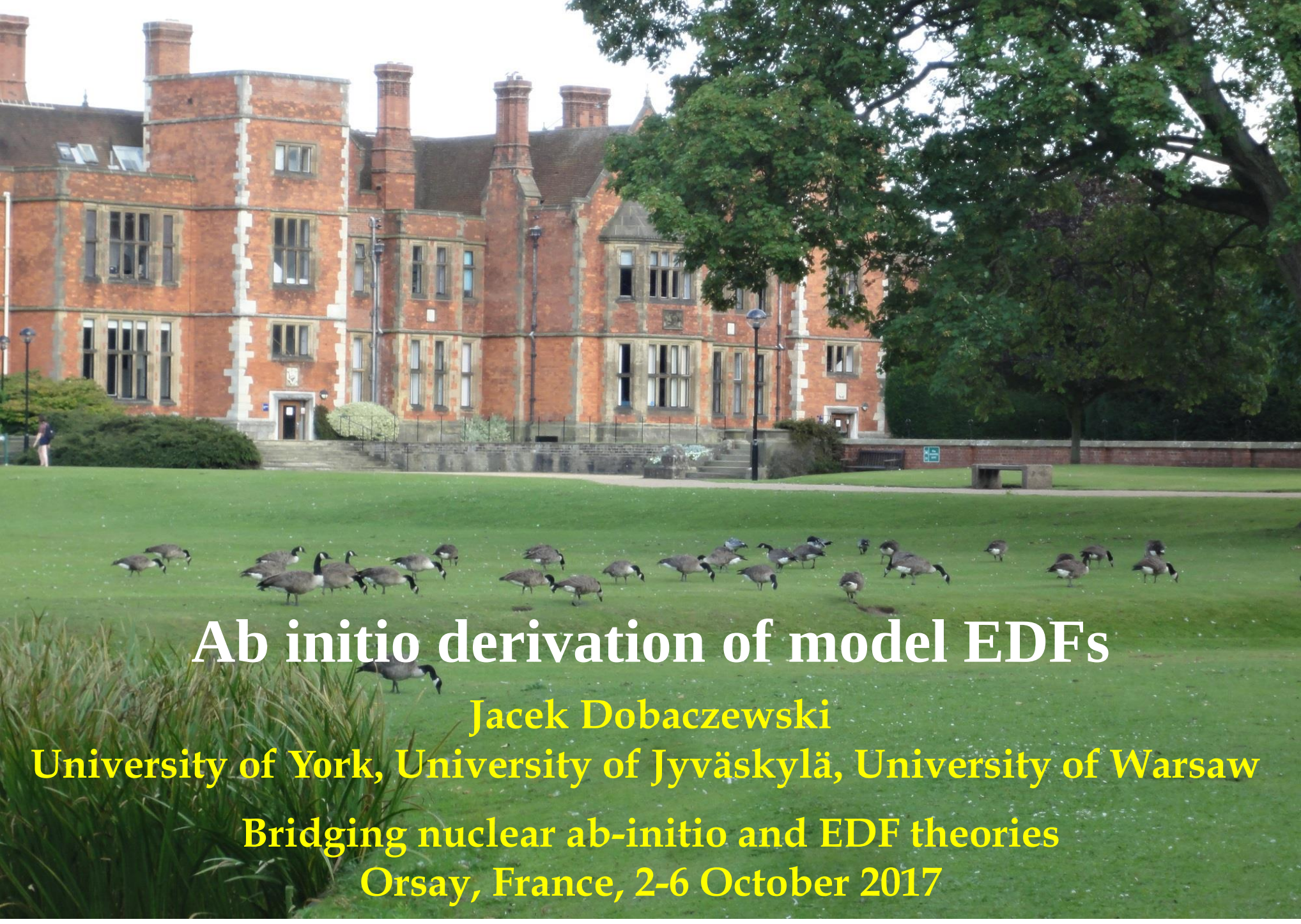

Ab initio derivation of model EDFs

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Bridging nuclear ab-initio and EDF theories

Orsay, France, 2-6 October 2017

Ab initio project in collaboration with:

- Gianluca Salvioni, Jyväskyla
- Karim Bennaceur, Lyon
- Carlo Barbieri, Surrey
- Andrea Idini, Surrey
- Gillis Carlsson, Lund
- Alessandro Pastore, York

Outline

1. *Ab initio* DFT
2. *Ab initio* derivations of nuclear DFT
3. Conclusions

What is DFT?

