Local approximation to the pairing field

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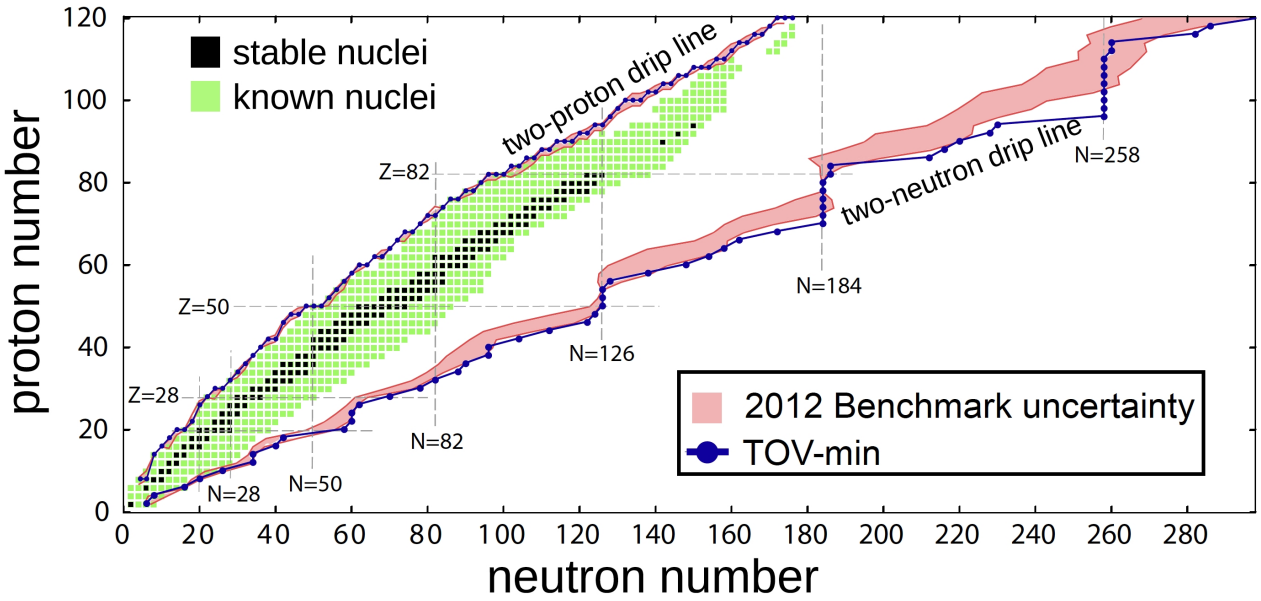
Saclay, May 2013

Introduction

New challanges for nuclear structure



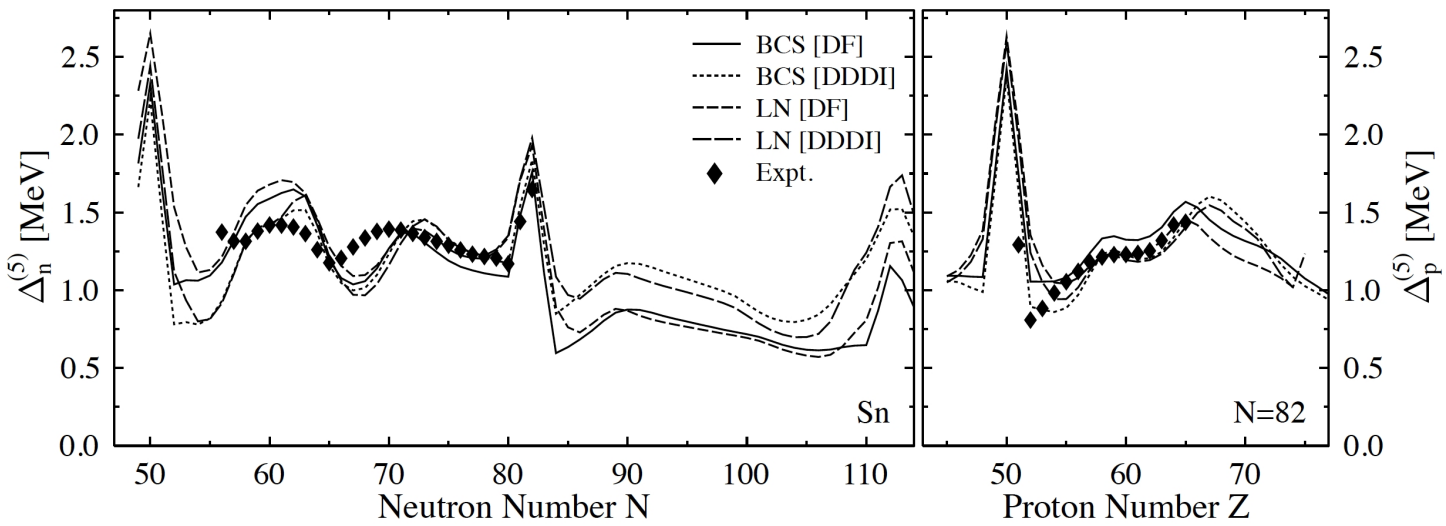
[J. Erler et al., Nature **486** 509 (2012)]

... toward exotic nuclei ...

Experimental data for $|N - Z|/A < 0.2/0.3$

Introduction

Nuclear superfluidity plays a crucial for the structure of exotic nuclei.



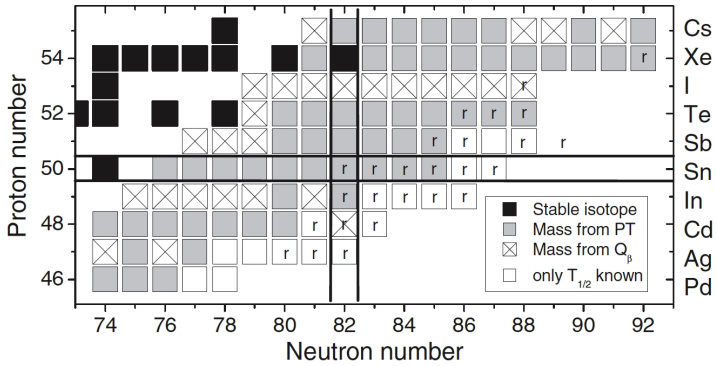
[M. Bender et al.,EPJA **8** 59-75 (2000)]

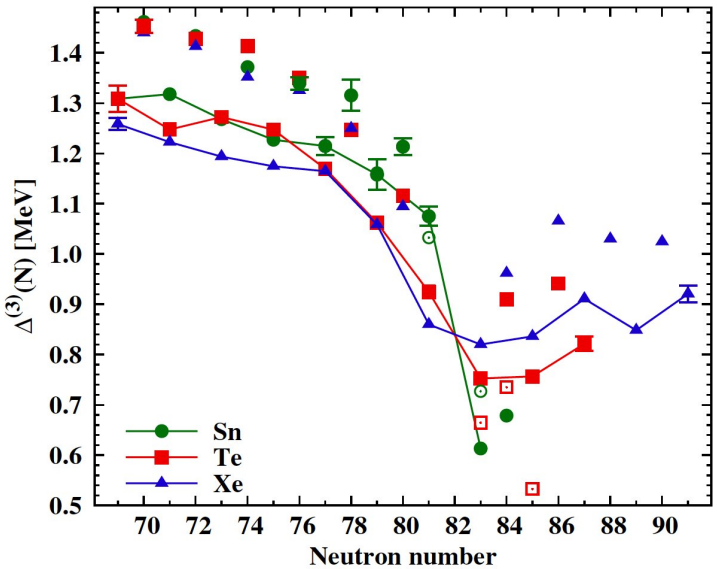
What do we know about pairing interaction?

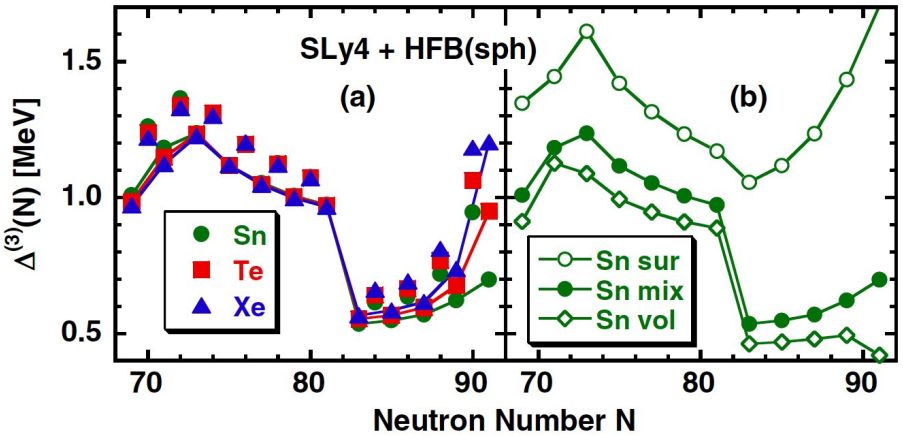
- What happens when we go to neutron rich nuclei?

