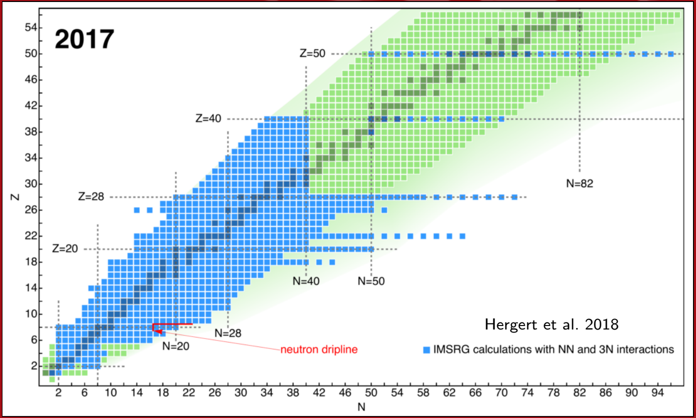
Onward and upward:

Prospects for applying ab initio methods to the structure of medium-heavy nuclei



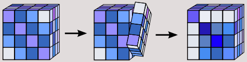
Hergert et al. 2018

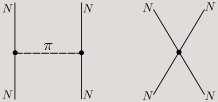
Ragnar Stroberg

Reed College

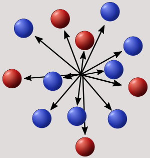
Ariel Science Workshop
Vancouver, BC
July 17, 2018

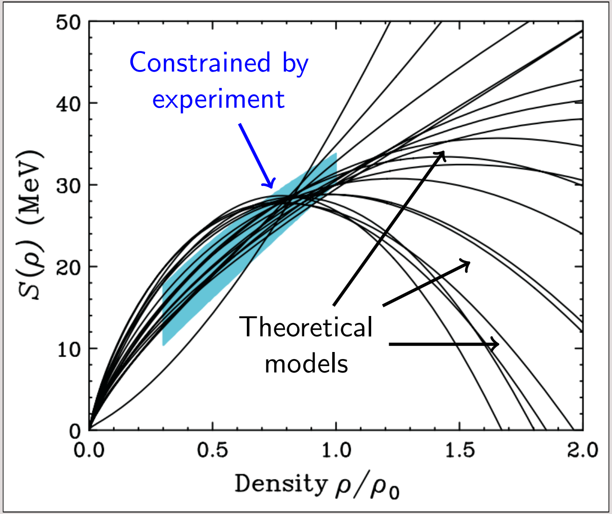
Outline





1. Motivation
    - Predictive power beyond existing data
2. Methods
    - Effective field theory (EFT)
    - Ab initio many-body methods
3. Selected results
    - Binding energies / dripline
    - β decay
4. Reaching beyond $A = 100$



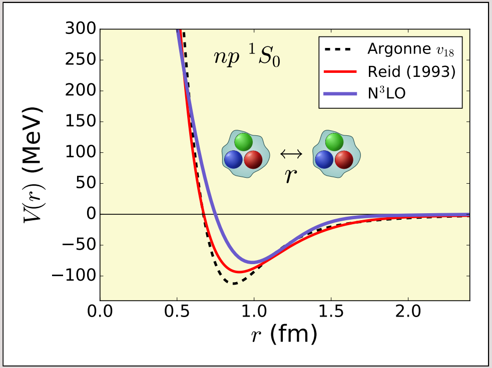


Fit to data
$\neq$
predictive power

Tsang et al. 2012

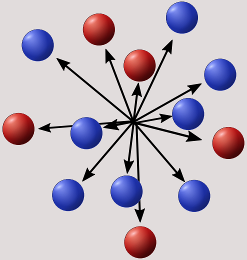
Difficulties in nuclear structure

Nuclear forces



Spin/isospin-dependence, tensor force, 3N forces…

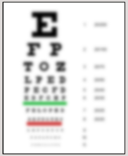
The many body problem

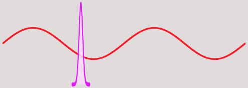


- Pauli-principle → antisymmetrized wave function
- Short-range repulsion → correlations, configuration mixing

Effective field theory (EFT)

- To begin, choose degrees of freedom and write down the most general theory allowed by the relevant symmetries.
- At low momenta $\sim Q$, high-momentum physics ($\sim \Lambda$) is not resolved





- Organize the infinite number of terms in the theory in powers of $\left(\frac{Q}{\Lambda}\right)$
- Higher powers should be less important

Weinberg 1990; Ordóñez and Kolck 1992; Bedaque and VanKolck 2002; Kaplan, Savage, and Wise 1996; Epelbaum 2010; Machleidt and Entem 2011. . .

