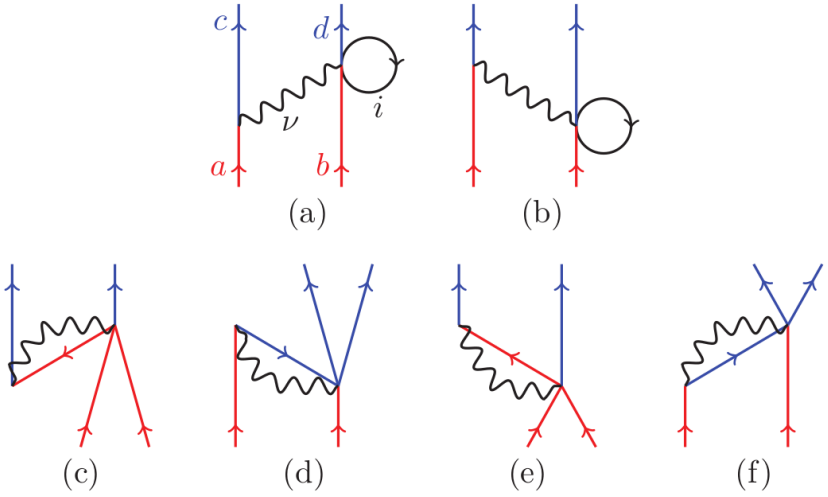
Approximate 2b current as effective 1b current



Quenching reduced to $\sim 20\%$ at $p \sim m_\pi$ for $0\nu\beta\beta$ decay

JM et al. PRL107 062501(2011)

Approximate 4b operator as effective 3b operator



Estimated effect $\sim 10\%$

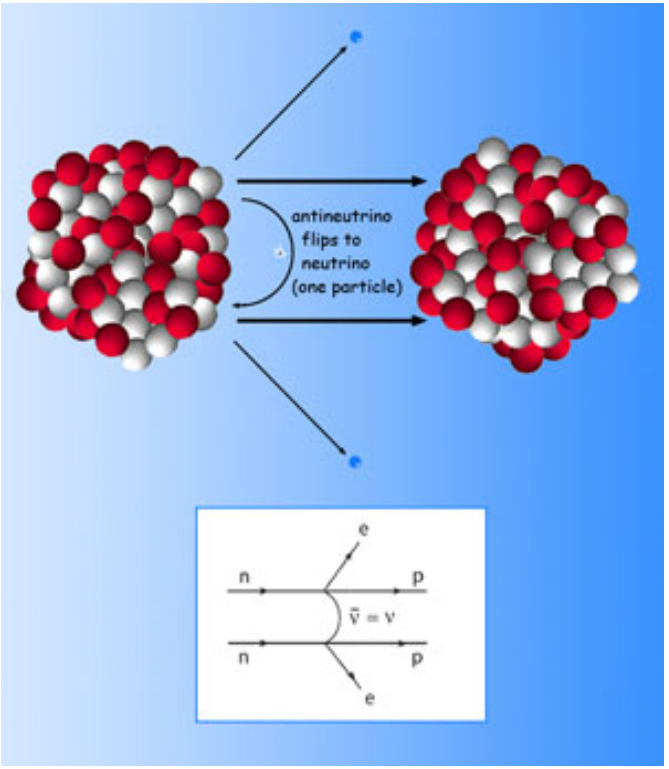
Wang et al. PRC98 031301 (2018)

Estimations suggest that 2b currents smaller in $0\nu\beta\beta$ than β decay

Summary

Nuclear matrix elements key
for the design of next-generation tonne-scale $0\nu\beta\beta$ decay experiments
and for fully exploiting the experimental results

- First principles calculations
  solve much of β decay "quenching" puzzle:
  (almost) no need for "quenching"
  when calculations include
  additional correlations and two-body currents
- Ab initio ^{48}Ca NMEs quite small,
  extension to heavier $\beta\beta$ nuclei in progress
  using several many-body methods
- First principles ^{12}Be NME quite small
  due to cancellation between
  short- and long-range contributions



Double Gamow-Teller strength distribution

Measurement of Double Gamow-Teller (DGT) resonance
in double charge-exchange reactions ^{48}Ca(pp,nn)^{48}Ti proposed in 80's

