



# Convergence of density-matrix expansions for nuclear interactions

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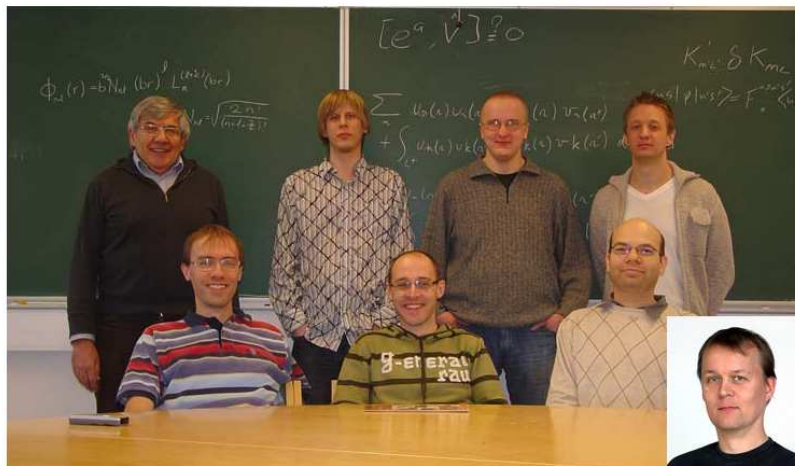
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in collaboration with

**Jacek Dobaczewski and the FIDIPRO team**

# Team

The FiDiPro team:



# Plan for this talk

## Generalized Skyrme functionals with higher order derivatives

- How to construct them [1]
- New computer code (HOSPHE) [2,3]

## Density matrix expansions, method to derive the coupling constants

- Test of DMEs using the Gogny force [4,5]
- Direct term (Hartree) - Gradient expansion
- Exchange term (Fock) - quasi-local expansion
- First test of convergence properties (beyond 2nd order)
- New DME method proposed

[1] B.G. Carlsson, J. Dobaczewski and M. Kortelainen *et. al.* Phys. Rev. **C78**, 044326 (2008)

[2] B.G. Carlsson, J. Dobaczewski, J. Toivanen and P. Vesely, To appear in Comp. Phys. Comm., arXiv:0912.3230 (2010)

[3] J. Toivanen, *et al.*, To appear in PRC, arXiv:0912.3234v1

[4] J. Dobaczewski, B.G. Carlsson and M. Kortelainen, Submitted to J. Phys. G, arXiv:1002.3646v1 (2010)

[5] B.G. Carlsson and J. Dobaczewski, submitted to PRL, arXiv:1003.2543v1 (2010)

# Ansatz for a nuclear density functional

The EDF is assumed to have the form

$$\mathcal{E} = \int d^3\mathbf{r} \mathcal{H}_E(\mathbf{r}),$$

where

$$\mathcal{H}_E(\mathbf{r}) = \frac{\hbar^2}{2m} \tau_0 + \mathcal{H}(\mathbf{r}).$$

we focus on the potential energy density  $\mathcal{H}(\mathbf{r})$

- expansion in derivatives of the one-body density
- consistent with symmetries of the nucleon-nucleon force

## One-body density matrix

Separation into standard scalar and vector parts,

$$\rho(\mathbf{r}\sigma, \mathbf{r}'\sigma') = \frac{1}{2}\rho(\mathbf{r}, \mathbf{r}')\delta_{\sigma\sigma'} + \frac{1}{2}\sum_a \langle \sigma | \sigma_a | \sigma' \rangle s_a(\mathbf{r}, \mathbf{r}'),$$

Building blocks in the spherical representation:

$$\begin{aligned} \rho_{00}(\mathbf{r}, \mathbf{r}') &= \rho(\mathbf{r}, \mathbf{r}'), \\ \mathbf{s}(\mathbf{r}, \mathbf{r}') &= -i \left\{ \frac{1}{\sqrt{2}} (s_x(\mathbf{r}, \mathbf{r}') - is_y(\mathbf{r}, \mathbf{r}')), s_z(\mathbf{r}, \mathbf{r}'), \right. \\ &\quad \left. \frac{-1}{\sqrt{2}} (s_x(\mathbf{r}, \mathbf{r}') + is_y(\mathbf{r}, \mathbf{r}')) \right\}, \\ \nabla &= -i \left\{ \frac{1}{\sqrt{2}} (\nabla_x - i\nabla_y), \nabla_z, \frac{-1}{\sqrt{2}} (\nabla_x + i\nabla_y) \right\}, \\ \mathbf{k} &= -i \left\{ \frac{1}{\sqrt{2}} (k_x - ik_y), k_z, \frac{-1}{\sqrt{2}} (k_x + ik_y) \right\}. \end{aligned}$$

