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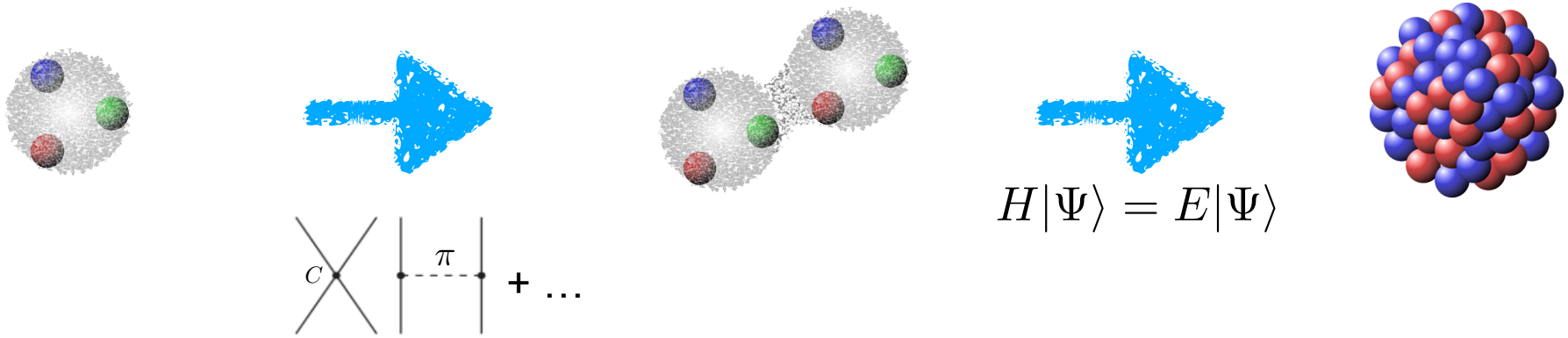
In-medium similarity renormalization group for valence-space problems



Supported by
ERATO TOMOE

Takayuki Miyagi (University of Tsukuba)

Many-Body Theory: Nuclear Physics Meets Quantum Chemistry

@ MITP, JGU, Mainz, Germany (Aug. 24 - Sep. 4, 2026)

Nuclear landscape

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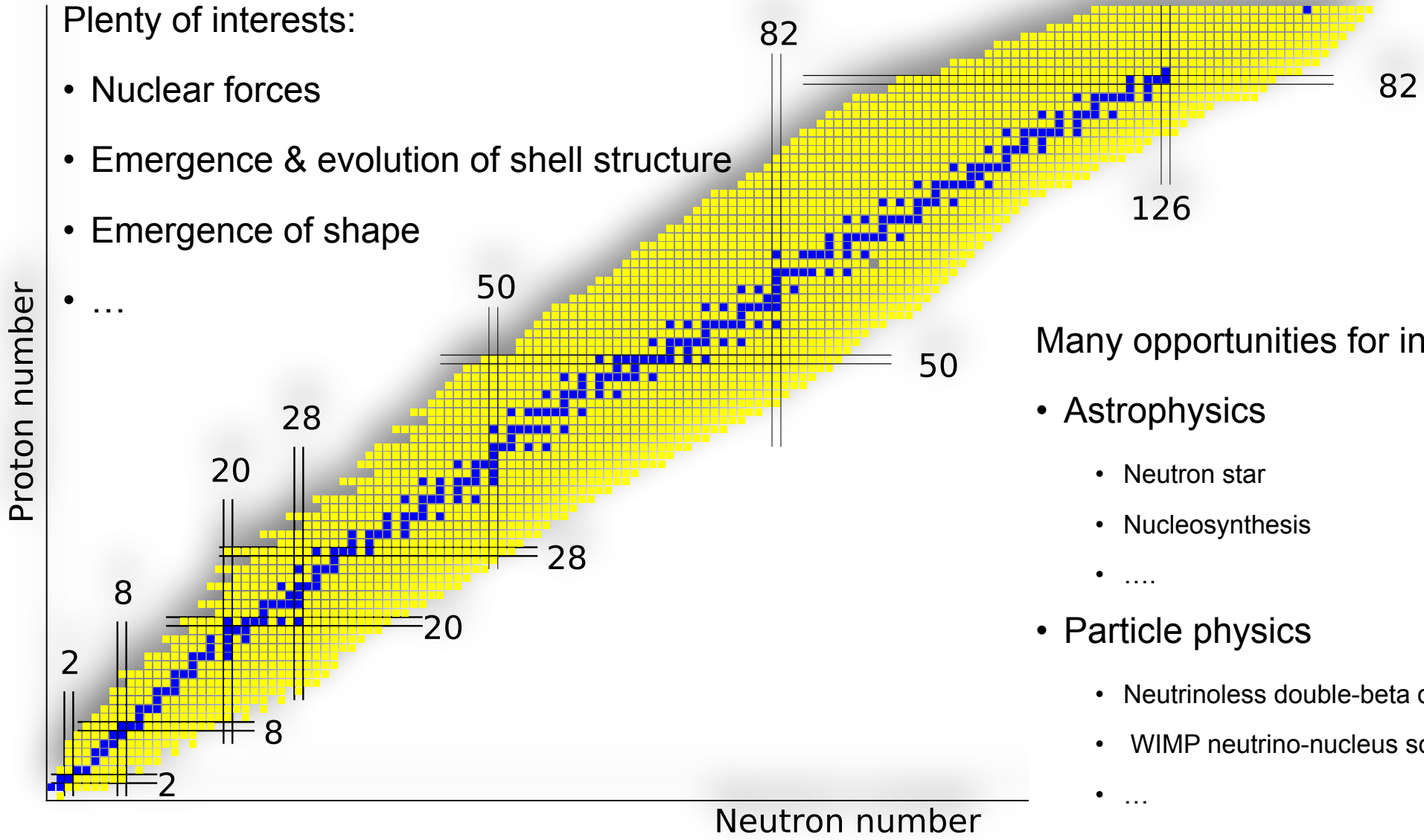
Plenty of interests:

- Nuclear forces
- Emergence & evolution of shell structure
- Emergence of shape
- …



Many opportunities for interdisciplinary studies!

- Astrophysics
  - Neutron star
  - Nucleosynthesis
  - ….
- Particle physics
  - Neutrinoless double-beta decay
  - WIMP neutrino-nucleus scattering
  - …

K. Murano et al., Prog. Theor. Phys. 125, 1225 (2011).
S. Aoki and T. Doi, Front. Phys. 8, (2020).
T. Otsuka et al., Rev. Mod. Phys. 92, 015002 (2020).
A. N. Andreyev et al., Nature 405, 430 (2000).

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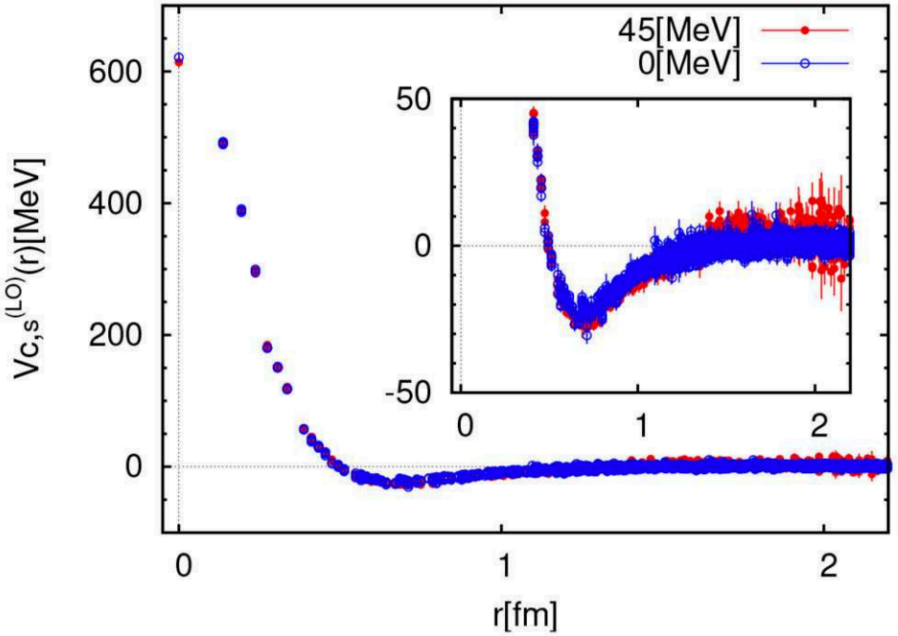

