Non-Empirical Pairing Functional

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Outline

Introduction : Non-empirical Energy Density Functional

- EDF: only general method applicable to the heavier nuclei
- ✘ Empirical in nature: limited to observables used for fitting
- ➡ Long-term goal: build a nuclear EDF (partly) from first principles

- Pairing part
  - ✘ Parameters hard to constrain (esp. isovector dependence)
  - ✔ Dominated by $^1S_0$ channel at low density
  - ➡ Starting point: use perturbative $V_{\text{low } k}$ at first order

- Origin of superfluidity
  - Relative importance of bare $V_{\text{low } k, \text{ NN}}$?

- Assess first-order $V_{\text{low } k, \text{ NN}}$ contribution to pairing gaps by using
  - $V_{\text{low } k, \text{ NN}}$ (pp channel)
  - A Skyrme EDF with consistent $m^* = m^*_{\text{HF, INM}}$ (ph channel)

Introduction : EDF with pairing

- Starting from effective zero-range, momentum-dependent vertices :

$$\mathcal{E}[\rho,\kappa^*,\kappa] \equiv \sum_{ij} t_{ij}\,\rho_{ij} + \frac{1}{2}\sum_{ijkl} \overline{V}^{\rho\rho}_{ijkl}\,\rho_{ik}\,\rho_{jl} + \frac{1}{4}\sum_{ijkl} \overline{V}^{\kappa\kappa}_{ijkl}\,\kappa^*_{ij}\,\kappa_{kl}$$

$$\rho_{ij} = \langle\Phi|c^\dagger_j c_i|\Phi\rangle, \qquad \kappa_{ij} = \langle\Phi|c_j c_i|\Phi\rangle$$

- Bogolyubov-de Gennes equations

$$\begin{pmatrix} h-\lambda & \Delta \\ -\Delta^* & -h^*+\lambda \end{pmatrix}\begin{pmatrix} U_i \\ V_i \end{pmatrix} = E_i \begin{pmatrix} U_i \\ V_i \end{pmatrix},$$

$$h_{ij} = \frac{\delta\mathcal{E}}{\delta\rho_{ji}}, \qquad \Delta_{ij} = \frac{\delta\mathcal{E}}{\delta\kappa^*_{ij}}$$

- Quasiparticle energy $E_i = \sqrt{(h_{ii}-\lambda)^2 + \Delta^2_{i\bar{i}}}$ (i: q.p. or canonical state)

➡ Odd-mass nucleus $\sim$ 1-q.p. state: linked to odd-even mass difference

$$\Delta^{(3)}_{\rm n} = \frac{(-1)^N}{2}\left[\mathcal{E}(N-1) - 2\mathcal{E}(N) + \mathcal{E}(N+1)\right] \simeq \Delta^{\rm n}_{\rm LCS}(N) \;(N\text{odd})$$

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Introduction : "Skyrme" EDF

- Kohn-Sham-like approach : Minimize $\mathcal{E}[\rho,\kappa]$, with ρ and κ characterizing a Bogolyubov quasiparticle vacuum (BCS state) $|\Phi\rangle$.
- Form of the functional (particle-hole)
  - Integral of an energy density bilinear in ρ + "density-dependent" terms
  - Local + up to 2[nd]-order derivatives

$$\mathcal{H}_{\text{Skyrme}} = \sum_{t=0,1} \left\{ C_t^{\rho}[\rho_0]\,\rho_t^2 + C_t^{\Delta\rho}\,\rho_t\Delta\rho_t + C_t^{\tau}\,\rho_t\tau_t + \frac{1}{2}\,C_t^{J}\,\vec{J}_t^{\,2} + C_t^{\nabla\cdot J}\,\rho_t\nabla\cdot\vec{J}_t \right\}$$

