Deuteron-nucleus reaction in NCSM/RGM framework* + Nonlocal nuclear Energy Density Functionals**

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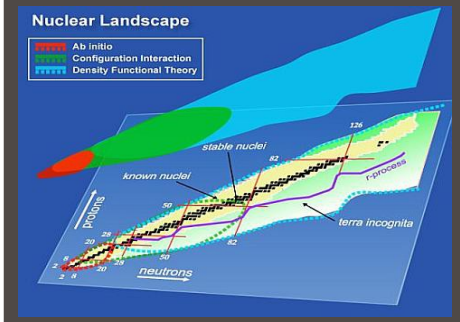
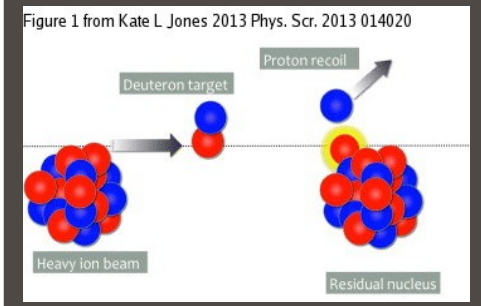


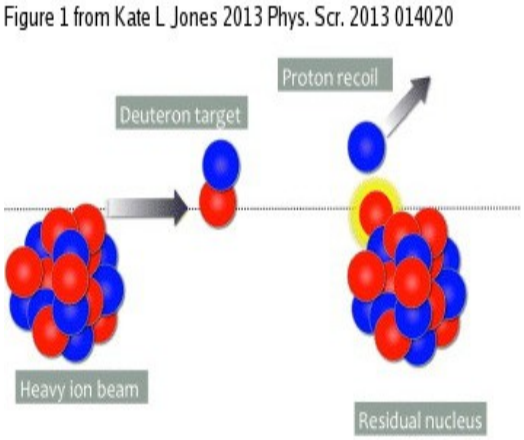


Outline

- ✔ Motivations
- ✔ NCSM/RGM Formalism
- ✔ Diagonal & transfer kernels

- ✔ Nuclear DFT
- ✔ (quasi)Local and nonlocal higher-order functionals
- ✔ Applications of ET principles to EDF

Deuteron-nucleus reaction: motivations



(d,p) reaction in inverse kinematics

Availability of exotic nuclei beams in RIB facilities:

- Structure of exotic nuclei (ex. ^{11}Be(d,p)^{12}Be at ISAC - TRIUMF)
- Nucleosynthesis and nuclear fusion applications (ex. ^{3}H(d,n)^{4}He reaction)
- Surrogate for (p/n) capture reactions (^{14C}(d,p)^{15}C as surrogate of ^{14}C(n, gamma)^{15}C)

Benchmark for *ab initio* theory:

- Microscopic Hamiltonian (test for chiral effective nuclear forces)
- Comparison with different approaches as DWBA, CDCC, etc

ab initio description of nuclear reactions

- Inter-nucleon realistic force:
  - SRG-evolved chiral NN potential
  - Chiral and SRG-induced NNN forces not included yet
- Detailed nuclear structure description (all nucleons in the system are active degrees of freedom):
  - Nuclear target wavefunction obtained within *ab initio* method

$$\hat{H}^{A-2}\psi_\alpha(r_1, r_2, .., r_{A-2}) = E_\alpha^{A-2}\psi_\alpha(r_1, r_2, .., r_{A-2})$$

  - Expansion in A-body harmonic oscillator basis
  - Pauli principle and translational invariance preserved
- Full antisymmetrization of the total wavefunction

$$\hat{A}_{\alpha,\beta}\psi_\alpha(r_1, r_2, .., r_{A-2})\psi_\beta(r_{A-1}, r_A)$$

No Core Shell Model with Resonating group method (NCSM-RGM formalism)

- Ansatz for the wavefunction:

$$|\Psi^{J^\pi T}\rangle = \sum_\nu \int dr\, r^2 \frac{g_\nu^{J^\pi T}(r)}{r} \hat{\mathcal{A}}_\nu \left|\Phi_{\nu r}^{J^\pi T}\right\rangle$$