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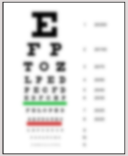

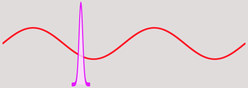

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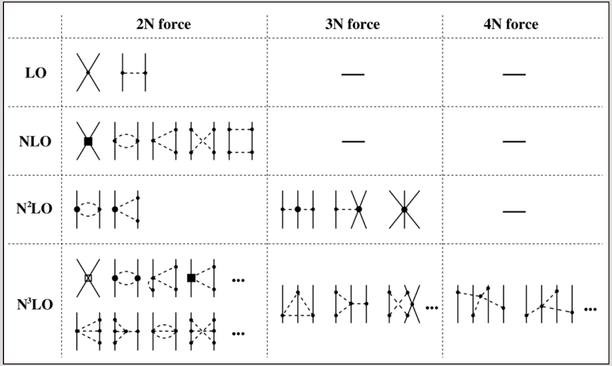
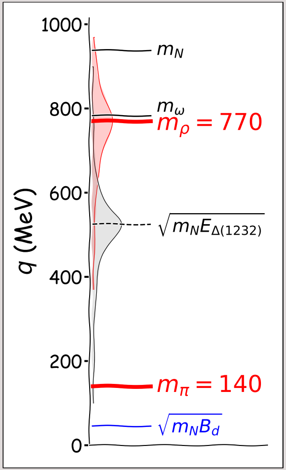
Low-energy nuclear physics

- Degrees of freedom: nucleons and pions
- Typical scale: $Q \sim k_F \lesssim m_\pi \sim 200$ MeV
- Breakdown scale: $\Lambda \sim m_\rho \sim 700$ MeV

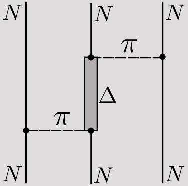


Weinberg 1990; Ordóñez and Kolck 1992; Bedaque and VanKolck 2002; Kaplan, Savage, and Wise 1996; Epelbaum 2010; Machleidt and Entem 2011...

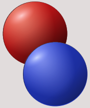
Challenges: Power counting

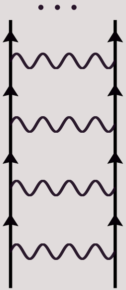


$\Delta(1232)$ resonance



$$\boxed{E(\Delta)\text{-}E(N) \approx 300 \text{ MeV}}$$





Bound states → IR divergences

Deuteron BE $= 2.22$ MeV $\ll m_\pi$

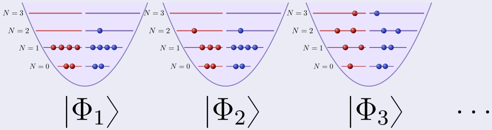
And of course, $2\pi \sim m_\rho / m_\pi \ \ldots$

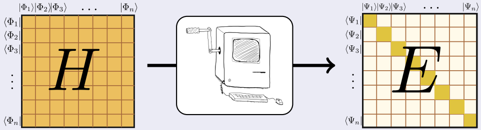
$$H|\Psi\rangle = E|\Psi\rangle$$

- An *exact* solution to an *exact* problem
- A *systematically improvable* solution to a *systematically improvable* problem
- The problem (i.e. the Hamiltonian) should not know or care about the solution (many-body method)

Ab initio methods for light systems

No Core Shell Model
(diagonalization in HO basis)

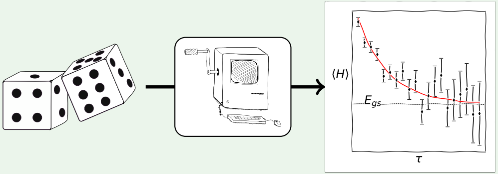




Scaling: $\binom{n}{A} = \frac{n!}{A!(n-A)!}$

Quantum Monte Carlo

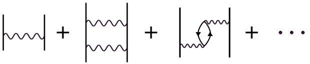
$$|\Psi\rangle \propto \lim_{\tau\to\infty} e^{-\tau H}|\Phi\rangle$$



Scaling: $2^A \frac{A!}{N!Z!}$

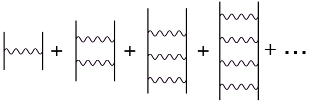
Ab initio methods for medium-mass systems

Many-body Perturbation Theory



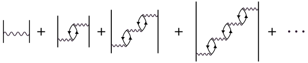
Scaling: νth order $\sim \mathcal{O}(n^{2\nu})$