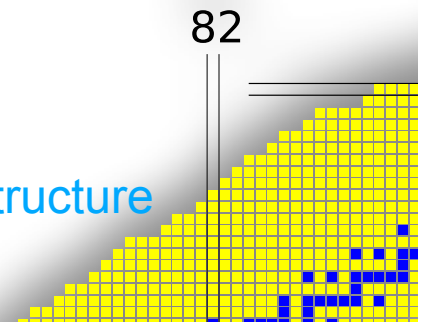

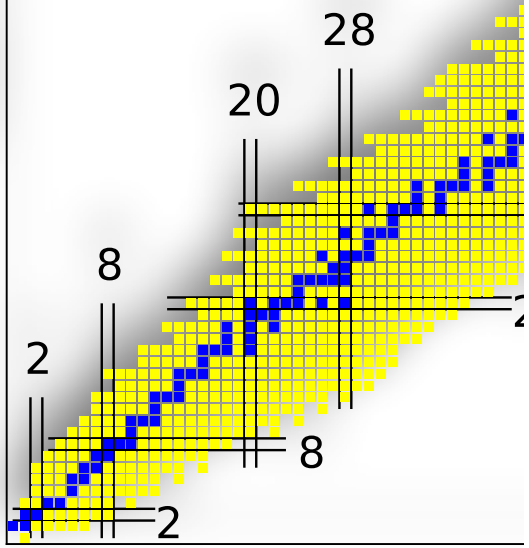

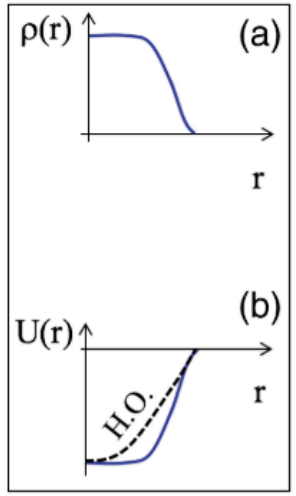

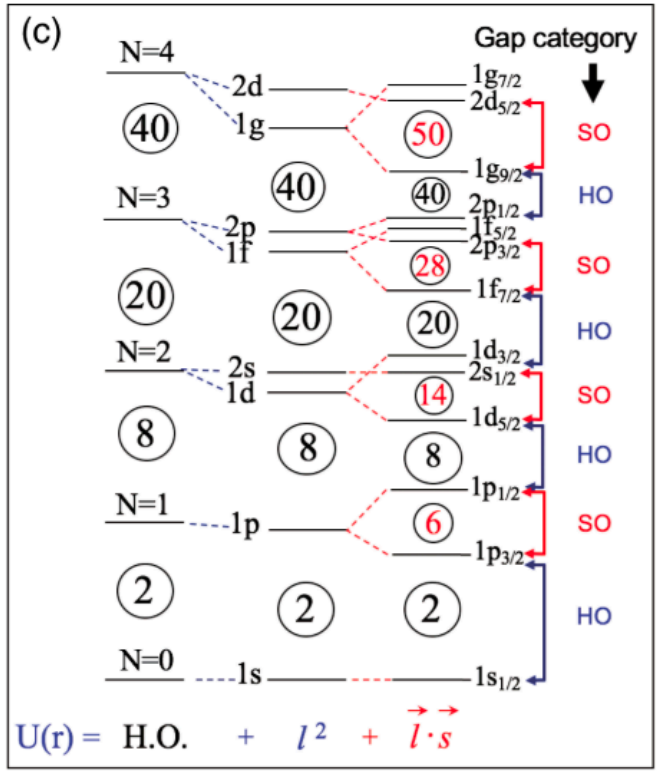

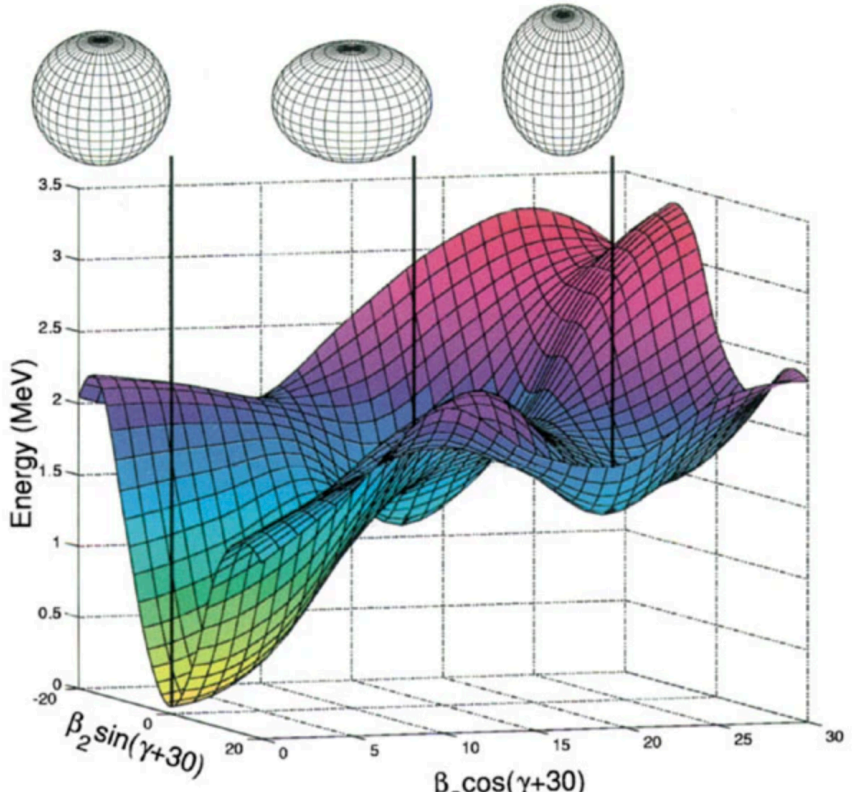

Motivations

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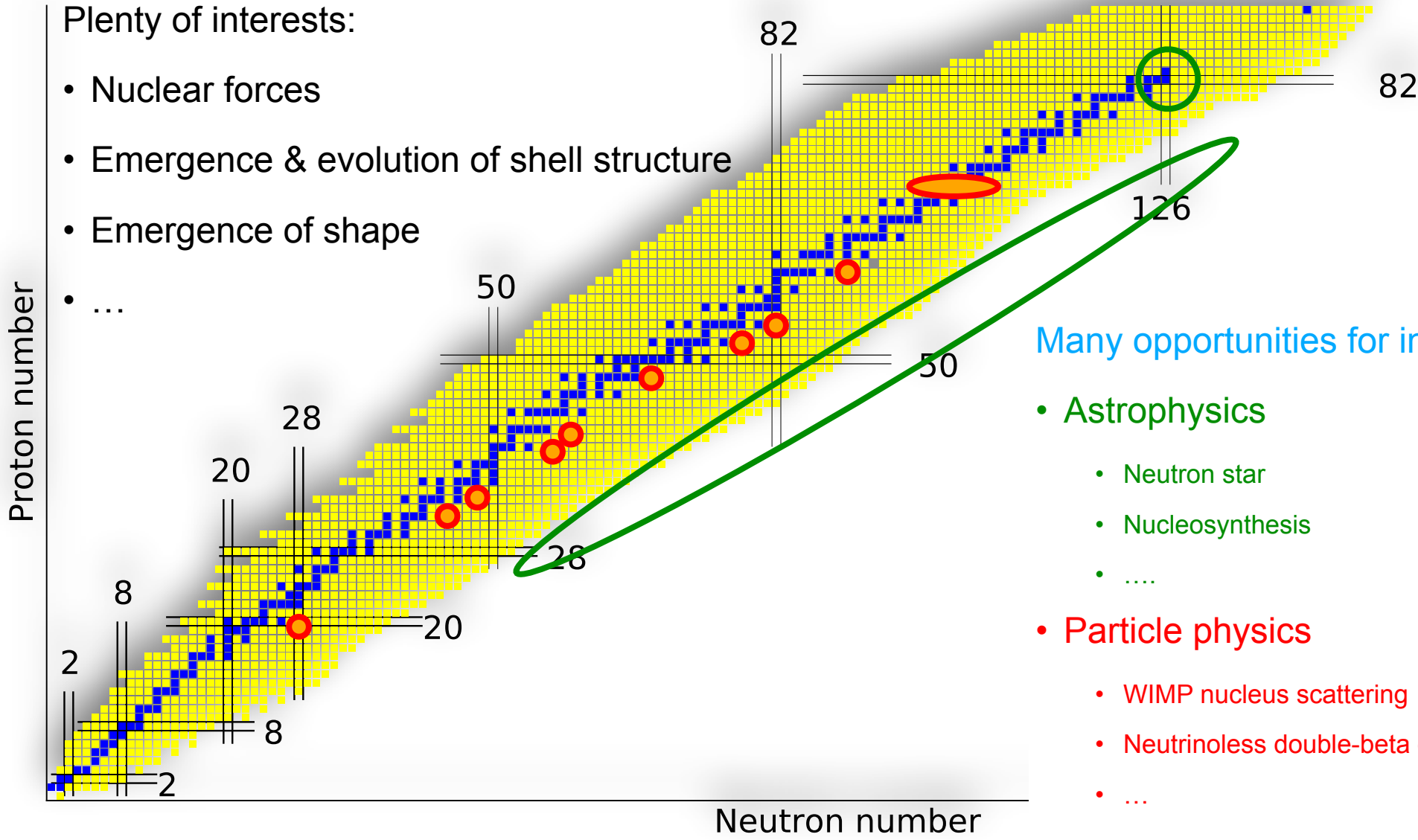

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  - ….
- Particle physics
  - WIMP nucleus scattering
  - Neutrinoless double-beta decay
  - …

Ab initio calculation for atomic nuclei

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- How can we make a prediction?

*If the importance of models is known, combining models should also be possible.

  - A probability distribution of target unknown data $\tilde{D}$ conditioned on known data D, based on a model I: $P(\tilde{D}\,|\,D, I)$
  - It can be realized with the help of model predictions:

$$P(\tilde{D}|D,I) = \int d\boldsymbol{\theta} P(\tilde{D}|\boldsymbol{\theta},I) P(\boldsymbol{\theta}|D,I)$$

Model parameters | Model prediction | Posterior parameter dist.

- Posterior parameter distribution
  - One can use Bayes' theorem: $P(\boldsymbol{\theta}|D,I) \propto P(D|\boldsymbol{\theta},I) P(\boldsymbol{\theta})$ (Likelihood; Prior parameter dist.)
  - In practice, a sampling method is needed, for example Markov-chain Monte Carlo (MCMC) method.
- **Uncertainty quantification** is necessary in **model predictions** and **Likelihood evaluations**!
  - **Systematically improvable theory** is required.

Ab initio calculation for atomic nuclei

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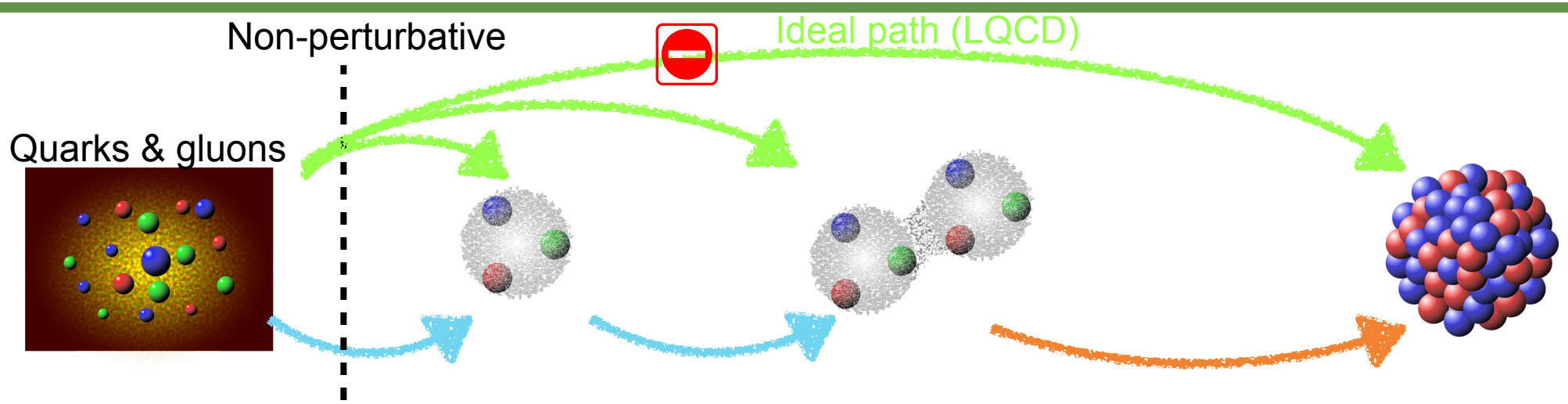

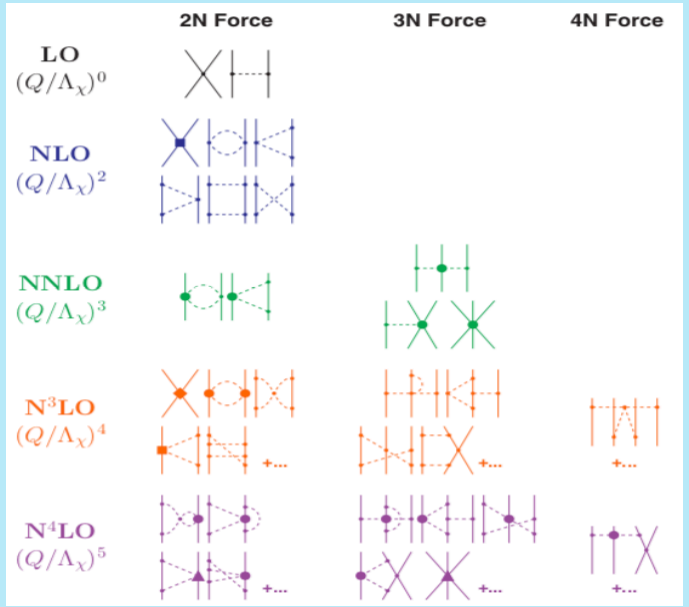

Nuclear many-body problem

- 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

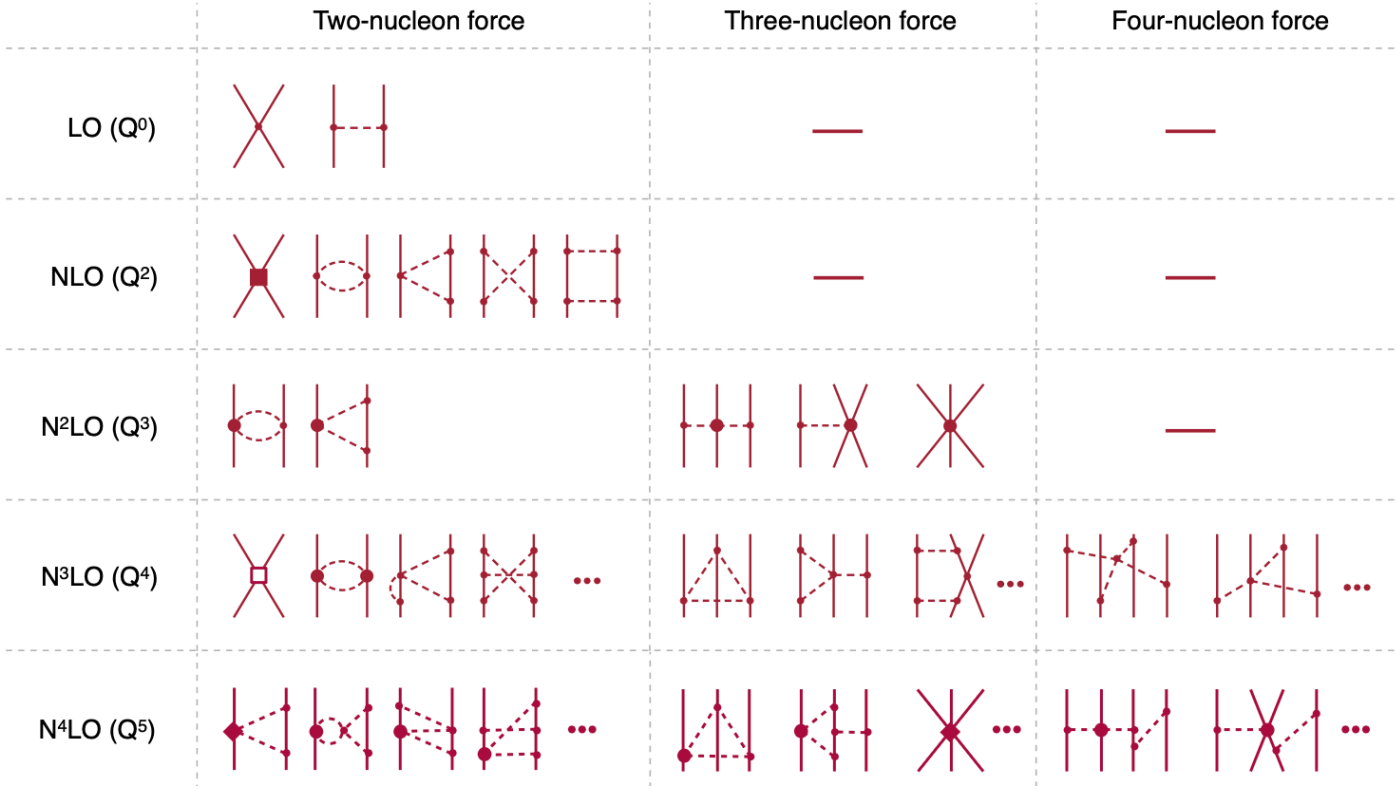

Figure is from E. Epelbaum, H. Krebs, and P. Reinert, Front. Phys. 8, 1 (2020).