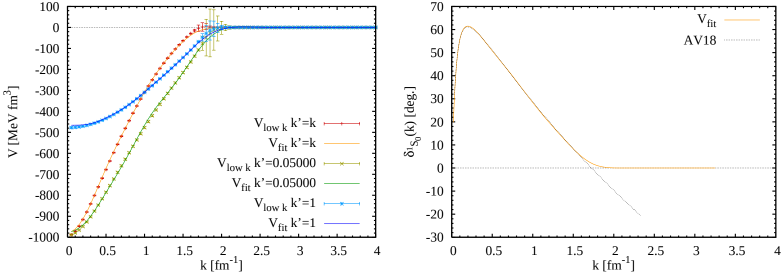
Outline

Separable representation of $V_{\text{low k}}(\Lambda) + V_{\text{Coulomb}}$

- High precision separable representation of rank n

$$V_n^{^1S_0}(k,k';\Lambda) \;=\; \sum_{\alpha=1}^{n} g_\alpha(k)\;\lambda_\alpha\;g_\alpha(k')$$

- Fit of $g_\alpha(k)$ and λ_α to $V_{\text{low k}}^{^1S_0}(k,k';\Lambda)$ and $T_{\text{low k}}^{^1S_0}(k,k';k^2;\Lambda)$
- For $\Lambda = 1.8/4.0/\text{"}\infty\text{"}\ \text{fm}^{-1}$ (rank 2/4/9) and smooth cutoff



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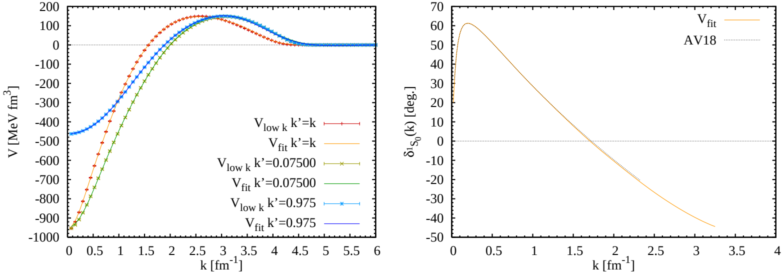

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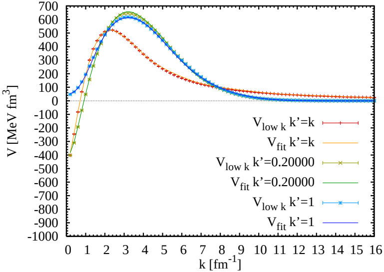

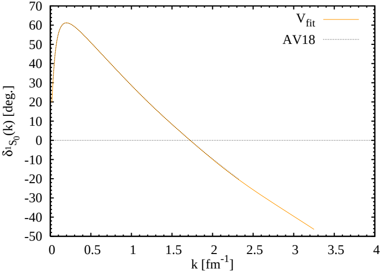

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EDF calculations in spherical nuclei

- Separable force in coordinate-space

$$\langle \mathbf{r}_1' \mathbf{r}_2' | V^{^1S_0} | \mathbf{r}_1 \mathbf{r}_2 \rangle = \sum_\alpha G_\alpha(s') \, \lambda_\alpha \, G_\alpha(s) \, \delta(\mathbf{R}' - \mathbf{R}),$$

$$\mathbf{s} = \mathbf{r}_1 - \mathbf{r}_2, \quad \mathbf{R} = (\mathbf{r}_1 + \mathbf{r}_2)/2$$

- Coordinate-space form factor $G_\alpha(s)$: Fourier transform $g_\alpha(k)$
- "Pseudo-local" pairing functional

$$E_{\text{pair}}[\kappa^*, \kappa] = \frac{1}{2} \int d^3\mathbf{R} \sum_{\alpha=1}^{n} \breve{\chi}_\alpha^*(\mathbf{R}) \, \lambda_\alpha \, \breve{\chi}_\alpha(\mathbf{R})$$

- The effective pair densities $\breve{\chi}_\alpha(\mathbf{R})$ contain the finite range/non-locality of the pairing vertex

$$\breve{\chi}_\alpha(\mathbf{R}) = \int d^3\mathbf{s} \sum_\sigma (-)^{\frac{1}{2}-\sigma} G_\alpha(s) \, \kappa\left(\mathbf{R} + \tfrac{\mathbf{s}}{2}, \sigma; \mathbf{R} - \tfrac{\mathbf{s}}{2}, -\sigma\right)$$