where  $\mathbf{k} = \frac{\nabla_{\mathbf{r}'} - \nabla_{\mathbf{r}''}}{2i}$

# Higher-order derivative operators

Independent derivative operators to 6th order

No.	tensor $D_{nL}$	order $n$	rank $L$
1	1	0	0
2	$\nabla$	1	1
3	$[\nabla\nabla]_0$	2	0
4	$[\nabla\nabla]_2$	2	2
5	$[\nabla\nabla]_0\nabla$	3	1
6	$[\nabla[\nabla\nabla]_2]_3$	3	3
7	$[\nabla\nabla]_0^2$	4	0
8	$[\nabla\nabla]_0[\nabla\nabla]_2$	4	2
9	$[\nabla[\nabla[\nabla\nabla]_2]_{3,4}]$	4	4
10	$[\nabla\nabla]_0^2\nabla$	5	1
11	$[\nabla\nabla]_0[\nabla[\nabla\nabla]_2]_3$	5	3
12	$[\nabla[\nabla[\nabla[\nabla\nabla]_2]_{3,4}]_5]$	5	5
13	$[\nabla\nabla]_0^3$	6	0
14	$[\nabla\nabla]_0^2[\nabla\nabla]_2$	6	2
15	$[\nabla\nabla]_0[\nabla[\nabla[\nabla\nabla]_2]_{3,4}]$	6	4
16	$[\nabla[\nabla[\nabla[\nabla[\nabla\nabla]_2]_{3,4}]_5]_6]$	6	6

Replacing  $\nabla \leftrightarrow \mathbf{k}$  gives  $K_{nL}$

## Local densities

formed by acting several times on the scalar and vector non-local densities with the relative momentum operator and taking limit  $\mathbf{r}' = \mathbf{r}$

$$\rho_{nLvJ}(\mathbf{r}) = \left\{ [K_{nL}\rho_v(\mathbf{r}, \mathbf{r}')]_J \right\}_{\mathbf{r}'=\mathbf{r}},$$

where the  $n$ th-order and rank- $L$  relative derivative operator  $K_{nL}$  acts on the scalar ( $v = 0$ ) or vector ( $v = 1$ )

Labeled using time-reversal ( $T$ ) and space-inversion ( $P$ ) parities defined as,

$$T = (-1)^{n+v},$$

$$P = (-1)^n.$$

## Local-densities from the scalar density matrix

No.		$\rho_{nLvJ} = \text{density}$	$n$	$L$	$\nu$	$J$	$T$	$P$
1	★ ●	$\rho_{0000} = [\rho]_0$	0	0	0	0	1	1
2	★	$\rho_{1101} = [k\rho]_1$	1	1	0	1	-1	-1
3	★ ●	$\rho_{2000} = [[kk]_0\rho]_0$	2	0	0	0	1	1
4	★ ●	$\rho_{2202} = [[kk]_2\rho]_2$	2	2	0	2	1	1
5	★	$\rho_{3101} = [[kk]_0k\rho]_1$	3	1	0	1	-1	-1
6	★	$\rho_{3303} = [[k[kk]_2]_3\rho]_3$	3	3	0	3	-1	-1
7	★ ●	$\rho_{4000} = [[kk]_0^2\rho]_0$	4	0	0	0	1	1
8	★ ●	$\rho_{4202} = [[kk]_0[kk]_2\rho]_2$	4	2	0	2	1	1
9		$\rho_{4404} = [[k[k[kk]_2]_3]_4\rho]_4$	4	4	0	4	1	1
10	★	$\rho_{5101} = [[kk]_0^2k\rho]_1$	5	1	0	1	-1	-1
11		$\rho_{5303} = [[kk]_0[k[kk]_2]_3\rho]_3$	5	3	0	3	-1	-1
12		$\rho_{5505} = [[k[k[k[kk]_2]_3]_4]_5\rho]_5$	5	5	0	5	-1	-1
13	★ ●	$\rho_{6000} = [[kk]_0^3\rho]_0$	6	0	0	0	1	1
14		$\rho_{6202} = [[kk]_0^2[kk]_2\rho]_2$	6	2	0	2	1	1
15		$\rho_{6404} = [[kk]_0[k[k[kk]_2]_3]_4\rho]_4$	6	4	0	4	1	1
16		$\rho_{6606} = [[k[k[k[k[kk]_2]_3]_4]_5]_6\rho]_6$	6	6	0	6	1	1