Odd-even mass staggering

New mass measurements

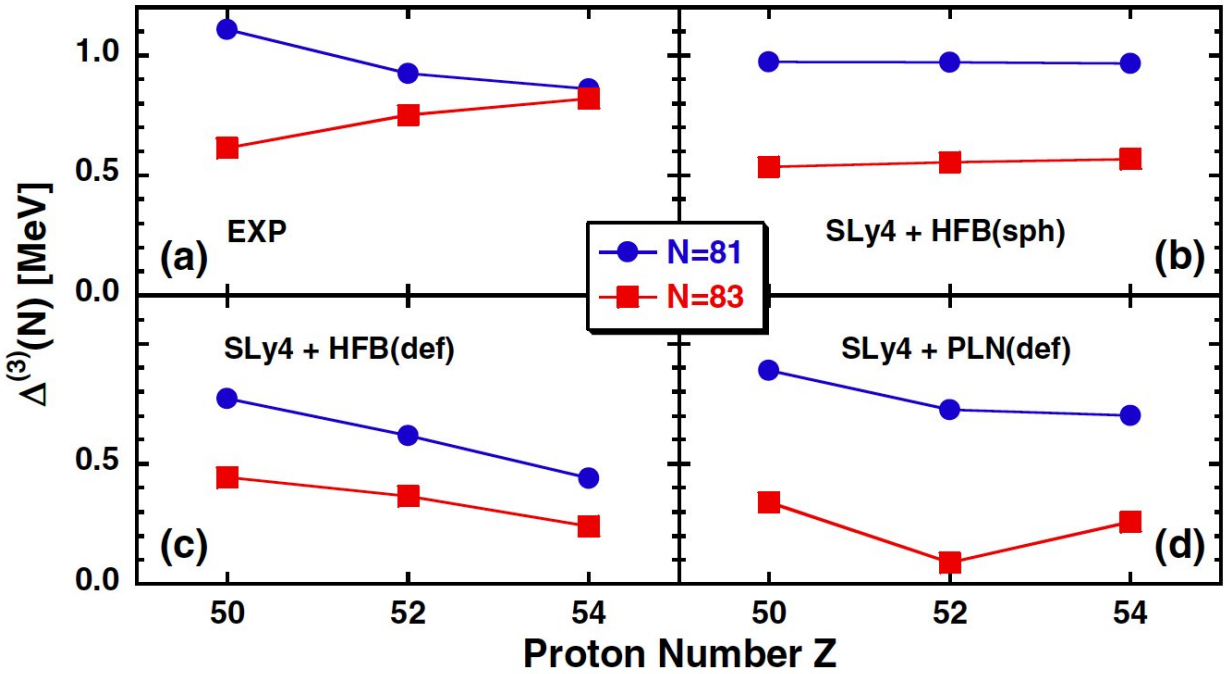






[J. Hakala et al.,PRL **109**, 032501 (2012)]

Odd-even mass staggering II



[J. Hakala et al.,PRL **109**, 032501 (2012)]

New challanges

- State of the art SR calculations are not capable to explain new data

Outline

Quantal calculation

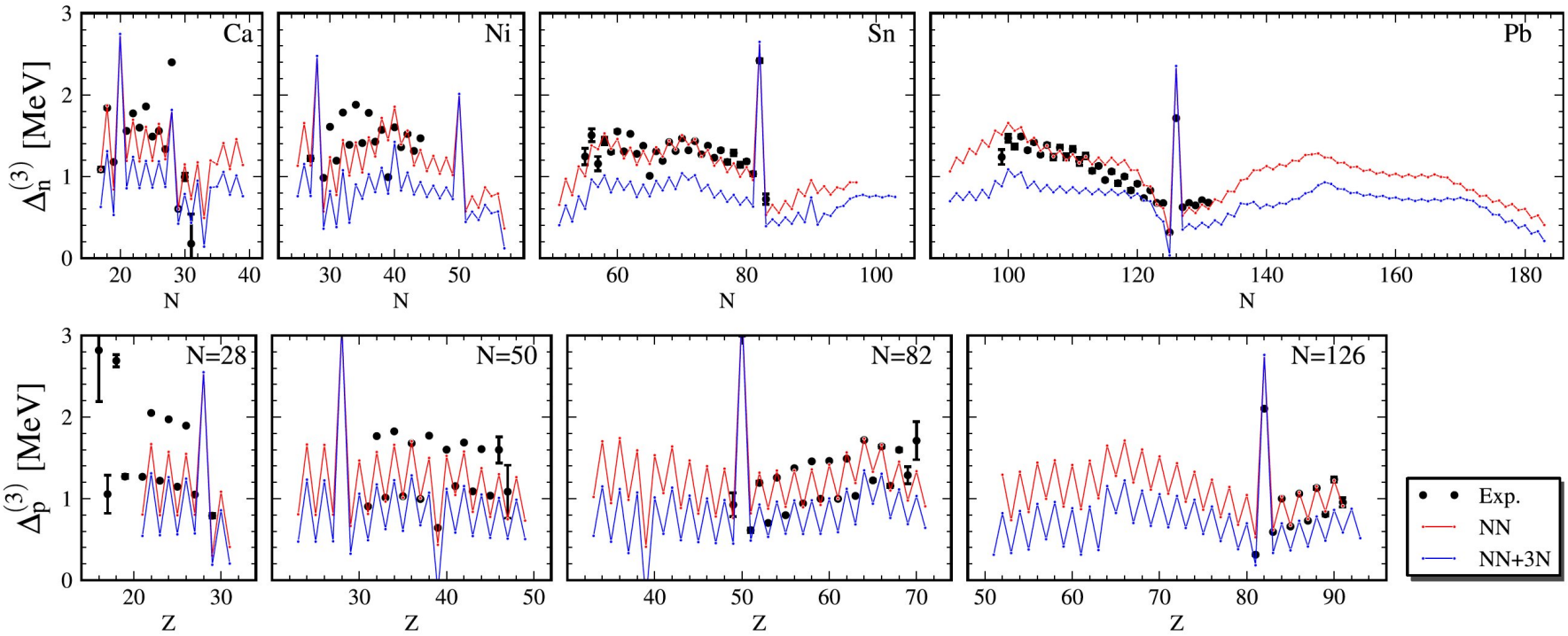
HFB in spherical symmetry

$$\sum_{n'}(h^q_{n'nlj} - e_{F,q})U^i_{n'lj} + \sum_{n'}\Delta^q_{nn'lj}V^i_{n'lj} = E^i_{lj}U^i_{nlj},$$
$$\sum_{n'}\Delta^q_{nn'lj}U^i_{n'lj} - \sum_{n'}(h^q_{n'nlj} - e_{F,q})V^i_{n'lj} = E^i_{lj}V^i_{nlj}, \quad q = p, n$$

Properties of the calculation

- Skyrme MHF in the ph channel [K. Hebeler et al., Phys. Rev. C (2009)]
- Separable rank-1 $\langle k|v^{^1S_0}|k'\rangle$ in the pp channel [T. Duguet, Phys. Rev. C (2004)]
- Box size = 24 fm , bessel basis cut off 4 fm^{-1} [T. Lesinski et al., Eur. Phys. J. A (2008)]
- ^{1}S$_0$ pairing only [S. Baroni et al. arxiv (2009), Phys. Rev C (in print)]
- Coulomb treated in pp channel [T. Lesinski et al., Eur. Phys. J. A (2008)]

Separable interactions



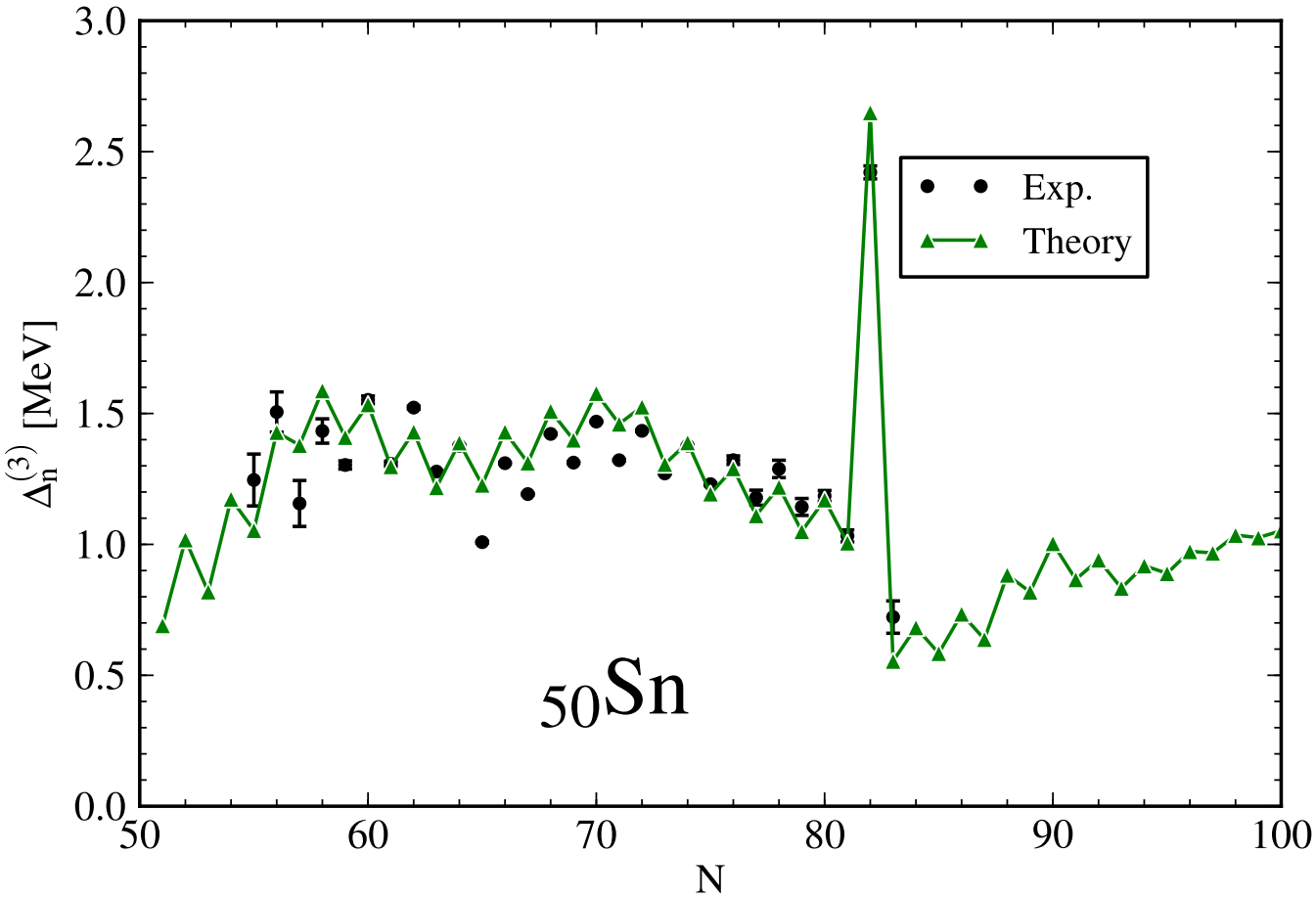
[T. Lesinski et al.,J. Phys. G **39**, 015108 (2012)]