- (A-2,2) binary cluster:

$$\left|\Phi_{\nu r}^{J^\pi T}\right\rangle = \left[\left(\left|A{-}2\,\alpha_1 I_1^{\pi_1} T_1\right\rangle \left|2\,\alpha_2 I_2^{\pi_2} T_2\right\rangle\right)^{(sT)} \times Y_\ell\left(\hat{r}_{A-2,2}\right)\right]^{(J^\pi T)} \frac{\delta\left(r - r_{A-2,2}\right)}{r r_{A-2,2}}$$

- Uncoupled SD channel states:

$$\left|A{-}2\,\alpha_1 I_1 M_1 T_1 M_{T_1}\right\rangle_{\mathrm{SD}} \left|n_a \ell_a j_a m_{j_a} \frac{1}{2} m_{t_a}\right\rangle \left|n_b \ell_b j_b m_{j_b} \frac{1}{2} m_{t_b}\right\rangle$$

'Target' nucleus

Deuteron

NCSM-RGM Formalism II

- Many-body Schrödinger equation:

$$\sum_{\nu} \int dr\, r^2 \left[\mathcal{H}^{J^\pi T}_{\nu'\nu}(r', r) - E\, \mathcal{N}^{J^\pi T}_{\nu'\nu}(r', r) \right] \frac{g^{J^\pi T}_{\nu}(r)}{r} = 0$$

$$\left\langle \Phi^{J^\pi T}_{\nu' r'} \middle| \hat{\mathcal{A}}_{\nu'} H \hat{\mathcal{A}}_{\nu} \middle| \Phi^{J^\pi T}_{\nu r} \right\rangle$$

Hamiltonian kernel

$$\left\langle \Phi^{J^\pi T}_{\nu' r'} \middle| \hat{\mathcal{A}}_{\nu'} \hat{\mathcal{A}}_{\nu} \middle| \Phi^{J^\pi T}_{\nu r} \right\rangle$$

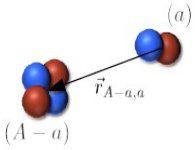
Norm kernel

- Potential part of the Hamiltonian kernel:

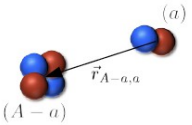
$$\mathcal{V}^{J^\pi T}_{\nu'\nu}(r', r) = \frac{1}{2} \left\langle \Phi^{J^\pi T}_{\nu' r'} \middle| \hat{\mathcal{A}}_{(A-1,1)} \hat{\mathcal{A}}_{(A-2,2)} \mathcal{V}_{\rm rel} + \mathcal{V}_{\rm rel} \hat{\mathcal{A}}_{(A-1,1)} \hat{\mathcal{A}}_{(A-2,2)} \middle| \Phi^{J^\pi T}_{\nu r} \right\rangle$$

1-body and 2-body partition intercluster antisymmetrizers enforce Pauli principle via permutation operators

Three-body density Hamiltonian kernel



$$\left\langle \Phi^{J^\pi T}_{k'_{ab}} \right| \left(V_{A,A-4} \hat{P}_{A-2,A-1} \hat{P}_{A-3,A} \right) \left| \Phi^{J^\pi T}_{k_{ab}} \right\rangle$$



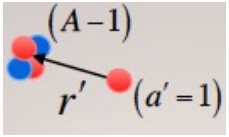
$$_{\rm SD}\langle A{-}2\alpha' | \hat{a}^\dagger_{\beta_{A-4}} \hat{a}^\dagger_a \hat{a}^\dagger_b \hat{a}_{b'} \hat{a}_{\beta'_{A-3}} \hat{a}_{\beta'_{A-4}} | A{-}2\alpha \rangle_{\rm SD} \; _a\langle \beta_{A-4}, a' | V_{A,A-4} | \beta'_{A-4} \beta'_{A-3} \rangle_a$$

Three-body density matrix

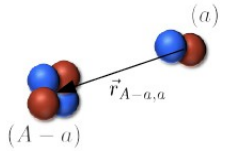
Two-body potential

- Number of three-body density matrix elements increases fast with basis size (separated calculations of them is not efficient)
- Optimized numerical algorithm: On-fly calculation of the needed three-body matrix elements for a given target nucleus (see Langhammer talk)

