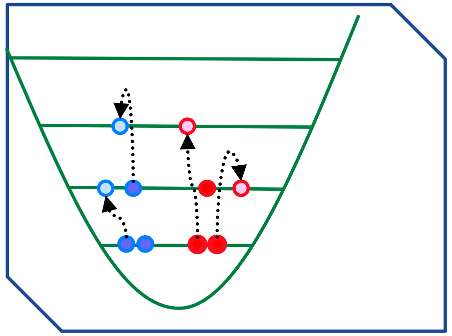
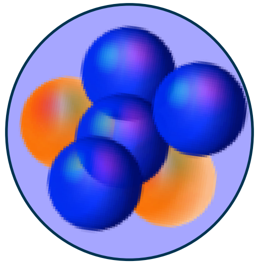


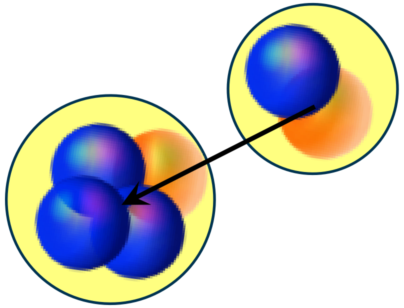


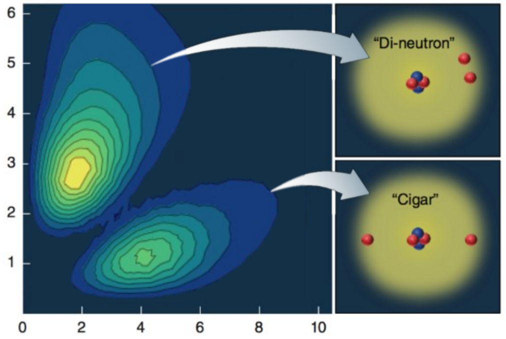
Guillaume Hupin, CNRS IJClab

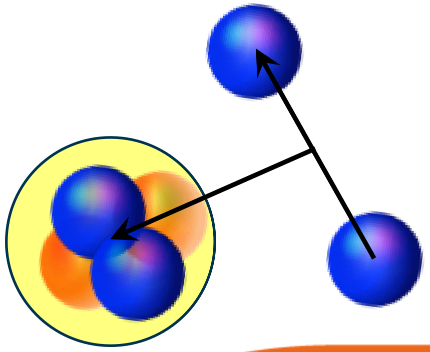
“Nuclear theory projects”

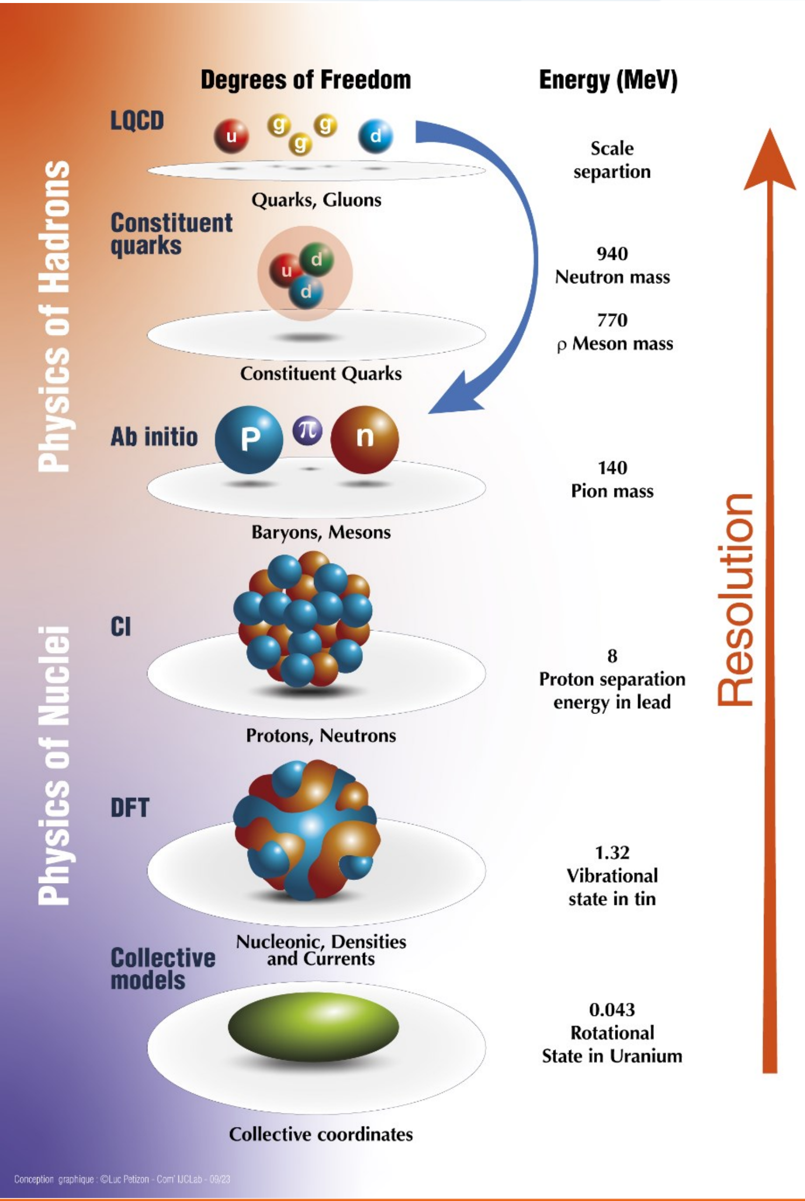
Collaborators

D. Becht (CEA)
J. Herko (TRIUMF)
P. Navratil (TRIUMF)
K.H.D. Nguyen (CNRS/IJCLab)
N. Pillet&P. Indelicato (CEA&CNRS/LKB)
O. Yaghi (PhD, now industry)