Nuclear currents from Chiral EFT

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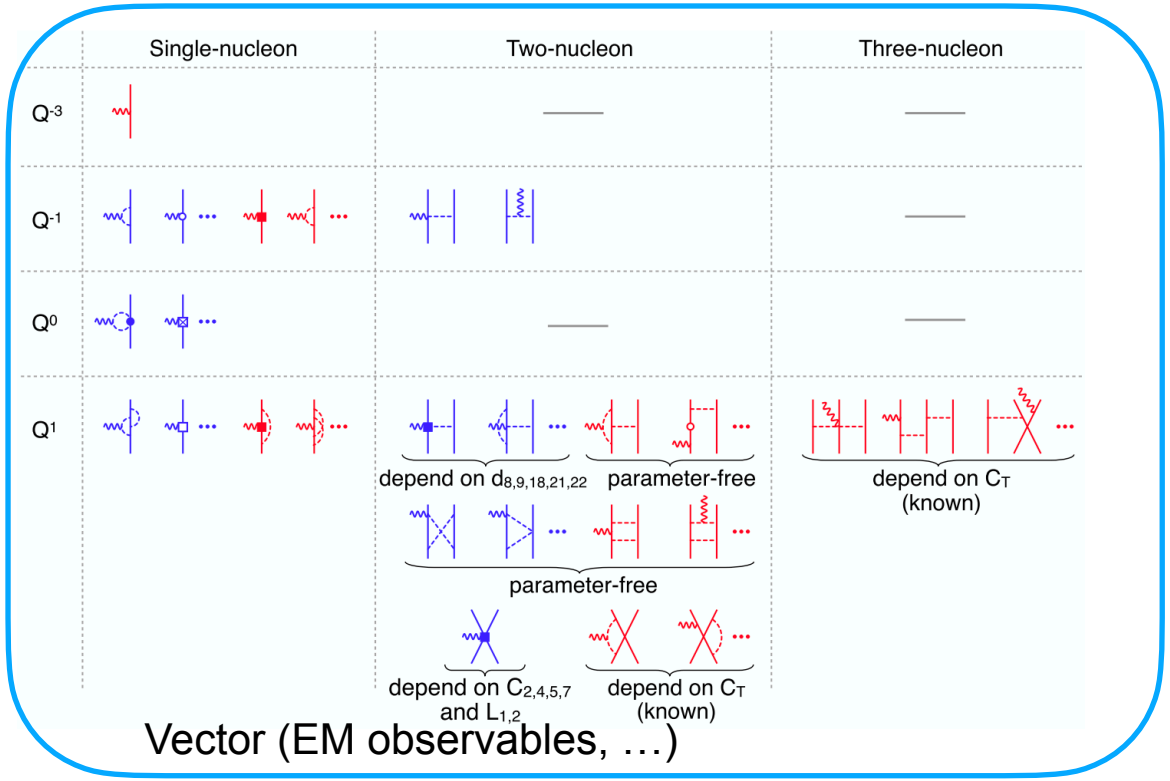
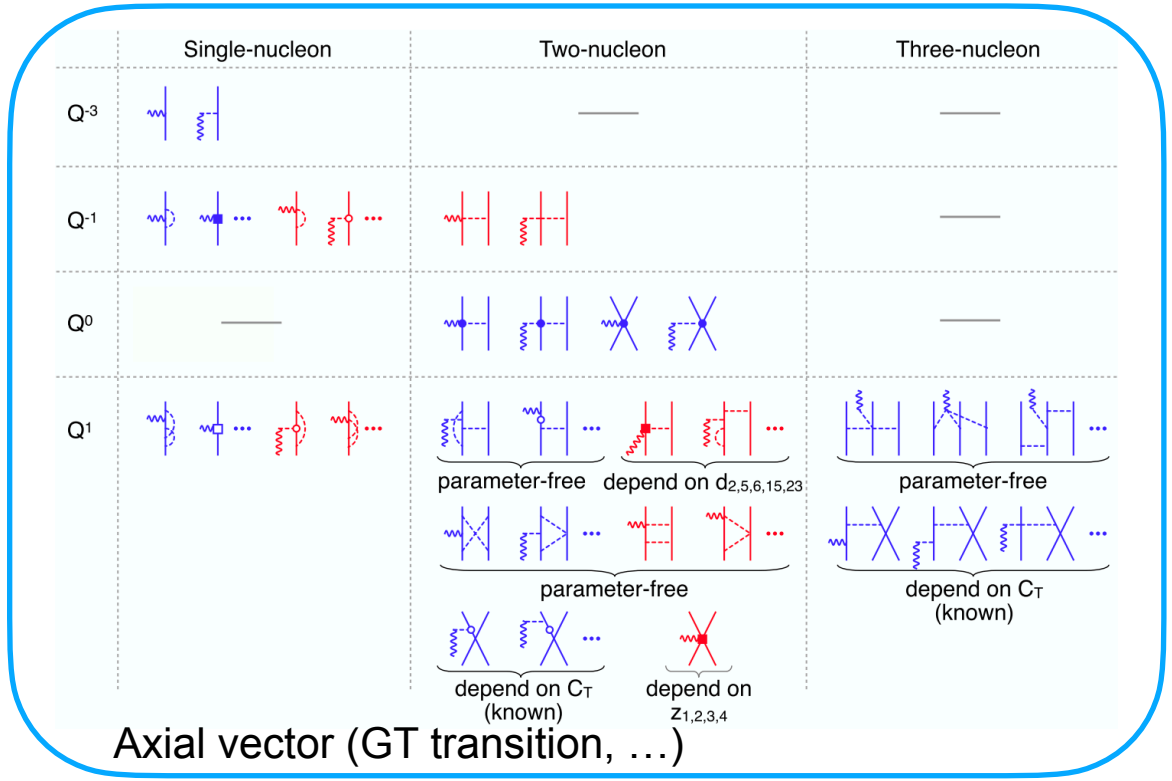
- Electroweak properties are related to current operators. $\mathcal{H} \propto l_\mu J^\mu_{\rm nucl}$
- Chiral EFT allows us a systematic expansion for charge and current operators.



Vector (EM observables, …)



Axial vector (GT transition, …)

E. Epelbaum, arXiv:1908.09349.

Many-body problem

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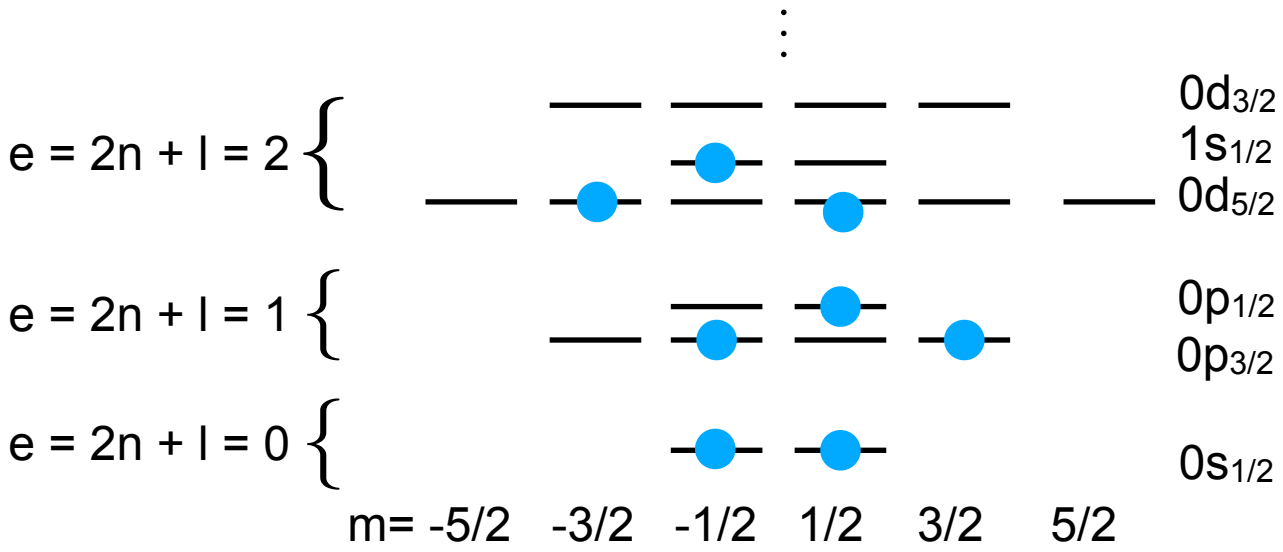
- Having a Hamiltonian, we need to solve the non-relativistic Schrödinger equation $H|\Psi_n\rangle = E_n|\Psi_n\rangle$
- Hamiltonian in the 2nd quantization form

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

- Single-particle index: the eigenstate of the spherical harmonic oscillator (HO) Hamiltonian



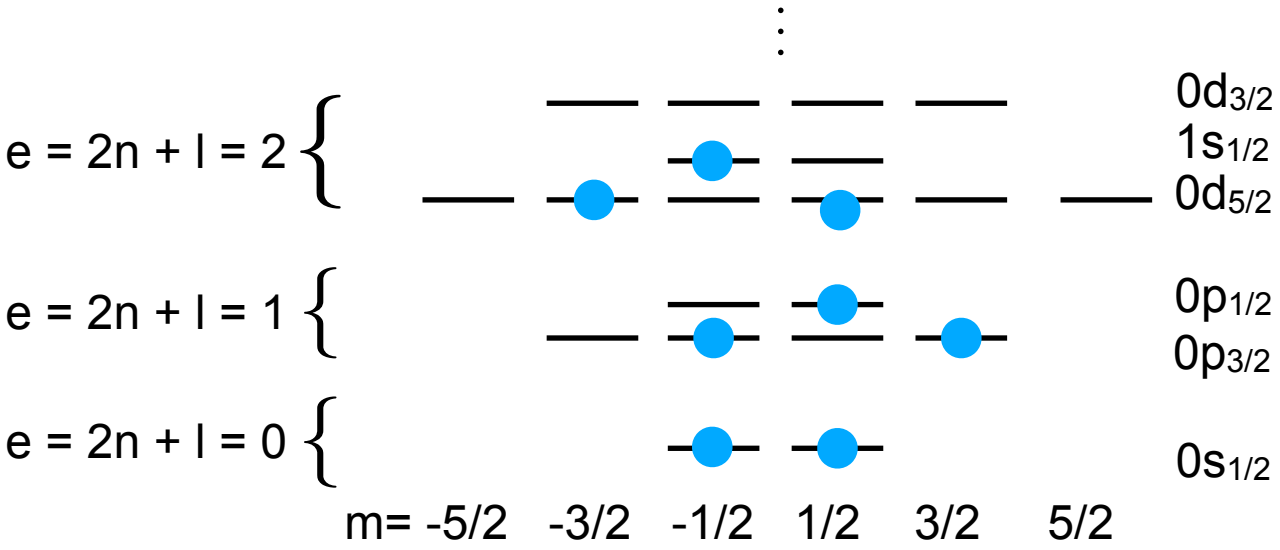
$$\langle \boldsymbol{r}|a_p^\dagger|0\rangle \propto x^{l_p} L_{n_p}^{(l_p+1/2)}(x^2) e^{-x^2/2} \Omega_{l_p j_p m_p}(\boldsymbol{r})$$

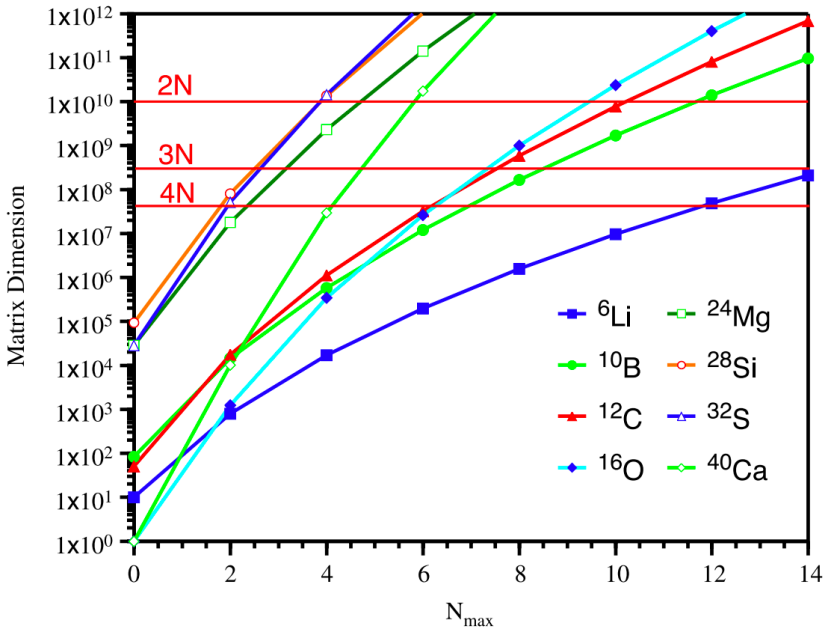
$$\Omega_{l_p j_p m_p}(\boldsymbol{r}) = \sum_{m_l s} \mathcal{C}^{j_p m_p}_{l_p m_l \frac{1}{2} s} Y_{l_p m_l}(\boldsymbol{r}) \chi_s$$

$$x^2 = \frac{\hbar r^2}{m\omega}$$

Many-body problem

- A straightforward way is to expand the wave function $|\Psi_n\rangle = \sum_i c_{ni} |\Phi_i\rangle$, where $|\Phi_i\rangle$ is the single Slater determinant state built with the HO single-particle state (full configuration interaction, FCI)
- Applications are limited to A ~ 20.