Derived from realistic N3LO forces

No free parameters to adjust on data of atomic nuclei

Separable interactions: rank-1

- Corresponding gaps in finite nuclei (NN only)



[T. Lesinski (private)]

Outline

Introduction: part I

Scheme

	Semiclassical	Quantal
Local	$\Delta^{\mathrm{LDA}}(\vec{R})$	$\Delta^{\mathrm{LOC}}(\vec{R})$
	$\uparrow k=k_F(R)$	$\uparrow k=k_F(R)$
Non-Local	$\Delta_{\mathrm{semi}}(\vec{R},\vec{k})$	$\xleftarrow{\hbar\to 0}$ $\Delta_{\mathrm{full}}(\vec{R},\vec{k})$

1. $\Delta_{\mathrm{full}}(\vec{R},\vec{k})$ = non-local pairing field from full HFB calculation
2. $\Delta_{\mathrm{semi}}(\vec{R},\vec{k})$ = semiclassical non-local pairing field from Infinite Matter
3. $\Delta^{\mathrm{LOC}}(\vec{R})$ = local pairing field derived from Δ_{full}
4. $\Delta^{\mathrm{LDA}}(\vec{R})$ = local pairing field from Local Density Approximation

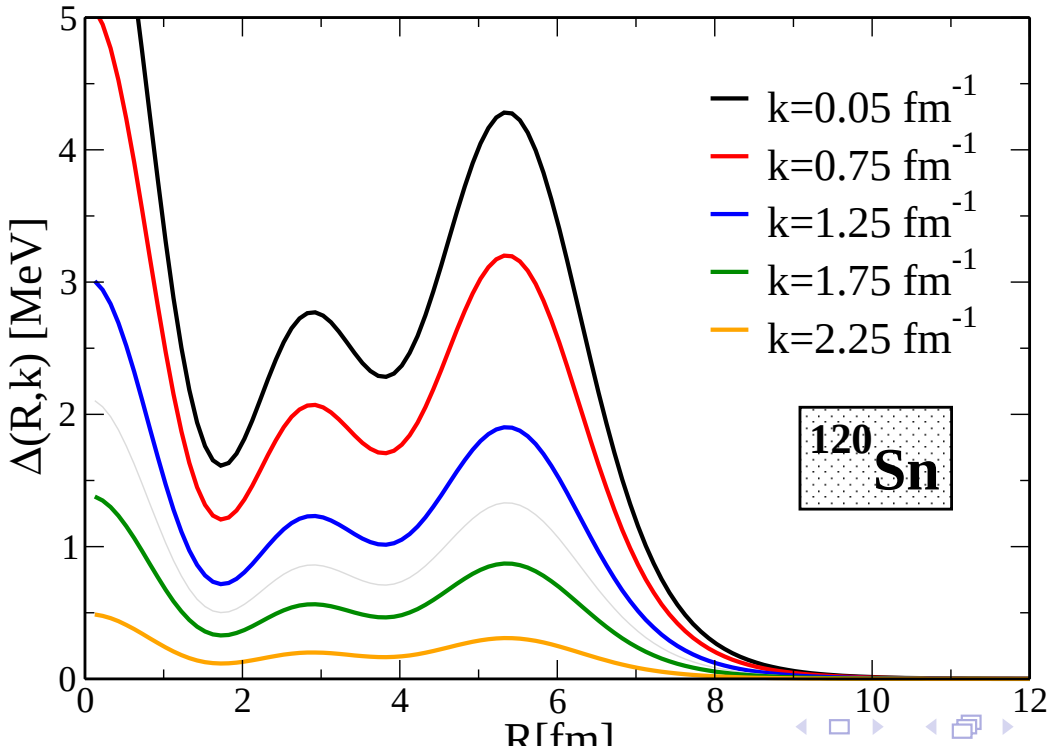
Extended Thomas-Fermi

New improved version of simple LDA [X. Viñas *et al.*, J. Phys.: Conf. Series **321**, 012024, (2011)]

Wigner transform

1. Non-local pairing field $\Delta(\vec{r}_1, \vec{r}_2)$ from HFB calculation
2. $\Delta(\vec{R}, \vec{k})$ from Wigner transform

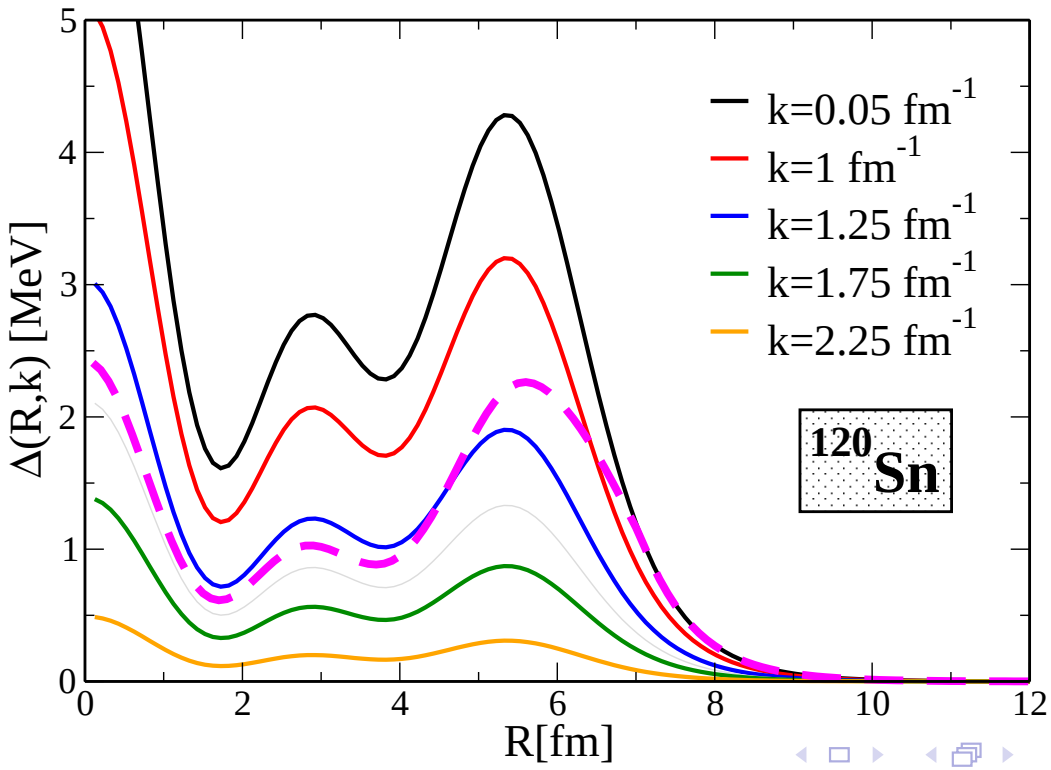
$$\Delta(\vec{R}, \vec{k}) = \frac{1}{(2\pi)^3} \int d^3 r e^{i\vec{k}\cdot\vec{r}} \Delta(\vec{R}, \vec{r}).$$



Local approximation to the pairing field

1) Local pairing field

- $\hbar^2 k_F^2(R) \equiv 2m_q^*(R)(e_F - U(R))$ [A.P. et al., Phys. Rev. C (2008)]
- $\Delta^{\mathrm{LOC}}(R) \equiv \begin{cases} \Delta(R, k_F(R)) & R \leq R_t; \\ \Delta(R, k=0) & R > R_t. \end{cases}$