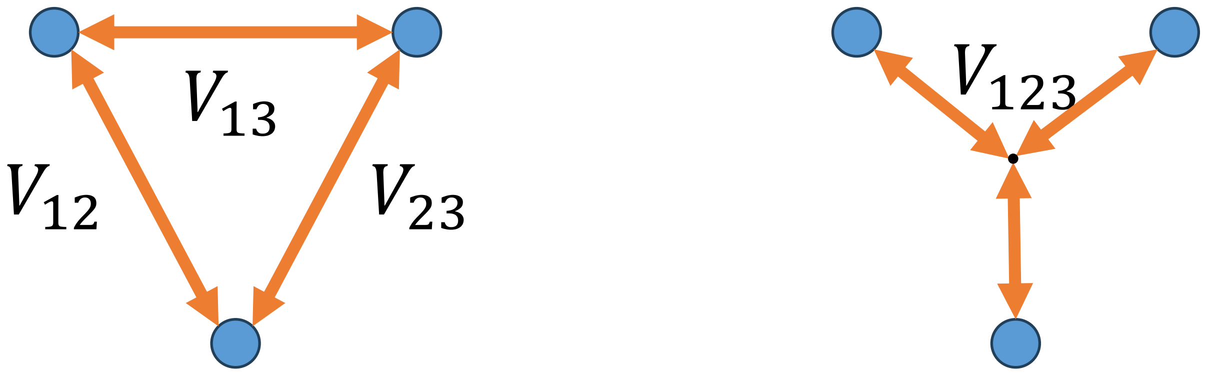


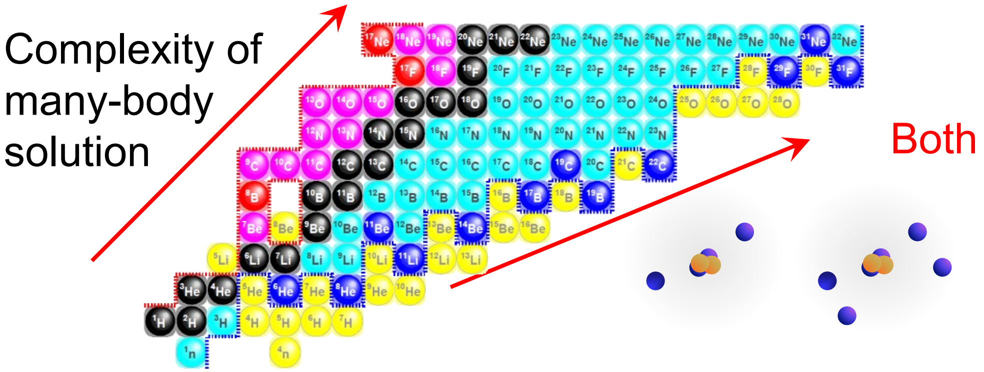


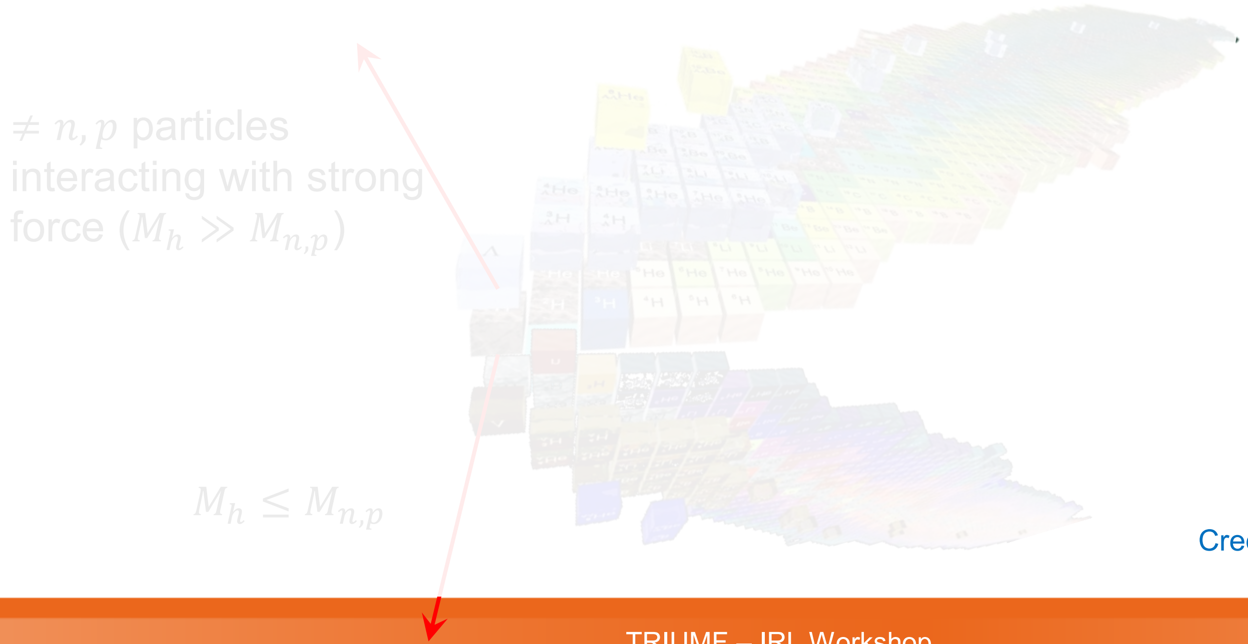
- Goal: Solving the Schrodinger equation (SE) for an A-body system:

$$H|\psi^{J^\pi T}> = E|\psi^{J^\pi T}>$$

- Nucleons are considered as point-like particles.
- The SE is solved by considering two and many-body interactions between nucleons



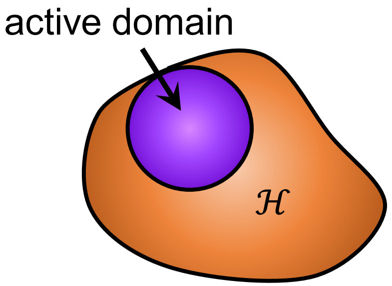




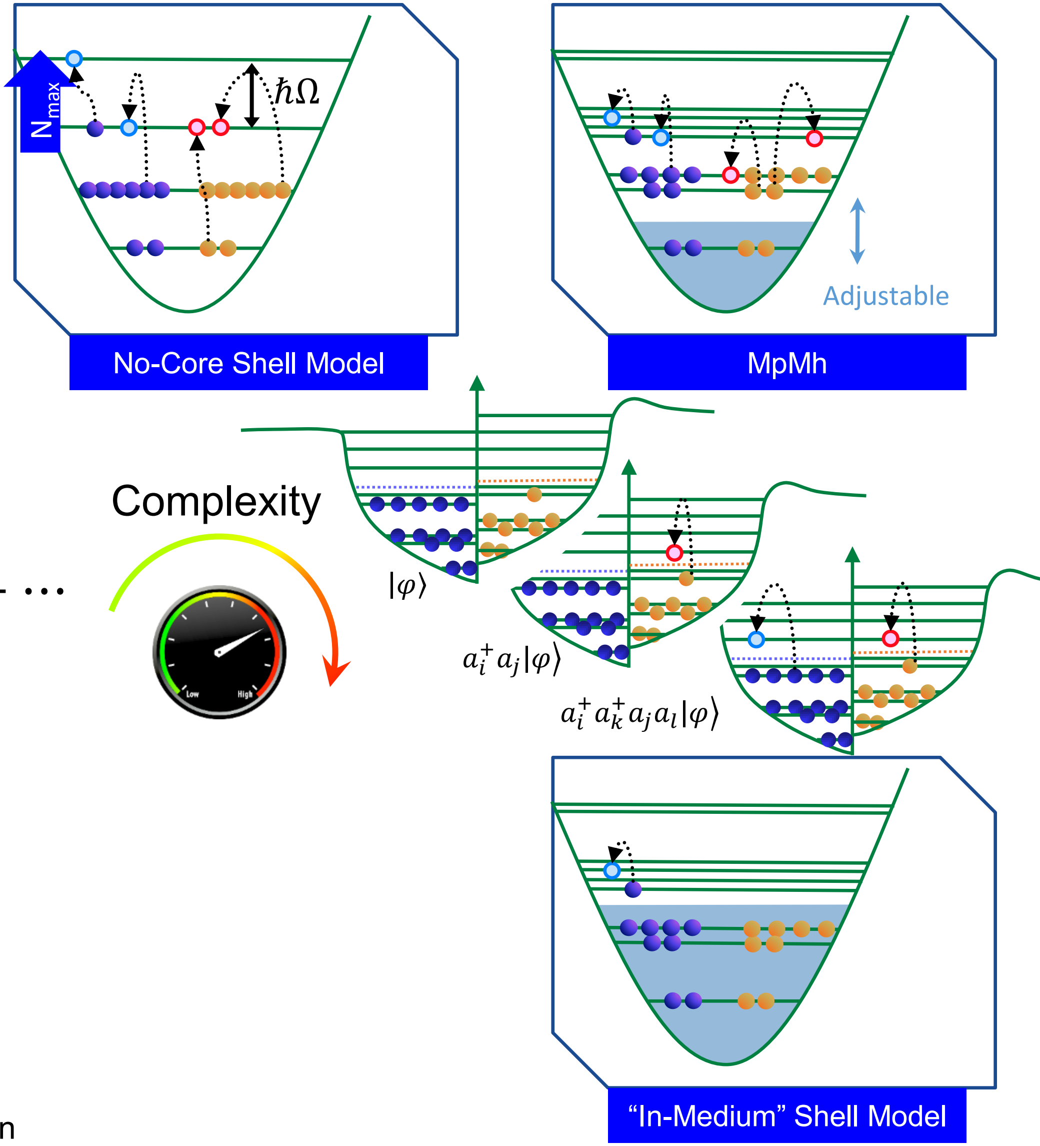
- 😐 Nuclear theory is **data driven**.
- ☹ The lack of accuracy of *ab initio* structure methods impedes the development of reactions modeling.

Credits H. Lenske

Configuration interaction methods suited for $A \gg 1$



- Variational;
- Orthonormal basis;
- Controllable parameters (N_{max}, $E1_{\mathrm{max}}$ etc…);
- UV/IR convergence.

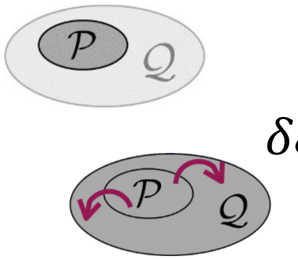


Superposition of Slater determinants:

$$|\Psi^A\rangle = \sum_\alpha c_\alpha \Phi_\alpha^\varphi(\vec{r}_1, \dots, \vec{r}_A) = A_0 \left|\Phi_{0p0h}^0\right\rangle + \sum_{\alpha'} A_{\alpha'} \left|\Phi_{1p1h}^{\alpha'}\right\rangle + \cdots$$

NCSM
IM-SH
MpMh

Optimization of mixing coefficients, one-body Hilbert space:



$$\delta\mathcal{E}[\Psi]_{/\{A_\alpha^*\}} = 0 \Longrightarrow \sum_\beta A_\beta \langle \Phi_\alpha | \hat{H} | \Phi_\beta \rangle = E A_\alpha$$

$$\delta\mathcal{E}[\Psi]_{/\{\varphi_\alpha^*\}} = \langle \Psi | [\hat{H}, \hat{T}] | \Psi \rangle = 0 \Leftrightarrow [\hat{h}(\rho), \hat{\rho}] = \hat{G}(\sigma)$$