Coupling Hamiltonian kernel



$$\left\langle \Phi^{J^\pi T}_{k'_a} \middle| \left(V_{A-3,A-2} \hat{P}_{A-2,A} \right) \middle| \Phi^{J^\pi T}_{k_{ab}} \right\rangle$$



$$_{\mathrm{SD}}\langle A-1\alpha' | \hat{a}^\dagger_{\beta_{A-3}} \hat{a}^\dagger_b \hat{a}^\dagger_a \hat{a}_{\beta'_{A-2}} \hat{a}_{\beta'_{A-3}} | A-2\alpha \rangle_{\mathrm{SD}} \; {}_a\langle \beta_{A-3}, a' | V_{A-3,A-2} | \beta'_{A-3} \beta'_{A-2} \rangle_a$$

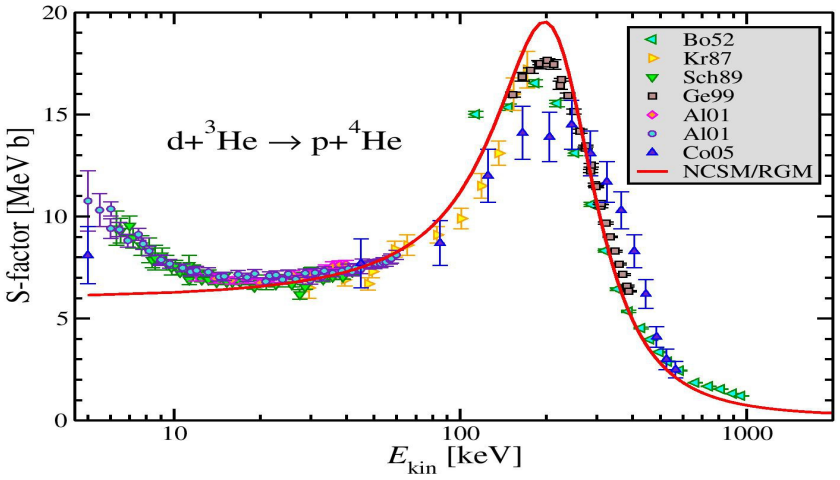
"Not-diagonal" density matrix

Two-body potential

(A-2,2) mass partition in the entrance channel
(A-1,1) mass partition in the exit channel

- Inclusion of coupling kernel describing the dominant channel in a (d,p/n) transfer reaction

Benchmark and tests



P. Navrátil, S. Quaglioni
PRL **108**, 042503 (2012)

Parallel projects:
- Explicit treatment of deuteron breakup (three-cluster formalism)
- Inclusion of the NCSMC coupling
- Inclusion of the NNN forces

- Benchmark of the new implementation with previous calculation on A=5,6 system
  - Diagonal kernels tested in (d,^{4}He) channel
  - Coupling kernels under test in ^{3}He(d,p)^{4}He reaction
- Next step: study of the transfer reaction for p-shell target nuclei (^{12}C(d,p)^{13}C, ^{7}Li(d,p)^{8}Li)

Conclusions & Perspectives

Extension of the capabilities of the NCSM-RGM for deuteron-projectile reaction:

- Inclusion of the coupling channel in the description of transfer reactions with deuteron projectile
- Implement the capability of calculation of scattering observables for p-shell nuclei (under test)

Possible perspectives:

- Extend the applications of the novel computational algorithm to other Hamiltonian kernels for heavier clusters
- Inclusion of NNN force
- Explicit treatment of three-body breakup

Nuclear Energy Density Functional

$$E\left[\rho(\mathbf{r})\right] = \frac{\hbar^2}{2m}\int d\mathbf{r}\,\tau(\mathbf{r}) + E^{int}\left[\rho(\mathbf{r})\right] - \lambda\int d\mathbf{r}\,\rho(\mathbf{r})$$

- EDF depends on the matter distribution of the nucleus
- Powerful tool in reproducing GS properties of the nuclear systems
- The existence of the EDF is predicted by a theorem (Hohenberg-Kohn theorem) but we do not know the exact form of it
- EDF is the only low-energy theory that can be applied across the entire table of nuclei
- Ground-state energy obtained through variational principle

$$E_{GS} = \mathrm{Min}_{\rho}\, E\left[\rho(\mathbf{r})\right]$$

Phenomenological nuclear EDF

- Only nucleonic degrees of freedom are explicitly included
- The connection to the strong interaction is limited to the role of symmetries in building the relevant terms of the EDF
- Coupling constants are fitted to the experimental data