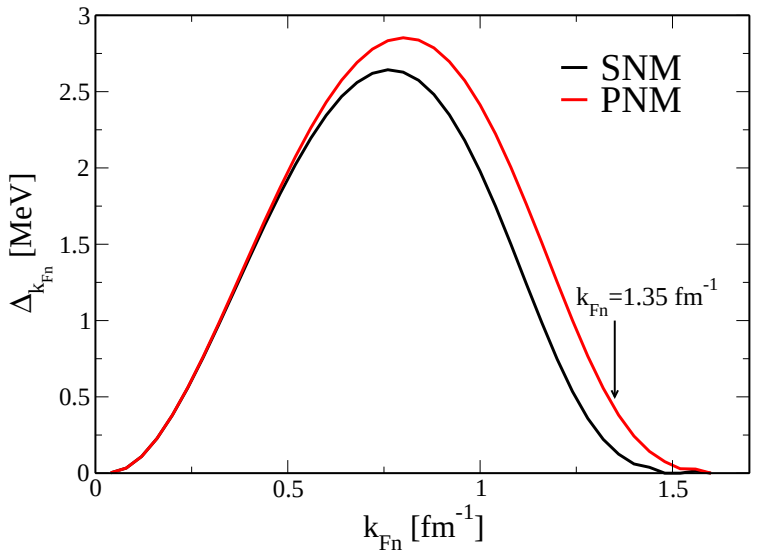
Limit $\hbar \longrightarrow 0$ (Infinite Matter with HF spectrum)

2) Thomas-Fermi limit

- Gap equation [R. Bengtsson and P. Schuck Phys. Lett. (1979)]

$$\Delta(\mathbf{R},\mathbf{k}) = \frac{1}{2}\int \frac{d^3\mathbf{k}'}{(2\pi)^3}\langle k|v^{\,^1S_0}|k'\rangle \frac{\Delta^{\text{semi}}(\mathbf{k}',\mathbf{R})}{[(k^2/2m^*(\mathbf{R}) - e_{Fn}(\mathbf{R}))^2 + \Delta^{\text{semi}}(\mathbf{k}',\mathbf{R})^2]^{1/2}}$$

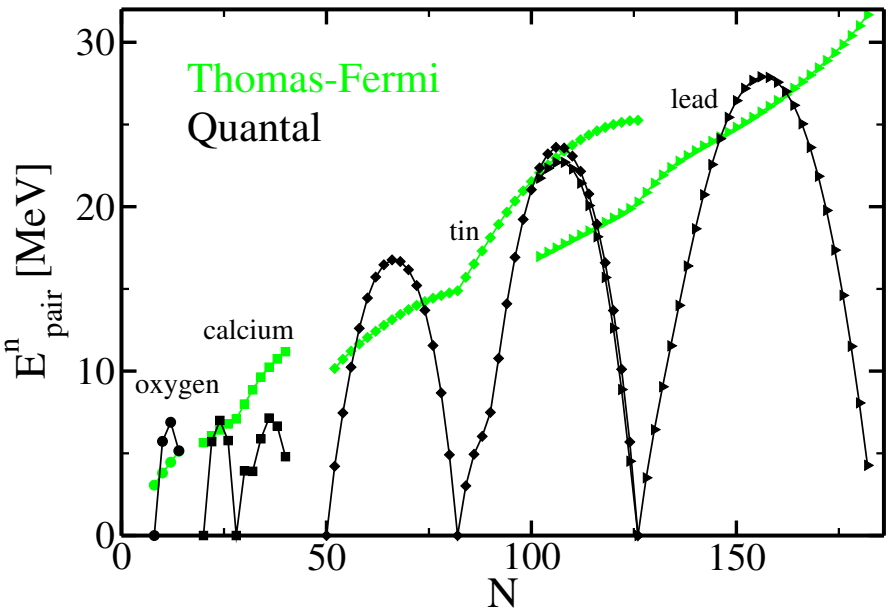
- Approximation of $m^*(R)$ at local isospin asymmetry $\beta(R) = \frac{\rho_n(R)-\rho_p(R)}{\rho_n(R)+\rho_p(R)}$



Pairing energy

Not an observable!!!

$$E_{pair} = \int \frac{d^3\mathbf{k}d^3\mathbf{R}}{(2\pi)^3}\Delta_{semi}(\mathbf{R},\mathbf{k})k(\mathbf{R},\mathbf{k}) \qquad k(\mathbf{R},\mathbf{k}) = \frac{\Delta_{semi}(\mathbf{R},\mathbf{k})}{2E_{\mathbf{R},\mathbf{k}}}$$

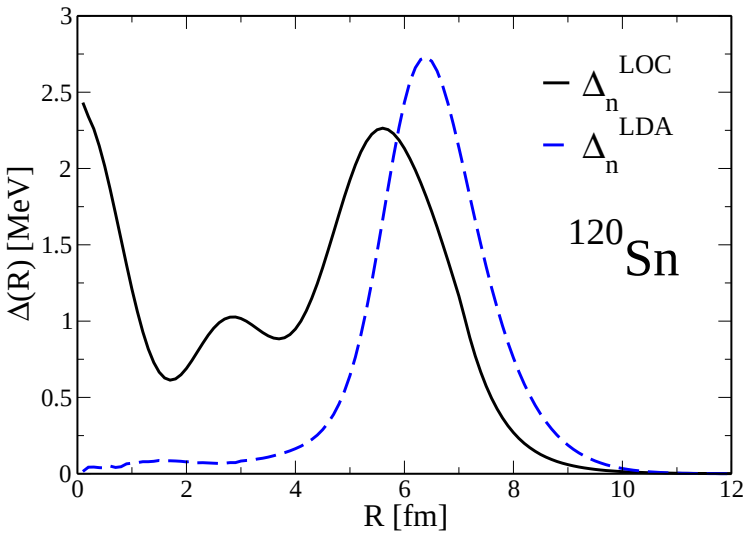


- Thomas Fermi reproduces the average quantal calculation

Local Density Approximation

local pairing field from IM

$$\Delta^{\text{LDA}}(R) = \Delta^{\text{semi}}(\vec{R}, \vec{k}_F(R))$$



- Δ^{LDA} is strongly surface peaked
- Δ^{LDA} loses quantal effects

Comparing both local approximations

Skyrme-HFB equations in position space for spherical symmetry

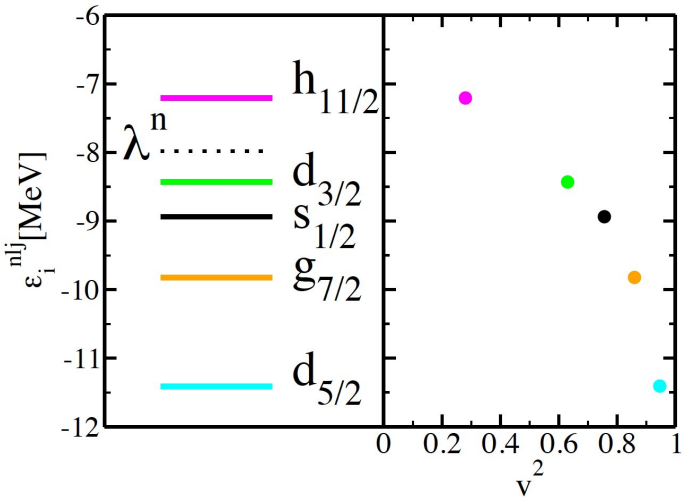
$$\left(\frac{d^2}{dR^2} - \frac{l(l+1)}{R^2} + \frac{2m^*}{\hbar^2}[e_F + E_{qp} - U(R)]\right) u_{lj}(R) + \frac{2m^*}{\hbar^2}\left(\frac{\hbar^2}{2m^*}\right)' u'_{lj}(R) - \frac{2m^*}{\hbar^2}\Delta(R) v_{lj}(R) = 0,$$

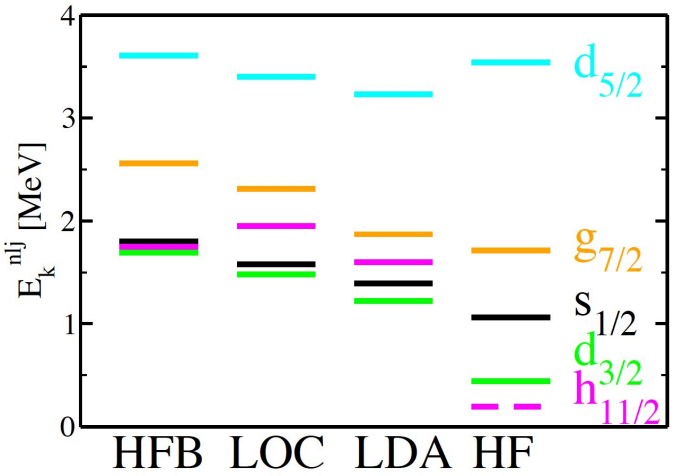
$$\left(\frac{d^2}{dR^2} - \frac{l(l+1)}{R^2} + \frac{2m^*}{\hbar^2}[e_F - E_{qp} - U(R)]\right) v_{lj}(R) + \frac{2m^*}{\hbar^2}\left(\frac{\hbar^2}{2m^*}\right)' v'_{lj}(R) + \frac{2m^*}{\hbar^2}\Delta(R) u_{lj}(R) = 0.$$