Valence-space approach

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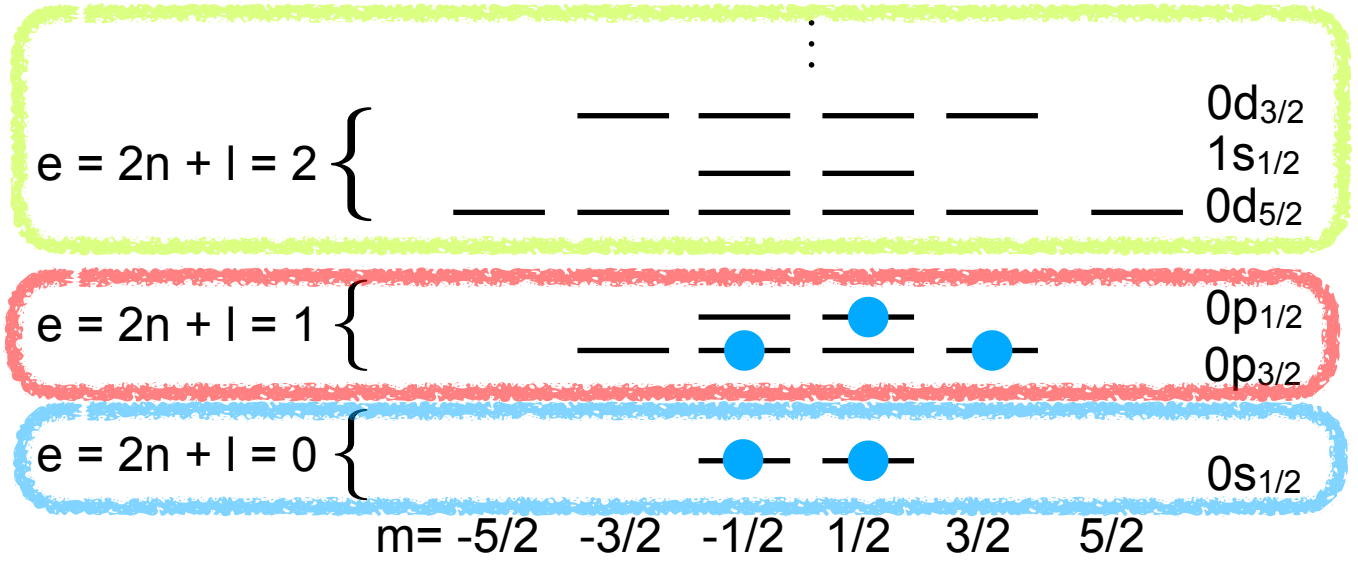
- Valence-space (or active-space) problem
- Hamiltonian is adjusted to reproduce the known experimental data
  - e=1 space: Cohen-Kurath potential, …
  - e=2 space: USD series, …
  - e=3 space: KB3G, GXPF1, …
- Methods:
  - Lanczos
  - DMRG
  - Monte-Carlo shell model (MCSM)
  - …



Issues:
Connection to starting Hamiltonian
Effective operators
Valence-space IMSRG

E. Caurier et al., Rev. Mod. Phys. 77, 427 (2005).

Valence-space approach

- Monte-Carlo shell model (MCSM)
- Variational method (NOT QMC)
- Good approximation for the exact shell-model diagonalization
- Wave function

$$|\Psi_{\mathrm{MCSM}}\rangle = \sum_{n=1}^{N_b} f_n \sum_{K=-J}^{J} g_K^{(n)} P_{MK}^{J\pi} |\Phi_n\rangle$$

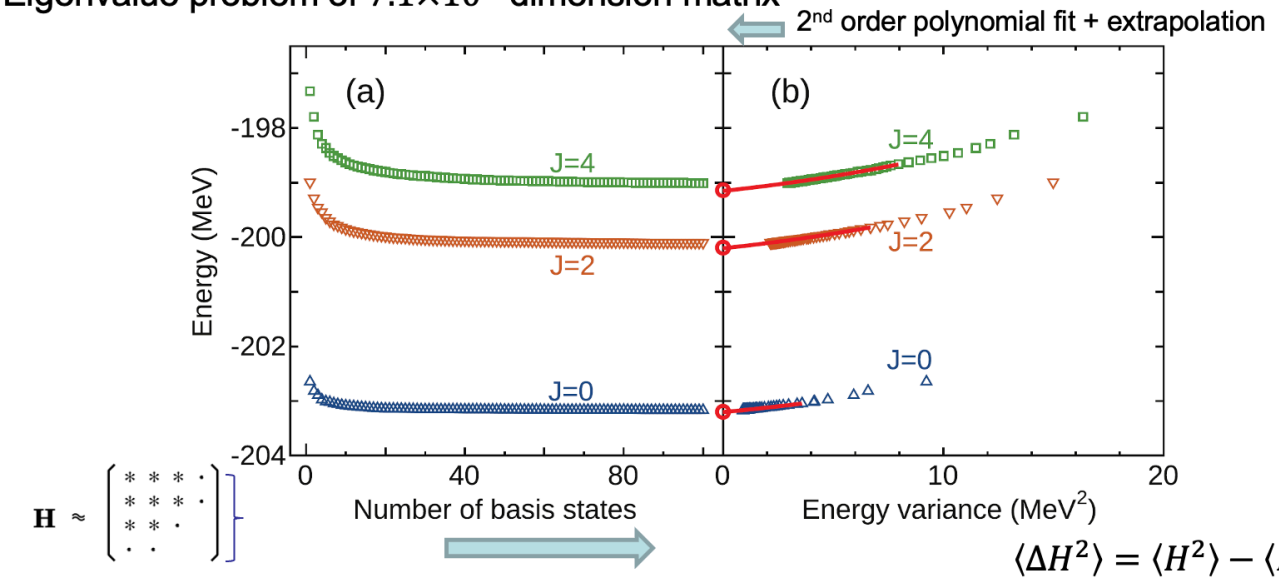
Deformed SD

Superposition

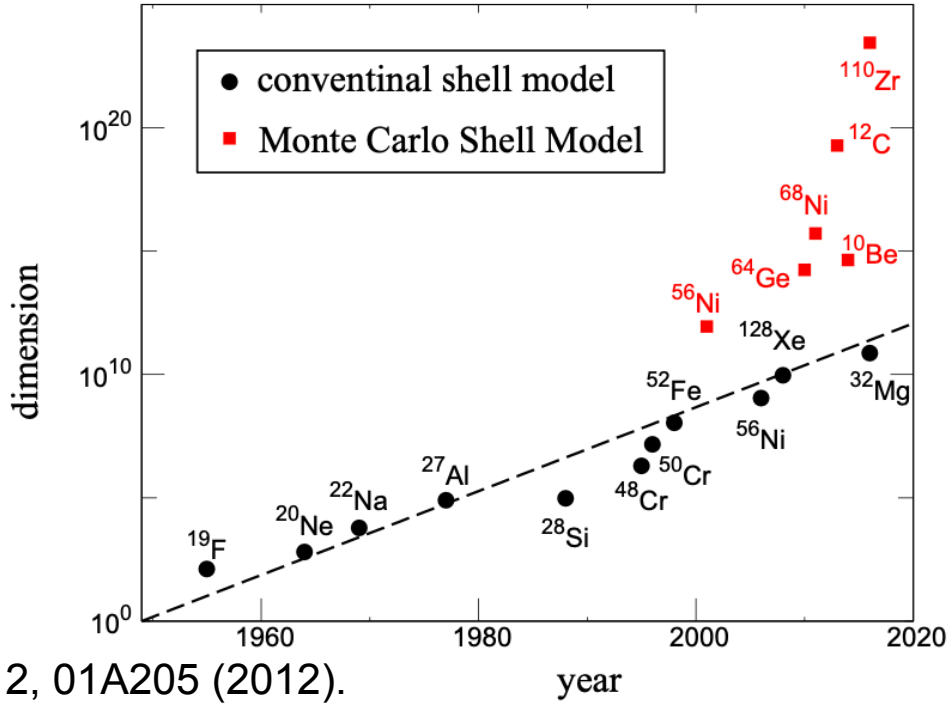
Angular momentum and parity projection

- Extrapolation wrt energy variance
- More than 10^{20} dimension problem is accessible

^{56}Ni with ^{40}Ca core, FPD6 int.
Eigenvalue problem of 7.1×10^{7}-dimension matrix



$$\langle \Delta H^2 \rangle = \langle H^2 \rangle - \langle H \rangle^2$$



N. Shimizu et al., Prog. Theor. Exp. Phys. 2012, 01A205 (2012).

Normal ordering and two-body approximation

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

1N 2N 3N

- Normal ordering

$$\langle \mathrm{HF} | \{ a_1^\dagger \dots a_n \} | \mathrm{HF} \rangle = 0$$

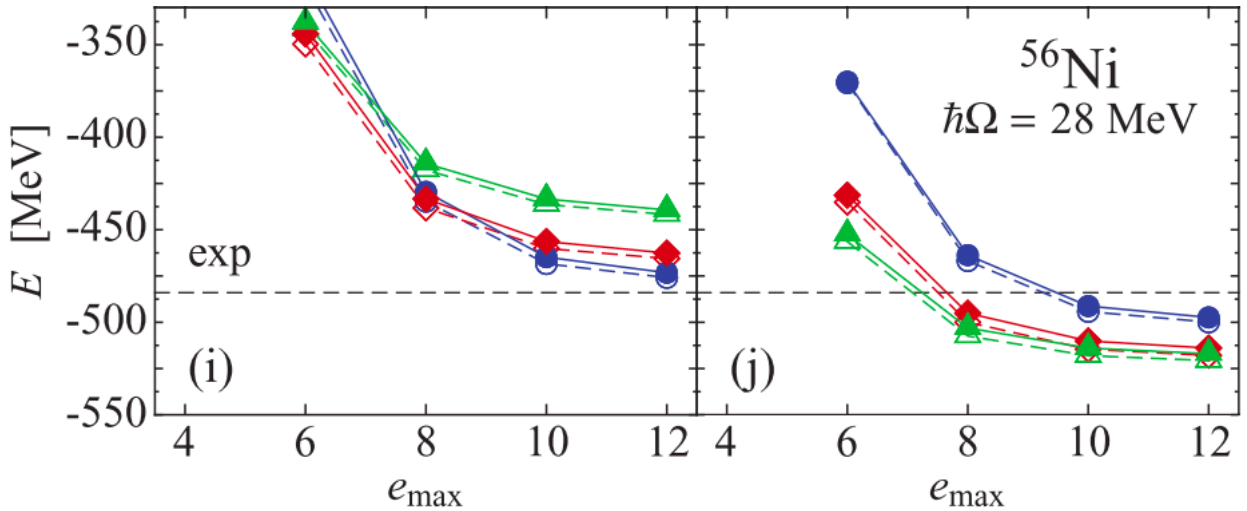
$$H = E_0 + \sum_{p'p} f_{p'p} \{ a_{p'}^\dagger a_p \} + \frac{1}{4} \sum_{p'q'pq} \Gamma_{p'q'pq} \{ a_{p'}^\dagger a_{q'}^\dagger a_q a_p \} + \frac{1}{36} \sum_{p'q'r'pqr} W_{p'q'r'pqr} \{ a_{p'}^\dagger a_{q'}^\dagger a_{r'}^\dagger a_r a_q a_p \}$$

Residual 3N

Input of post mean-field calc. (NO2B)

- Effect of residual 3N

CC calculations from S. Binder et al., Phys. Rev. C 87, 021303 (2013).



Solid: with W term
Dashed: without W term

W term: only ~ 1% of the total gs energy!

NO2B approximation (neglect W term)

In-medium similarity renormalization group approach

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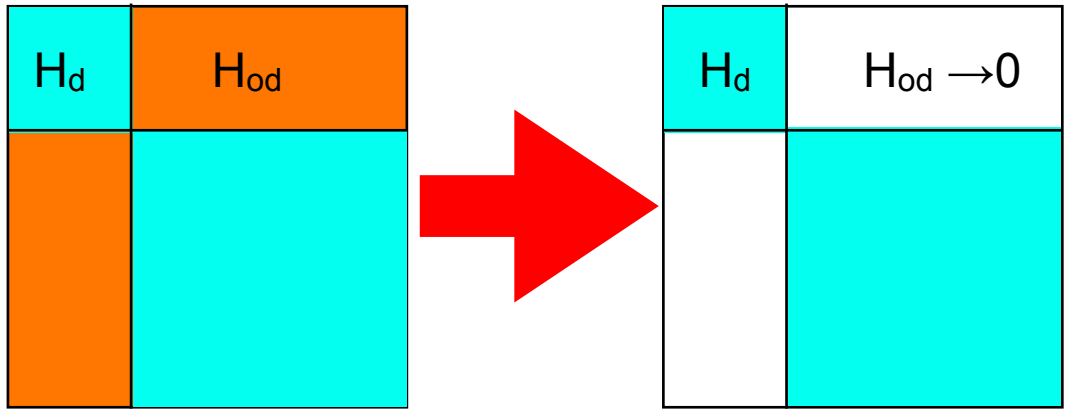
- Similarity renormalization group

H. Hergert et al., Phys. Rep. 621, 165 (2016).
S. R. Stroberg et al., Annu. Rev. Nucl. Part. Sci. 69, 307 (2019).

$$H(s) = U(s)H(s=0)U^\dagger(s)$$

$$\eta(s) \equiv \frac{dU(s)}{ds}U^\dagger(s)$$

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



- The anti-Hermitian generator η(s) is arbitrary.
- How can we choose the functional form to suppress the off-diagonal MEs?