Brueckner G-matrix



Scaling: $\mathcal{O}(n^4)$

Random Phase Approximation



Scaling: $\mathcal{O}(n^3) - \mathcal{O}(n^4)$

Coupled Cluster

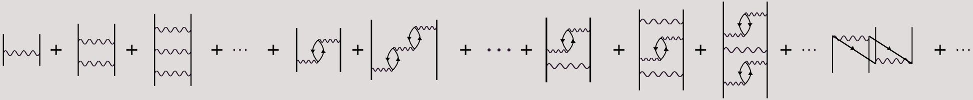
$$|\Psi\rangle = e^{\hat{T}}|\Phi\rangle$$

Self-Consistent Green's Function

$$g(\omega) = g^{(0)}(\omega) + \Sigma^*(\omega)\, g^{(0)}(\omega)$$

In-Medium Similarity Renormalization Group

$$\frac{d}{ds}H(s) = [\eta(s), H(s)]$$



Scaling: $\mathcal{O}(n^6)$, higher corrections $\sim \mathcal{O}(n^7)$, etc.

Selected Results

Ab initio[†] results with interactions from χ_{EFT}[‡]

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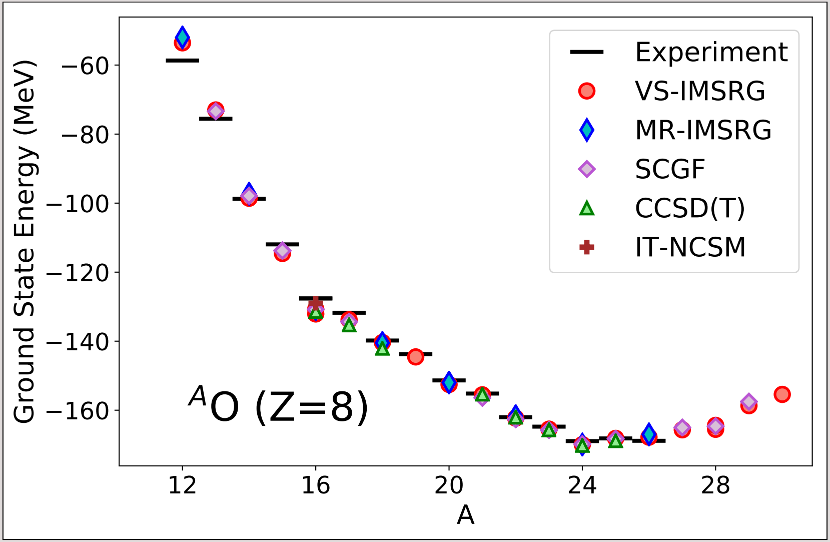
† Generally without error estimation; ‡ Generally with inconsistent power counting

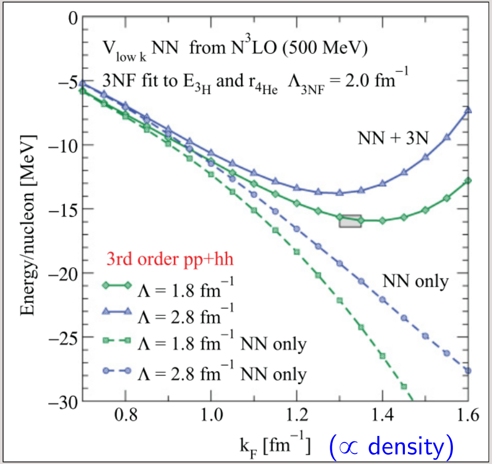
Oxygen



Hagen et al. 2009; Roth et al. 2012; Cipollone, Barbieri, and Navrátil 2013; Hergert et al. 2013; Jansen et al. 2014; Stroberg et al. 2017; (&refs therein)