Skyrme force at higher order

Skyrme force as generator of quasi-local nuclear EDF

$$E\left[\rho(\mathbf{r}),\tau(\mathbf{r}),j(\mathbf{r}),\cdots\right]=\int d\mathbf{r}\, C^{\rho}\rho(\mathbf{r})^2+C^{\tau}\rho(\mathbf{r})\tau(\mathbf{r})+C^{j}j(\mathbf{r})^2+\cdots$$

- Bilinear terms composed by local densities (equipped with coupling constants)
- Order of each term given by the number of derivatives (up to NLO)

The two-body term of the Skyrme interaction

$$\begin{aligned}t(\mathbf{k}',\mathbf{k}) &= t_0(1+x_0P^{\sigma})+\tfrac{1}{2}t_1(1+x_1P^{\sigma})(\mathbf{k}'^2+\mathbf{k}^2)\\ &+ t_2[1+x_2(P^{\sigma}-\tfrac{4}{5})]\mathbf{k}'\cdot\mathbf{k}\\ &+ \tfrac{1}{2}T[\boldsymbol{\sigma}_1\cdot\mathbf{k}\boldsymbol{\sigma}_2\cdot\mathbf{k}-\tfrac{1}{3}\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2\mathbf{k}^2+\text{conj.}]\\ &+ \tfrac{1}{2}U[\boldsymbol{\sigma}_1\cdot\mathbf{k}'\boldsymbol{\sigma}_2\cdot\mathbf{k}-\tfrac{1}{3}\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2\mathbf{k}'\cdot\mathbf{k}+\text{conj.}]\\ &+ V[i(\boldsymbol{\sigma}_1+\boldsymbol{\sigma}_2)\cdot\mathbf{k}'\times\mathbf{k}],\end{aligned}$$

- Expansion in relative momenta of a finite-range interaction (low-momentum range)
- Consistent with the symmetries of the nucleon-nucleon interaction
- Contact force (easier calculation) fitted to experimental data

Extended Skyrme interaction: higher-order pseudopotential

$$\hat{V} = \sum_{\substack{\tilde{n}'\tilde{L}', \\ \tilde{n}\tilde{L}, v_{12}S}} C^{\tilde{n}'\tilde{L}'}_{\tilde{n}\tilde{L}, v_{12}S} \hat{V}^{\tilde{n}'\tilde{L}'}_{\tilde{n}\tilde{L}, v_{12}S}$$

strength parameter corresponding to the term of the pseudopotential

$$\hat{V}^{\tilde{n}'\tilde{L}'}_{\tilde{n}\tilde{L}, v_{12}S} = \frac{1}{2} i^{v_{12}} \left([[K'_{\tilde{n}'\tilde{L}'} K_{\tilde{n}\tilde{L}}]_S S_{v_{12}S}]_0 + (-1)^{v_{12}+S} [[K'_{\tilde{n}\tilde{L}} K_{\tilde{n}'\tilde{L}'}]_S S_{v_{12}S}]_0 \right)$$

$$\times \left(1 - \hat{P}^M \hat{P}^\sigma \hat{P}^\tau \right) \hat{\delta}_{12}(r'_1 r'_2; r_1 r_2)$$

- Locality and zero-range character ensured by the Dirac delta function
- Exchange term explicitely embedded in the pseudopotential
- Terms up to next-to-next-to-next-to-leading order (N^3LO)
- (Skyrme interaction corresponds to a NLO expansion)

TRIUMF

Derivation of EDF from the pseudopotential

The EDF is obtained by averaging the pseudopotential over the Slater determinant

$$\langle C^{\tilde{n}'\tilde{L}'}_{\tilde{n}\tilde{L},v_{12}S}\hat{V}^{\tilde{n}'\tilde{L}'}_{\tilde{n}\tilde{L},v_{12}S}\rangle = \sum C_\alpha T_\alpha \equiv \int d\mathbf{r}\mathcal{H}[\rho(\mathbf{r})]$$

Main results:

- Reduction of the free coupling constants of the functional (useful in view of the optimization procedure)
- Solution of the self-interaction problem for the functional
- Link between the validity of continuity equation and the gauge invariance of the functional