Density Functional Theory:

A variational method that uses a two-step variational procedure.

J. D., J. Phys.: Conf. Ser. 312, 092002 (2011)

Levy and Lieb construction,
see Chapter 3.4 in R.G. Parr and W. Yang
Density-Functional Theory of Atoms and Molecules
(New York, Oxford University Press, 1989)

A two-step variation

I	23	22	19	34	21		42	22	21	34	20	19
II	21	25	43	24	21		32	32	18	31	29	18
III	38	27	30	24	23		27	22	42	23	32	22
IV	21	23	31	32	27		35	20	21	26	37	20
V	32	22	36	25	22		23	21	25	34	33	21
VI	32	20	21	32	35		36	27	31	22	21	20
VII	31	33	42	32	25		31	42	29	31	23	23
VIII	24	29	24	32	42		23	34	45	32	27	23

What is DFT?

Density Functional Theory:

A variational method that uses a two-step variational procedure.

Divide all states into groups that have the same densities, an then:

1. **Find the lowest energy in each group (very, very, difficult)**
2. **Find the lowest energy among all groups (relatively easy)**

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What is DFT?

Density Functional Theory:

A variational method that uses observables as variational parameters.

$$\delta\langle \hat{H} - \lambda \hat{Q} \rangle = 0$$

$$\Downarrow$$

$$E = E(Q)$$

for $E(\lambda) \equiv \langle \hat{H} \rangle$ and $Q(\lambda) \equiv \langle \hat{Q} \rangle$

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Which DFT?

$$\delta\langle \hat{H} - \lambda \hat{Q} \rangle = 0 \Longrightarrow E = E(Q)$$

$$\delta\langle \hat{H} - \sum_k \lambda_k \hat{Q}_k \rangle = 0 \Longrightarrow E = E(Q_k)$$

$$\delta\langle \hat{H} - \int \mathrm{d}q\, \lambda(q) \hat{Q}(q) \rangle = 0 \Longrightarrow E = E[Q(q)]$$

$$\delta\langle \hat{H} - \int \mathrm{d}\vec{r}\, \lambda(\vec{r}) \hat{\rho}(\vec{r}) \rangle = 0 \Longrightarrow E = E[\rho(\vec{r})]$$

$$\text{for} \quad \hat{\rho}(\vec{r}) = \sum_{i=1}^{A} \delta(\vec{r} - \vec{r}_i)$$

$$\delta\langle \hat{H} - \int\int \mathrm{d}\vec{r}\mathrm{d}\vec{r}\,' \lambda(\vec{r}, \vec{r}\,') \hat{\rho}(\vec{r}, \vec{r}\,') \rangle = 0 \Longrightarrow E = E[\rho(\vec{r}, \vec{r}\,')]$$

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What is DFT?

Density Functional Theory:

Exact: A variational method that uses a two-step variational procedure with observables used for the variational parameters.

Practical: Build a model of density functional.

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Nuclear energy density functionals

How the nuclear EDF is built?

$$E[\rho(\vec{r}_1,\vec{r}_2)] = \int\int \mathrm{d}\vec{r}_1 \mathrm{d}\vec{r}_2\, \mathcal{H}(\rho(\vec{r}_1,\vec{r}_2))$$

Energy Density Functional (EDF)

Energy Density

$$\mathcal{H}(\rho(\vec{r}_1,\vec{r}_2)) = V(\vec{r}_1-\vec{r}_2)\Big[\rho(\vec{r}_1)\rho(\vec{r}_2) - \rho(\vec{r}_1,\vec{r}_2)\rho(\vec{r}_2,\vec{r}_1)\Big]$$