Solve using

1. HFBRAD [K. Bennaceur and J. Dobaczewski, Comp. Phys. Comm. (2005)]
2. Fixed ph potential form full HFB calculation
3. Insert $\Delta^{\text{LDA}}(R)$ or $\Delta^{\text{LOC}}(R)$ as pairing field
4. Particle number fixed using the same box and same mesh

Quasi particle spectrum ^{120}Sn





		full		LOC		LDA	
l	$2j$	E_{qp}[MeV]	v^2	E_{qp}[MeV]	v^2	E_{qp}[MeV]	v^2
2	3	1.692	0.631	1.483	0.597	1.229	0.601
5	11	1.750	0.280	1.951	0.265	1.591	0.199
0	1	1.800	0.757	1.591	0.744	1.398	0.767
4	7	2.560	0.859	2.315	0.866	1.894	0.933

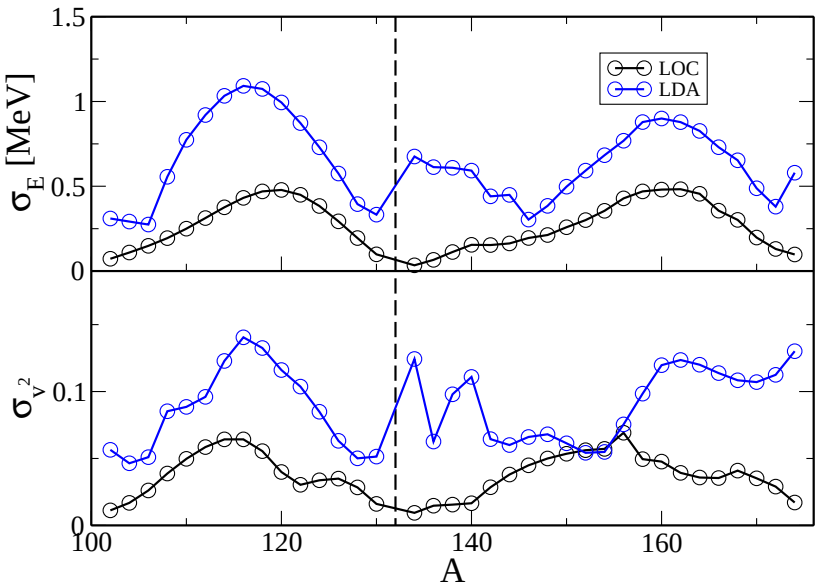
- LOC gives better description then LDA
- Both modify the pattern of quasi particle spectrum

Spectra

Systematic error along tin isotopic chain

$$\sigma_E = \sqrt{\sum_{(E_{nlj}<5\text{MeV})} (E_{full} - E_x)^2}$$

$$\sigma_{v^2} = \sqrt{\sum_{(E_{nlj}<5\text{MeV})} (v^2_{full} - v^2_x)^2} \quad x = \text{LOC/LDA}$$

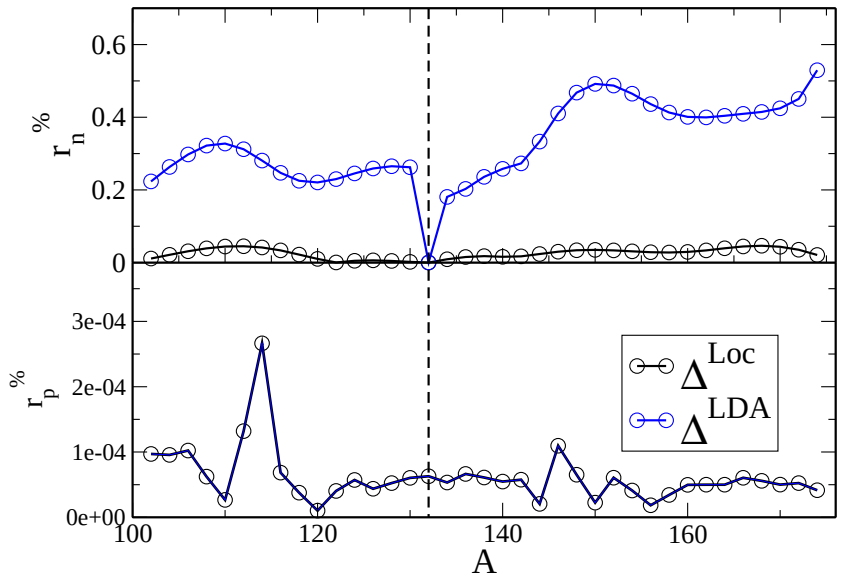


Error comparable with the intrinsic error of the theory [M. Kortelainen et al., Phys. Rev. C (2008)]

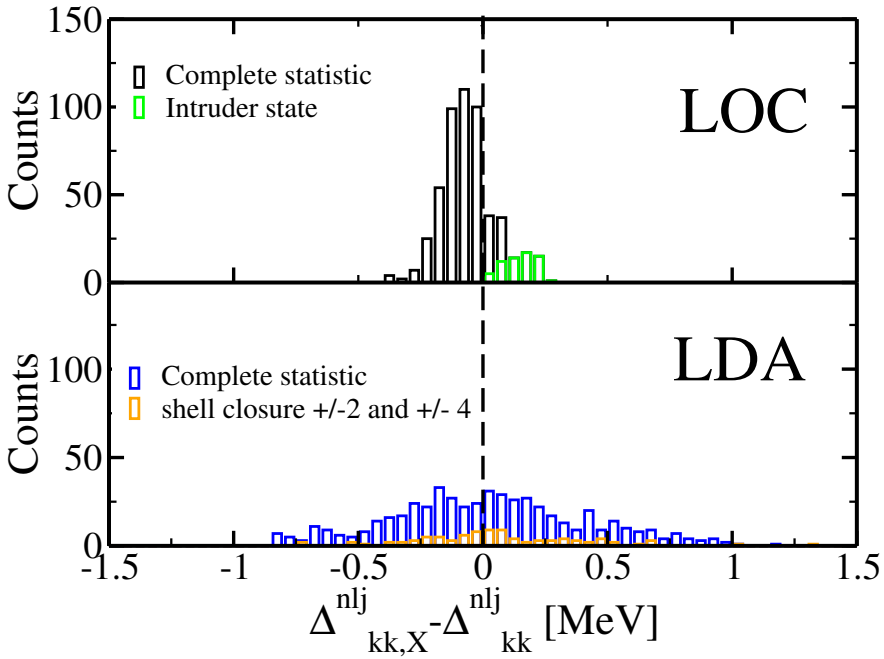
Sn chain: radii

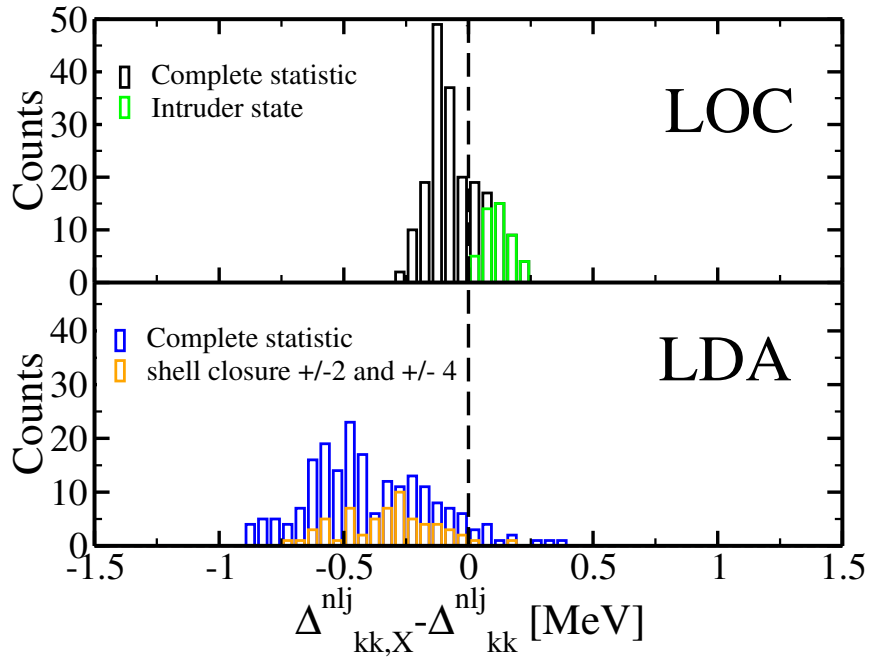
Error on the average radius

$$
\begin{aligned}
r_q &= \frac{\int dr 4\pi r^4 \rho_p(r)}{\int dr 4\pi r^2 \rho_p(r)} \\
r_q^{\%} &= \frac{|r_q^{Full} - r_q^{type}|}{r_q^{Full}} \cdot 100
\end{aligned}
$$