## Terms in the energy density

Terms in the EDF are required to be

- quadratic in densities
- time reversal invariant
- space-inversion invariant
- invariant with respect to rotations

A general term can be written

$$T_{ml,nLvJ,Q}^{m'l',n'l'v'j'}(\mathbf{r}) = C[[D_{m'l'}\rho_{n'l'v'j'}(\mathbf{r})]_Q [D_{ml}\rho_{nLvJ}(\mathbf{r})]_Q]_0,$$

With density-independent coupling-constants P.I gives

$$T_{ml,nLvJ}^{n'l'v'j'}(\mathbf{r}) = C[\rho_{n'l'v'j'}(\mathbf{r})[D_{ml}\rho_{nLvJ}(\mathbf{r})]_{j'}]_0,$$

## Skyrme terms

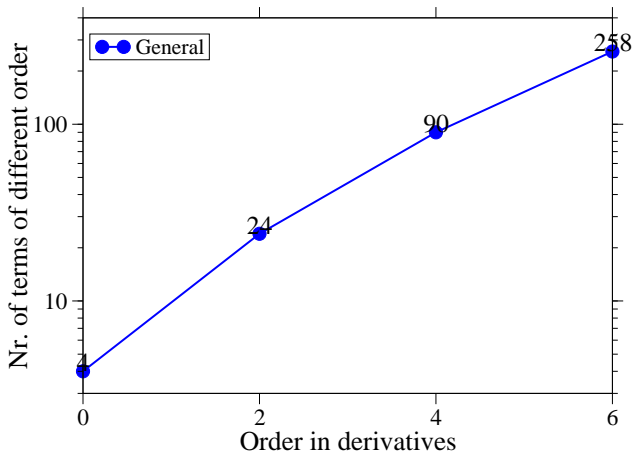
Second order expansion is equivalent to the Skyrme functional

No.	$C_{ml,nLvJ}^{n'l'v'j'}$	Spherical	Cartesian
1	• $C_{00,0000}^{0000}$	$[\rho\rho]_0$	$= \rho^2$
2	$C_{00,0011}^{0011}$	$[ss]_0$	$= \frac{1}{\sqrt{3}} s^2$
3	• $C_{20,0000}^{0000}$	$[\rho[(\nabla\nabla)_0\rho]_0]_0$	$= \frac{1}{\sqrt{3}} \rho\Delta\rho$
4	• $C_{00,2000}^{0000}$	$[\rho[[kk]_0\rho]_0]_0$	$= \frac{1}{\sqrt{3}} \left( \rho\tau - \frac{1}{4}\rho\Delta\rho \right)$
5	$C_{00,1110}^{1110}$	$[[ks]_0[ks]_0]_0$	$= \frac{1}{3} \left( J^{(0)} \right)^2$
6	• $C_{00,1111}^{1111}$	$[[ks]_1[ks]_1]_0$	$= \frac{1}{\sqrt{12}} J^2$
7	$C_{00,1112}^{1112}$	$[[ks]_2[ks]_2]_0$	$= \frac{1}{\sqrt{5}} \sum_{ab} J_{ab}^{(2)} J_{ab}^{(2)}$
8	• $C_{11,1111}^{0000}$	$[\rho[\nabla[ks]_1]_0]_0$	$= \frac{1}{\sqrt{6}} \rho \nabla \cdot \mathbf{J}$
9	$C_{00,1101}^{1101}$	$[[k\rho]_1[k\rho]_1]_0$	$= \frac{1}{\sqrt{3}} \mathbf{j}^2$
10	$C_{20,0011}^{0011}$	$[s[(\nabla\nabla)_0s]_1]_0$	$= \frac{1}{3} \mathbf{s}\Delta\mathbf{s}$
11	$C_{22,0011}^{0011}$	$[s[(\nabla\nabla)_2s]_1]_0$	$= \frac{-1}{\sqrt{5}} \left( (\nabla \cdot \mathbf{s})^2 + \frac{1}{3} \mathbf{s}\Delta\mathbf{s} \right)$
12	$C_{00,2011}^{0011}$	$[s[[kk]_0s]_1]_0$	$= \frac{1}{3} \left( \mathbf{s} \cdot \mathbf{T} - \frac{1}{4} \mathbf{s}\Delta\mathbf{s} \right)$
13	$C_{00,2211}^{0011}$	$[s[[kk]_2s]_1]_0$	$= \frac{1}{\sqrt{5}} \left( \mathbf{s} \cdot \mathbf{F} + \frac{1}{4} (\nabla \cdot \mathbf{s})^2 \right)$
14	$C_{11,0011}^{1101}$	$[[k\rho]_1[\nabla s]_1]_0$	$= -\frac{1}{3} \mathbf{s} \cdot \mathbf{T} + \frac{1}{12} \mathbf{s}\Delta\mathbf{s} - \frac{1}{\sqrt{6}} \mathbf{j} \cdot \nabla \times \mathbf{s}$