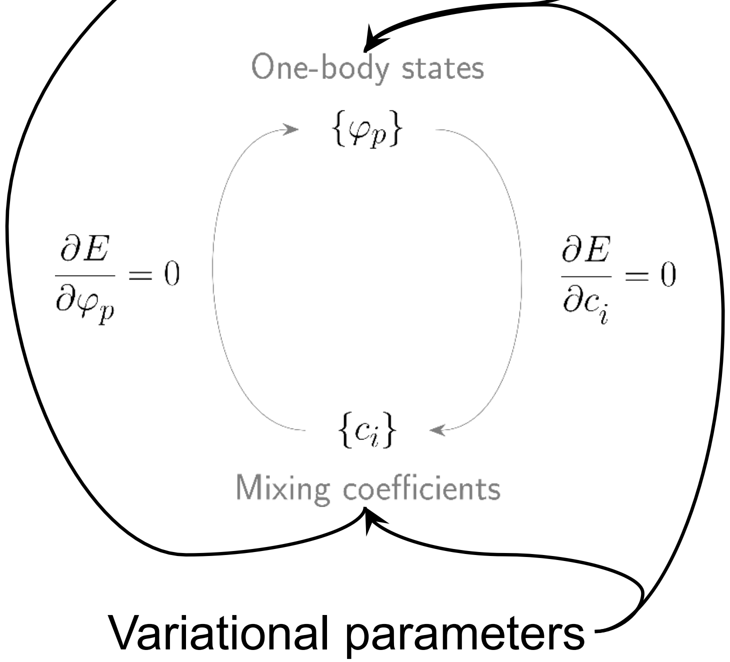
Generalized Brillouin (GB) equation

One-body Hamiltonian:

$$\left(c\,\vec{\alpha}.\vec{p} + \beta c^2 + V(r)\right)\varphi_p(x) = 0,$$

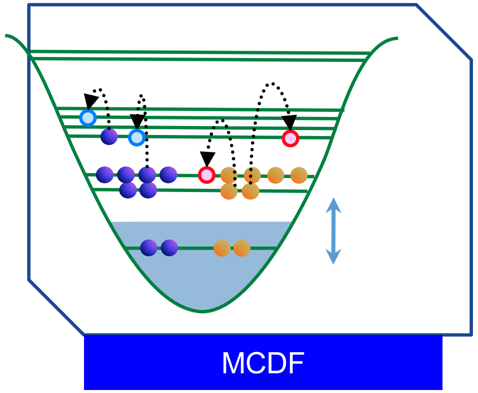
Many body atomic wave function

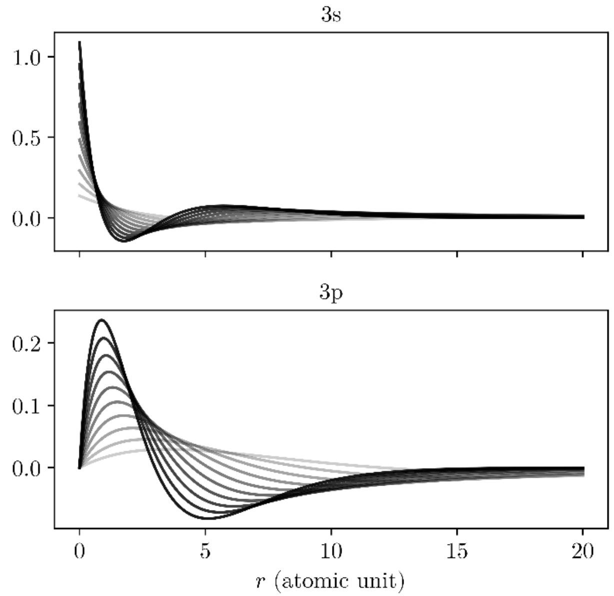
$$|\Psi^n\rangle = \sum_i c_i \Phi_i^{\varphi}(\vec{r}_1, \dots, \vec{r}_A).$$

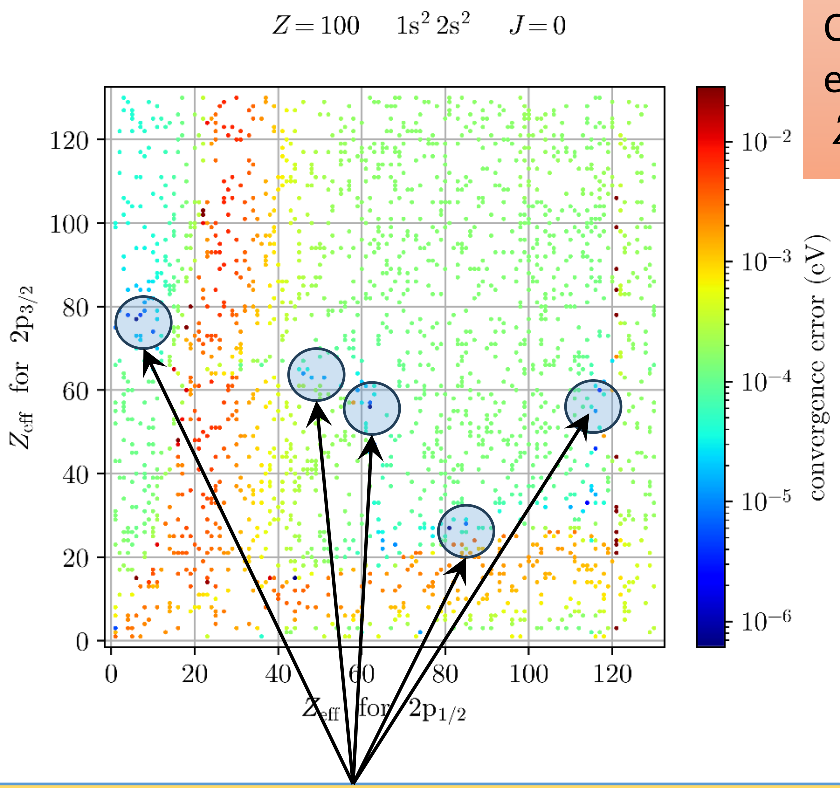


- Initial one-body states are hydrogenlike.
- To guesstimate the effect of many body correlation, orbitals are adjusted with an effective proton number Z_{eff}.

  bad Z_{eff} leads to no convergence
- Finding a good combination of Z_{eff} is time consumming.







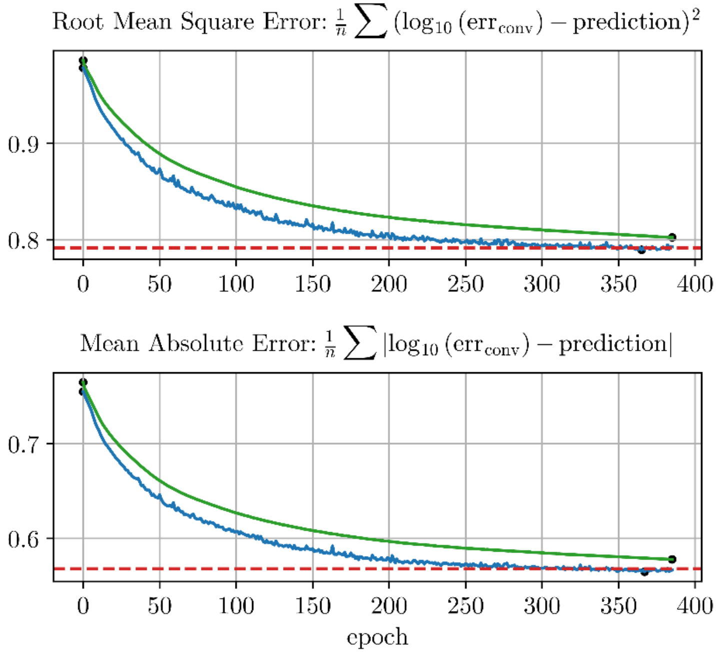
Correlation plot of the convergence error estimate as a function of the Z_{eff} of $2p_{\frac{3}{2}}$ and $2p_{\frac{1}{2}}$ of Be-like Fm.

☺ This is an excellent candidate problem for **machine learning**.

☹ The physicist (or software user) is therefore required to **manually predict** the **hyperparameter** Z_{eff} for each successive atomic orbital of every atomic state, making the procedure very cumbersome.

Generating data:

Features	Labels
⋮	⋮
state, $Z_{\text{eff(s)}}$	$\log(\text{err}_{\text{conv}})$
⋮	⋮



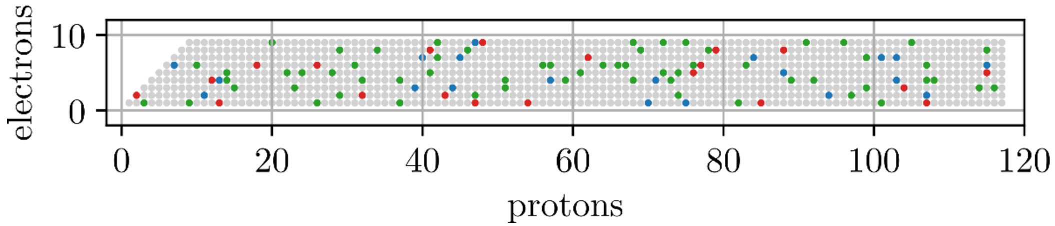
Select a target dataset:

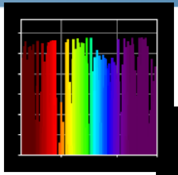
$$1 \leq n_{\text{protons}} \leq 118 \quad 1 \leq n_{\text{electrons}} \leq 10$$

Train a neural network on 10% of it:

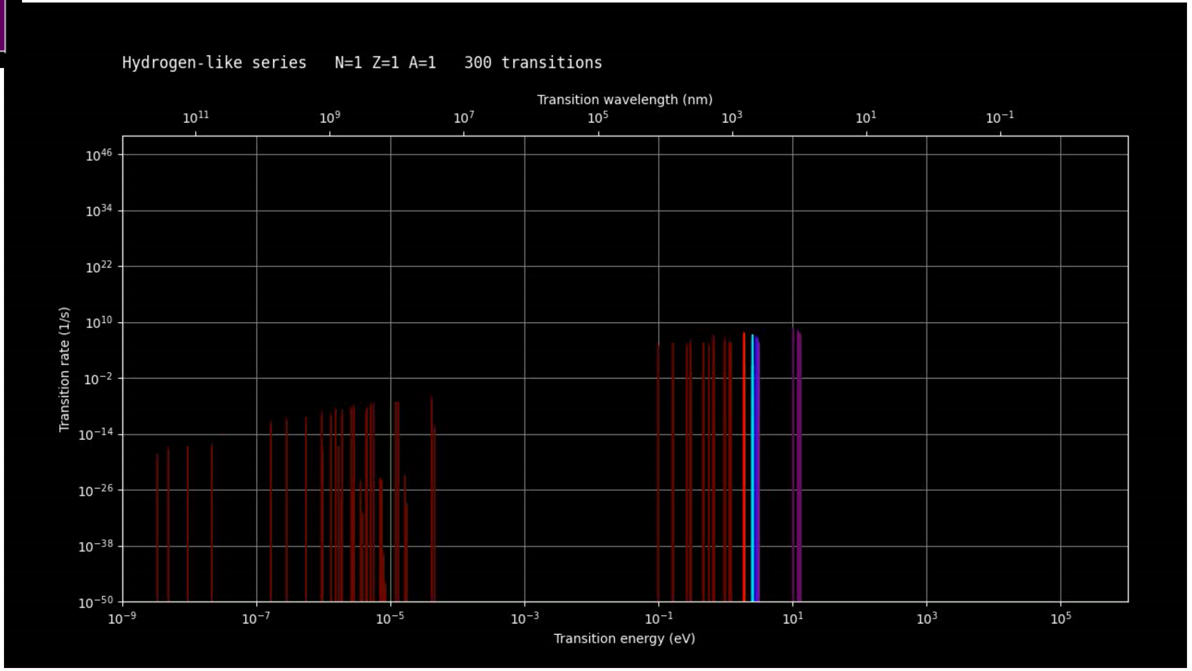
training + validation + test = 10% of target

Use trained model for remaining 90%





Datatom: public repository (soon)



The dataset co-generated by AI is substantially larger than the NIST repository and opens the way to applications such as:

- opacity calculations for stellar objects,
- spectroscopic identification of stellar events,
- the study of metastable states relevant to lasers and atomic clocks…

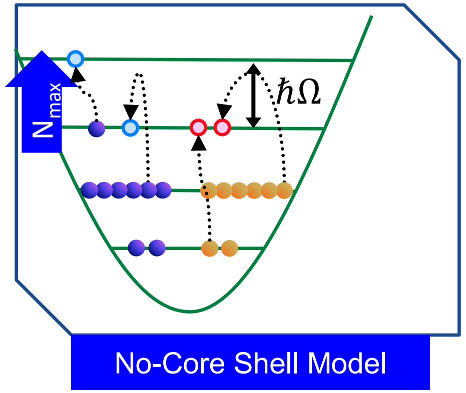
One-body basis states:

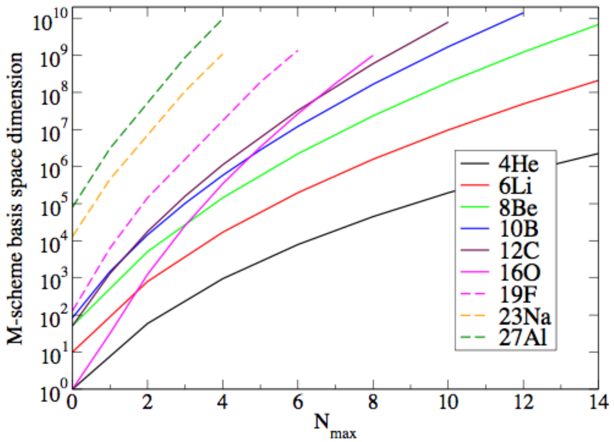
$$\varphi_{nl\frac{1}{2}j}(\vec{x},\vec{\sigma}) = \left[R_{nl}(x)Y_l(\hat{x})\chi_{\frac{1}{2}}(\vec{\sigma})\right]^J,$$

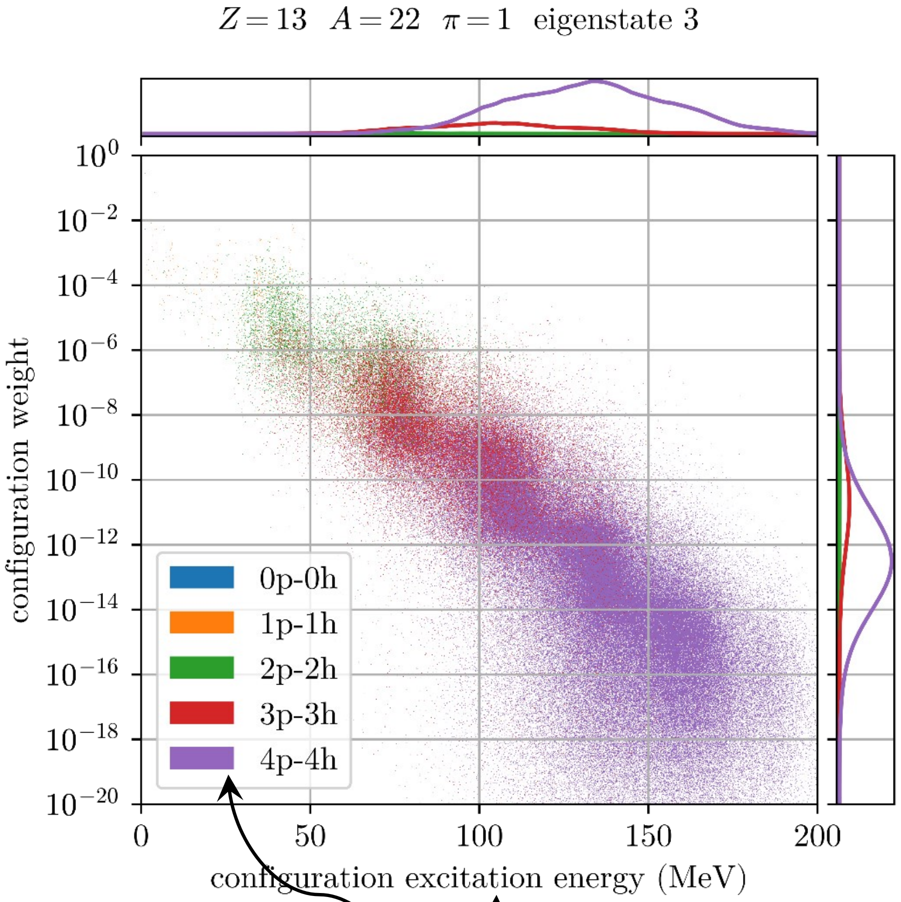
Many body nuclear wave function

$$|\Psi^n\rangle = \sum_i c_i \Phi_i^{\varphi}(\vec{r}_1,\dots,\vec{r}_A).$$

$$\phi_n^A = \frac{1}{\sqrt{A!}}\begin{vmatrix} \phi_i(\vec{r}_1) & \dots & \phi_i(\vec{r}_A) \\ \vdots & \ddots & \vdots \\ \phi_l(\vec{r}_1) & \dots & \phi_l(\vec{r}_A) \end{vmatrix} = a_l^\dagger \dots a_i^\dagger |0\rangle$$







Usual truncation schemes:

- Excitation order
- Excitation energy
- Importance truncation

Usual schemes:

- Excitation order
- Excitation energy

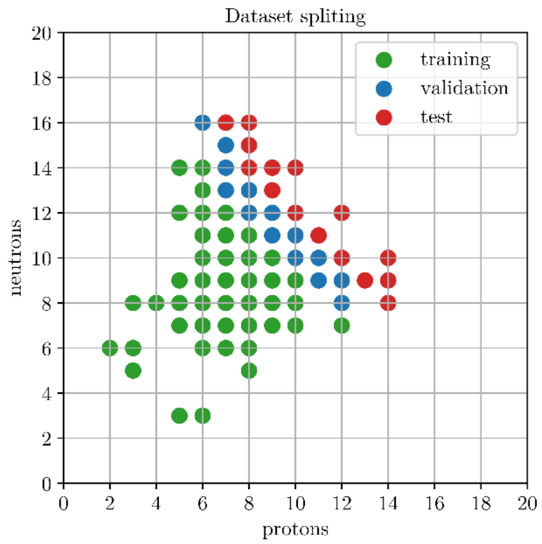
Importance truncation

Select a target dataset (exact solution):

$$1 \le n_{\text{protons}}, n_{\text{neutrons}} \le 14; A \le 18$$

Train a neural network on 10% of it:

training + validation + test

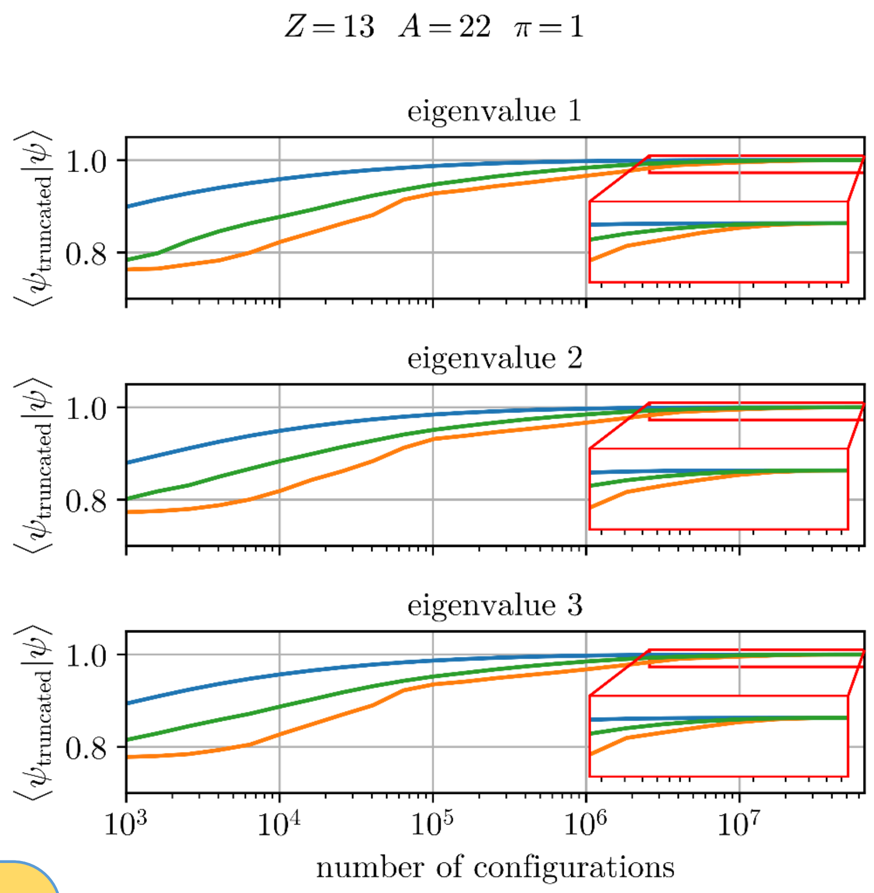


Generating data:

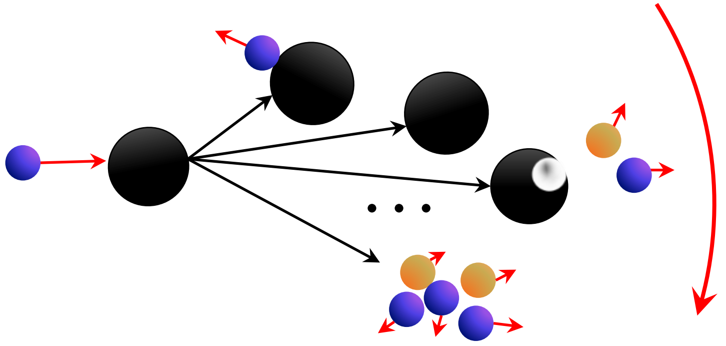
Features	Labels
⋮	⋮
state, $\vert \text{config}_i \rangle$	$\log_{10}(c_i{}^2)$
⋮	⋮

Each Slater determinants configuration are encoded via a transformer layer

The AI augments, **rather than replaces**, the MB solver by automatically selecting the relevant subspace for diagonalization, with state-dependent variations.



Using real weights: $c_i^2 \ge cste$;
Using model;
Using excitation energies: $E_i \le cste$



- 😐 Nuclear theory is **data driven**.
- ☹ Few-body techniques scale **very bad** with the number of constituents in the continuum.

Credits H. Lenske

We want to develop a unique tool applicable to both nuclear structure and reactions, to enhance our understanding of the strong force at low energy.

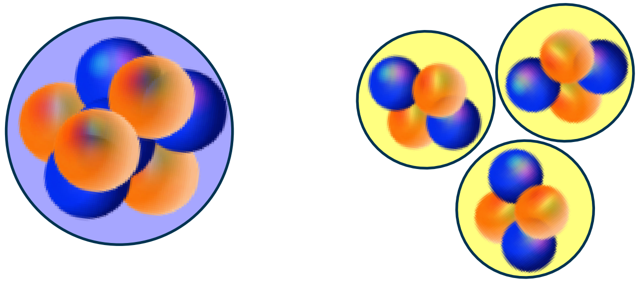
Structure

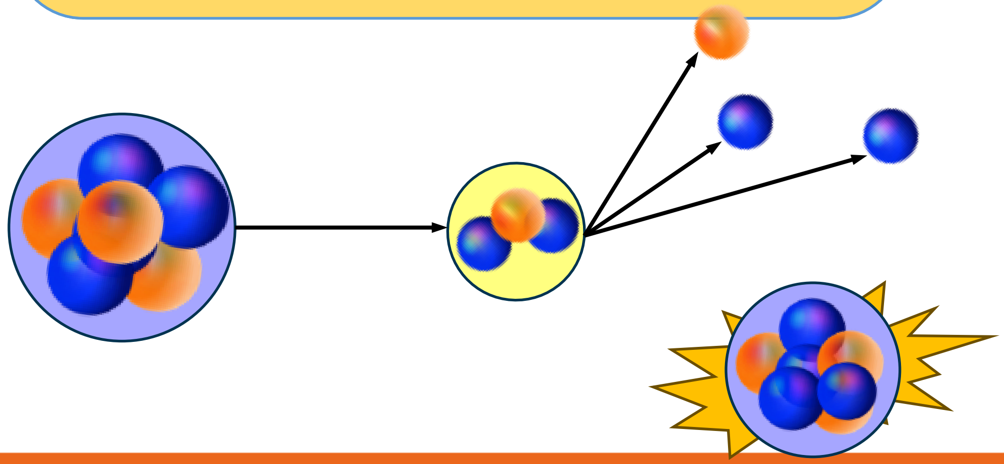
☺ Extraction of resonance properties for fine tuning interactions and applications to astrophysics.

Reactions

☺ Enabling us to study nuclear breakup reactions including Final State Interaction (FSI)

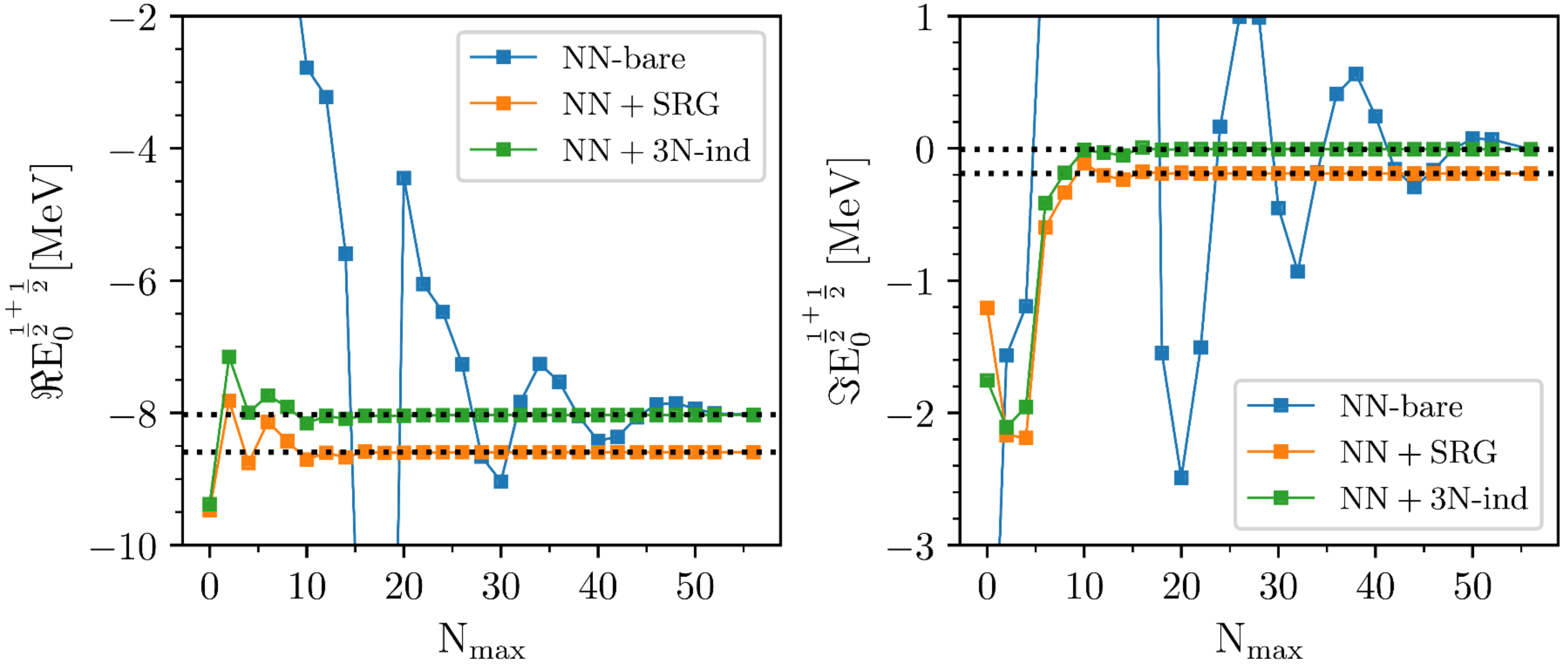
☺ Calculation of complex charged (and multi-neutron) nuclear decay.