TRIUMF

Regularized pseudopotential

$$\delta(r) = \lim_{a\to 0} g_a(r) = \lim_{a\to 0} \frac{e^{-\frac{r^2}{a^2}}}{(a\sqrt{\pi})^3}$$

The expansion scale a is introduced

Central two-body regularized pseudopotential

$$V(r_1', r_2'; r_1, r_2) = \sum_{i=1}^{4} \hat{P}_i \hat{O}_i(k, k') \delta(r_1' - r_1) \delta(r_2' - r_2) g_a(r_1 - r_2)$$

Skyrme-like interaction

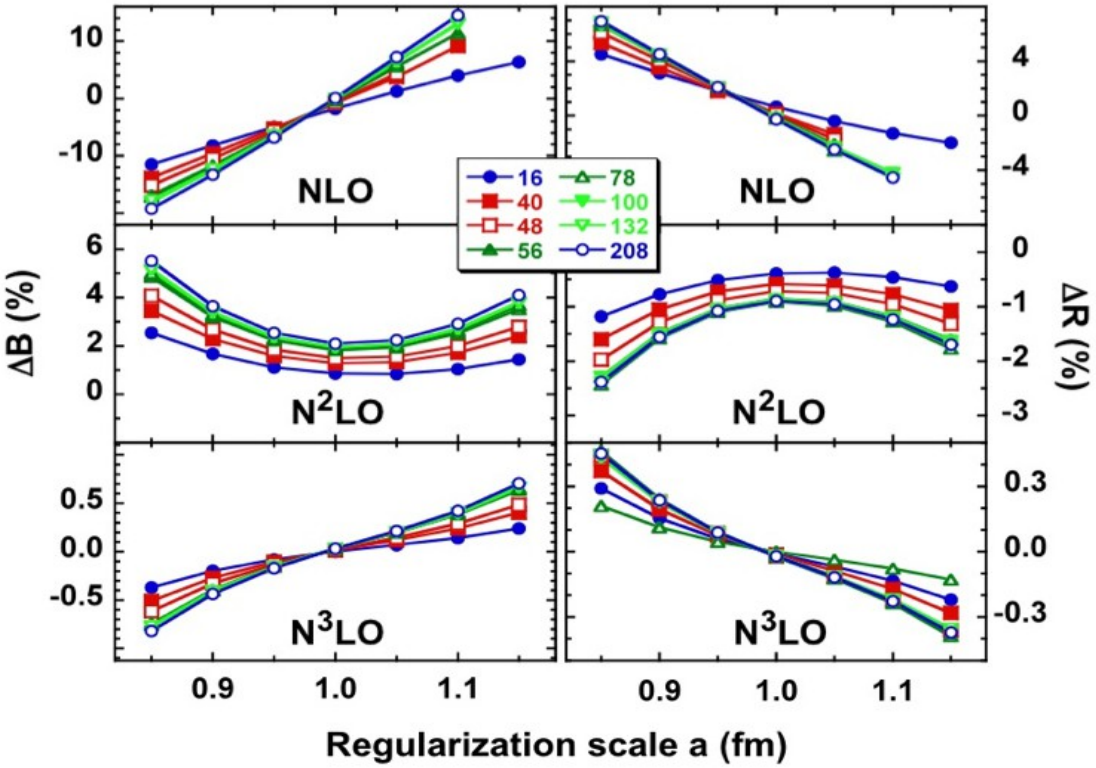
Gogny-like interaction

Local central two-body regularized pseudopotential

$$V(r) = \sum_{i=1}^{4} \hat{P}_i \hat{O}_i(k) g_a(r) = \sum_{i=1}^{4} \hat{P}_i \sum_{n=0}^{n_{\max}} V_{2n}^{(i)} \Delta^n g_a(r)$$