In-medium similarity renormalization group approach

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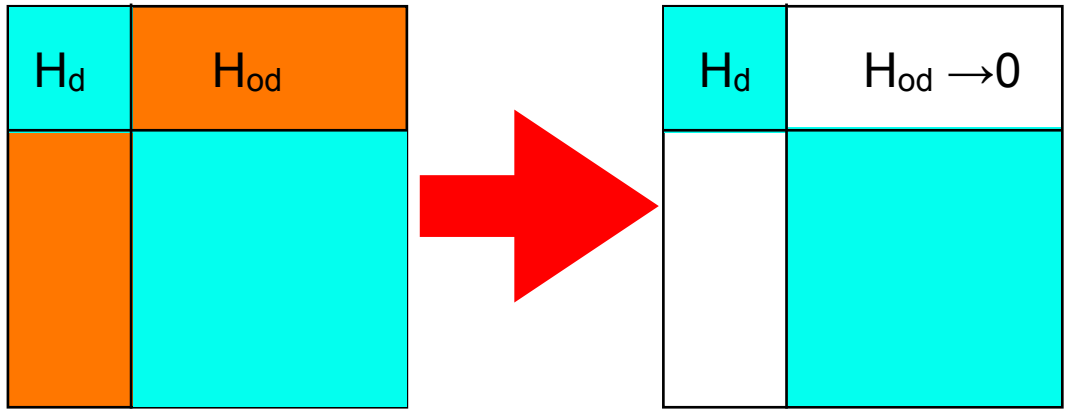

- A simple example:
  - 2 x 2 Hamiltonian

$$H(s) = \begin{pmatrix} c+z & x \\ x & c-z \end{pmatrix} = cI + z(s)\sigma_3 + x(s)\sigma_1 \qquad \eta(s) = \frac{i}{2}\frac{x(s)}{z(s)}\sigma_2$$

$$\frac{dx(s)}{ds} = -x(s) \rightarrow x(s) = x(0)\exp(-s)$$ Exponential decay of the off-diagonal ME.

$$\text{note} : [\sigma_2, \sigma_3] = 2i\sigma_1$$

In-medium similarity renormalization group approach

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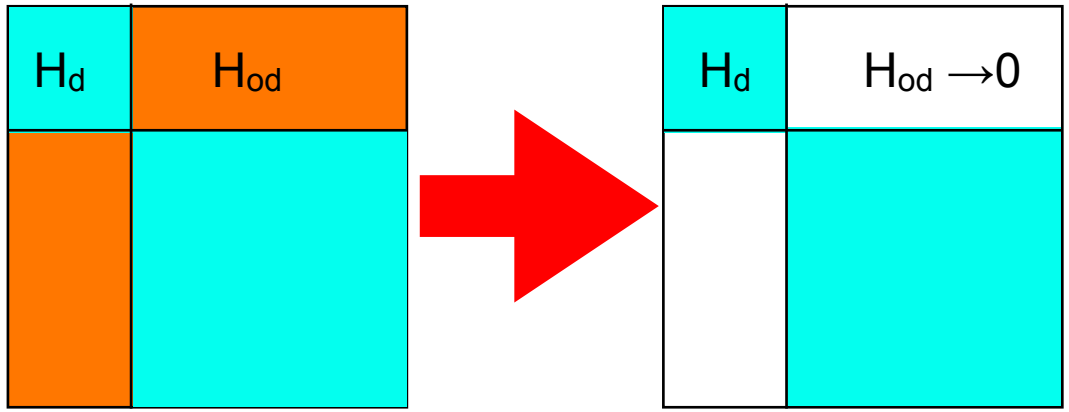

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$$\frac{dx(s)}{ds} = -x(s) \rightarrow x(s) = x(0)\exp(-s)$$ Exponential decay of the off-diagonal ME.

- An expected form

$$\eta(s) = \frac{i}{2}\frac{x(s)\sigma_2}{z(s)}$$ → $$\frac{\text{Off-diagonal MEs need to be suppressed}}{\text{Energy gap from the diagonal MEs}}$$ (Anti-Hermitian)

Magnus formalism

- One can solve $\eta(s) = \frac{dU(s)}{ds}U^\dagger(s)$, instead of $\frac{dH(s)}{ds} = [\eta(s), H(s)]$

- Exponential ansatz: $U(s) = e^{\Omega(s)}$ $\rightarrow$ flow equation for $\Omega(s)$

$$\frac{d\Omega(s)}{ds} = \sum_{n=0} \frac{B_n}{n!}[\Omega(s), \eta(s)]^{(n)}, \quad [\Omega(s), \eta(s)]^{(0)} = \eta(s), \quad [\Omega(s), \eta(s)]^{(n)} = [\Omega(s), [\Omega(s), \eta(s)]^{(n-1)}]$$

- Hamiltonian and other operators can be obtained as

$$H(s) = e^{\Omega(s)} H e^{-\Omega(s)} = \sum_{n=0} \frac{1}{n!}[\Omega(s), H]^{(n)}$$

$$O(s) = e^{\Omega(s)} O e^{-\Omega(s)} = \sum_{n=0} \frac{1}{n!}[\Omega(s), O]^{(n)}$$

In-medium similarity renormalization group approach

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$$\frac{d\Omega}{ds} = \eta(s) - \frac{1}{2}[\Omega(s), \eta(s)] + \cdots$$

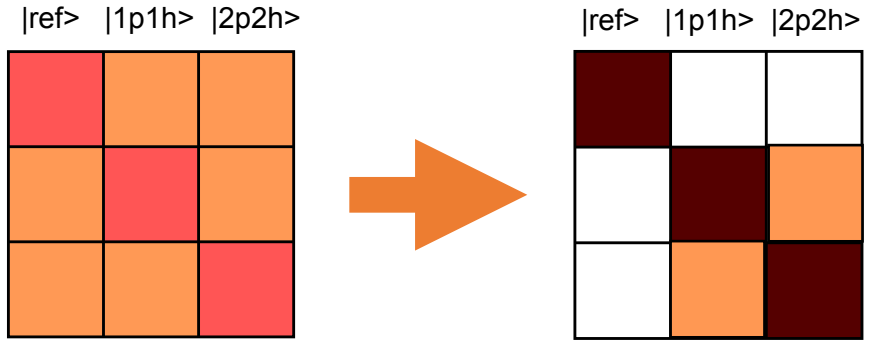
$$H(s) = e^{\Omega(s)} H(s=0) e^{-\Omega(s)} \approx E(s) + \sum_{12} f_{12}(s)\{a_1^\dagger a_2\} + \frac{1}{4}\sum_{1234} \Gamma_{1234}(s)\{a_1^\dagger a_2^\dagger a_4 a_3\}$$

$$\eta(s) = \sum_{12} \eta_{12}(s)\{a_1^\dagger a_2\} + \sum_{1234} \eta_{1234}(s)\{a_1^\dagger a_2^\dagger a_4 a_3\}$$

$$\eta_{12} = \frac{1}{2}\arctan\left(\frac{2f_{12}}{f_{11} - f_{22} + \Gamma_{1212}}\right)$$

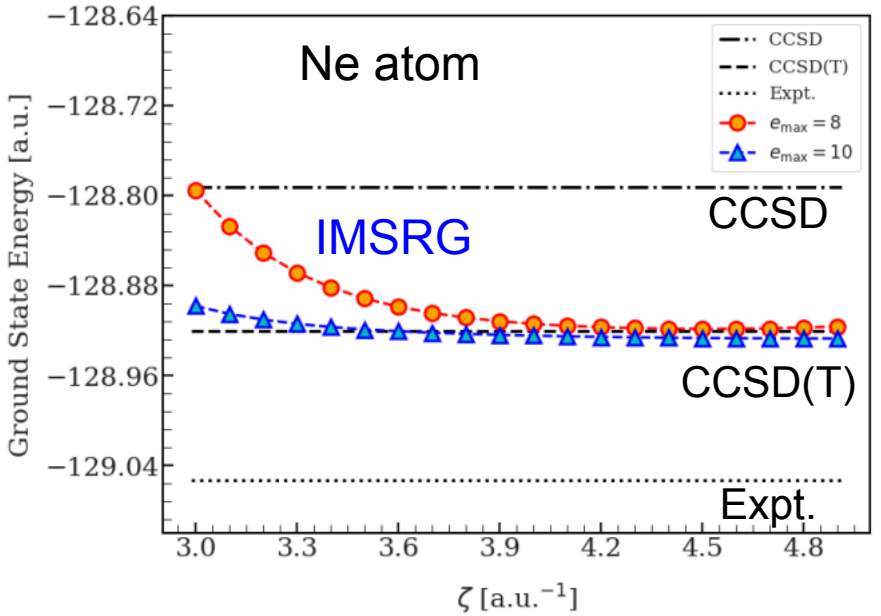
$$\eta_{1234} = \frac{1}{2}\arctan\left(\frac{2\Gamma_{1234}}{f_{11} + f_{22} - f_{33} - f_{44} + A_{1234}}\right)$$

$$A_{1234} = \Gamma_{1212} + \Gamma_{3434} - \Gamma_{1313} - \Gamma_{2424} - \Gamma_{1414} - \Gamma_{2323}$$



G. Tenkila et al., arXiv:2212.08188

- Ne atom example
  - Basis function: $\phi_p(\boldsymbol{r}) \propto \left(\frac{2r}{\zeta}\right)^{l_p} L_{n_p}^{(2l_p+2)}\left(\frac{2r}{\zeta}\right) e^{-\frac{r}{\zeta}} \Omega_{l_p j_p m_p}(\boldsymbol{r})$
  - e_{max} = max(n+l)



Valence-Space Operators from IMSRG

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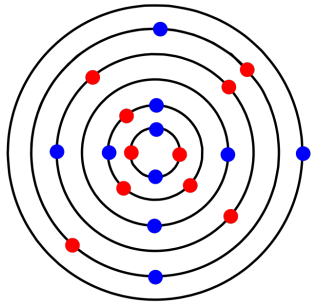
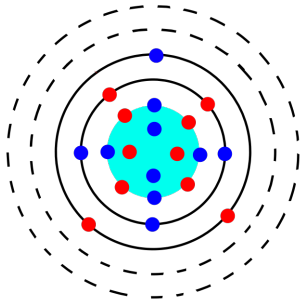
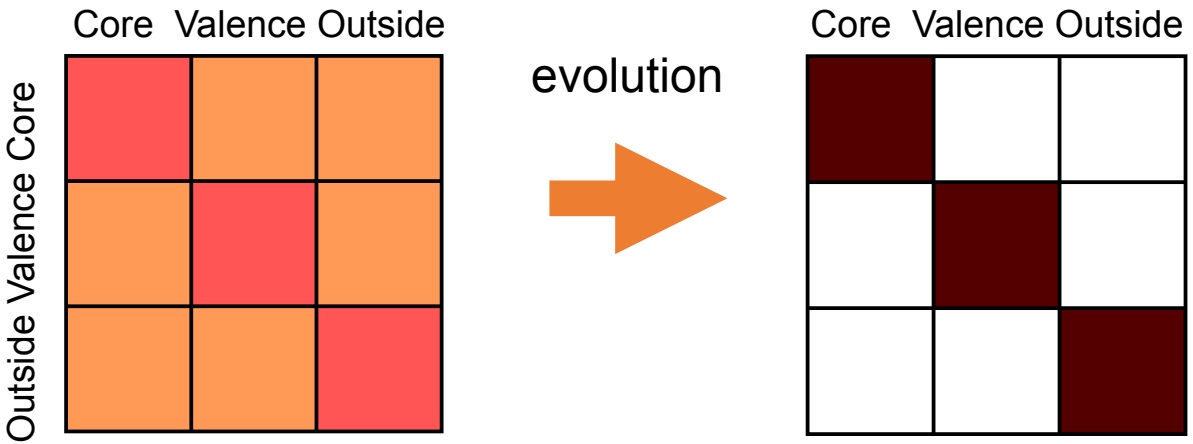




● : frozen core
— : valence
--- : outside



Similarity transformation

$$H \qquad H(s) = e^{\Omega(s)} H e^{-\Omega(s)}$$

$$\frac{d\Omega}{ds} = \eta(s) - \frac{1}{2}[\Omega(s), \eta(s)] + \cdots$$

$$\eta(s) = \sum_{12} \eta_{12}(s)\{a_1^\dagger a_2\} + \sum_{1234} \eta_{1234}(s)\{a_1^\dagger a_2^\dagger a_4 a_3\}$$

$$\eta_{12} = \frac{1}{2}\arctan\left(\frac{2f_{12}}{f_{11} - f_{22} + \Gamma_{1212} + \Delta}\right)$$

$$\eta_{1234} = \frac{1}{2}\arctan\left(\frac{2\Gamma_{1234}}{f_{11} + f_{22} - f_{33} - f_{44} + A_{1234} + \Delta}\right)$$

$$A_{1234} = \Gamma_{1212} + \Gamma_{3434} - \Gamma_{1313} - \Gamma_{2424} - \Gamma_{1414} - \Gamma_{2323}$$

f_{12}, Γ_{1234} : matrix elements to be suppressed

$$H(s) \approx E(s) + \sum_{12} f_{12}(s)\{a_1^\dagger a_2\} + \frac{1}{4}\sum_{1234} \Gamma_{1234}(s)\{a_1^\dagger a_2^\dagger a_4 a_3\}$$

$$\mathcal{O}(s) = e^{\Omega(s)}\mathcal{O}e^{-\Omega(s)} \approx \mathcal{O}^{[0]}(s) + \sum_{12} \mathcal{O}_{12}^{[1]}(s)\{a_1^\dagger a_2\} + \frac{1}{4}\sum_{1234} \mathcal{O}_{1234}^{[2]}(s)\{a_1^\dagger a_2^\dagger a_4 a_3\}$$

s: flow parameter

H. Hergert, S. K. Bogner, T. D. Morris, A. Schwenk, and K. Tsukiyama, Phys. Rep. **621**, 165 (2016).
S. R. Stroberg, H. Hergert, S. K. Bogner, and J. D. Holt, Annu. Rev. Nucl. Part. Sci. **69**, 307 (2019).