➡ Non-local potential and pairing field

EDF calculations in spherical nuclei (2)

- Define a reduced two-body wave function

$$\breve{\Psi}^{\alpha}_{i\hat{j}}(\mathbf{R}) = \int d^3\mathbf{s}\; G_\alpha(s)\Psi_{i\hat{j}}(\mathbf{R}+\mathbf{s}/2, \mathbf{R}-\mathbf{s}/2)$$

$$\Psi_{ij}(\mathbf{r},\mathbf{r}') = \sum_{\sigma} (-)^{s-\sigma}\phi_i(\mathbf{r},\sigma)\phi_j(\mathbf{r}',-\sigma).$$

- The ϕ_i are basis functions : the $\breve{\Psi}^{\alpha}_{i\hat{j}}(\mathbf{R})$ are computed once
- Build densities and pairing field matrix elements

$$\breve{\chi}_\alpha(\mathbf{R}) = \sum_{ij;\; i>0, j<0} \breve{\Psi}^{\alpha}_{ij}(\mathbf{R})\,\kappa_{ij}$$

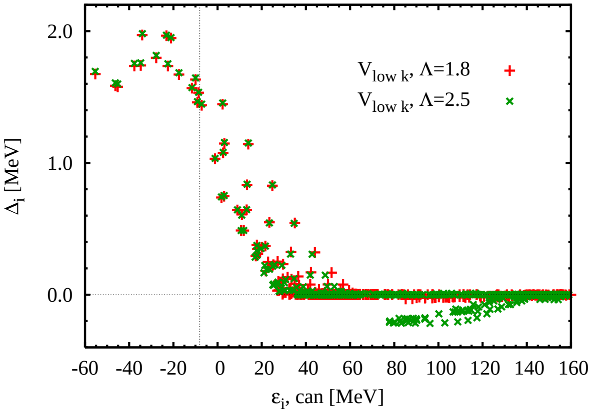
$$\Delta_\alpha(\mathbf{R}) = \frac{1}{2}\sum_{\alpha} \lambda_\alpha\,\breve{\chi}_\alpha(\mathbf{R})$$

$$\Delta_{ij} = \sum_{\alpha} \int d^3\mathbf{R}\,\breve{\Psi}^{\alpha}_{ij}(\mathbf{R})\,\Delta_\alpha(\mathbf{R})$$

- Basic tool: CoM/relative coordinate separation in spherical symmetry
  - Basis of spherical Bessel functions $j_\ell(kr)$, $k < k_{\mathrm{max}} = \Lambda + 1.0\ \mathrm{fm}^{-1}$
  - ✔ Natural representation for continuum states (→ drip line...)

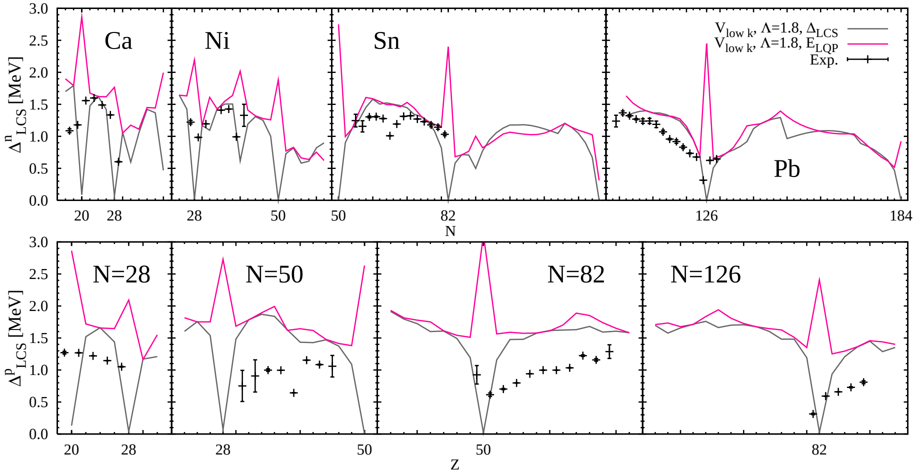
Outline

Results: State-dependent gaps (^{120}Sn)