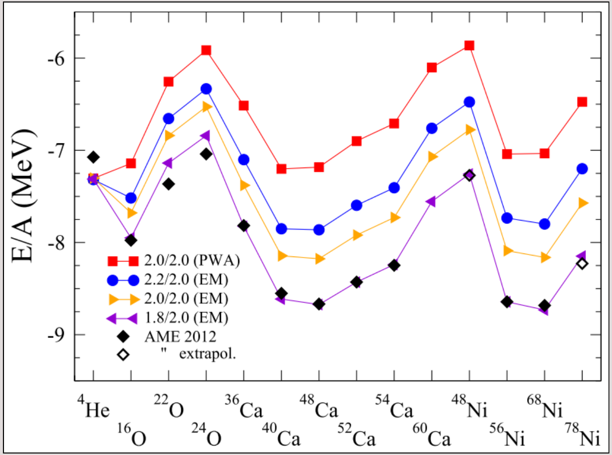
Saturation and binding energies

Nuclear matter



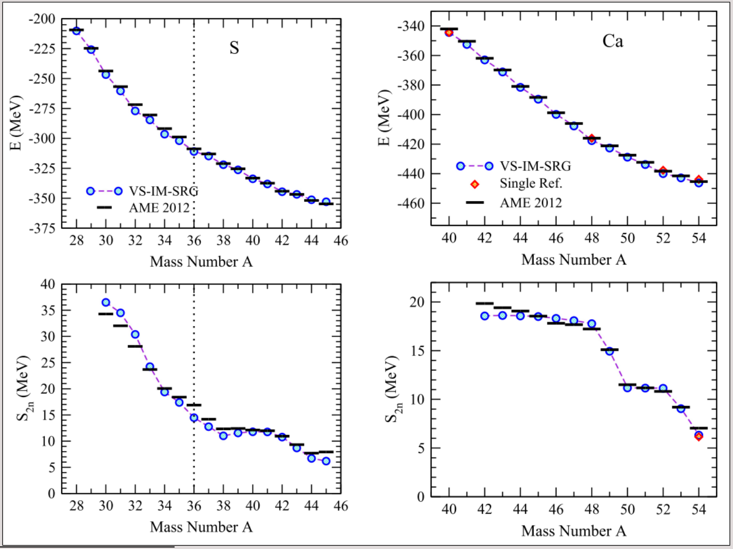
($\propto$ density)

Finite nuclei



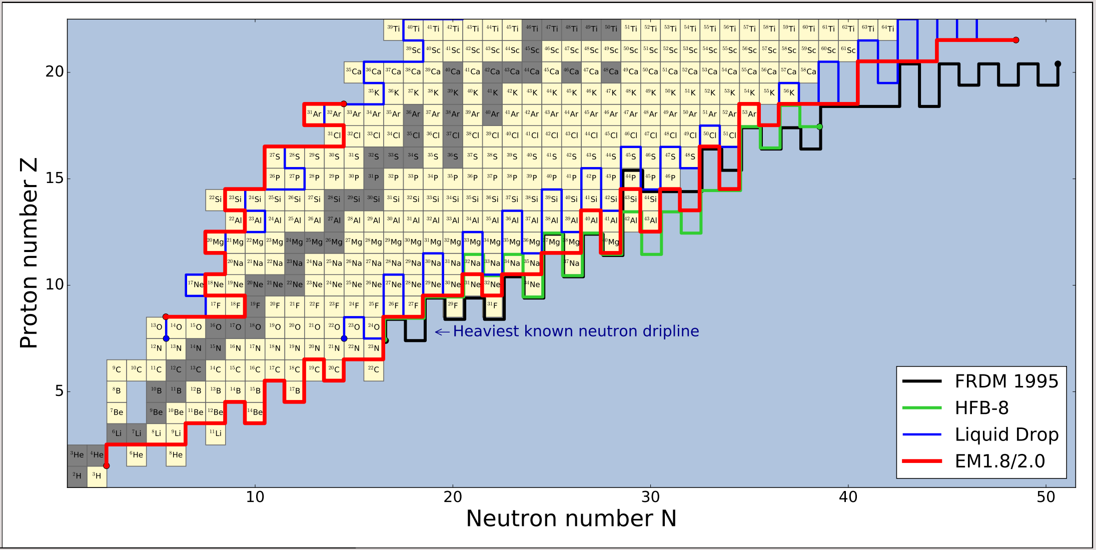
Hebeler et al. 2011; Simonis et al. 2017; [see also Hagen et al. 2014; Carbone, Rios, and Polls 2014; Drischler, Hebeler, and Schwenk 2016; Tews et al. 2016]