## Time-even 4th order terms

No.		$C_{nl, nLvJ}^{n' L' v' J'}$	$\rho_{n' L' v' J'}$ Time-even	$D_{ml}$	$\rho_{nLvJ}$ Time-even
1	•	$C_{40,0000}^{0000}$	$[\rho]_0$	$[\nabla\nabla]_0^2$	$[\rho]_0$
2	•	$C_{20,2000}^{0000}$	$[\rho]_0$	$[\nabla\nabla]_0$	$[[kk]_0\rho]_0$
3	•	$C_{22,2202}^{0000}$	$[\rho]_0$	$[\nabla\nabla]_2$	$[[kk]_2\rho]_2$
4	•	$C_{00,4000}^{0000}$	$[\rho]_0$	1	$[[kk]_0^2\rho]_0$
5	•	$C_{00,2000}^{2000}$	$[[kk]_0\rho]_0$	1	$[[kk]_0\rho]_0$
6	•	$C_{00,2202}^{2202}$	$[[kk]_2\rho]_2$	1	$[[kk]_2\rho]_2$
7		$C_{20,1110}^{1110}$	$[ks]_0$	$[\nabla\nabla]_0$	$[ks]_0$
8		$C_{22,1112}^{1110}$	$[ks]_0$	$[\nabla\nabla]_2$	$[ks]_2$
9		$C_{00,3110}^{1110}$	$[ks]_0$	1	$[[kk]_0ks]_0$
10	•	$C_{20,1111}^{1111}$	$[ks]_1$	$[\nabla\nabla]_0$	$[ks]_1$
11	•	$C_{22,1111}^{1111}$	$[ks]_1$	$[\nabla\nabla]_2$	$[ks]_1$
12		$C_{22,1112}^{1111}$	$[ks]_1$	$[\nabla\nabla]_2$	$[ks]_2$
13	•	$C_{00,3111}^{1111}$	$[ks]_1$	1	$[[kk]_0ks]_1$
14		$C_{20,1112}^{1112}$	$[ks]_2$	$[\nabla\nabla]_0$	$[ks]_2$
15		$C_{22,1112}^{1112}$	$[ks]_2$	$[\nabla\nabla]_2$	$[ks]_2$
16		$C_{00,3112}^{1112}$	$[ks]_2$	1	$[[kk]_0ks]_2$
17		$C_{00,3312}^{1112}$	$[ks]_2$	1	$[[k[kk]_2]_3s]_2$
18	•	$C_{31,1111}^{0000}$	$[\rho]_0$	$[\nabla\nabla]_0\nabla$	$[ks]_1$
19	•	$C_{11,3111}^{0000}$	$[\rho]_0$	$\nabla$	$[[kk]_0ks]_1$
20	•	$C_{11,1111}^{2000}$	$[[kk]_0\rho]_0$	$\nabla$	$[ks]_1$
21	•	$C_{11,1111}^{2202}$	$[[kk]_2\rho]_2$	$\nabla$	$[ks]_1$
22		$C_{11,1112}^{2202}$	$[[kk]_2\rho]_2$	$\nabla$	$[ks]_2$