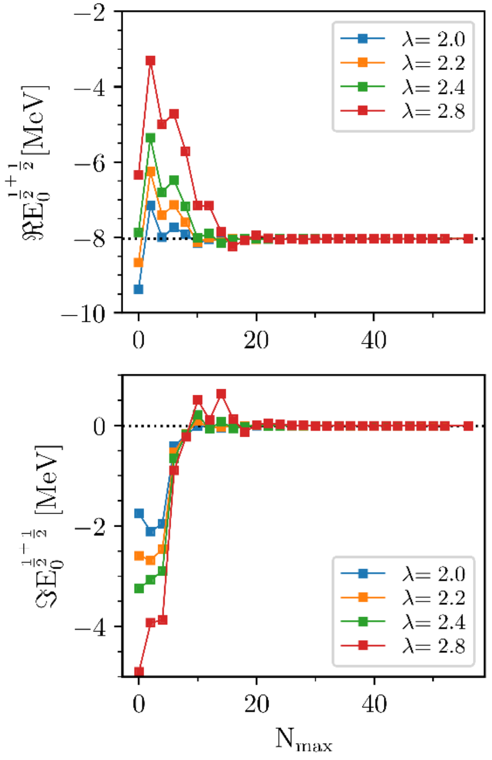




Quality of the rotated Hamiltonian evaluated in A=3

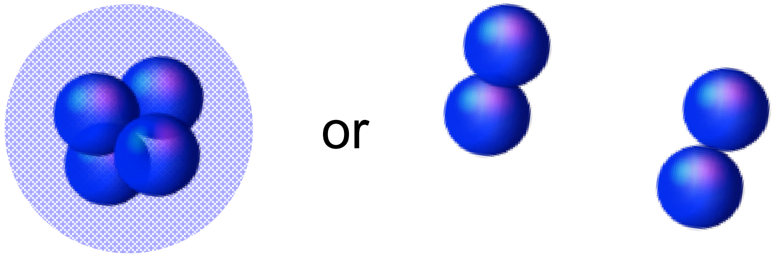
Triton g.s. convergence with CS-Hamiltonian (θ = 0.3 rad)



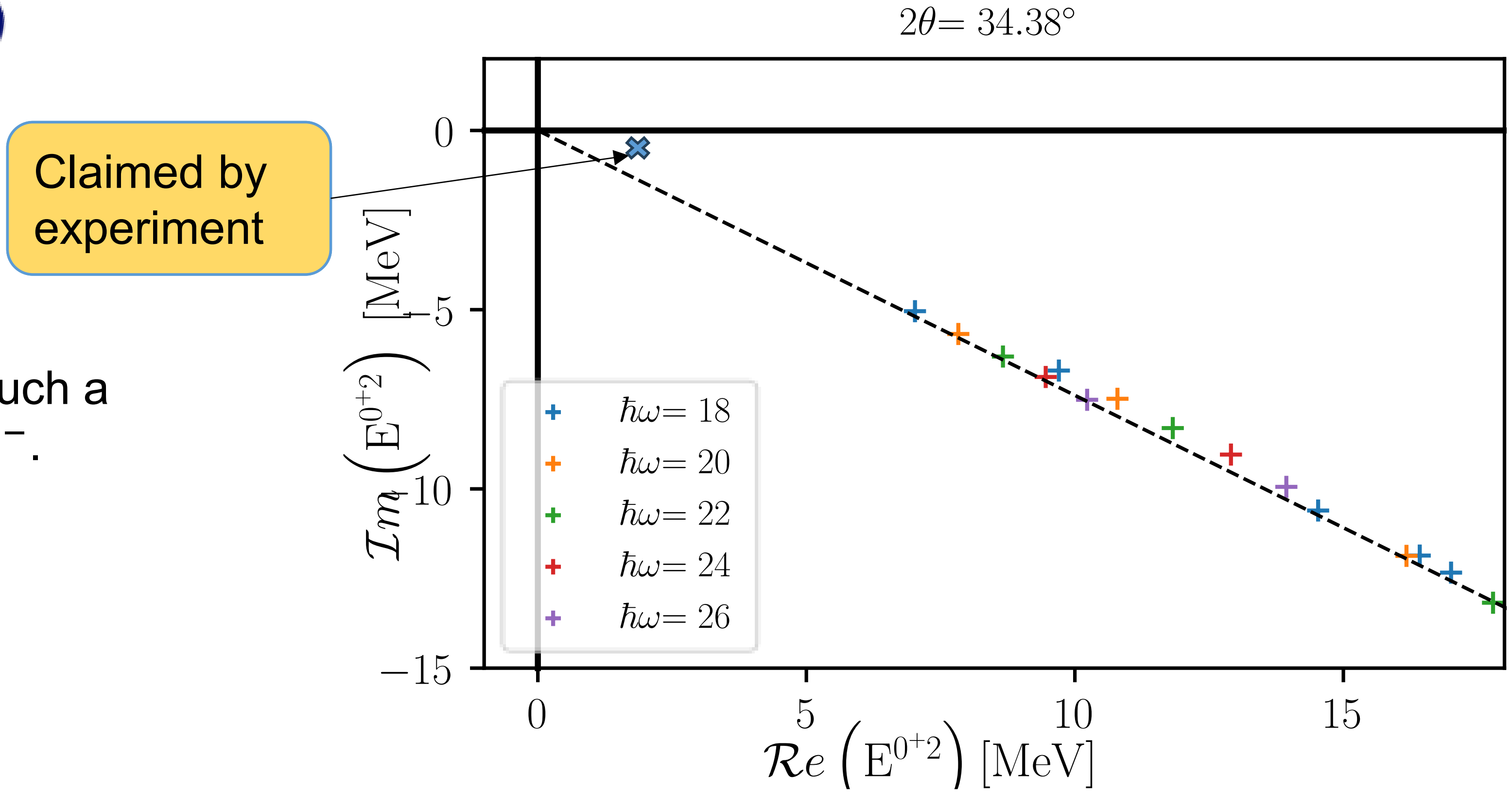


Maximum model space achievable $N_{\max}$~60 (30 nodes a box in excess of 15 fm)

- SRG leads to faster convergence;
- Induced 3N-interaction needs to be accounted for (as expected from literature).



or



CS shows no indication of such a resonance in 1^+, 1^-, 0^+ or 0^-.

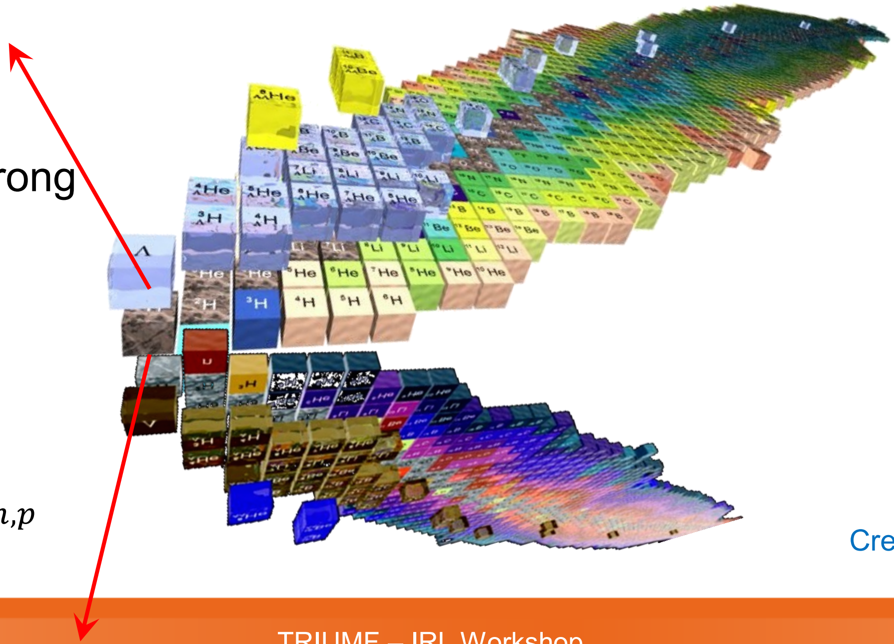
Lower bound of :

$$\Gamma_r = 1.9\, E_r$$

or :

$$\Gamma_r = 4.5\, MeV$$

$\neq n, p$ particles interacting with strong force ($M_h \gg M_{n,p}$)



$M_h \leq M_{n,p}$

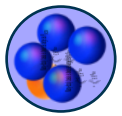
- 😐 Nuclear theory is **data driven**.
- ☹ Global optical models (NN or $N\bar{p}$ or $N\pi$ scattering) are not applicable to exotic systems.