EDF generator

Direct

Exchange

Standard EDF generators

- Gogny*

$$V(\vec{r}_1\vec{r}_2;\vec{r}\,'_1\vec{r}\,'_2) = \delta(\vec{r}_1-\vec{r}\,'_1)\delta(\vec{r}_2-\vec{r}\,'_2)V(\vec{r}_1-\vec{r}_2),$$

where,

$$V(\vec{r}_1-\vec{r}_2) = \sum\nolimits_{i=1,2} e^{-(\vec{r}_1-\vec{r}_2)^2/\mu_i^2} \times (W_i + B_iP_\sigma - H_iP_\tau - M_iP_\sigma P_\tau)$$
$$+t_3(1+P_\sigma)\delta(\vec{r}_1-\vec{r}_2)\rho^{1/3}\left[\tfrac{1}{2}(\vec{r}_1+\vec{r}_2)\right].$$

$P_\sigma=\frac{1}{2}(1+\vec{\sigma}_1\cdot\vec{\sigma}_2)$ and $P_\tau=\frac{1}{2}(1+\vec{\tau}_1\cdot\vec{\tau}_2)$ are, respectively, the spin and isospin exchange operators of particles 1 and 2, $\rho(\vec{r})$ is the total density of the system at point $\vec{r}$, and μ_i=0.7 and 1.2 fm, W_i, B_i, H_i, M_i, and t_3 are parameters.

- Skyrme*

$$V(\vec{r}_1\vec{r}_2;\vec{r}\,'_1\vec{r}\,'_2) = \Big\{t_0(1+x_0P^\sigma) + \tfrac{1}{6}t_3(1+x_3P^\sigma)\rho^\alpha\left(\tfrac{1}{2}(\vec{r}_1+\vec{r}_2)\right)$$
$$+\tfrac{1}{2}t_1(1+x_1P^\sigma)[\vec{k}'^{*2}+\vec{k}^2] + t_2(1+x_2P^\sigma)\vec{k}'^{*}\cdot\vec{k}\Big\}\,\delta(\vec{r}_1-\vec{r}\,'_1)\delta(\vec{r}_2-\vec{r}\,'_2)\delta(\vec{r}_1-\vec{r}_2),$$

where the relative-momentum operators read $\hat{\vec{k}} = \frac{1}{2i}\left(\vec{\nabla}_1-\vec{\nabla}_2\right)$, $\hat{\vec{k}}' = \frac{1}{2i}\left(\vec{\nabla}\,'_1-\vec{\nabla}\,'_2\right)$.

*We omit the spin-orbit and tensor terms for simplicity.

Ab initio derivation of model EDFs

Jyväskylä – York – Surrey – Lyon collaboration

A few remarks are in order:

- In the standard derivation of the DFT, the first-step constrained variation corresponds to probing the system with an external one-body field. By inverting the obtained relation $\rho[U]$ and inserting it into the functional $E[U]$, one can, again in principle, obtain the final exact EDF, $E[\rho]$.
- The second-step variation, with respect to the density, $\delta_{\rho(r)}E[\rho]=0$, obviously then gives the exact ground-state energy and the exact ground-state local one-body density.
- The EDF is always meant to be minimized with respect to the density, and thus its detailed form beyond the minimum is not essential.
- Therefore, for the model functionals built from the generators, the manifold of meaningful ground-state densities is not really infinite dimensional, but it can be parametrized by the coupling constants, so it has a finite number of dimensions.
- If we use model functionals, then instead of probing the system with all possible one-body potentials of an arbitrary shape, it is enough to probe it within the finite set of the EDF generators.

Ab initio derivation of model EDFs

The goal is to provide an *ab initio* derivation within a certain class of model EDFs $\tilde{E}[\rho]$:

$$\tilde{E}[\rho] = \sum_{i=1}^{m} C^i V_i[\rho],$$

where C^i are coupling constants and $V_i[\rho]$ are the EDF generators.