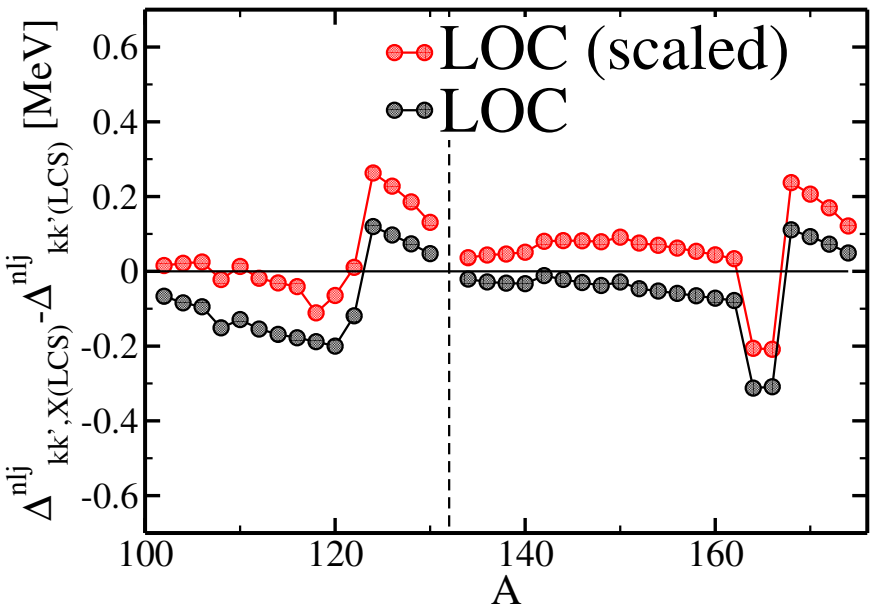
Semimagic nuclei

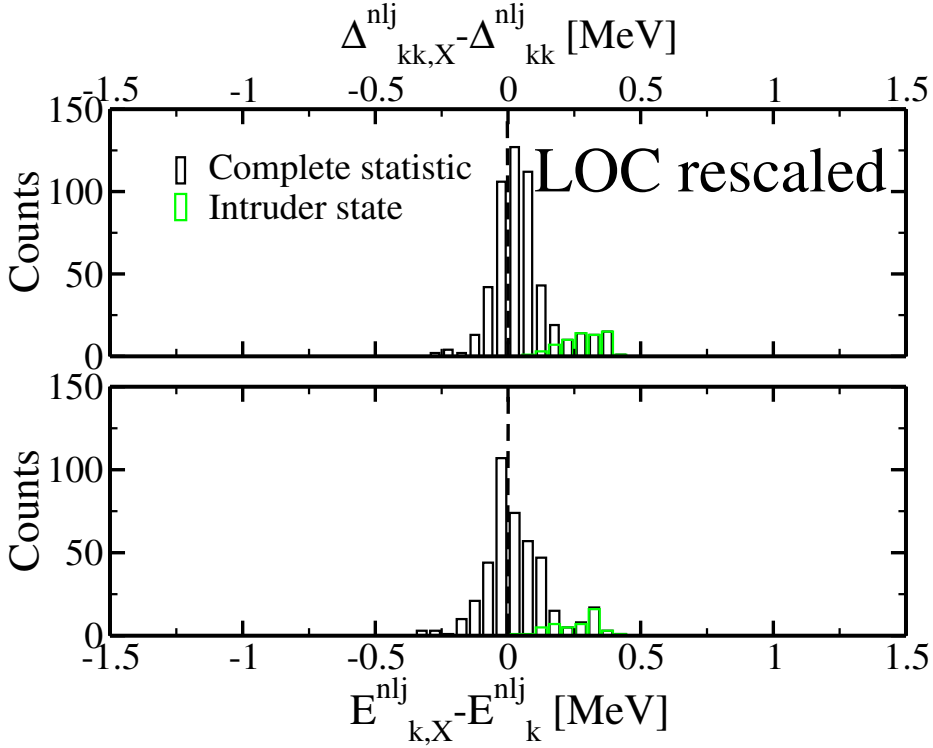




- The LDA distribution is more spread
- The LDA spread is shifted towards an underestimation for proton gaps (-500 KeV)

Semimagic nuclei





It is possible to rescale $\Delta^{\mathrm{LOC}}(R)$ to improve the average error

Outline

Non-empirical local functional

Rank-1 separable interaction in momentum space

$$v(k,k') = \mu g(k) g(k') \qquad g(k) = e^{-\alpha^2 k^2/2}$$

$$\begin{aligned}
E_{\text{pair}} &= \sum_q \frac{1}{4} \int d\vec{R} \mu_q \left| \hat{\tilde{\rho}}_q(\vec{R}) \right|^2 \\
\hat{\tilde{\rho}}_q(\vec{R}) &= -\sum_{ij}^{E_{cut}} \hat{\psi}^q_{ij}(\vec{R}) k_{ij} \\
\psi^q_{ij}(\vec{R},\vec{r}) &= \sum_\sigma 2\sigma \phi_i(\vec{R} + \frac{\vec{r}}{2}\sigma q) \phi_j(\vec{R} - \frac{\vec{r}}{2}\sigma q) \\
\hat{\psi}^q_{ij}(\vec{R}) &= \int \frac{d\vec{k}}{(2\pi)^2} g(r) \psi^q_{ij}(\vec{R},\vec{r})
\end{aligned}$$

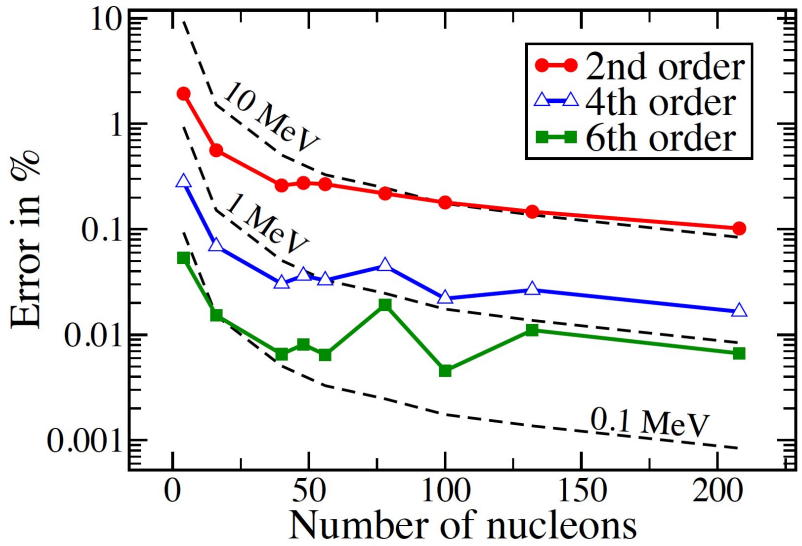
Density matrix expansion

Standard scheme

$$\rho(\mathbf{R},\mathbf{r}) = \rho(\mathbf{R}) + i r_a j_a(\mathbf{R}) + \frac{1}{2} r_a r_b \left[\frac{1}{4}\nabla_a \nabla_b \rho(\mathbf{R}) - \tau_{ab}(\mathbf{R})\right] + \ldots$$

Implicit summation over cartesian indices a, b

- To ensure $\rho(\mathbf{R},\mathbf{r}) \to 0$ for large $\mathbf{r}$ we introduce $\pi_0(r), \pi_1(r), \pi_2(r)$



[G. Carlsson et al., Phys. Rev. Lett. **105**,122501 (2010)]

Density matrix expansion

Non-standard scheme

$$\psi^q_{nn'}(\mathbf{R},\mathbf{r}) = \exp^{i\mathbf{r}\cdot\mathbf{k}} \exp^{\mathbf{r}|\nabla_{\mathbf{r}}-i\mathbf{k}|} \psi^q_{nn'}(\mathbf{R},\mathbf{r})\Big|_{\mathbf{r}=0}$$

- We consider just 0th order
- Shifted-expansion $\mathbf{k} \to \mathbf{k} + \alpha\mathbf{K}$
- No averaging functions $\pi_0(r), \pi_1(r), \pi_2(r)$

Separable interaction

$$\hat{\psi}^q_{nn'}(\mathbf{R}) \approx g([k^2_\alpha]_{nn'}(R))\ \psi^q_{nn'}(\mathbf{R},\mathbf{r})\Big|_{\mathbf{r}=0}$$

- Need to define the momentum scale
- g is the form factor of the rank-1 interaction
- Exact in infinite matter