Energy systematics of isotopic chains



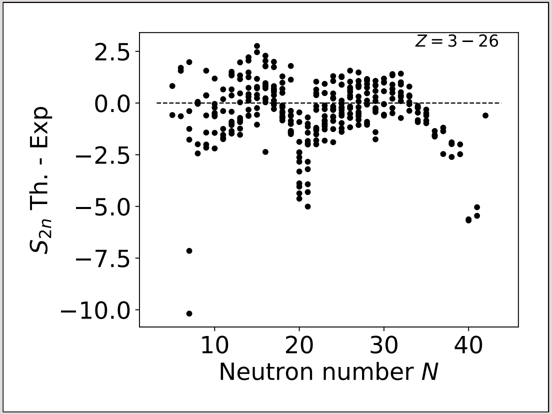
Simonis et al. 2017

The neutron dripline

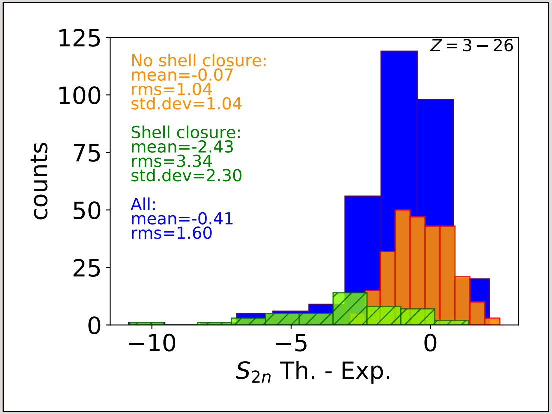


J.D. Holt et al. (in prep); Moller et al. 1995; Samyn et al. 2004

Deviation from experiment



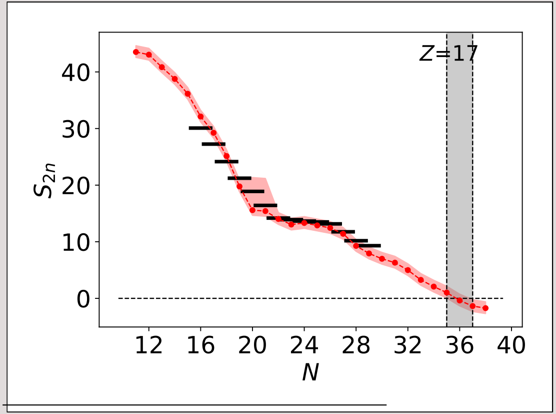
Distribution of errors



J.D. Holt et al. (in prep)

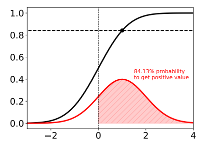
Dripline

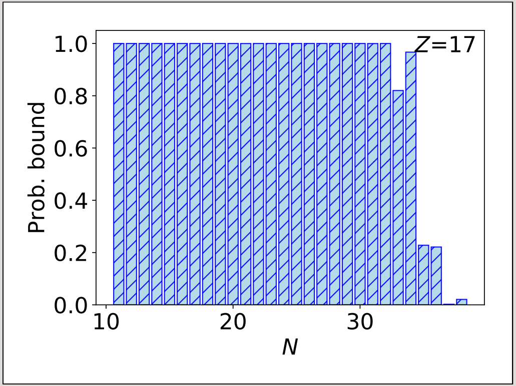
- Theory error bars based on rms deviation from experiment.
- Inflated error bars near shell closures.



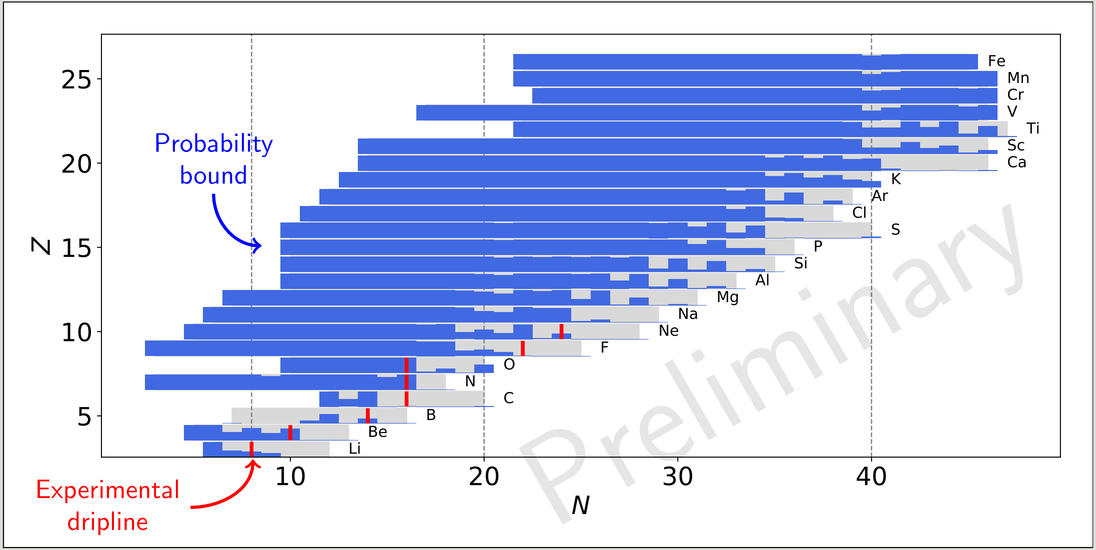
J.D. Holt et al. (in prep)

- Probability bound from Gaussian
- Total probability bound $= P_{1n} \times P_{2n}$