Instead of probing the system with all possible one-body potentials it is enough to probe it within the finite set of the EDF generators $-\hat{V}_j$, that is, to solve the constrained variational equation,

$$\delta E' = \delta \langle \Psi | \hat{H} - \sum_{j=1}^{m} \lambda^j \hat{V}_j | \Psi \rangle = 0,$$

for a suitable set of values of a finite number of Lagrange multipliers λ^i, which is perfectly manageable a task.

Solution of this equation gives us the exact ground-state energies $E(\lambda^j)$ and one-body non-local densities $\rho_{\lambda^j}(r_1, r_2)$, both as functions (not functionals!) of the Lagrange multipliers λ^j. Then we adjust the EDF coupling constants C^i so as to have,

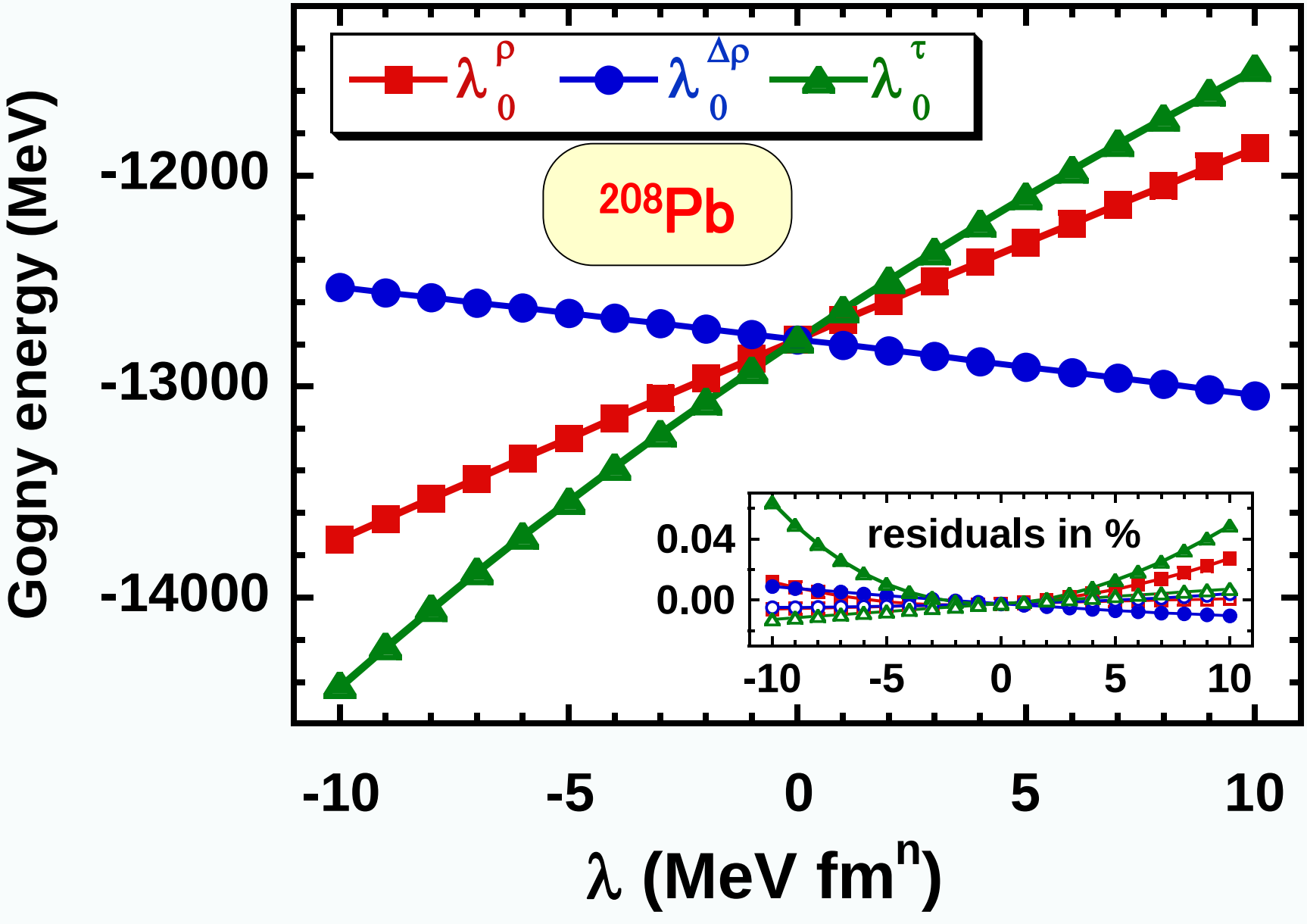
$$E(\lambda^j) = \sum_{i=1}^{m} C^i V_i[\rho_{\lambda^j}].$$