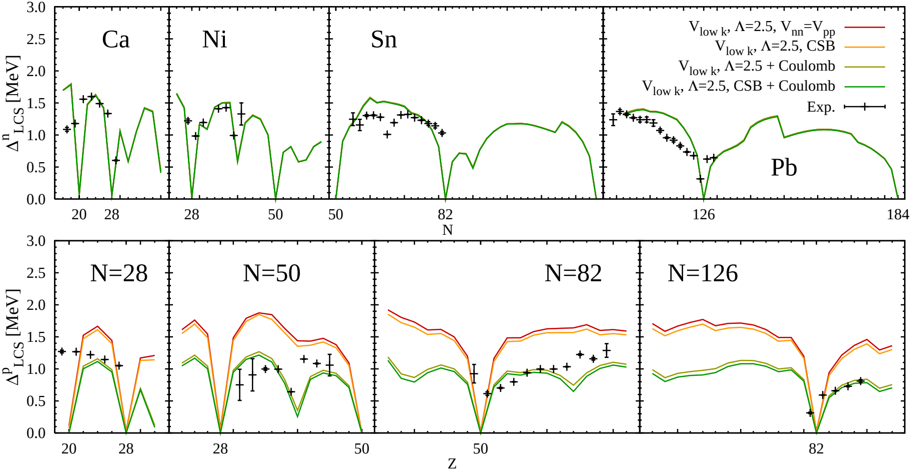
- SLy4, $m^*/m = 0.7$
- Gaps almost identical below $\varepsilon \simeq 60$ MeV
- $\Lambda = 2.5$ fm^{-1}: hint of a repulsive “core” at high energy

Results: LQP energies and LCS Gaps, no Coulomb, $V_{nn} = V_{pp}$



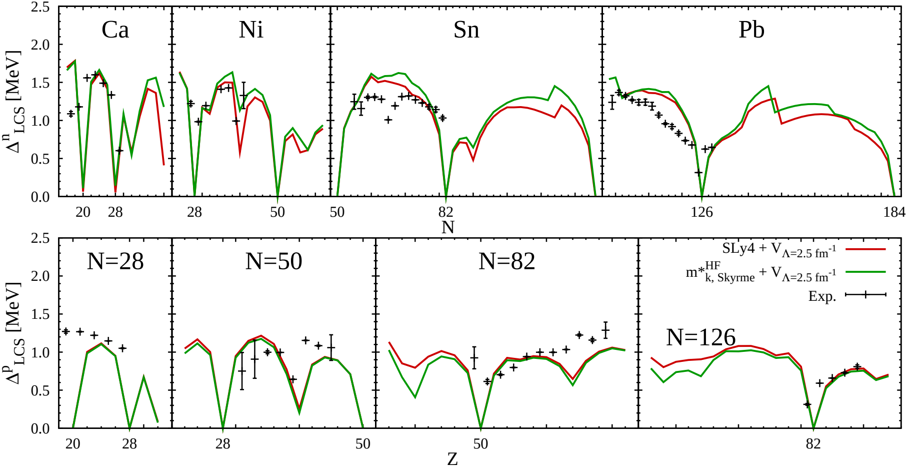
- $E_{\rm LQP}$: lowest quasiparticle energy,
  $\Delta_{\rm LCS}$: corresponding gap
- Theoretical $\Delta^n_{\rm LCS}$ close (n) or above (p) exp. $\Delta^{(3)}_{\rm odd}$ values

Results: LCS Proton gaps, CSB, Coulomb



- Coulomb decreases gaps by ∼ 30%
- V_{NN} (incl. Coulomb) at first order matches the magnitude of the gaps
- Coulomb effect consistent with Madrid group (Gogny)