Self-consistent mean field calculation

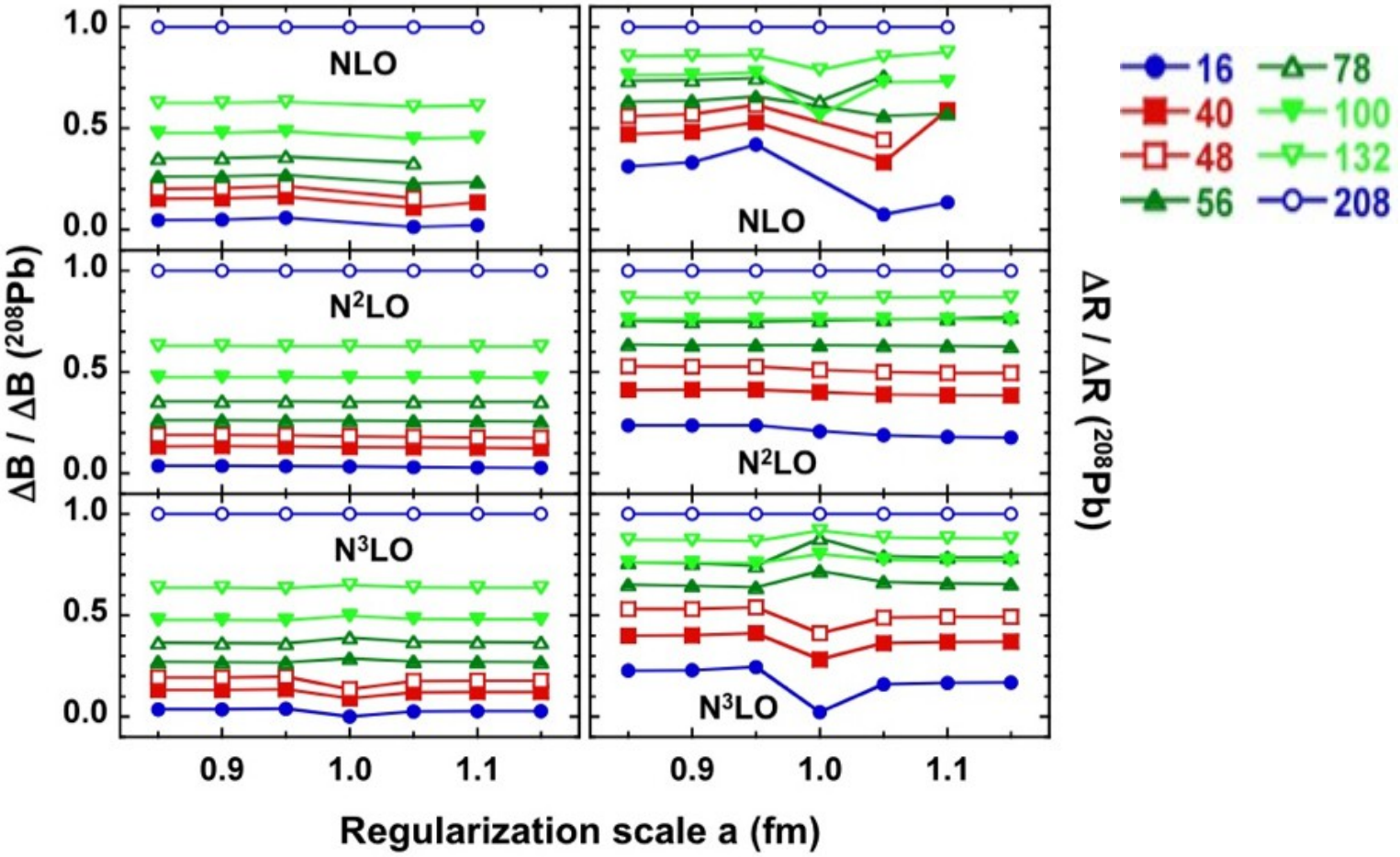
Eight doubly magic nuclei: ^{16}O, ^{40}Ca, ^{48}Ca, ^{56}Ni, ^{78}Ni, ^{100}Sn, ^{132}Sn and ^{208}Pb



Deviations of binding energies and radii relative to Gogny interaction results

- Convergence very rapid: decreasing by about a factor of four at each order
- Deviations below 1% at N^{3}LO