J.D., J. Phys. G: Nucl. Part. Phys. 43, 04LT01 (2016)

More remarks are in order:

- After adjustment of the best coupling constants, one obtains a true ab initio-equivalent model EDF.
- On the manifold of the exact one-body densities, the model EDF then gives the closest possible approximation to the exact energies.
- After the minimization in the space of all one-body densities (the second-step variation), the resulting approximate energies may deviate from the exact ones, and this may inform us about the quality of the proposed model EDF.
- Within the outlined method, only true two-, three-, or many-body operators can be used as functional generators. The obtained EDFs are than automatically self-interaction free and usable in the beyond-mean-field approaches.

Gogny-equivalent Skyrme EDF



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Gogny-equivalent Skyrme EDF

S1Se

		$t=0$	$t=1$
C_t^{ρ}	(MeV fm^3)	−605.41(16)	509(3)
$C_t^{\Delta\rho}$	(MeV fm^5)	−74.82(12)	41(2)
C_t^{τ}	(MeV fm^5)	79.73(16)	−98(2)

Table 1: Gogny-force D1S ground-state energies E_G (b) compared to energies E (c) calculated using the Skyrme EDF S1Se.

	E_G	E	δE	$\delta E/\lvert E\rvert$	$\delta E/\Delta E$
(a)	(b)	(c)	(d)	(e)	(f)
^{16}O	−129.626	−128.83(6)	0.79	0.61%	13
^{40}Ca	−344.663	−344.34(6)	0.32	0.09%	5
^{48}Ca	−416.829	−419.36(7)	−2.53	−0.61%	−37
^{56}Ni	−483.820	−485.83(7)	−2.01	−0.42%	−29
^{78}Ni	−640.598	−642.99(13)	−2.39	−0.37%	−18
^{100}Sn	−830.896	−832.60(10)	−1.70	−0.20%	−18
^{132}Sn	−1103.246	−1107.17(15)	−3.93	−0.36%	−26
^{208}Pb	−1638.330	−1641.26(16)	−2.93	−0.18%	−18
rms	n.a.	n.a.	2.34	0.40%	22

J.D., J. Phys. G: Nucl. Part. Phys. 43, 04LT01 (2016)