Separable interaction II

$$[k^2_\alpha]_{nn'}(R) = \left. \frac{\psi^{q*}_{nn'}(\mathbf{R},\mathbf{r})(\mathbf{k}+\alpha\mathbf{K})^2\psi^{q}_{nn'}(\mathbf{R},\mathbf{r})}{\psi^{q^*}_{nn'}(\mathbf{R},\mathbf{r})\psi^{q}_{nn'}(\mathbf{R},\mathbf{r})} \right|_{\mathbf{r}=0}$$

so we can write

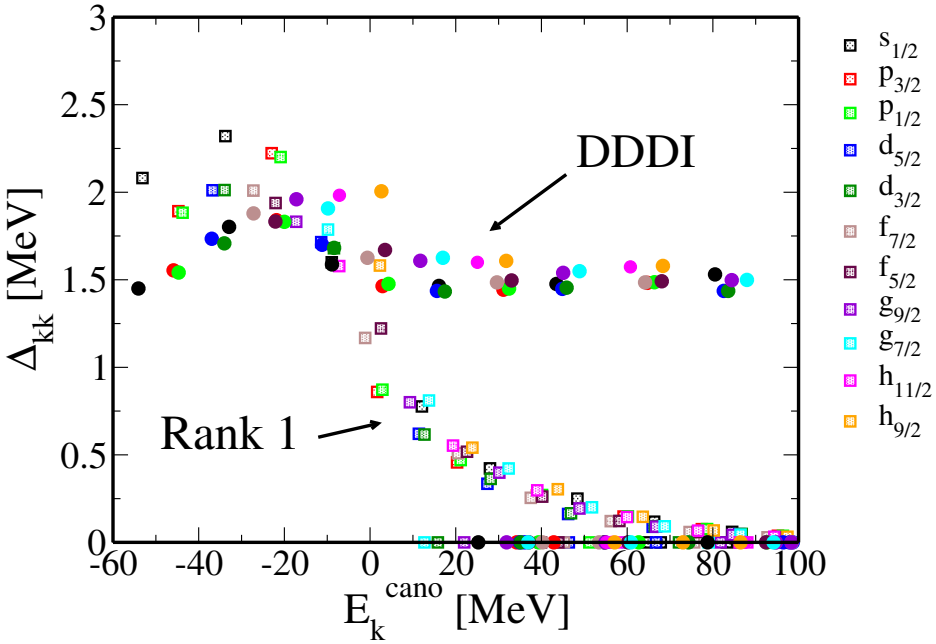
$$\tilde{\rho}^q_{loc}(\mathbf{R}) = \sum_{nn'} g([k^2_\alpha]_{nn'}(R))\psi^q_{nn'}(\mathbf{R})\kappa_{nn'}$$

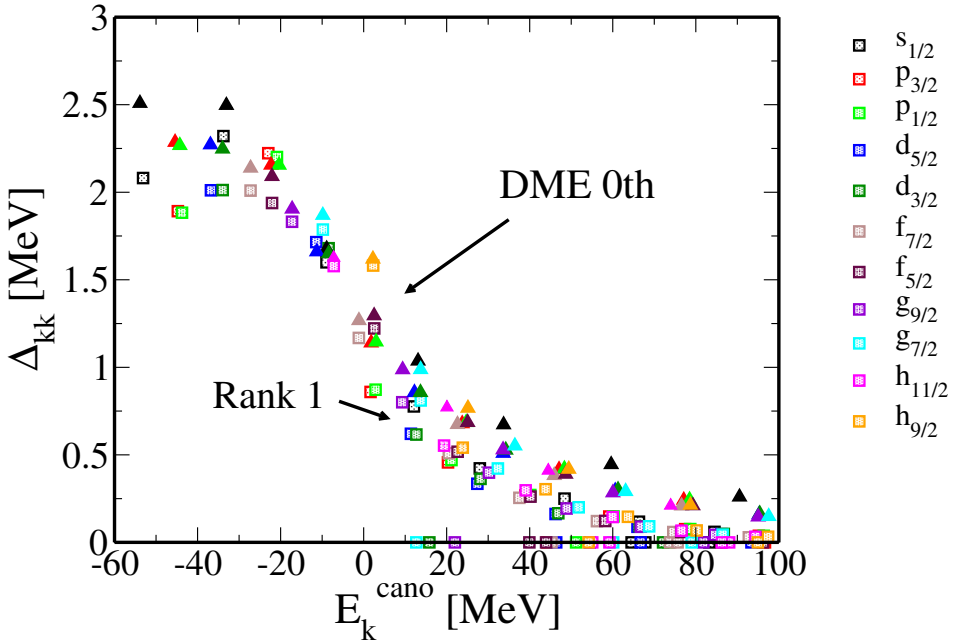
$$\Delta_{nn'}(\mathbf{R}) = -\frac{\mu}{2} g([k^2_\alpha]_{nn'}(R))\tilde{\rho}^q_{loc}(\mathbf{R})$$

No free parameters

- All the parameters come from rank-1
- The choice $\alpha = \frac{1}{2}$ guarantees $\tilde{\rho}^q_{loc}(\mathbf{R}) \to 0$ for large values of R.

Preliminary results: ^{120}Sn



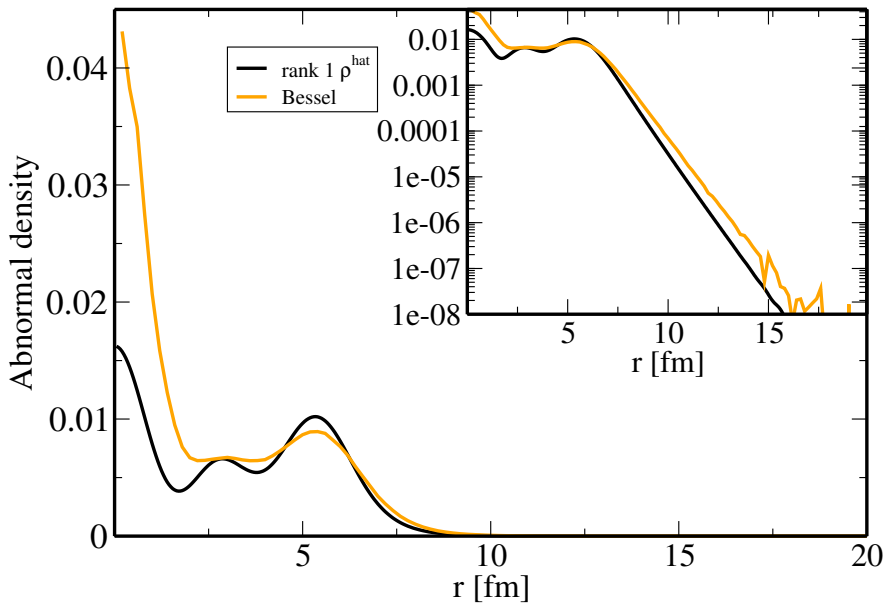


Some advantages

- The regulator $g_{ij}(k)$ improves the pattern of canonical gaps.
- DDDI is not able to reproduce the pattern (unless small pairing window)

Preliminary results: ^{120}Sn

The abnormal density takes the form



Abnormal density

- The regulator *do not work* for s-states and $R \to 0$
- Numerical problems (?) at $R \to +\infty$

Preliminary results: ^{120}Sn

Convergence (in MeV) as a function of q.p. states used in the HFB matrix

E_{qp-cut}	Δ_{LCS}	E_{tot}	E_{pair}	$\Delta_{LCS}^{\text{original}}$	$E_{tot}^{\text{original}}$	$E_{pair}^{\text{original}}$
30	1.376	-1017.250	-12.1450	1.472	-1017.552	-12.695
60	1.421	-1018.573	-15.363	1.645	-1018.820	-15.606
100	1.442	-1018.846	-15.994	1.674	-1019.041	-16.079
150	1.446	-1018.926	-16.1802	1.680	-1019.078	-16.156
250	1.446	-1018.966	-16.272	1.680	-1019.084	-16.167

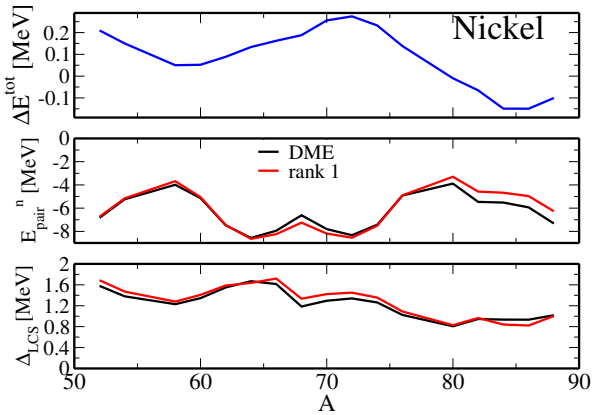
Convergence (in MeV) as a function of basis states used in the HFB matrix

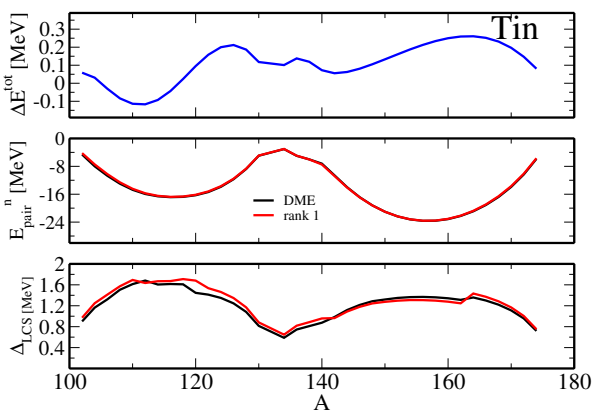
k_{max} [fm^{-1}]	Δ_{LCS}	E_{tot}	E_{pair}	$\Delta_{LCS}^{\text{original}}$	$E_{tot}^{\text{original}}$	$E_{pair}^{\text{original}}$
4	1.447	-1018.985	-16.304	1.680	-1019.081	-16.1675
5	1.447	-1018.995	-16.335	1.680	-1019.083	-16.1676
6	1.447	-1018.998	-16.346	1.680	-1019.084	-16.168
7	1.447	-1018.998	-16.348	1.680	-1019.084	-16.168