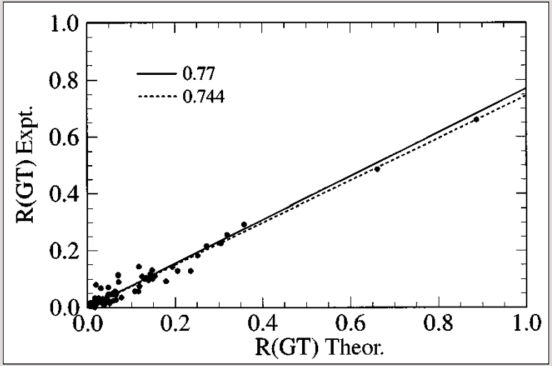


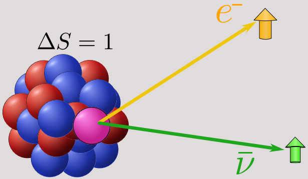
Dripline



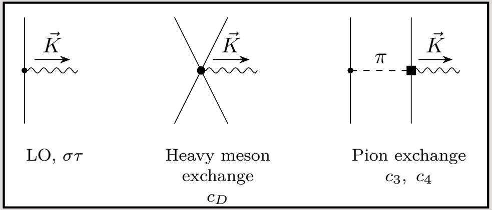
J.D. Holt et al. (in prep)

“Quenching” in Gamow-Teller decays





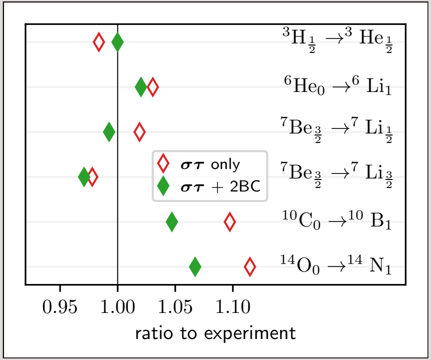
Currents from χEFT



Martínez-Pinedo et al. 1996; Gysbers et al., (under review)

Beta decay

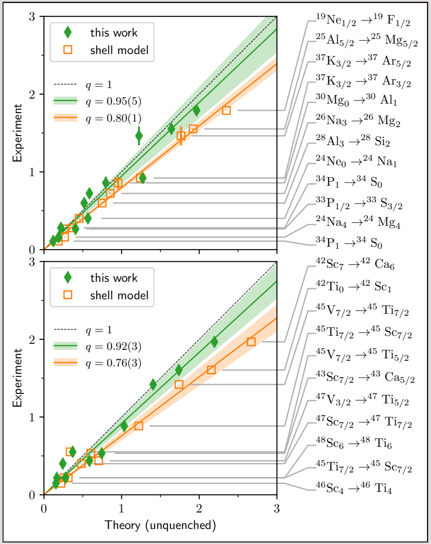
Light nuclei with NCSM



Medium-mass with VS-IMSRG

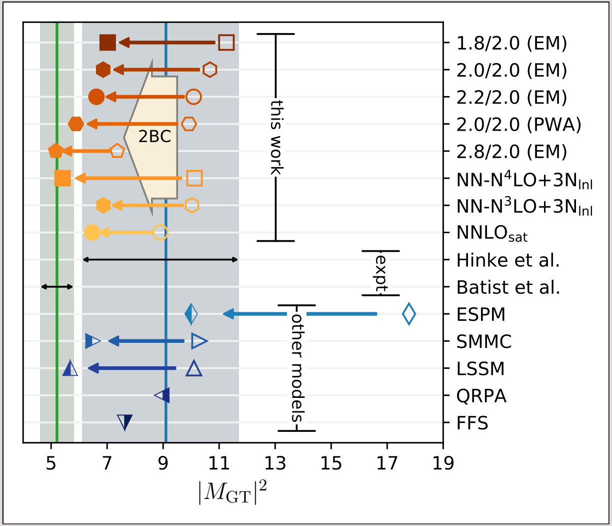
sd shell →

pf shell →



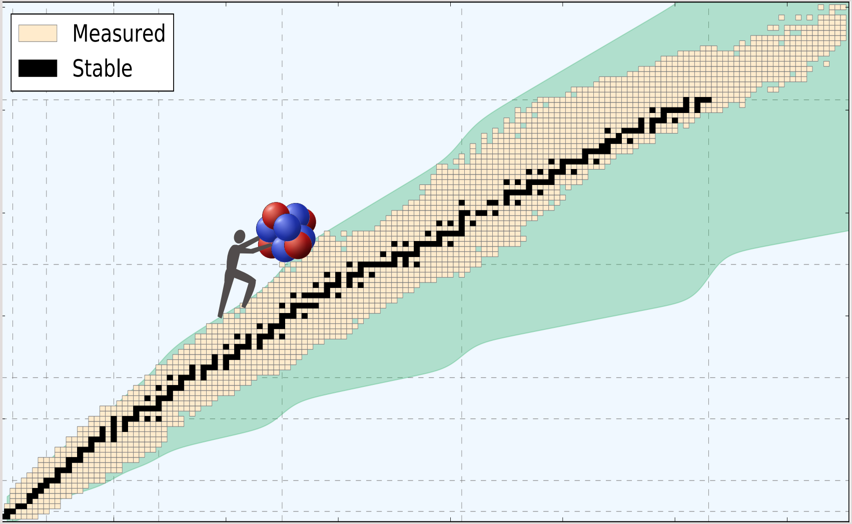
Gysbers et al. (under review)

“Superallowed” Gamow-Teller decay of ^{100}Sn ($N=Z=$50), calculated with coupled cluster method.