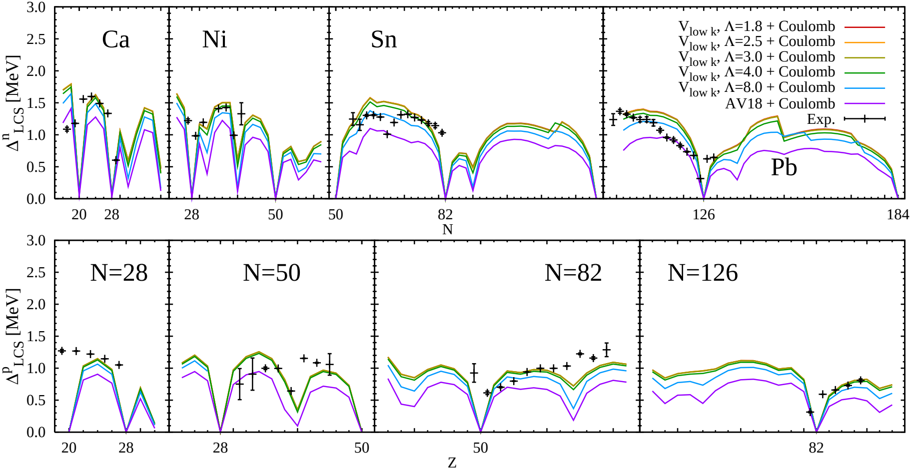
HF effective mass



Outline

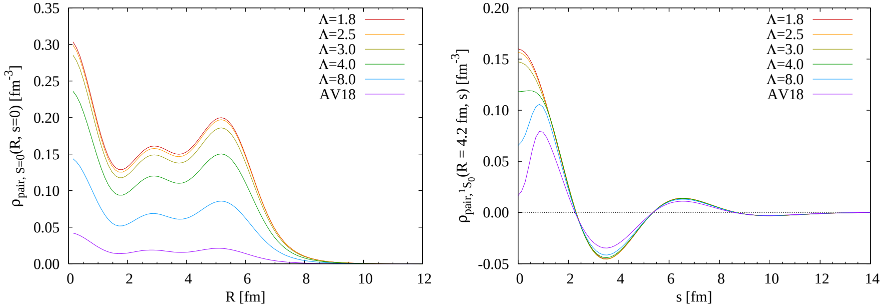
Λ-dependence: SLy4

- Milan group: SLy4 + Argonne v_{14} yields ca. 1 MeV gap in ^{120}Sn (A. Pastore et al. PRC 78 (2008) 024315)



Λ-dependence: SLy4

- Non-local pair density in ^{120}Sn
  - Short-range part Λ-dependent
  - Long-range part Λ-independent up to $\Lambda \simeq 4.0\ \mathrm{fm}^{-1}$



Some comments

- Missing in this calculation:
  - ▼ Higher partial waves
  - ▼ Three-body force
  - ▼ Two-body CoM correction (H. Hergert, R. Roth)
  - ▲ Phonon coupling
  - ▲ Coulomb screening ?
  - ▼ Blocking
- These effects seem to cancel out “near” the valley of stability
- ✘ Still valid in highly asymmetric nuclei ?
  - ➡ High isospin asymmetry ⇒ effect of NNN on proton gaps ?
  - ➡ Continuum effects beyond first order ?

- Λ-dependence: soft $\neq$ hard interactions
- Genuine disagreement likely
- Issue: effective-mass approximation (cf. Kai Hebeler yesterday)
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  - Reliable approximation with low-momentum V_{NN}
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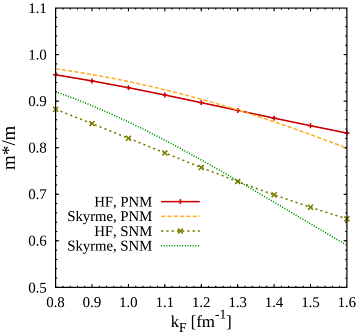
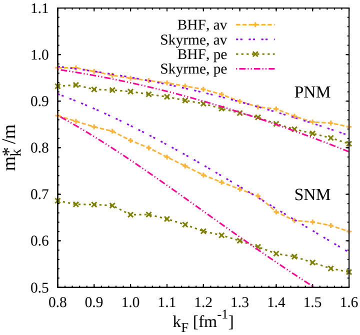
Effective-mass approximation