Auerbach, Muto, Vogel... 1980's, 90's

Recent experimental plans in RCNP, RIKEN (^{48}Ca), INFN Catania

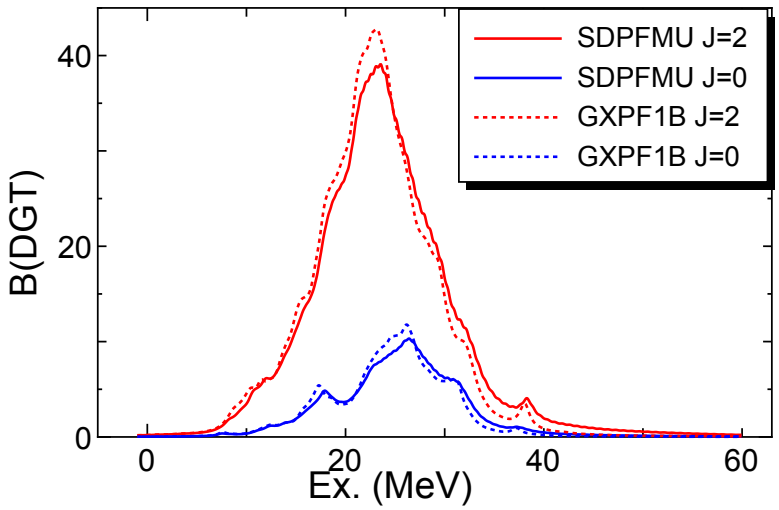
Takaki et al. JPS Conf. Proc. 6 020038 (2015)

Capuzzello et al. EPJA 51 145 (2015), Takahisa, Ejiri et al. arXiv:1703.08264

Promising connection to $\beta\beta$ decay,
two-particle-exchange process,
especially the (tiny) transition
to ground state of final state

Shell model calculation

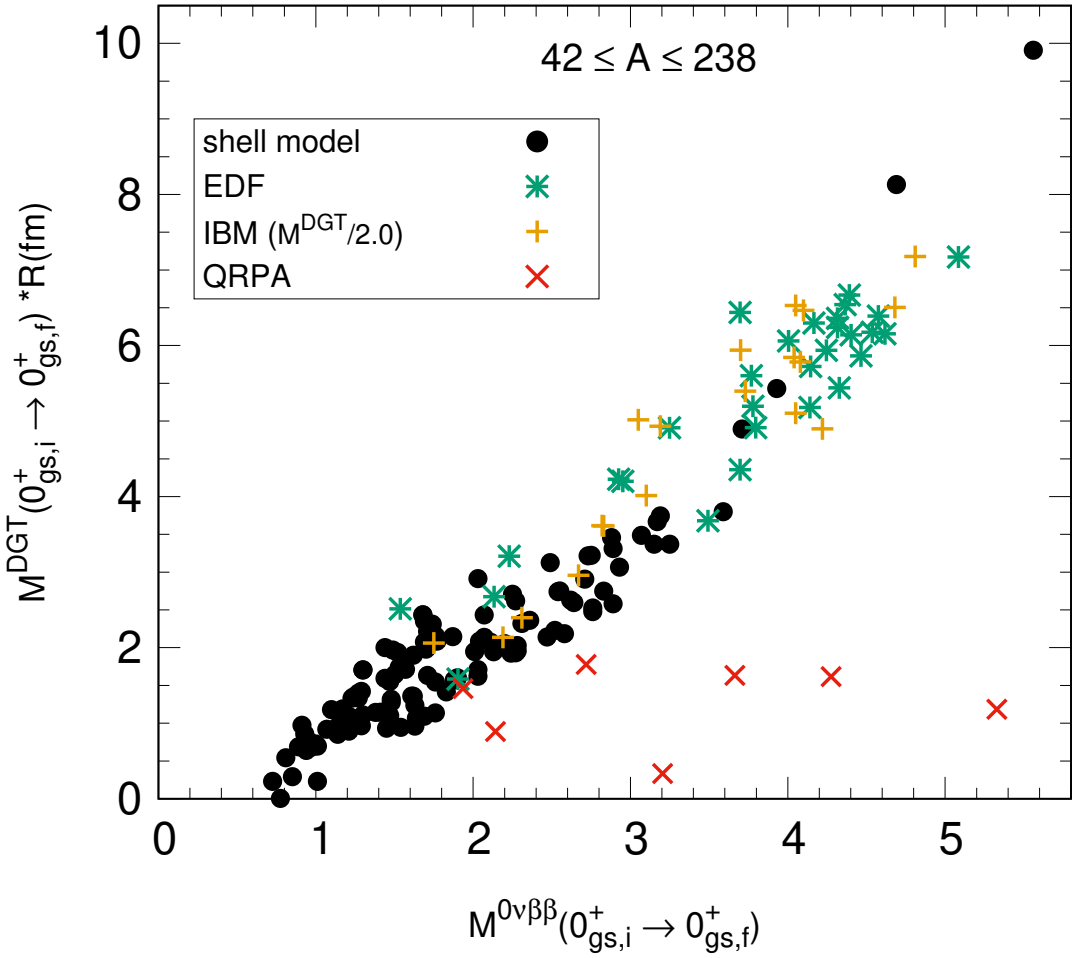
Shimizu, JM, Yako, PRL120 142502 (2018)



$$B(DGT^-;\lambda;i\to f)=\frac{1}{2J_i+1}\left|\left\langle {}^{48}\mathrm{Ti}\left\|\left[\sum_i \boldsymbol{\sigma}_i\tau_i^- \times \sum_j \boldsymbol{\sigma}_j\tau_j^-\right]^{(\lambda)}\right\|{}^{48}\mathrm{Ca}_{gs}\right\rangle\right|^2$$