# Number of terms increases exponentially



# More constraints, Galilean and gauge invariance

## Galilean invariance

Relativistic effects are neglected

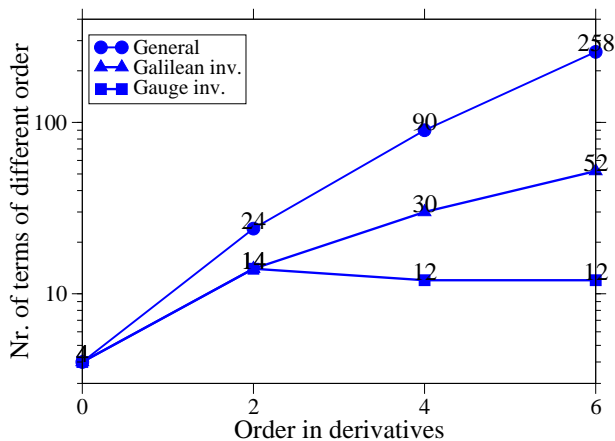
## Local gauge invariance

For local forces

$$v(\mathbf{r}'_1, \mathbf{r}'_2, \mathbf{r}_1, \mathbf{r}_2) = \delta(\mathbf{r}'_1 - \mathbf{r}_1) \delta(\mathbf{r}'_2 - \mathbf{r}_2) v(\mathbf{r}_1, \mathbf{r}_2)$$

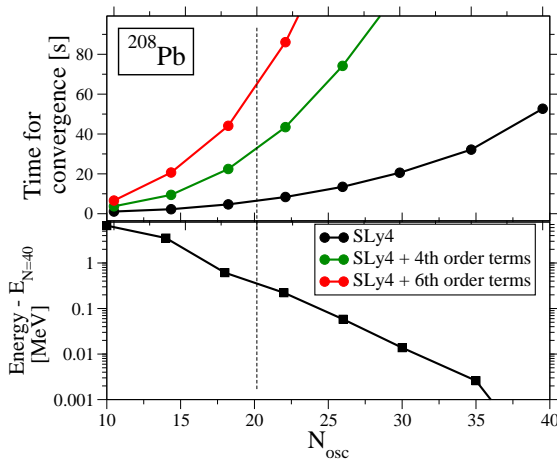
such as Gogny, Coulomb, and Yukawa.

# Symmetries introduce constraints between the parameters



# New code HOSPHE

- Spherical HO basis
- All terms up to 6th order in derivatives
- Mean field + linear response
- Density expanded in multipoles (zero multipole for MF and higher for LR)
- To appear in *Comp. Phys. Comm.*,  
B.G. Carlsson *et al*  
arXiv:0912.3230.



with no symmetry assumed  
(order, terms) = (2, 32), (4, 122), (6, 380)

# Summary empirical functional

- General sixth order EDF
- Restricted only by symmetries
- Elegant notation introduced
- Fourth order and (Galilean,Gauge)=(48,30) free parameters.  
Skyrme (2nd order) has 18
- Code publicly available

B. G. Carlsson *et. al.* Phys. Rev. **C78**, 044326 (2008)

B. G. Carlsson *et al*, To appear in Comp. Phys. Comm., arXiv:0912.3230. (2010)



# DME methods

- Introduced by Negele and Vautherin [1] to relate microscopic theory to Skyrme type models
- G-matrix to Skyrme functional
- Transforms direct and exchange energy to expansions in derivatives of the DM
- Corrective contributions to the Slater approximation for exchange
- Leads to much simpler and faster calculations for 2 and 3 body exchange parts

## New stuff

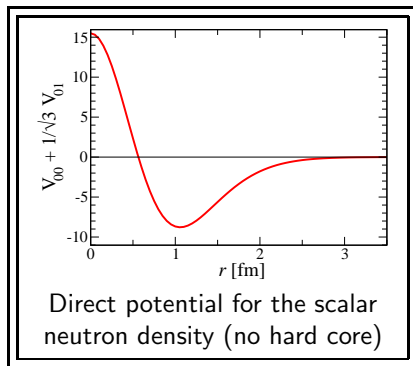
- Test convergence of DME methods (first time beyond 2nd order)
- new expansion method

[1] Negele and Vautherin PRC 5, 1472 (1972)

## Gogny effective interaction as test case

$$V_{12} = \text{Contact part} + \text{Coulomb part} \\ + \sum_{k=1}^2 e^{-(\mathbf{r}_1 - \mathbf{r}_2)^2 / \mu_k^2} (W_k + B_k P_\sigma - H_k P_\tau - M_k P_\sigma P_\tau)$$

- Accuracy for masses 0.798 MeV
- Range < 3 fm
- Good test for DME methods



## Gradient expansion of the direct term

Direct (Hartree) term (neglecting spin and isospin)

$$\mathcal{E}_{\text{dir}}^{\text{int}} = \frac{1}{2} \int \int \rho(\mathbf{r}_1) \rho(\mathbf{r}_2) v(\mathbf{r}_1, \mathbf{r}_2) d\mathbf{r}_1 d\mathbf{r}_2. \quad (1)$$