- Soft V_{NN}: HF m^*
- Hard V_{NN}: BHF k-mass, averaged over k or point-evaluated at k_F





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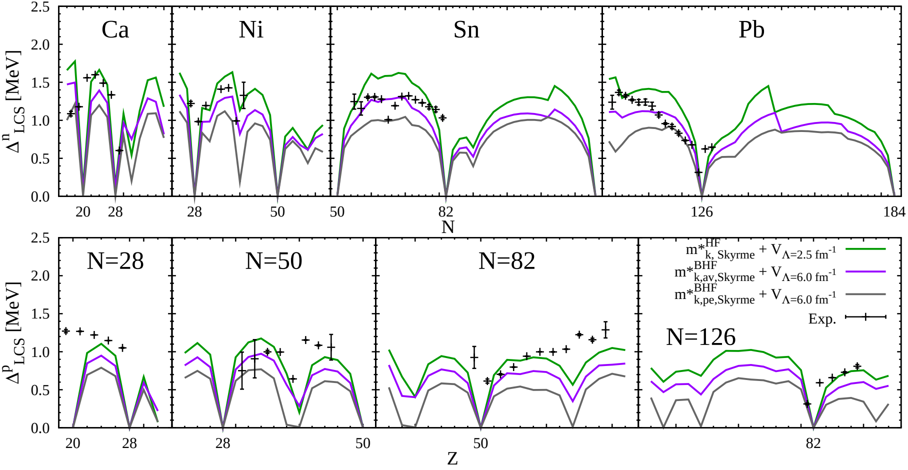
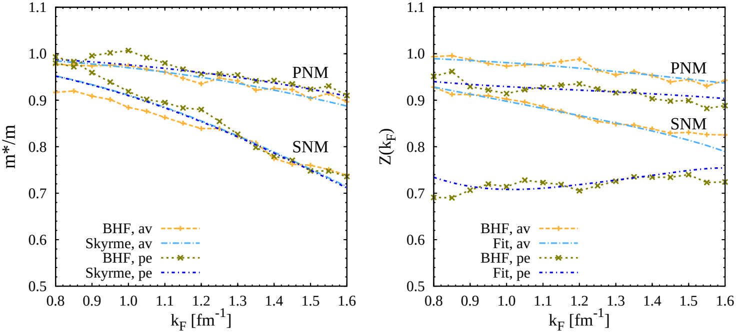


Effective-mass approximation – full self-energy

- Consistent treatment of self-energy effects: ω-dependence of $\Sigma(k,\omega)$
  - Pole approximation: $Z(k) = [1 + \partial_\omega \Sigma(k,\omega)|_{\omega=\varepsilon_k}]^{-1}$
- Soft interaction: HF m^*
- Hard interaction: BHF total m^* and $Z(k)$, averaged over k or point-evaluated



$$\hat{\Delta}(k) = \int \frac{p^2\,dp}{2\pi^2} \frac{Z(k)\,V(k,p)\,Z(p)\hat{\Delta}(p)}{2\sqrt{\varepsilon_p^2 + \hat{\Delta}(p)^2}}$$

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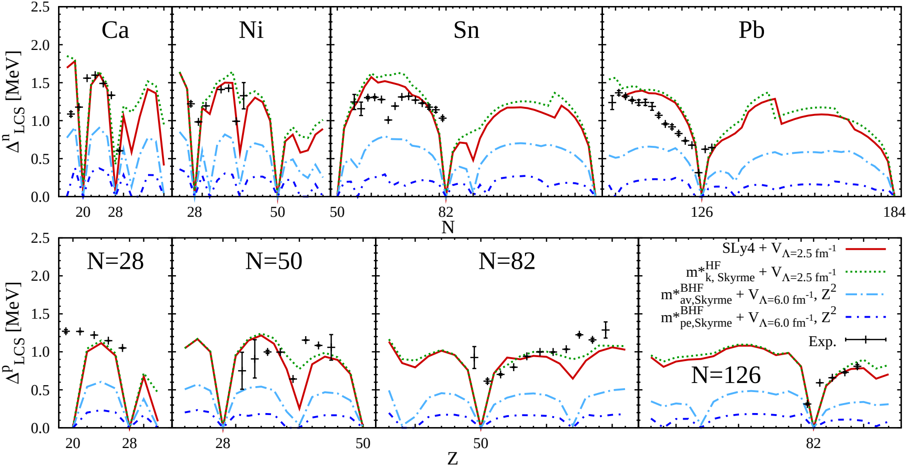