Correlation of $0\nu\beta\beta$ decay to DGT transitions

Double GT transition to ground state $M^{\mathrm{DGT}} = \langle \mathrm{F_{gs}} || [\sum_i \boldsymbol{\sigma}_i \tau_i^- \times \sum_j \boldsymbol{\sigma}_j \tau_j^-]^0 || \mathrm{I_{gs}} \rangle |^2$
very good linear correlation with $0\nu\beta\beta$ decay nuclear matrix elements



Double Gamow-Teller correlation with $0\nu\beta\beta$ decay holds across nuclear chart
Shimizu, JM, Yako
PRL120 142502 (2018)

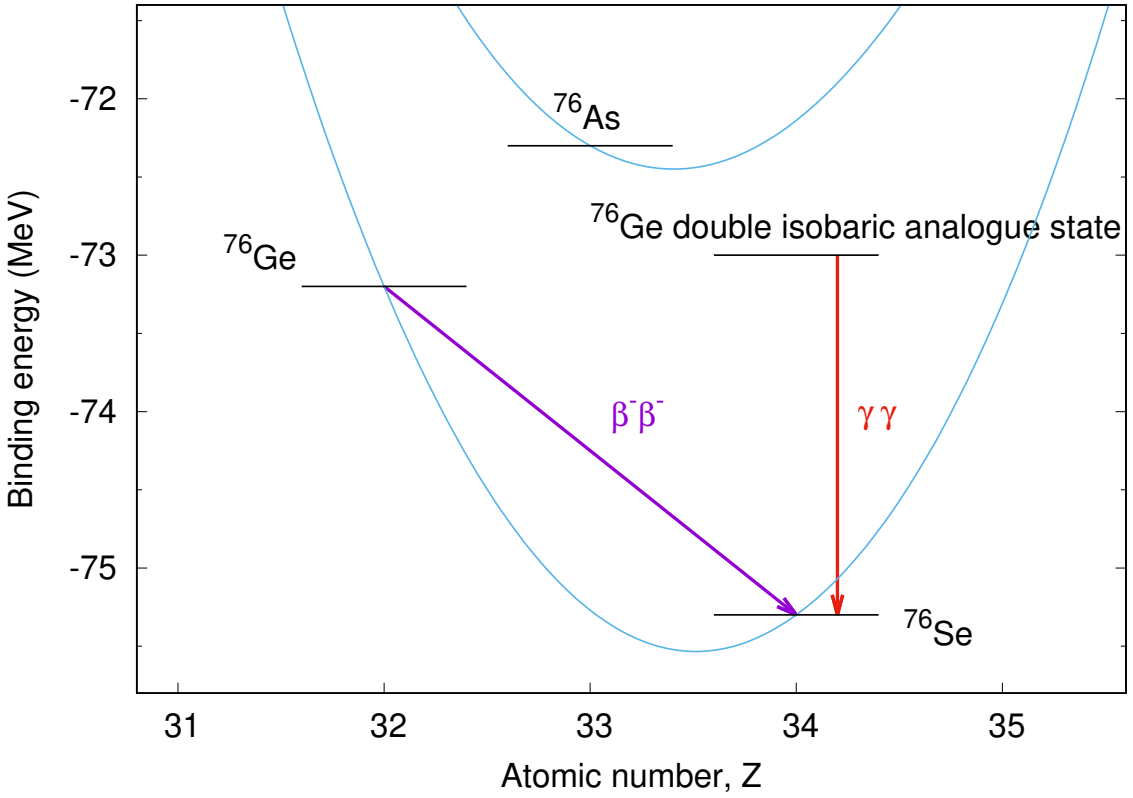
Common to shell model energy-density functionals interacting boson model, disagreement to QRPA

Experiments at RIKEN, INFN Catania may access DGT transitions

Similar $0\nu\beta\beta$ and $\gamma\gamma$ decays?