Credits H. Lenske

- One way to solve the many-body problem when two scales appear

$$\Psi^{(A)}_{NCSM} = |A\lambda J^{\pi} T\rangle = \sum_{\alpha} c_{\alpha} \, |A\alpha j_z{}^{\pi} t_z\rangle$$

Mixing coefficients (unknown) — A-body harmonic oscillator states



$|A\lambda J^{\pi} T\rangle_{SD} \phi_{00}(\vec{R}^{A}_{c.m.})$

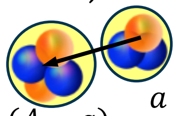
Second quantization

Can address bound and low-lying resonances (short range correlations)

$$\Psi^{(A)}_{RGM} = \sum_{\nu} \int d\vec{r}\, g_{\nu}(\vec{r})\, \hat{A}_{\nu} \left| \Phi^{(A-a,a)}_{\nu\vec{r}} \right\rangle$$

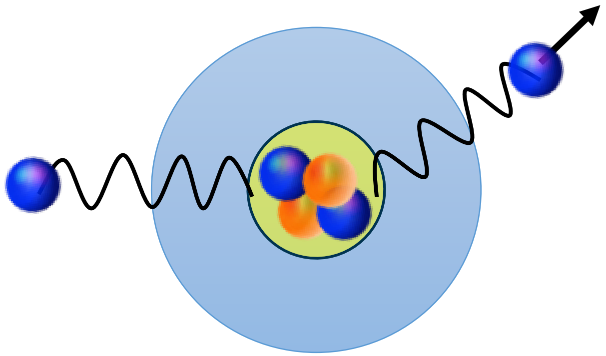
Relative wave function (unknown) — Antisymmetrizer — Channel basis

$\vec{r}_{A-a,a}$



$\psi^{(A-a)}_{\alpha_1} \psi^{(a)}_{\alpha_2} \, \delta(\vec{r} - \vec{r}_{A-a,a})$

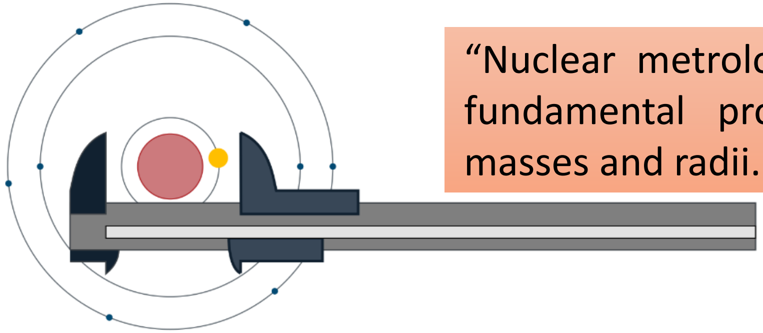
Cluster expansion technique



Many-body basis is twice as large as Ψ_{NCSM}

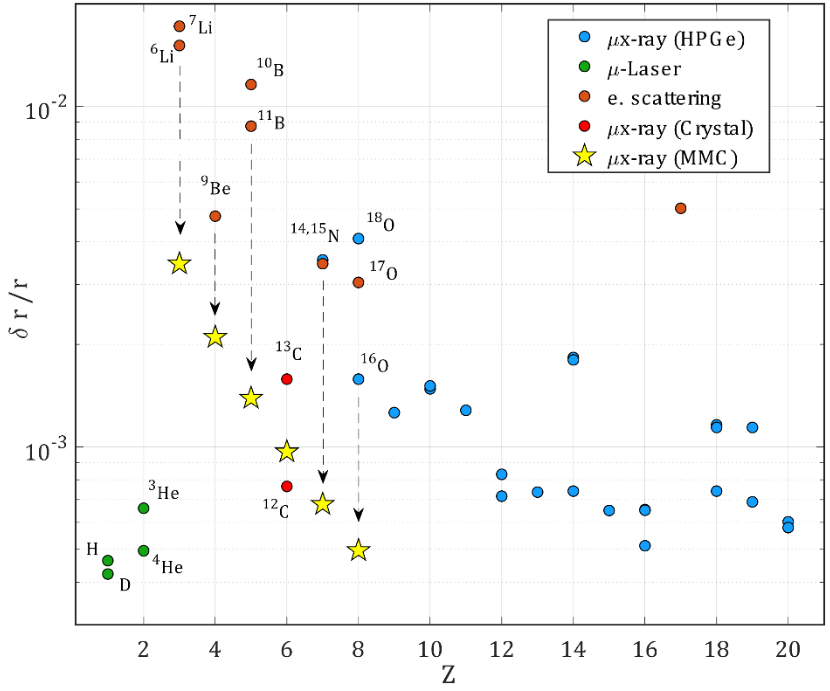
- $\psi^{(A-a)}_{\alpha_1} \in \mathcal{H}^{N_{\max}}$
- $\psi^{(a)}_{\alpha_2} \in \mathcal{H}^{N_{\max}}$

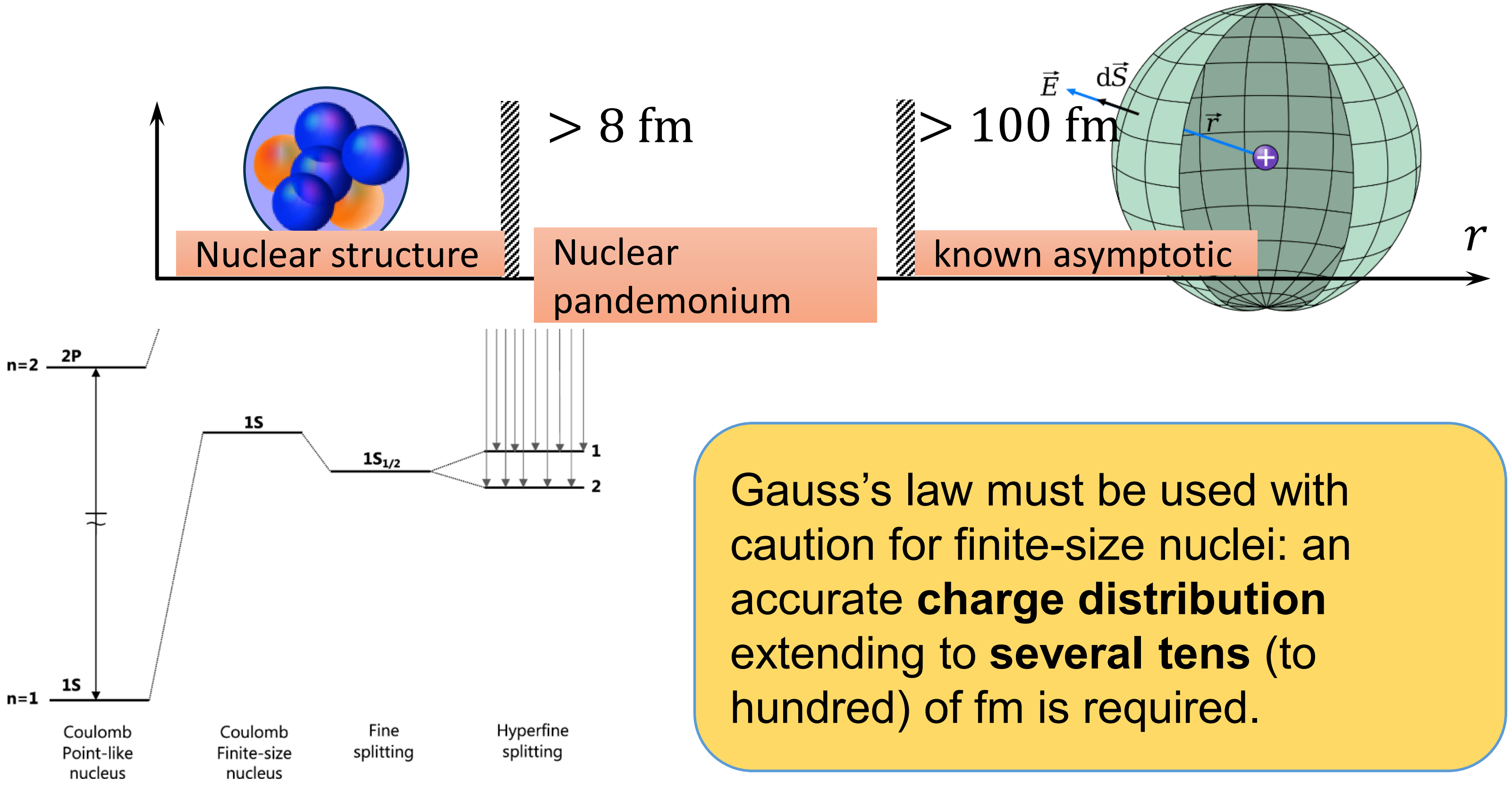
NCSM/RGM
Cluster formalism for elastic/inelastic



"Nuclear metrology": determining fundamental properties such as masses and radii..

The aims is to improve the measurement of absolute charge radii of light nuclei by a factor of 10 (**on light systems**!).