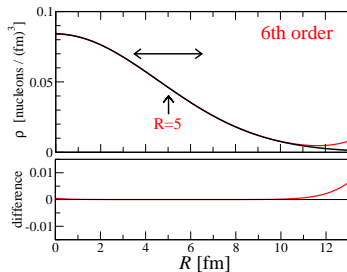
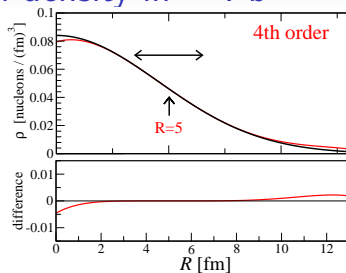
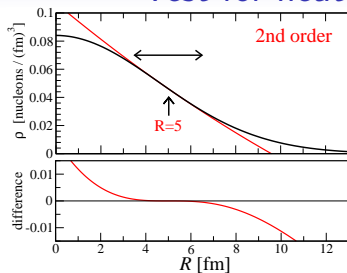
Taylor expansion in powers of  $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$  around  $\mathbf{R} = \frac{1}{2}(\mathbf{r}_1 + \mathbf{r}_2)$

$$\begin{aligned} \rho(\mathbf{r}_1) &= \rho\left(\mathbf{R} + \frac{\mathbf{r}}{2}\right) = e^{\frac{1}{2}\mathbf{r} \cdot \nabla} \rho(\mathbf{R}) = \sum_n \frac{1}{n!} \left(\frac{\mathbf{r}}{2} \cdot \nabla\right)^n \rho(\mathbf{R}) \\ &= \sum_{nL} a_{nL} r^n \left[ Y_L(\hat{r}), \hat{D}_{nL} \right]_0 \rho(\mathbf{R}). \end{aligned}$$

expanding both densities and inserting in Eq. 1 gives

$$\mathcal{E}_{\text{dir}}^{\text{int}} = \sum_{nn'L} \int \underbrace{\left( \int \frac{a_{nL} a_{n'L}}{\sqrt{1+2L}} r^{n+n'+2} v(r) dr \right)}_{C_L^{nn'}} [D_{nL}\rho(\mathbf{R}), D_{n'L}\rho(\mathbf{R})]_0 d\mathbf{R}$$

# Test for neutron density in $^{208}\text{Pb}$

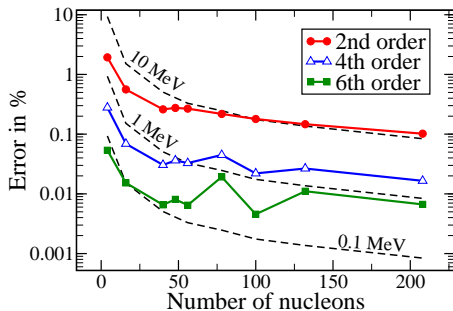


- Analytical HO with smeared occupancies from [1]
- Gradient expansion works well in this test case
- What about realistic cases with more wiggles ?

# Direct term accuracy for the Gogny D1S force

- Test with densities from Skyrme SLy4 functional
- nine nuclei:  ${}^4\text{He}$ ,  ${}^{16}\text{O}$ ,  ${}^{40,48}\text{Ca}$ ,  ${}^{56,78}\text{Ni}$ ,  ${}^{100,132}\text{Sn}$  and  ${}^{208}\text{Pb}$
- Exact direct energy versus gradient expansion

- First test going beyond second order
- Accuracy surprisingly good
- Total RMS at sixth order is 0.479 MeV



# Exchange term

The direct term can be calculated exactly but for the exchange term the DME makes calculations much faster.

Some proposals for the exchange part:

- NV: corrective factors to Slater using Bessel fkn expansion of  $\rho(\mathbf{r}_1, \mathbf{r}_2)$
- PSA: Recent proposal improving the NV expansion for the spin part [1]
- DT: Our method, improved convergence, works well for all channels without rotational averaging.