VS-IMSRG

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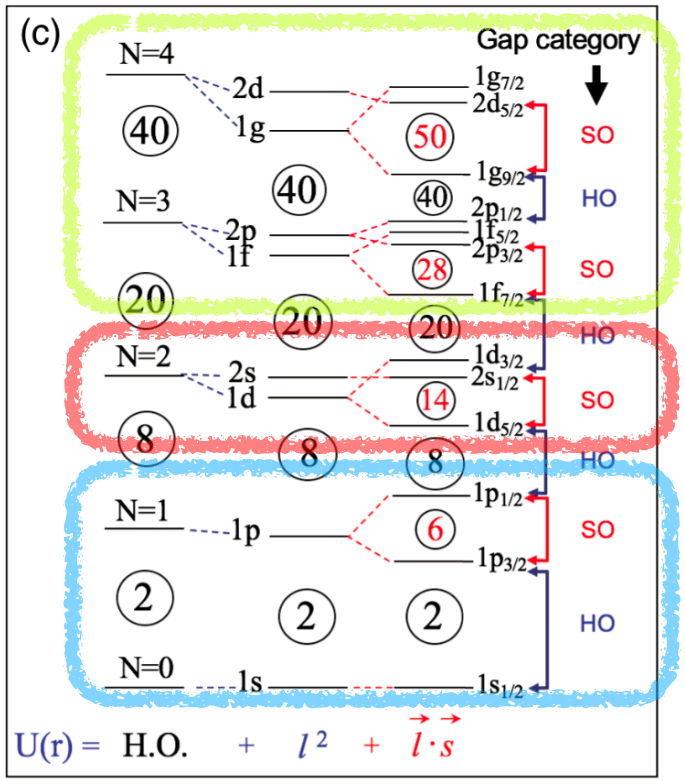
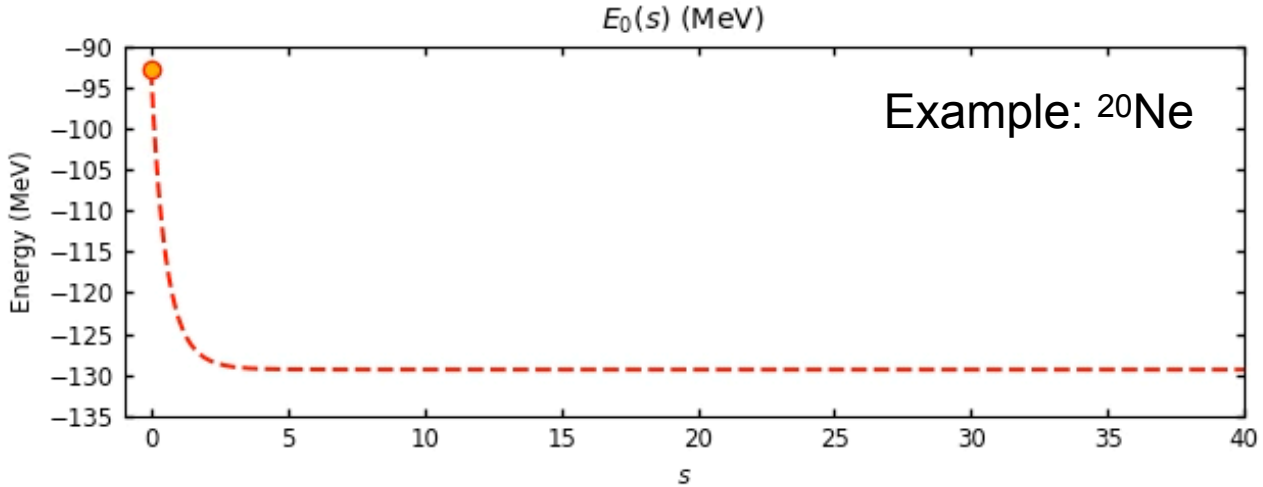
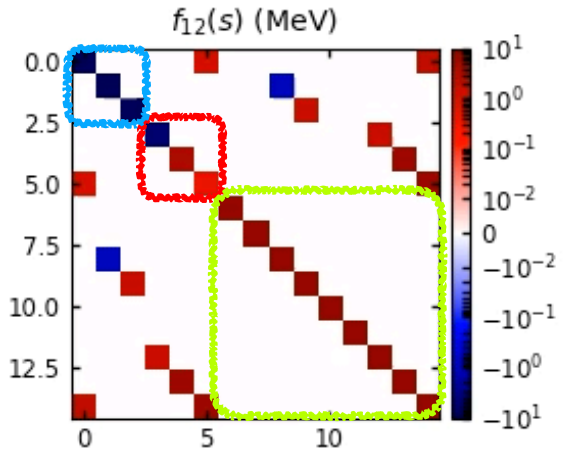
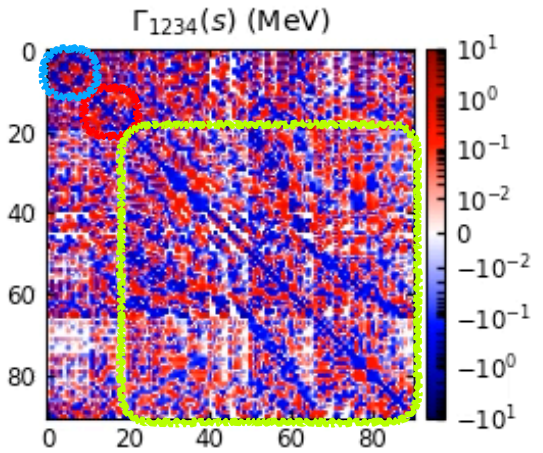
- IMSRG flow with valence-space formulation

$$H(s) \approx E(s) + \sum_{12} f_{12}(s)\{a_1^\dagger a_2\} + \frac{1}{4}\sum_{1234}\Gamma_{1234}(s)\{a_1^\dagger a_2^\dagger a_4 a_3\}$$









In-medium similarity renormalization group approach

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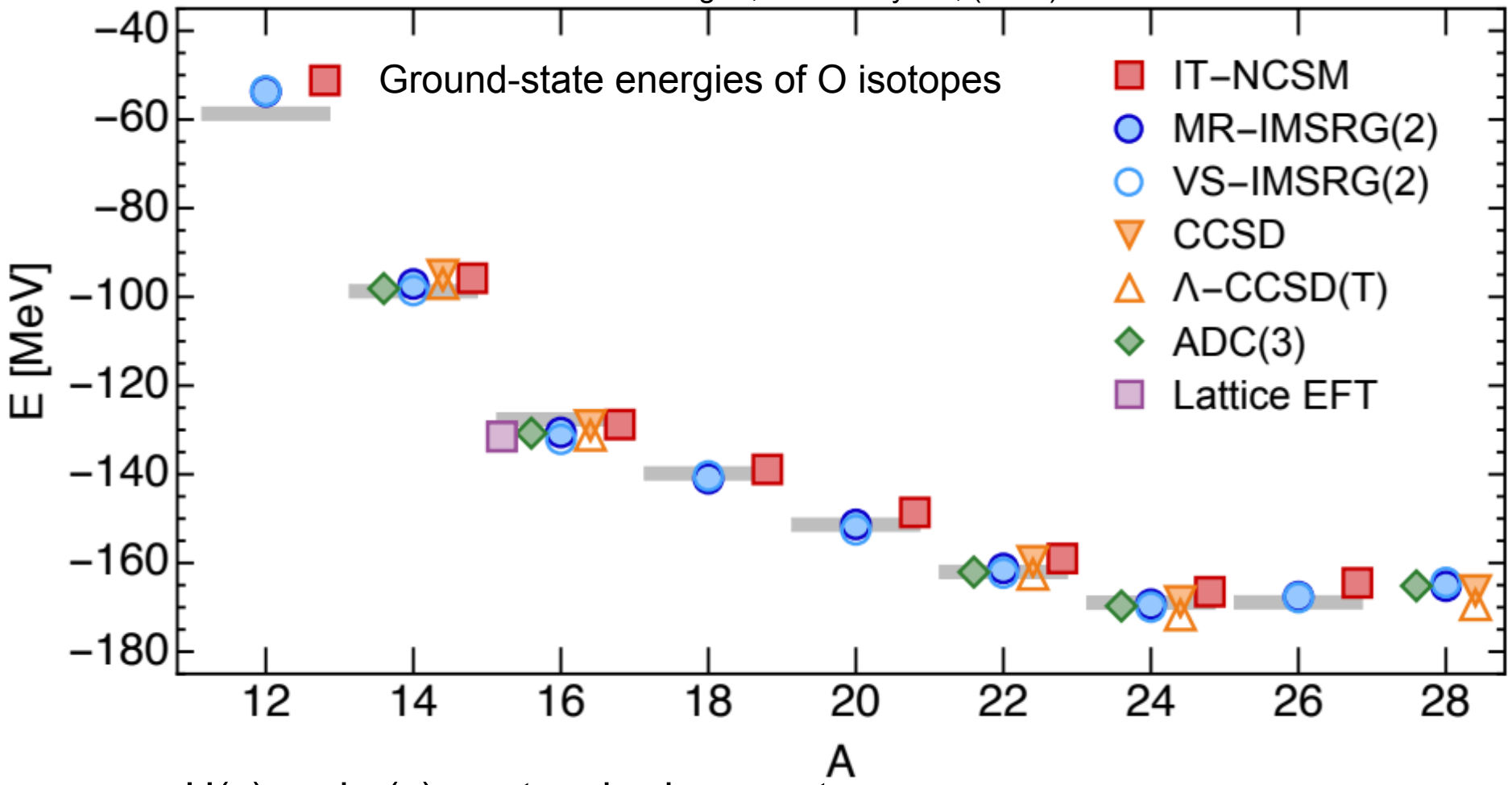
H. Hergert, Front. Phys. 8, (2020).



H(s) and η(s) are two-body operators.

A few % error in the ground-state energy and radius

In-medium similarity renormalization group approach

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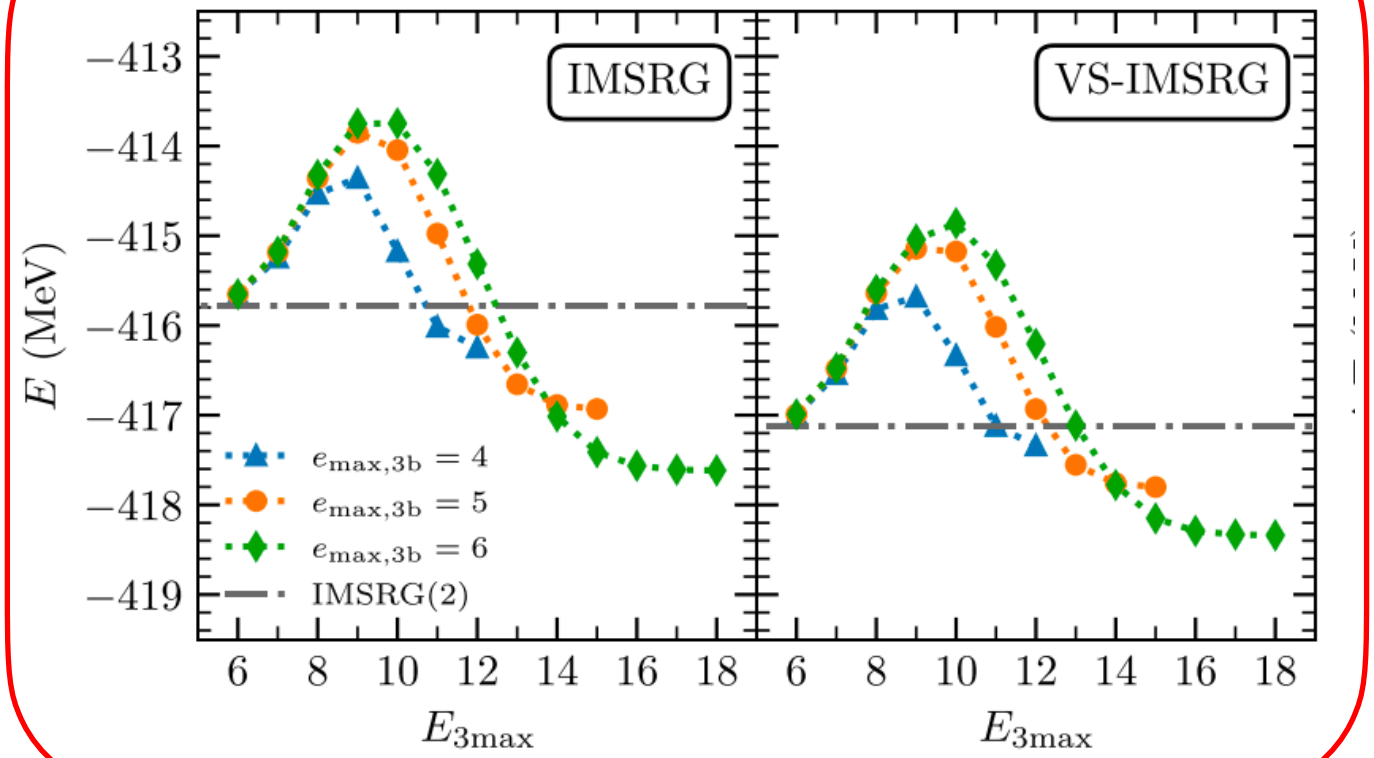
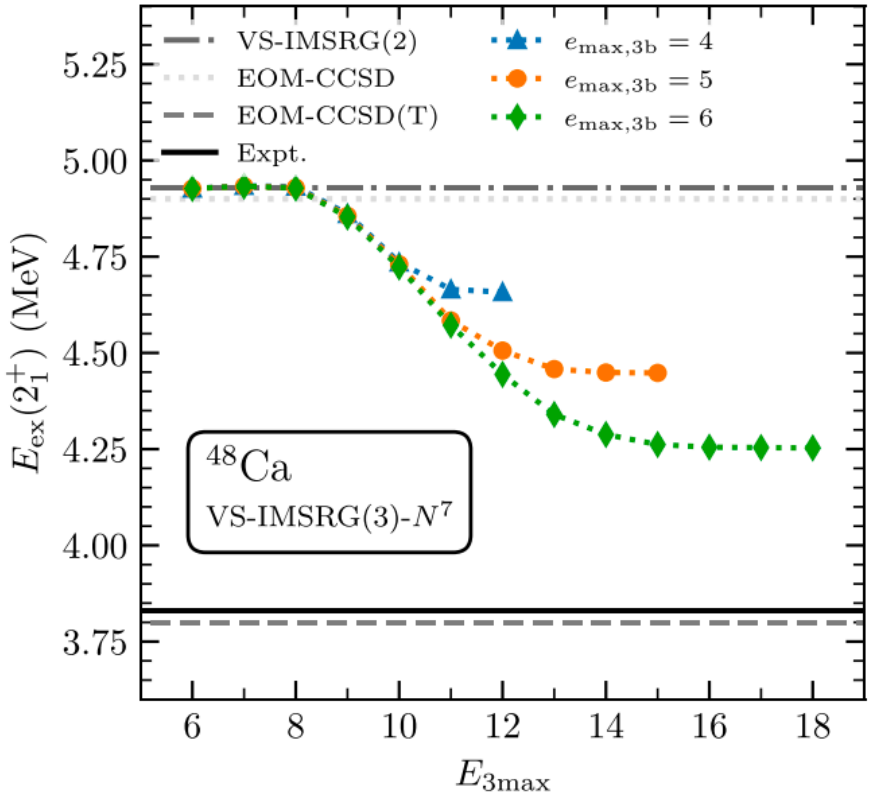
Ground-state energy

$$\frac{\Delta E_{\mathrm{corr}}}{E_{\mathrm{corr}}} \lesssim 0.01$$



First 2^+ excitation energy

$$\frac{\Delta Ex(^{48}\mathrm{Ca},2^+)}{Ex(^{48}\mathrm{Ca},2^+)} \lesssim 0.25\ (?)^*$$