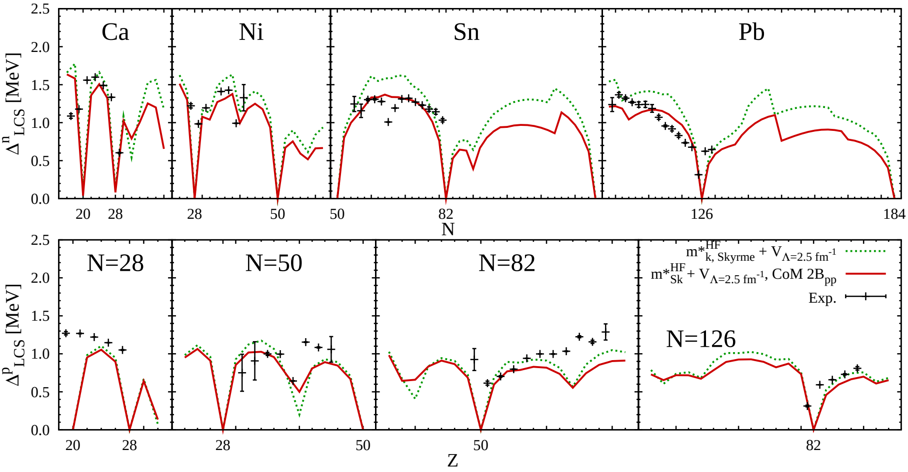
Outline

Summary and outlook

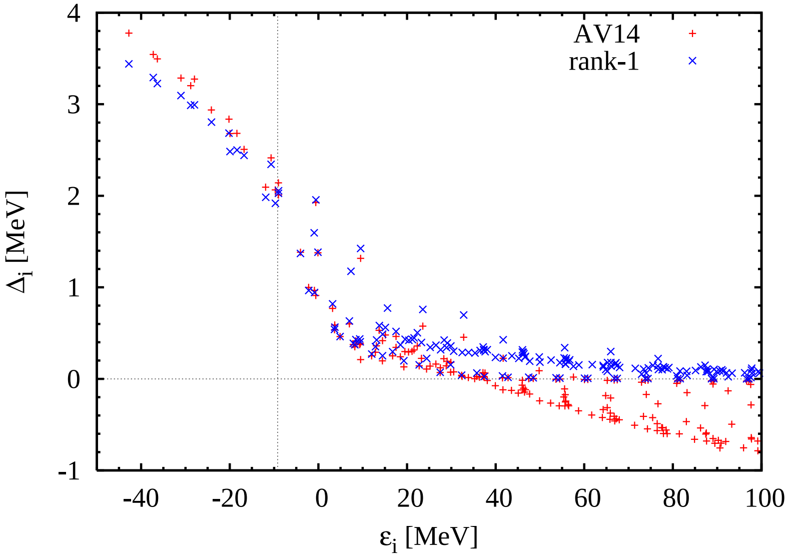
- Systematic calculation of pairing gaps in spherical nuclei
- ➡ Low-momentum NN interaction (including Coulomb potential) yields gaps of the order of exp. mass differences
  - ➡ Stong reduction of proton gaps due to Coulomb
  - ➡ Effects beyond present calculation cancel each other ?
  - Corrections at first order (NNN,CoM...) should leave room for higher orders
- Future work with separable forces
  - 3-body force, through an LDA or DME scheme (TL, K. Hebeler, A. Schwenk, T. Duguet)
  - DME: non-empirical local pairing functional (B. Gebremariam, S. Bogner, T.Duguet)
  - Other channels of the interaction ($^3P, ^1D$) to be added (S. Baroni)

Thank you !

Two-body CoM correction



$V_{\text{low } k}$ vs. Argonne



Coulomb / INM gaps