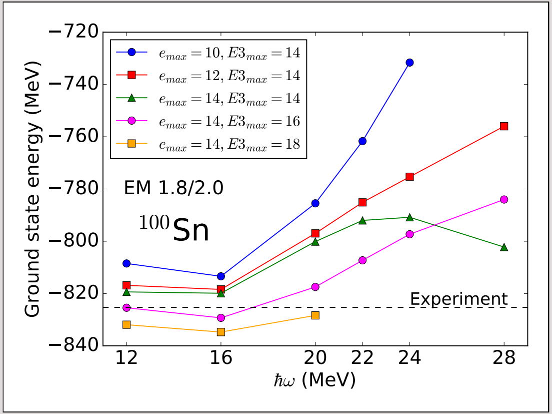


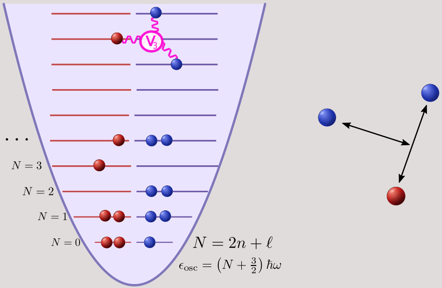
Gysbers et al. (under review)

Prospects for reliable calculations of nuclei with $A > 100$



The current limit: ^{100}Sn





Simonis et al. 2017; Binder et al. 2013; Roth et al. 2014; Binder et al. 2014; Lascar et al. 2017

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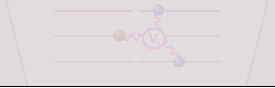
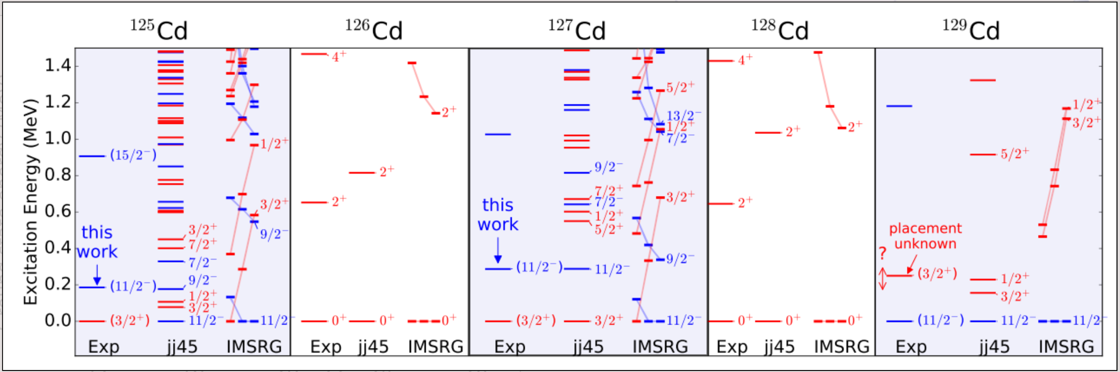
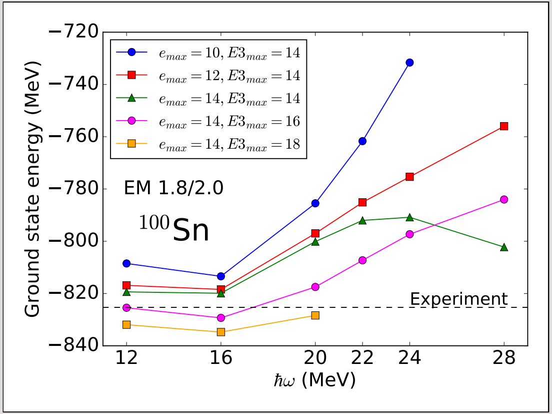


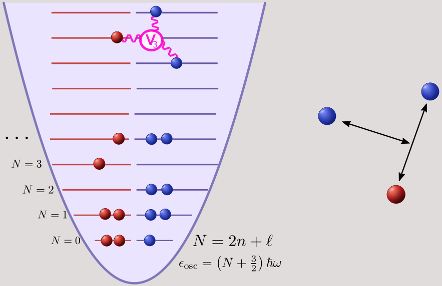


Simonis et al. 2017; Binder et al. 2013; Roth et al. 2014; Binder et al. 2014; Lascar et al. 2017