[1] B. Gebremarian *et. al.* arxiv 0910.4979 (2009)

## DT expansion for the exchange term

The density in the exchange (Fock) term

$$\mathcal{E}_{\text{exc}}^{\text{int}} = \frac{1}{2} \int \int \rho(\mathbf{r}_1, \mathbf{r}_2) \rho(\mathbf{r}_2, \mathbf{r}_1) v(|\mathbf{r}_1 - \mathbf{r}_2|) d\mathbf{r}_1 d\mathbf{r}_2$$

can be expanded in powers of  $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$  around  $\mathbf{R} = \frac{1}{2}(\mathbf{r}_1 + \mathbf{r}_2)$  as:

$$\begin{aligned} \rho(\mathbf{R}, \mathbf{r}) &= \bar{\rho}(\mathbf{R}, \mathbf{r}) + e^{-\frac{r^2}{a^2}} \left[ e^{i\mathbf{r} \cdot \hat{\mathbf{k}}} e^{\frac{(\mathbf{r}_1 - \mathbf{r}_2)^2}{a^2}} (\rho(\mathbf{r}_1, \mathbf{r}_2) - \bar{\rho}(\mathbf{r}_1, \mathbf{r}_2)) \right] \Big|_{\mathbf{r}_1 = \mathbf{r}_2 = \mathbf{R}} \\ &= \sum_{nLm} \pi_{nL}^m(r) \left[ Y_L(\hat{r}), \hat{K}_{nL} \rho(\mathbf{r}_1, \mathbf{r}_2) \Big|_{\mathbf{r}_1 = \mathbf{r}_2 = \mathbf{R}} \right]_0. \end{aligned}$$

around a model density (Slater mixed density)

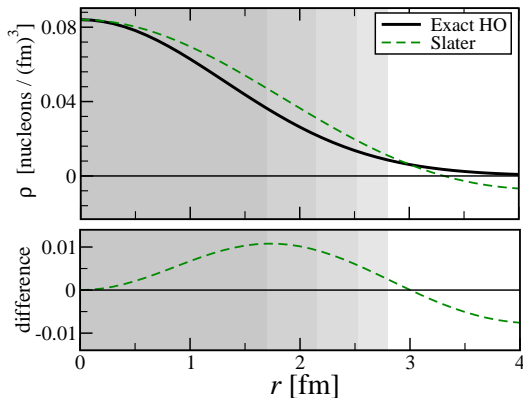
$$\bar{\rho}(\mathbf{r}_1, \mathbf{r}_2) = \rho(\mathbf{R}) \frac{3j_1(k_F r)}{k_F r}$$

Gives the exchange energy as quasi-local expansion

$$\mathcal{E}_{\text{exc}}^{\text{int}} \simeq \sum_{t, nn'L} \int d\mathbf{R} C_{nL}^{n'} [\rho_{n'L}(\mathbf{R}), \rho_{nL}(\mathbf{R})]_0,$$

## Idea behind the DT expansion

$\rho(\mathbf{r}_1, \mathbf{r}_2)$  as fkn of  $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$  for  $\mathbf{R} = 0$

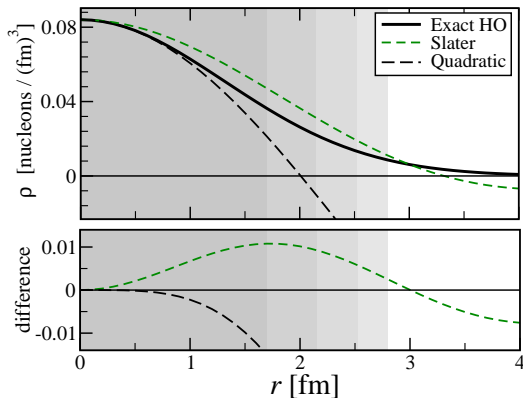


- Exact density from analytical model of HO with smeared occupancies
- The model density gives a good average approximation
- Shaded regions indicate relevant range



# Idea behind the DT expansion

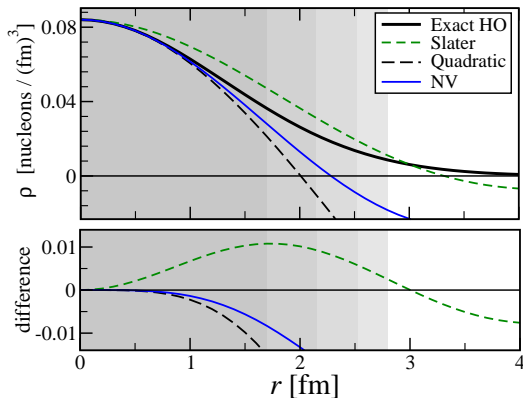
$\rho(\mathbf{r}_1, \mathbf{r}_2)$  as fkn of  $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$  for  $\mathbf{R} = 0$