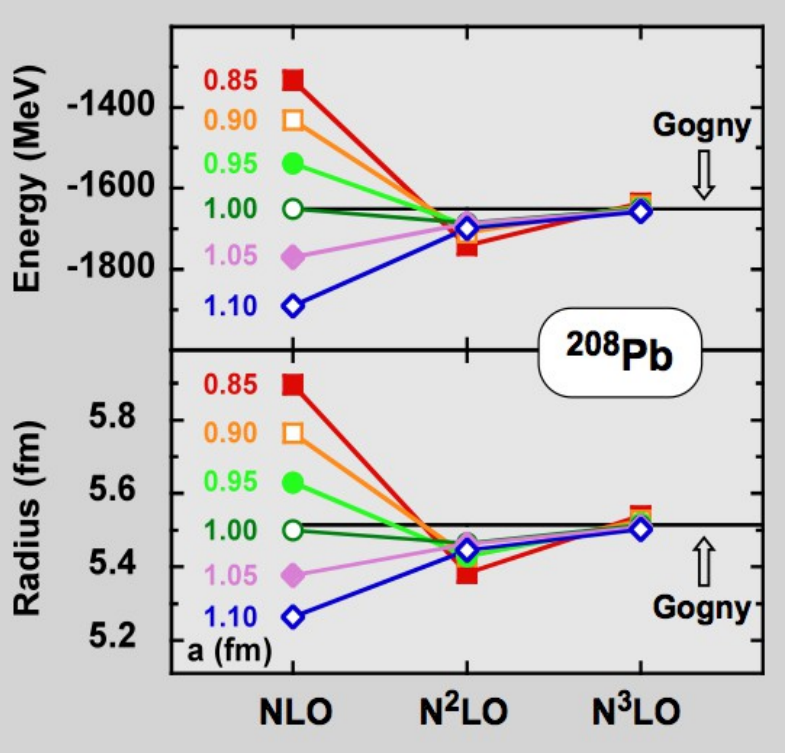
Independence of the regularization scale



Deviations of binding energies and radii relative to ^{208}Pb

- The flatness of lines shows a good degree of independence of the regularization scale

Convergence of the expansion (^{208}Pb)



Same properties of convergence and independence from scale for all nuclei calculated

- At N^{2}LO the independence with respect to the scale is reached
- At N^{3}LO the convergence of the energy and radius are reached

Higher-order finite-range pseudopotential

$$\hat{V} = \sum_{\substack{\tilde{n}'\tilde{L}',\tilde{t} \\ \tilde{n}\tilde{L},v_{12}\tilde{S}}} C^{\tilde{n}'\tilde{L}',\tilde{t}}_{\tilde{n}\tilde{L},v_{12}\tilde{S}} \hat{V}^{\tilde{n}'\tilde{L}',\tilde{t}}_{\tilde{n}\tilde{L},v_{12}\tilde{S}}$$

$C^{\tilde{n}'\tilde{L}',\tilde{t}}_{\tilde{n}\tilde{L},v_{12}\tilde{S}}$: strength parameter corresponding to the term of the pseudopotential

$$\hat{V}^{\tilde{n}'\tilde{L}',\tilde{t}}_{\tilde{n}\tilde{L},v_{12}S} = \frac{1}{2} i^{v_{12}} \left([[K'_{\tilde{n}'\tilde{L}'} K_{\tilde{n}\tilde{L}}]_S S_{v_{12}S}]_0 + (-1)^{v_{12}+S} [[K'_{\tilde{n}\tilde{L}} K_{\tilde{n}'\tilde{L}'}]_S S_{v_{12}S}]_0 \right)$$

$$\times \left(\hat{P}^\tau \right)^{\tilde{t}} \left(1 - \hat{P}^M \hat{P}^\sigma \hat{P}^\tau \right) \delta(r'_1 - r_1) \delta(r_2 - r_2) g_a(r)$$

- 100 terms up to N^{3}LO of central, spin-orbit, tensor parts of the pseudopotential
- At second order, 14 pseudopotential terms derived in both cartesian and spherical tensor formalism
- 1272 (for each isospin channel...) terms of the N^{3}LO nonlocal EDF derived from the finite-range pseudopotential
- At second order, 36 EDF terms derived in both cartesian and spherical tensor formalism

Conclusions & Perspectives

Study of both local and nonlocal higher-order EDFs:

- Relation of the functional to the N^3LO pseudopotential and reduction of the free coupling constants of the functional (useful in view of the optimization procedure)
- Solution of the self-interaction problem for the functional
- Application of the effective-theory principles to low-energy nuclear theory
- EOS in nuclear matter with preliminary parametrization (not covered in this talk)

Perspectives:

- Fitting of the higher-order EDFs
- Inclusion of finite-range NNN (at LO) phenomenological pseudopotential