*4-5% in ^{52}Ca

M. Heinz et al., Phys. Rev. C 111, 034311 (2025).

Application of VS-IMSRG

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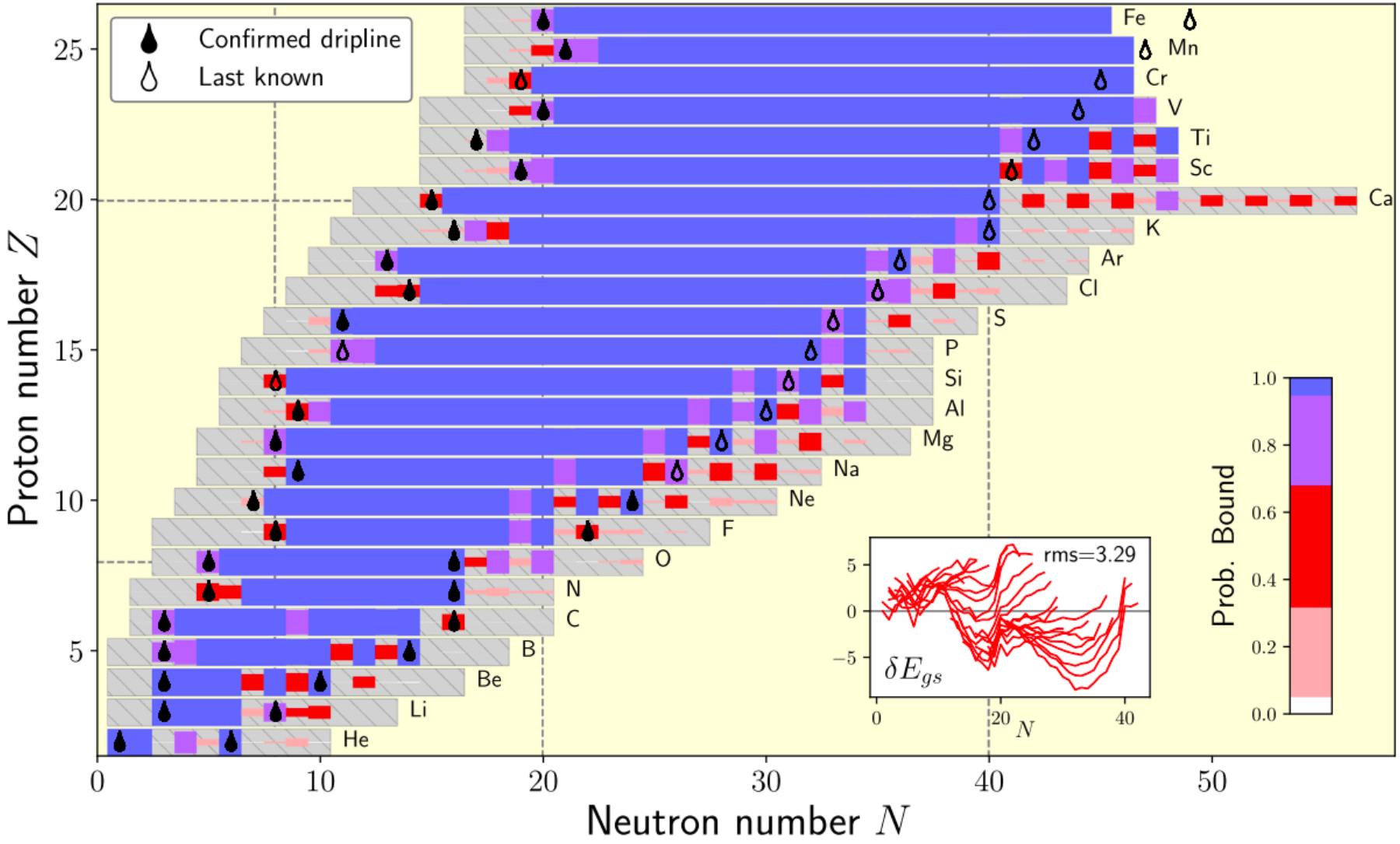
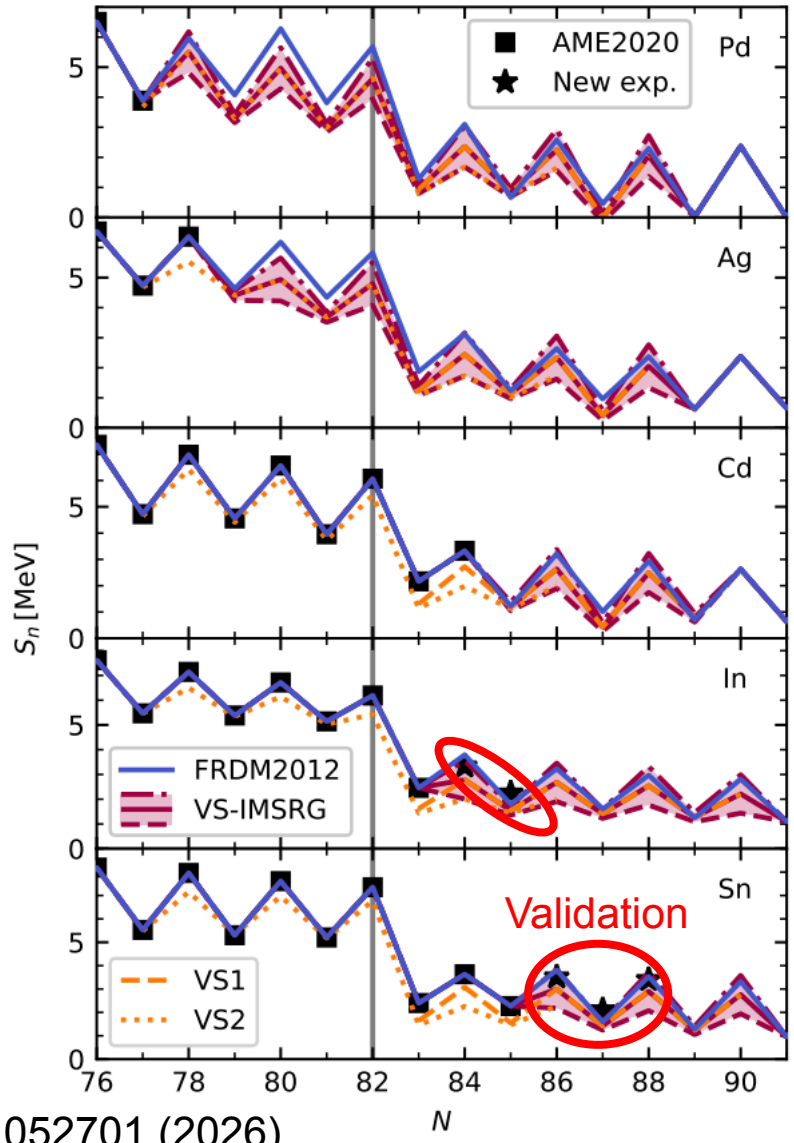
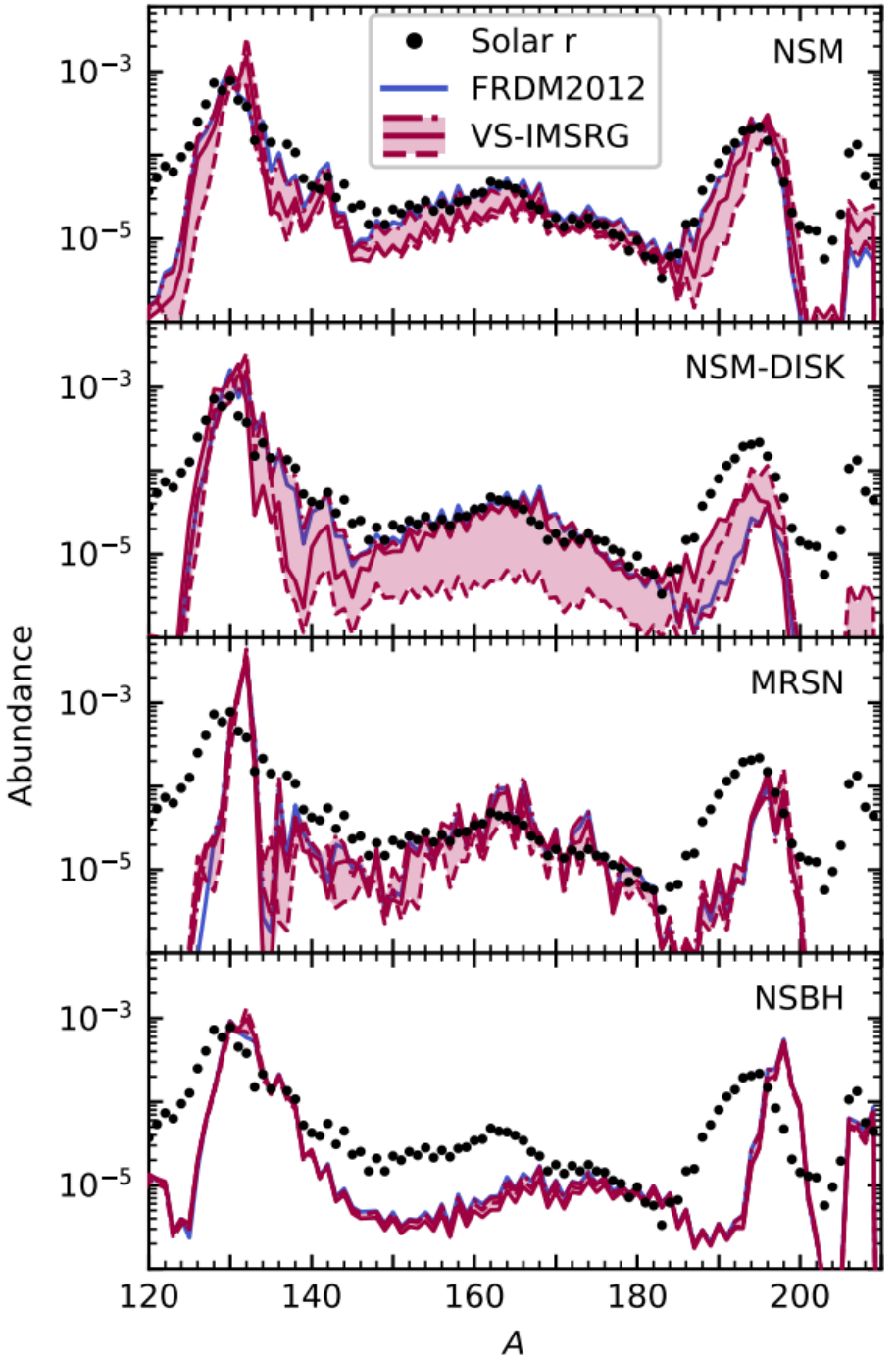


S. R. Stroberg et al., Phys. Rev. Lett. 126, 022501 (2021).

Application of VS-IMSRG

- Separation energies are adjusted to the last known AME2020.
- Uncertainty: VS1 and VS2 results
- The rest is FRDM12 + AME2020
- Ab initio masses makes r-process slower