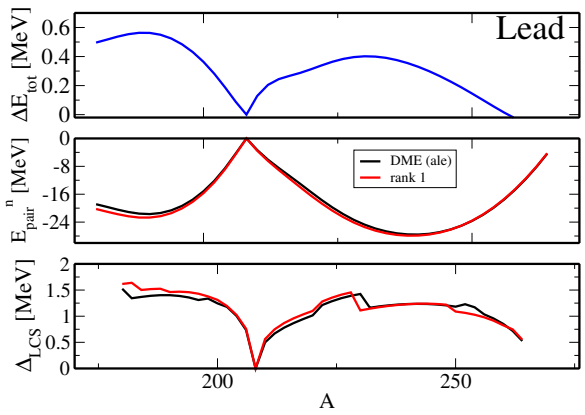
Some remarks

- The *convergence* is not too much affected by the problem with s-states.
- We can reproduce at the same time $E_{tot}, E_{pair}, \Delta_{LCS}$ within good accuracy
- We can use a typical basis size (≈ 60 MeV) as for a DDDI (within a given error)

Systematic calculations







Spherical calculations

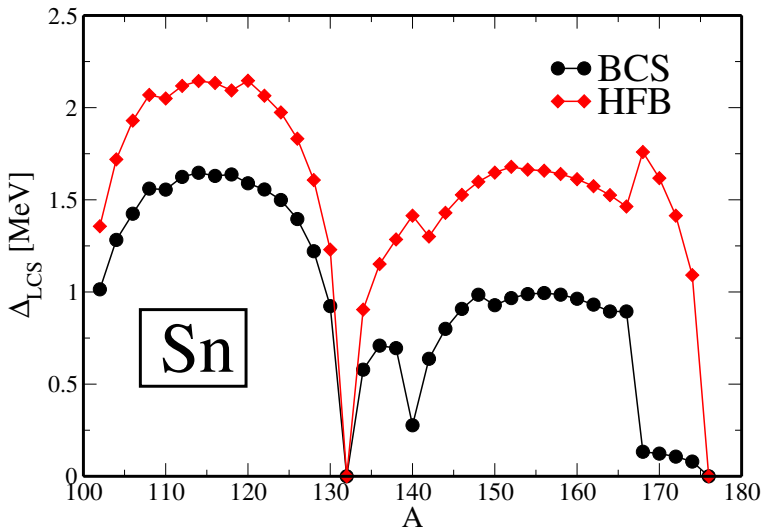
- The DME0th behaves well along 3 different isotopic chains
- Good reproduction of $E_{tot}, E_{pair}, \Delta_{LCS}$ on average

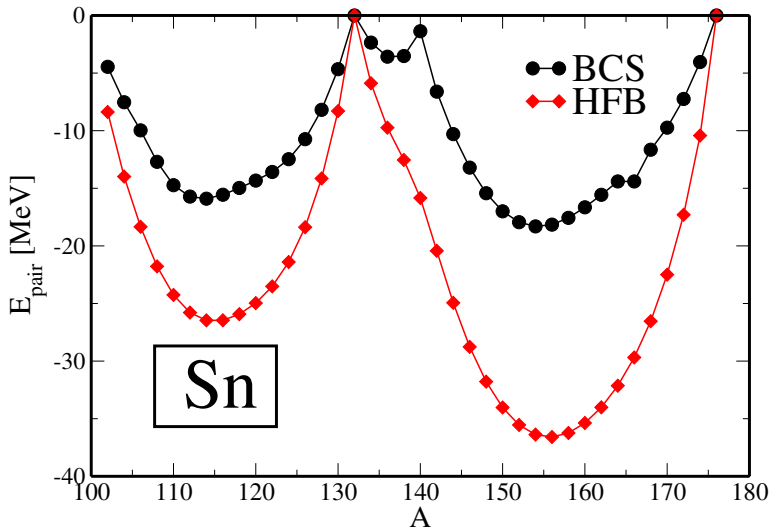
Outline

BCS approximation

Numerical details

- We use the Gogny D1 pairing interaction (separable form)
- The same code to perform HFB/BCS

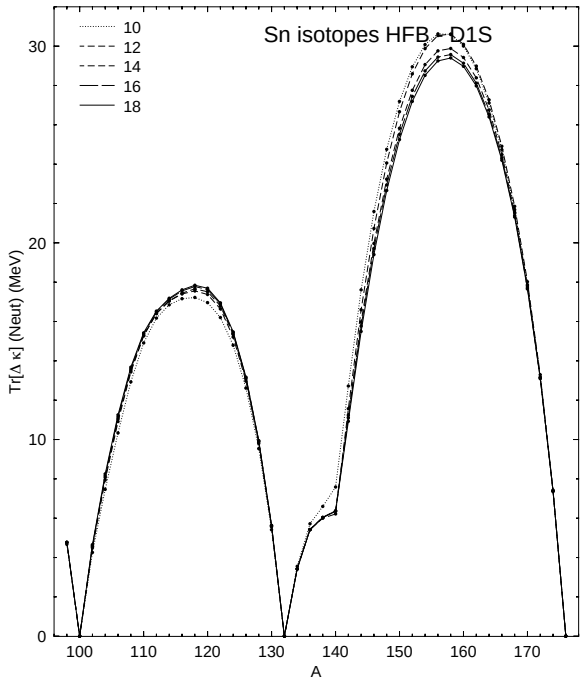


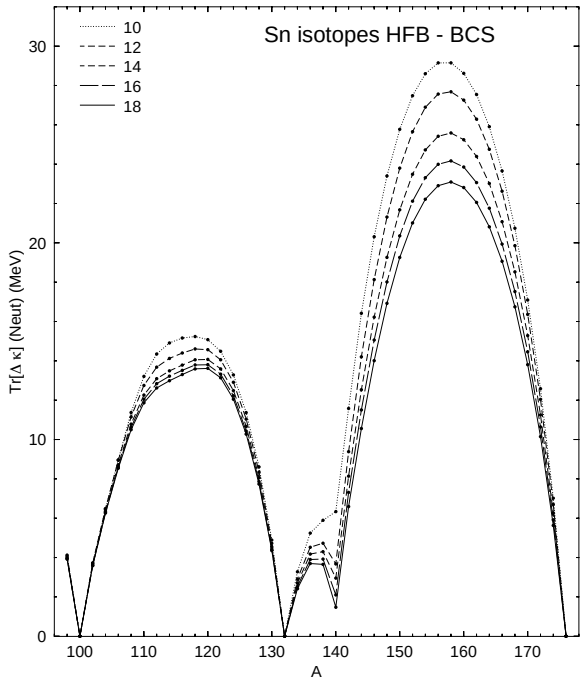


The BCS approximation gives a factor 2 difference!!!

Does BCS converge using finite-range forces?

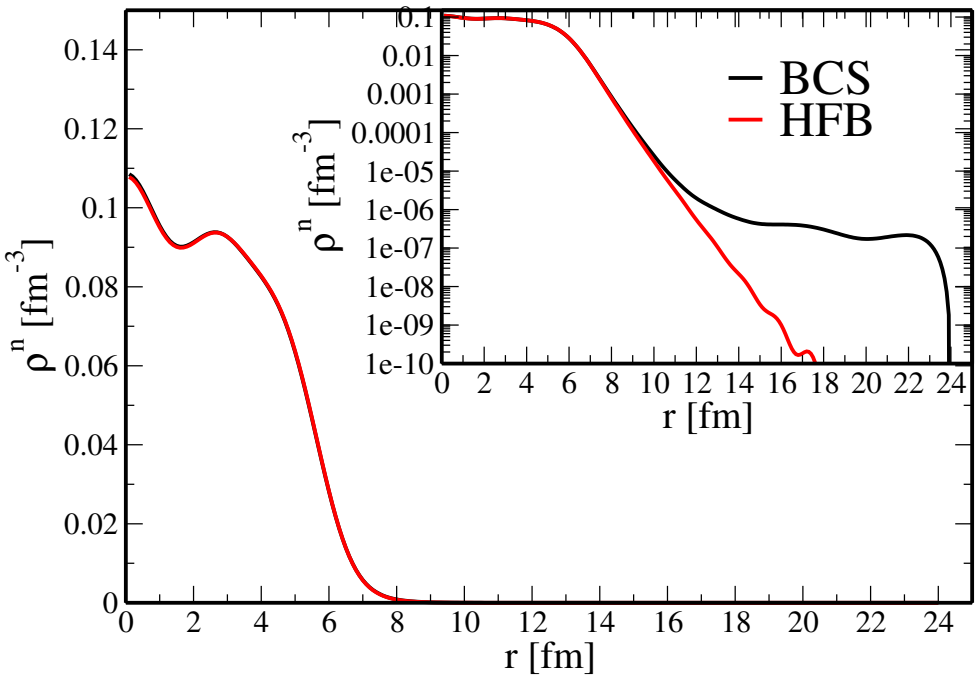
[L. Robledo (private)]





- Convergence problem!!!!
- BCS is NOT a good approximation for well stable nuclei for finite-range force!!!!

Neutron gas



- Within BCS ^{120}Sn presents an external neutron gas
- BCS favor occupations of unbound states!
- Using a small pairing-window ($\approx 1\hbar\omega$) we avoid such problem (stable nuclei)

Conclusions

- We have applied a non-standard DME approach to pairing problem
  - Numerical problem at the same level of standard DDDI
  - Accurate reproduction of main (pseudo)-observables
  - Systematic calculations
- No ultraviolet divergency
- Possible implementation in 3D code
- We need still some improvements

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... not only working on superfluidity...

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