- Quadratic Taylor expansion improves for  $r < 1.5$  fm

## Idea behind the DT expansion

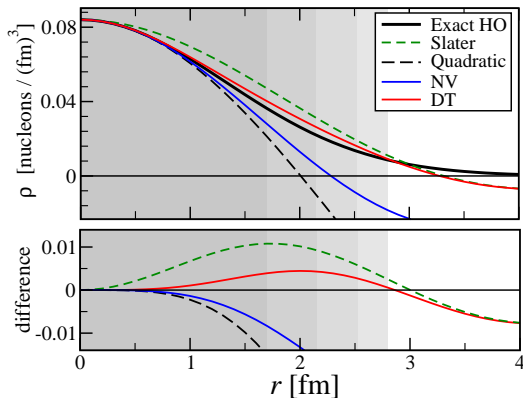
$\rho(\mathbf{r}_1, \mathbf{r}_2)$  as fkn of  $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$  for  $\mathbf{R} = 0$



- NV Bessel-function expansion is somewhat better

# Idea for the DT expansion

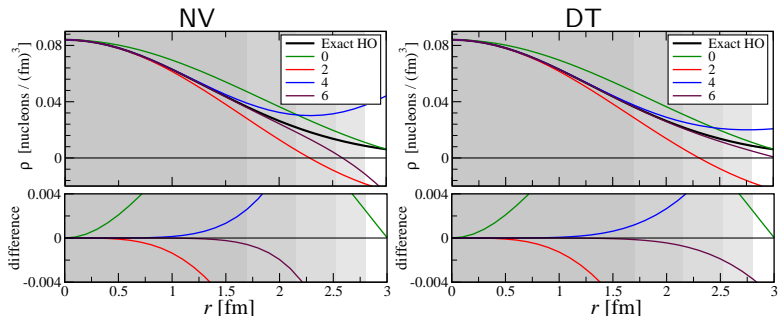
$\rho(\mathbf{r}_1, \mathbf{r}_2)$  as fkn of  $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$  for  $\mathbf{R} = 0$



- DT improves short range while preserving the long range part

## Comparison of NV and DT expansions

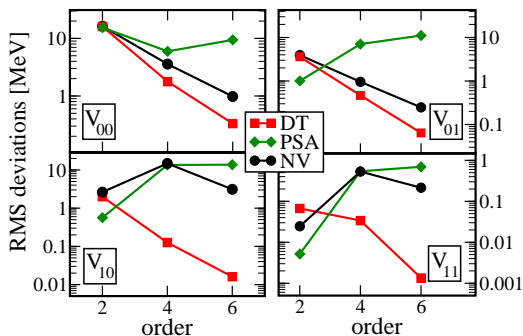
- We fix the damping width  $a$  in the DT by fitting the sixth order expansion to symmetric nuclear matter which gives  $a \approx 4/k_F$
- Better convergence than NV
- Avoids rotational averaging in the non-local direction, hence has the potential to be more accurate than NV



# Exchange term accuracy for the Gogny D1S force

Test case: SLy4 for nine nuclei:  ${}^4\text{He}$ ,  ${}^{16}\text{O}$ ,  ${}^{40,48}\text{Ca}$ ,  ${}^{56,78}\text{Ni}$ ,  ${}^{100,132}\text{Sn}$  and  ${}^{208}\text{Pb}$

- First test of convergence properties (beyond 2nd order)
- 2nd order: PSA best, RMS = 14.09 MeV
- 4th order: DT best, RMS = 1.54 MeV
- 6th order: DT best, RMS = 0.36 MeV



# Conclusions

- First test of DME methods beyond 2nd order
- new method with excellent convergence properties
- Can be used to approximate both direct and exchange
- at sixth order the number of active terms are doubled (gauge symmetry) compared to Skyrme calculations, hence the computer time only doubles.

B. G. Carlsson and J. Dobaczewski, submitted to PRL, arXiv:1003.2543v1 (2010)

J. Dobaczewski, B.G. Carlsson and M. Kortelainen, submitted to JPG, arXiv:1002.3646v1 (2010)

## Plans for the future

- Derive simple and fast Hartree-Fock functional from chiral effective field theory (in collaboration with T. Duguet)
- Add RPA correlations using iterative HOSPHE-LR (Monday presentation by J. Toivanen)
- Add remaining correlations using LDA (second Born, GW)
- sp states from the response function (Hedin style)

Thank You