Explore correlation between $0\nu\beta\beta$ and $\gamma\gamma$ decays, focused on double-M1 transitions

$$M^{\gamma\gamma}_{M1\,M1} = \sum_k \frac{\langle 0^+_f | \sum_n (g^l_n \boldsymbol{l}_n + g^s_n \boldsymbol{\sigma}_n)^{IV} | 1^+_k(\mathrm{IAS}) \rangle \langle 1^+_k(\mathrm{IAS}) | \sum_m (g^l_m \boldsymbol{l}_m + g^s_m \boldsymbol{\sigma}_m)^{IV} | 0^+_i(\mathrm{DIAS}) \rangle}{E_k - (M_i + M_f)/2}$$



Similar initial and final states but both in same nucleus for electromagnetic transition

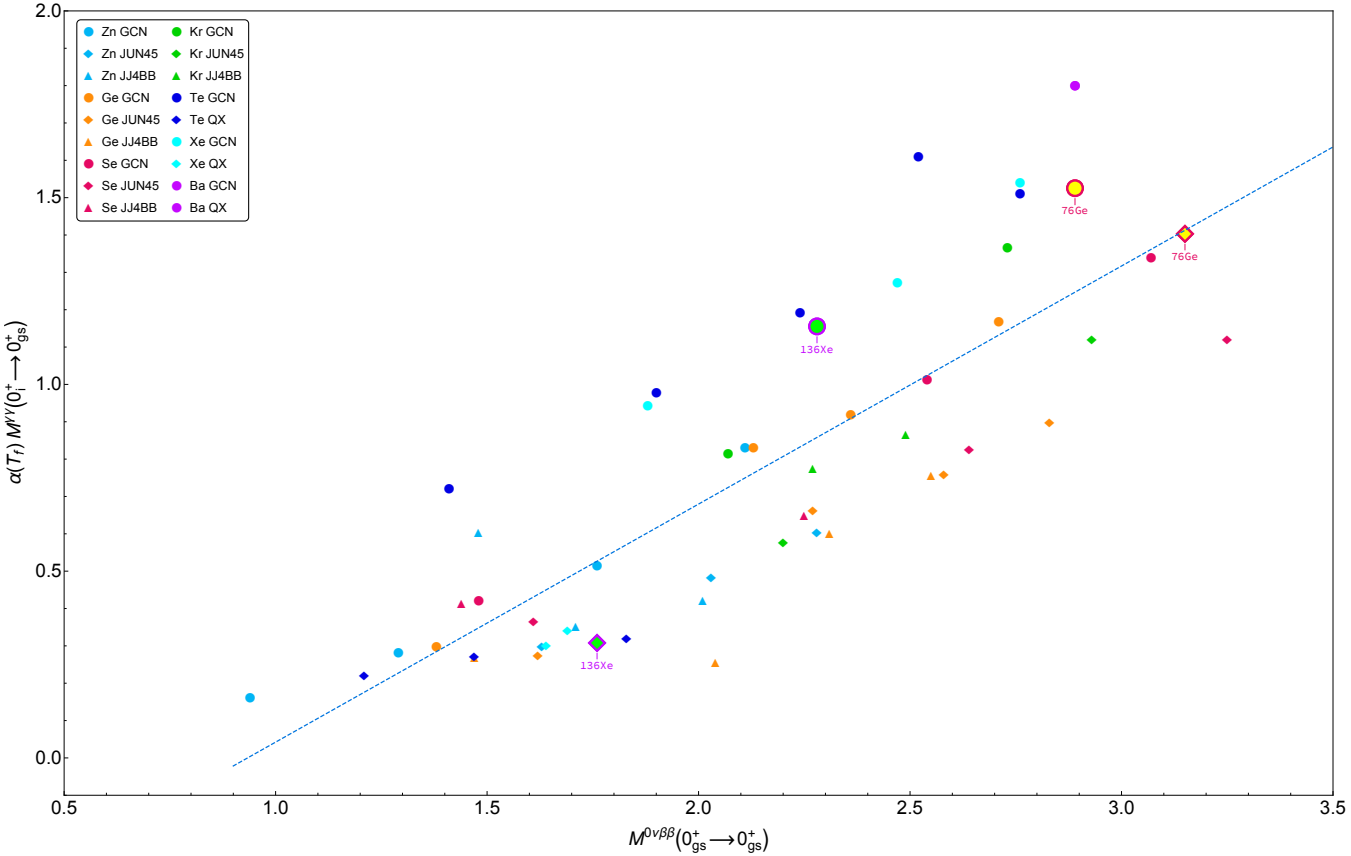
M1 and GT operators similar, physics of spin operator
M1 also angular momentum

Different energy denominator

Romeo, JM, Peña-Garay, in progress

Correlation of $0\nu\beta\beta$ decay to $\gamma\gamma$ transitions

Good linear correlation between $\gamma\gamma$ M1M1 and $0\nu\beta\beta$ decays obtained with nuclear shell model, holds for nuclei with $A \sim 60 - 140$



Includes $\beta\beta$ nuclei: ^{76}Ge, ^{82}Se, ^{130}Te, ^{136}Xe

Romeo, JM, Peña-Garay, in progress

Measurements of $\gamma\gamma$ M1M1 decays could inform $0\nu\beta\beta$ NMEs!