Getting heavy

The current limit: ^{100}Sn





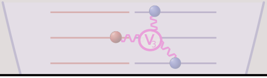
E_{3max}	Storage (GB)	Jacobi
14	5	0.05
16	20	0.15
18	100	0.33
20	300	0.70
22	950	1.50

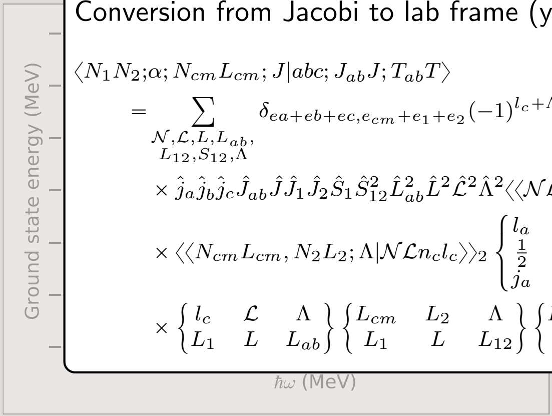
^{208}Pb requires $E_{3max} \geqslant 18$

Simonis et al. 2017; Binder et al. 2013; Roth et al. 2014; Binder et al. 2014; Lascar et al. 2017

Getting heavy

The current limit: ^{100}Sn





Conversion from Jacobi to lab frame (yikes!):

$$
\begin{aligned}
&\langle N_1 N_2;\alpha; N_{cm}L_{cm}; J | abc; J_{ab}J; T_{ab}T\rangle \\
&\quad = \sum_{\substack{\mathcal{N},\mathcal{L},L,L_{ab},\\ L_{12},S_{12},\Lambda}} \delta_{ea+eb+ec,e_{cm}+e_1+e_2}(-1)^{l_c+\Lambda+L_{ab}+L+S_{12}+L_1+J} \\
&\qquad \times \hat{j}_a\hat{j}_b\hat{j}_c\hat{J}_{ab}\hat{J}\hat{J}_1\hat{J}_2\hat{S}_1\hat{S}_{12}^2\hat{L}_{ab}^2\hat{L}^2\hat{\mathcal{L}}^2\hat{\Lambda}^2\langle\langle \mathcal{N}\mathcal{L}, N_1L_1; L_{ab}|n_bl_bn_al_a\rangle\rangle_1 \\
&\qquad \times \langle\langle N_{cm}L_{cm}, N_2L_2;\Lambda|\mathcal{N}\mathcal{L}n_cl_c\rangle\rangle_2 \begin{Bmatrix} l_a & l_b & L_{ab} \\ \frac{1}{2} & \frac{1}{2} & S_1 \\ j_a & j_b & J_{ab} \end{Bmatrix} \begin{Bmatrix} L_{ab} & l_c & L \\ S_1 & \frac{1}{2} & S_{12} \\ J_{ab} & j_c & J \end{Bmatrix} \begin{Bmatrix} L_1 & L_2 & L_{12} \\ S_1 & S_2 & S_{12} \\ J_1 & J_2 & J_{12} \end{Bmatrix} \\
&\qquad \times \begin{Bmatrix} l_c & \mathcal{L} & \Lambda \\ L_1 & L & L_{ab} \end{Bmatrix} \begin{Bmatrix} L_{cm} & L_2 & \Lambda \\ L_1 & L & L_{12} \end{Bmatrix} \begin{Bmatrix} L_{cm} & L_{12} & L \\ S_{12} & J & J_{12} \end{Bmatrix}
\end{aligned}
$$

22	950	1.50

^{208}Pb requires $E_{3max} \geqslant 18$

Simonis et al. 2017; Binder et al. 2013; Roth et al. 2014; Binder et al. 2014; Lascar et al. 2017

Summary

- EFT and ab-initio many-body methods allow the possibility to obtain theoretical predictions *with quantified uncertainties* where no experimental data exist.

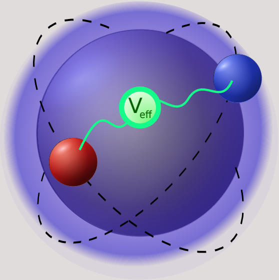
- Hurdles remain:
  - What is the optimal power counting?
  - How to rigorously estimate uncertainties of non-perturbative many-body methods?

- Application to probabilistic predictions of the dripline

- Consistent picture of quenching of GT strength from $A = 3$ to $A = 100$

- Algorithmic developent and/or approximation schemes needed to push beyond $A = 100$

Thank you!



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LLNL S. Quaglioni, K. Wendt

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