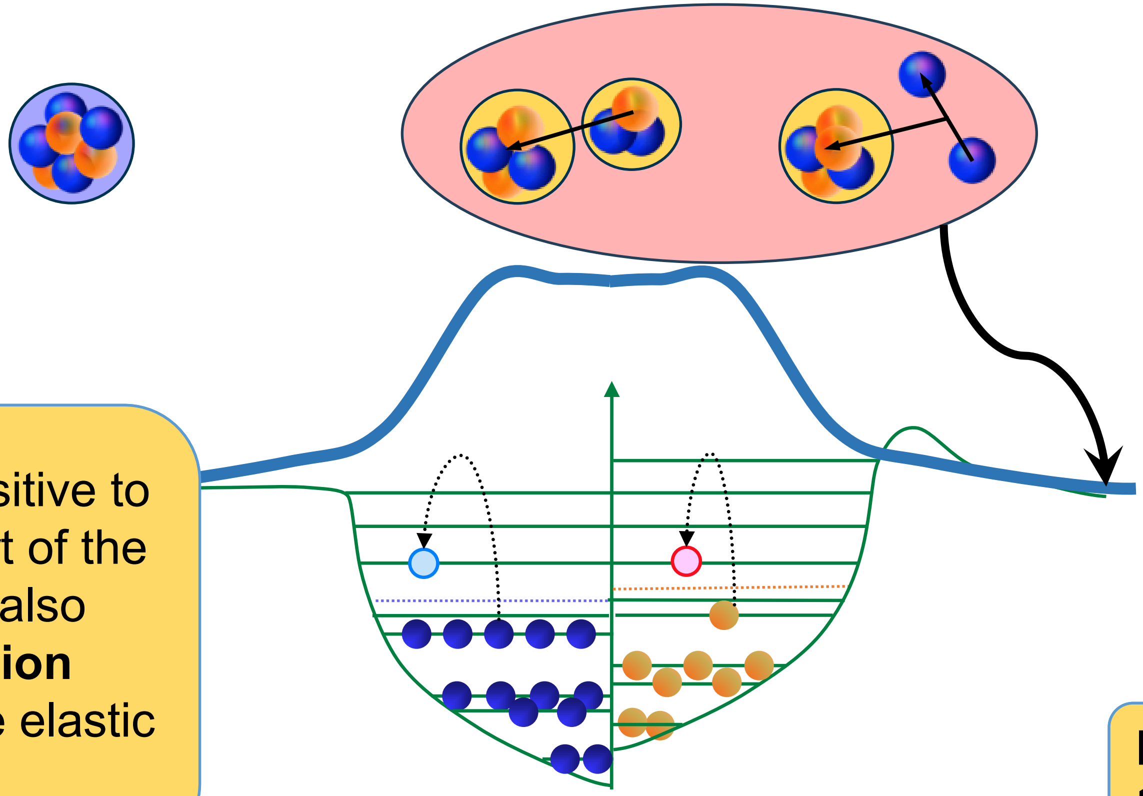


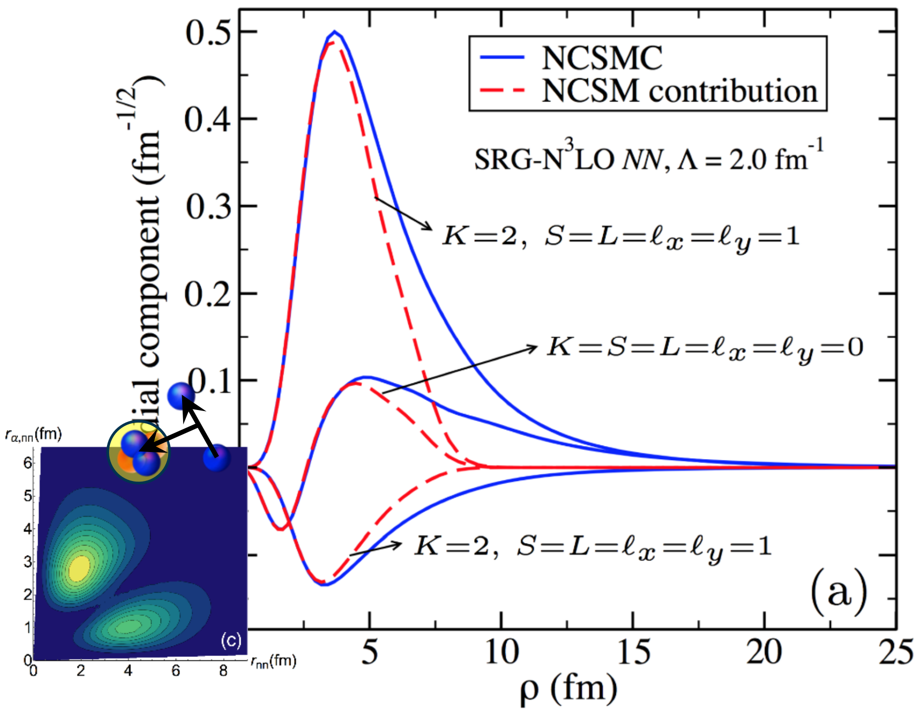


Gauss's law must be used with caution for finite-size nuclei: an accurate **charge distribution** extending to **several tens** (to hundred) of fm is required.

- The nuclear bound state wave function can be decomposed into all the neiboring reaction channels

$$\Psi^{(A)}_{\mathrm{NCSMC}} = \Psi^{(A)}_{\mathrm{NCSM}} + \Psi^{(A-1,1)}_{\mathrm{RGM}} + \cdots + \Psi^{(A-3,3)}_{\mathrm{RGM}} + \cdots \Psi^{(A-2,1,1)}_{\mathrm{RGM}} + \cdots$$





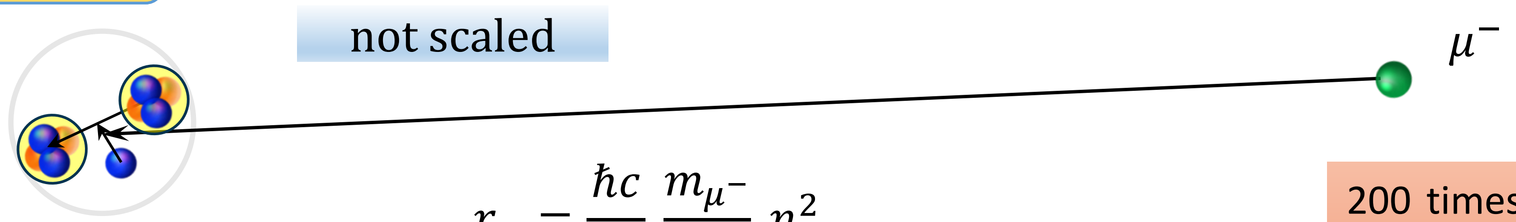
N_{max} =12 model space i.e. $r \approx 8$ fm HO spatial box

Observables sensitive to the long-range part of the wave function are also **sensitive to reaction channels** near the elastic threshold.

Long-distance components are mandatory to model ^{6}He.

Doable with continuum

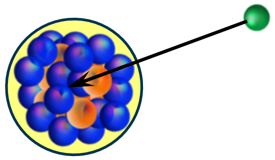
- Nuclear size 10^{-5} a.u.
- Muonic 1s Bohr radius 10^{-3} a.u.



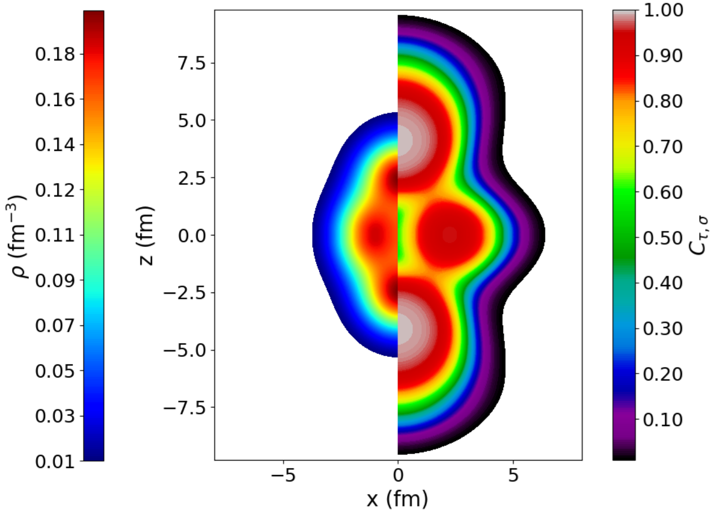
$$r_n = \frac{\hbar c}{Z\alpha}\frac{m_{\mu^-}}{2\mu}n^2$$

200 times closer than the electron, 10 times more sensitive to nuclear density

Maybe in 2326



- Bound state properties with continuum $\left\langle \Psi^{(A)}_{\mathrm{NCSMC}} \middle| \hat{O} \middle| \Psi^{(A)}_{\mathrm{NCSMC}} \right\rangle$ to obtain the charge density $\hat{\rho}(r)$ at large r and the magnetic distribution.
- We will also explore the interest of computing localization probabilities: $D_{\tau\sigma}(r) = \left(\tau_{\tau\sigma} - \frac{1}{4}\frac{(\nabla\rho_{\tau\sigma})^2}{\rho_{\tau\sigma}}\right)$



Phys. Rev. C **106**, 064330 (2022)

Link with DFT (new constraints)

Thank you !