J. Kuske et al., Phys. Rev. Lett. 137, 052701 (2026).

Capturing collective phenomena is challenging

- The collective nature of the wave function can be measured as

Proton/neutron effective charge

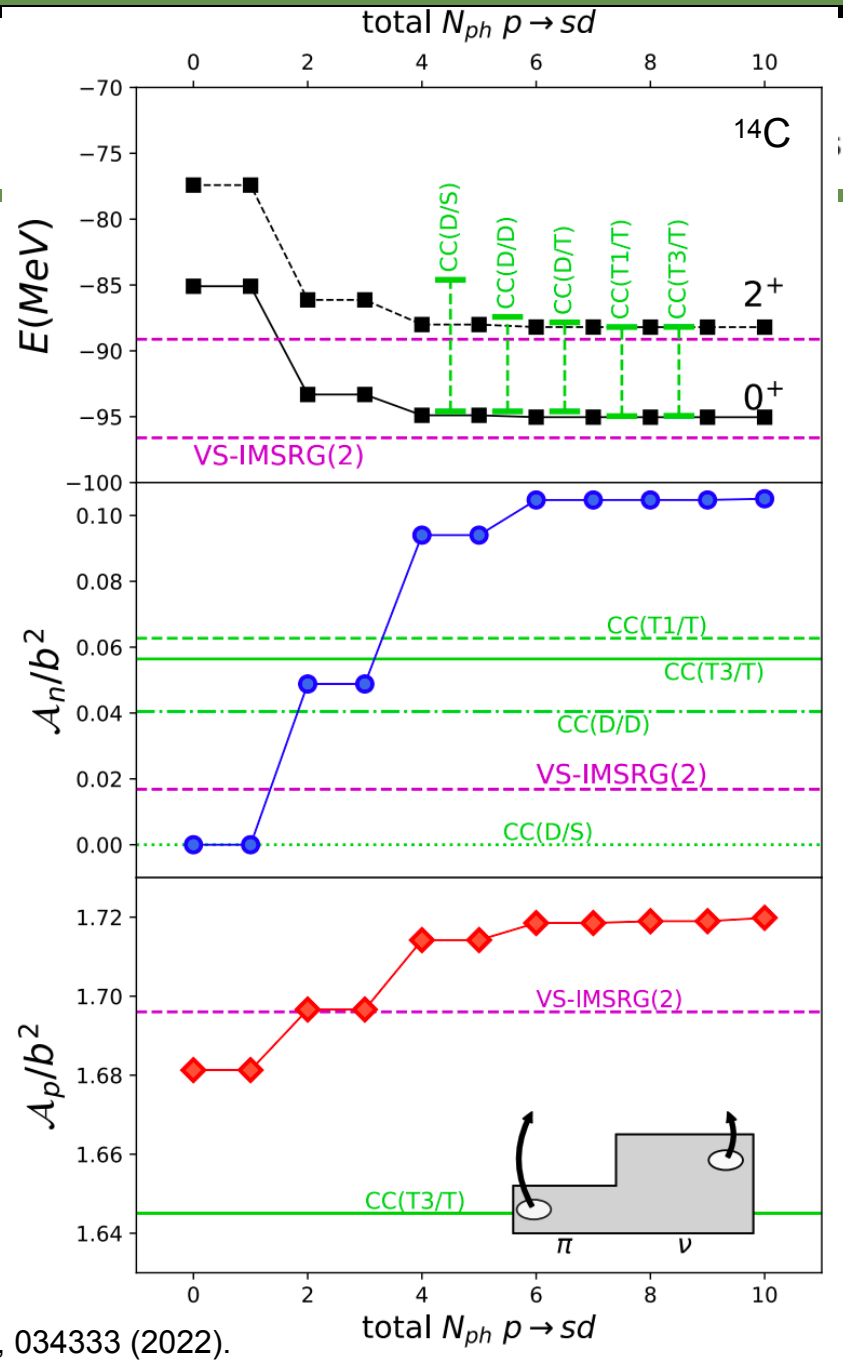
$$\langle J_f M_f | \sum_i e_i r_i^2 Y_{2,M_f - M_i}(\boldsymbol{r}_i) | J_i M_i \rangle = \mathcal{A}_p e_p + \mathcal{A}_n e_n$$

Proton/neutron amplitude

- Dimensionless amplitudes indicate that one needs to include up to 4p4h contributions.
- 4p4h naively corresponds to IMSRG(4). Maybe possible?

  Rongzhe Hu et al., arXiv: 2607.08830.

- Alternative approaches
  - ✦ Starting from a deformed reference?
  - ✦ A larger valence space?



S. R. Stroberg et al., Phys. Rev. C 105, 034333 (2022).

Toward a larger valence space

- In general, our lab-frame wave function should be

$$|\Psi\rangle = \sum_{iI} c_{iI} |\Psi_i^{\rm intr}\rangle \otimes |\Psi_I^{\rm CM}\rangle$$

- Earlier CC and IMSRG works suggest that the CM wave function is factorizable

G. Hagen et al., Phys. Rev. Lett. 103, 062503 (2009).
H. Hergert et al., Phys. Rep. 621, 165 (2016).
N. M. Parzuchowski et al., Phys. Rev. C 96, 034324 (2017).

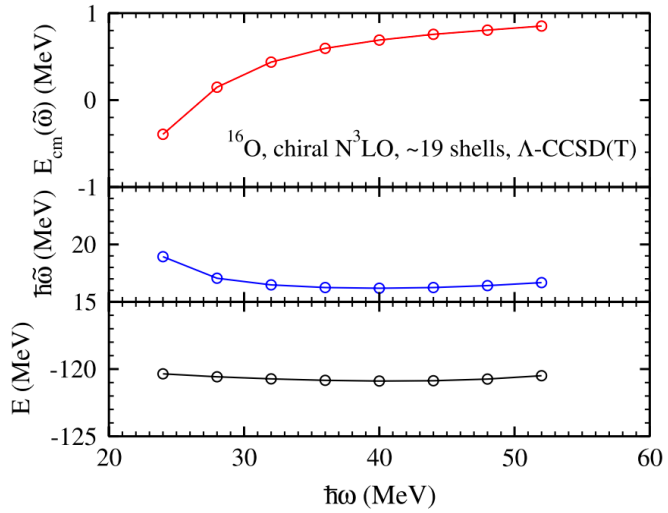
$$|\Psi\rangle \approx |\Psi_i^{\rm intr}\rangle \otimes |\Psi_I^{\rm CM}\rangle$$

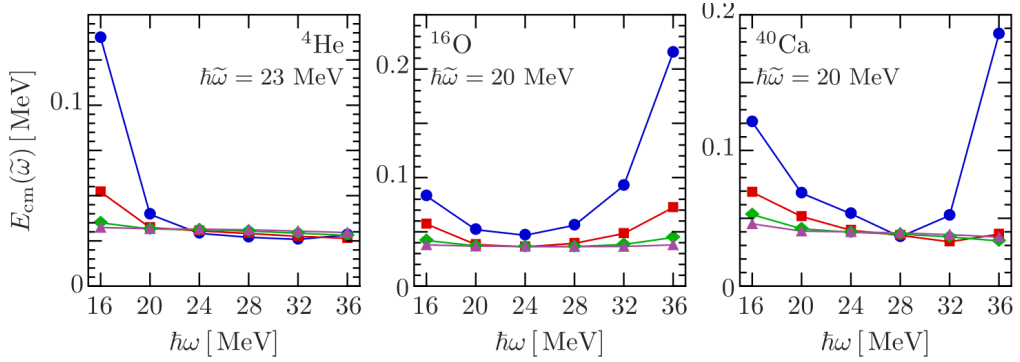
- To impose the CM wave function as Gaussian, one can add the CM term to the starting Hamiltonian

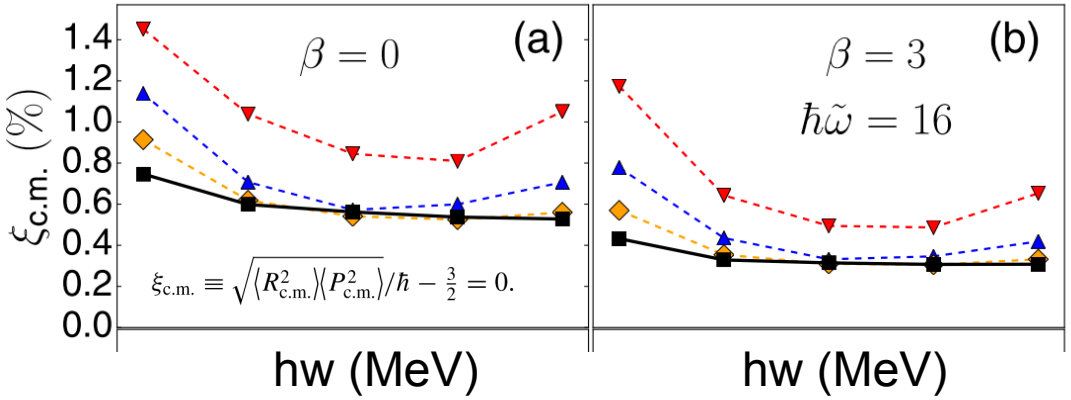
D. H. Gloeckner and R. D. Lawson, Phys. Lett. B 53, 313 (1974).

$$H \to H + \beta H_{\rm CM}, \quad H_{\rm CM} = \frac{\boldsymbol{P}^2}{2Am} + \frac{1}{2} Am\tilde{\omega}^2 \boldsymbol{R}^2 - \frac{3}{2}\hbar\tilde{\omega}$$

- Increase β until we find the β-independent results.

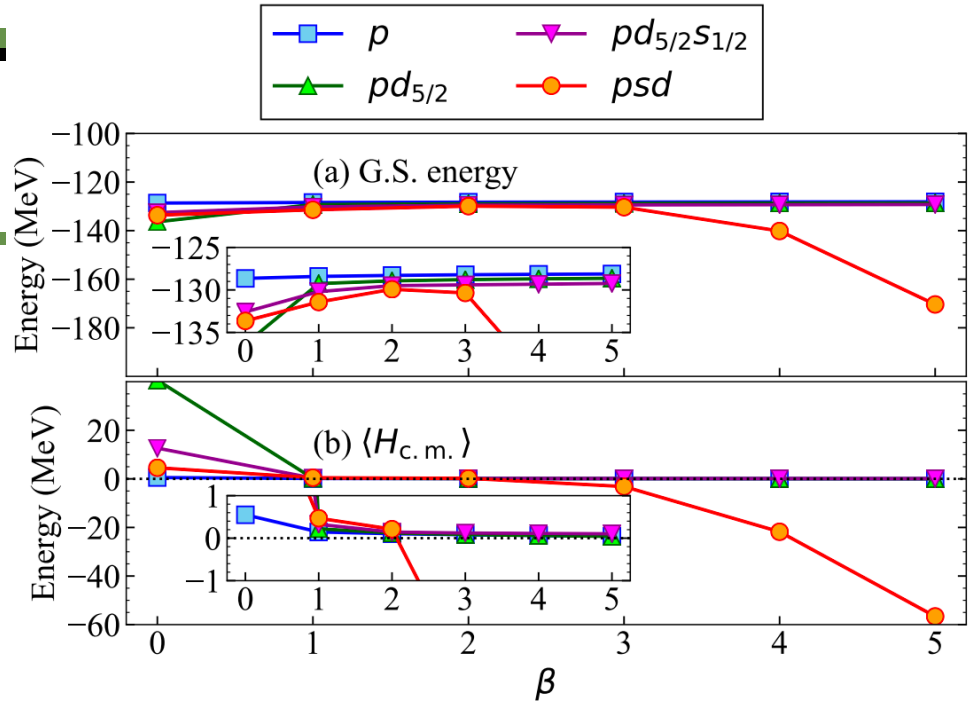






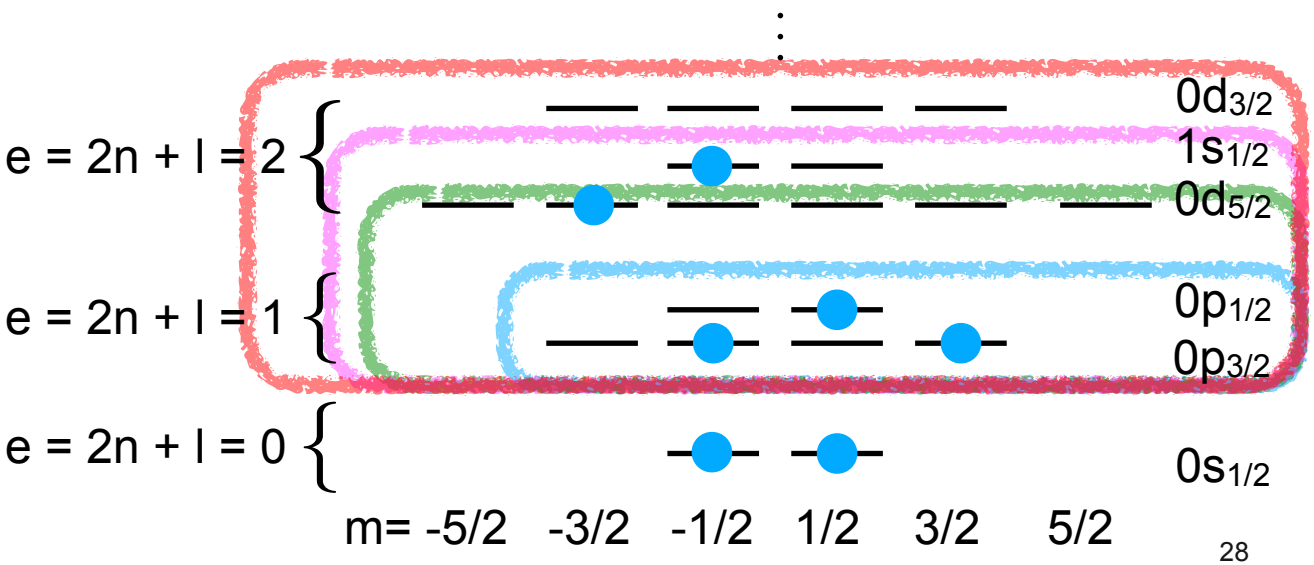
Toward a larger valence space

- Keep increasing the size of the valence space
  - ➡ Restore the original Hamiltonian.
  - ➡ Collective phenomena should be captured at some point.



^{16}O ground-state energy

- If we take the full 2 HO-shell valence space, we cannot find a plateau anymore.
- Also, the Hcm expectation value indicates a breakdown of the IMSRG(2) approximation.
- A similar issue in quantum chemistry?



TM et al., Phys. Rev. C 102, 034320 (2020).

Summary

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- Nuclear ab initio calculations are promising in many applications.
- Valence-space in-medium similarity renormalization (VS-IMSRG) is a powerful method to address open-shell systems and excited states.
  - VS-IMSRG(2) is the workhorse approximation
- Collective physics is difficult to capture within the 2-body level approximation
  - Starting from a deformed reference state
  - Higher-order approximation
  - A larger valence space
- The center-of-mass issue in an arbitrarily large valence-space decoupling.