Gogny-equivalent Skyrme EDF

S1Se

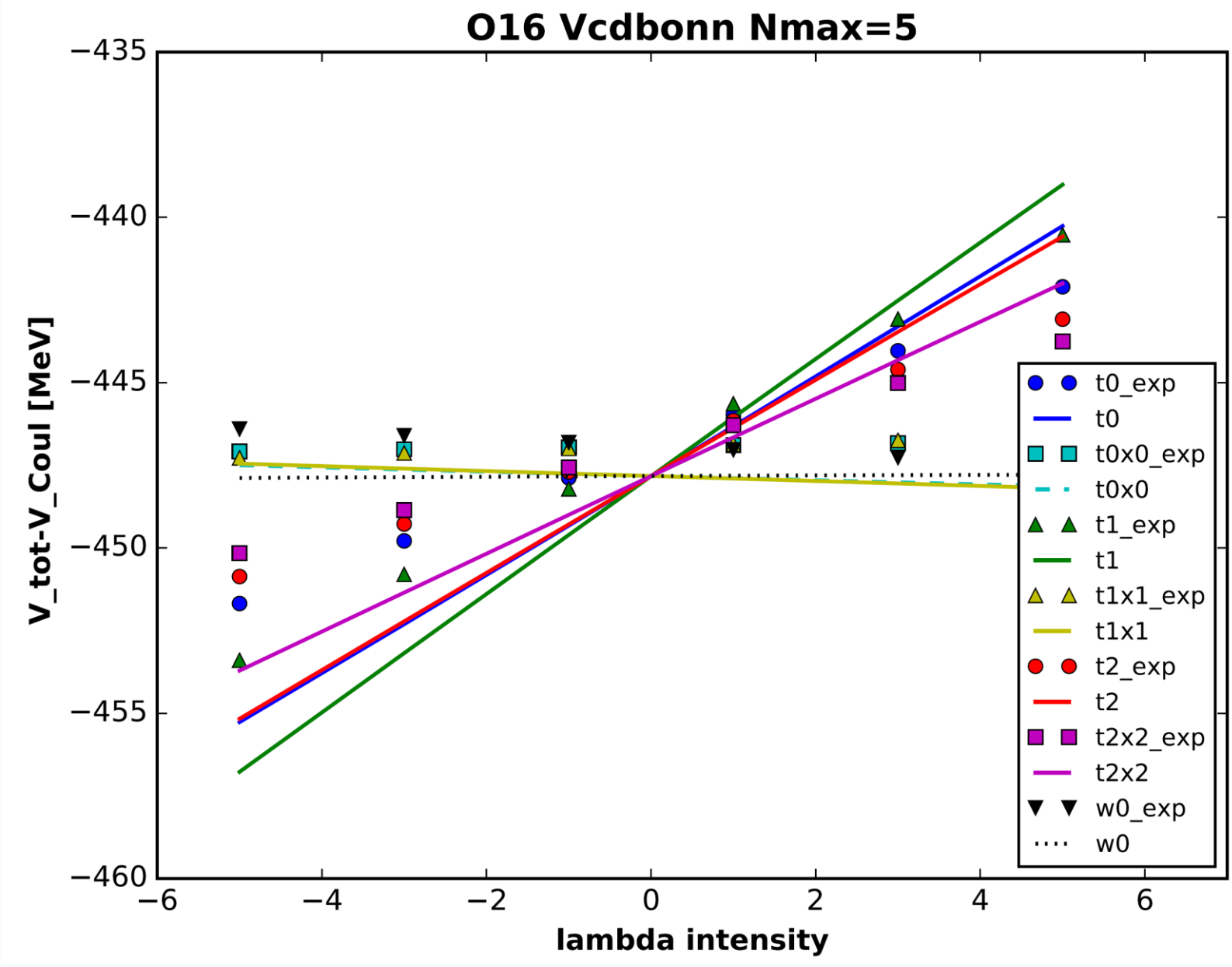
		$t=0$	$t=1$
C_t^{ρ}	(MeV fm^3)	−605.41(16)	509(3)
$C_t^{\Delta\rho}$	(MeV fm^5)	−74.82(12)	41(2)
C_t^{τ}	(MeV fm^5)	79.73(16)	−98(2)

Table 2: Gogny-force D1S ground-state radii R_G (b) compared to radii R (c) calculated using the Skyrme EDF S1Se.

	R_G	R	δR	$\delta R/R$	$\delta R/\Delta R$
(a)	(b)	(c)	(d)	(e)	(f)
^{16}O	2.6689	2.6350(7)	−0.0339	−1.27%	−48
^{40}Ca	3.4117	3.3860(8)	−0.0257	−0.75%	−31
^{48}Ca	3.4423	3.4347(10)	−0.0076	−0.22%	− 8
^{56}Ni	3.6773	3.6781(11)	0.0008	0.02%	1
^{78}Ni	3.9070	3.9222(10)	0.0151	0.39%	16
^{100}Sn	4.4070	4.4118(12)	0.0048	0.11%	4
^{132}Sn	4.6530	4.6694(11)	0.0164	0.35%	15
^{208}Pb	5.4365	5.4535(12)	0.0170	0.31%	14
rms	n.a.	n.a.	0.0183	0.57%	22

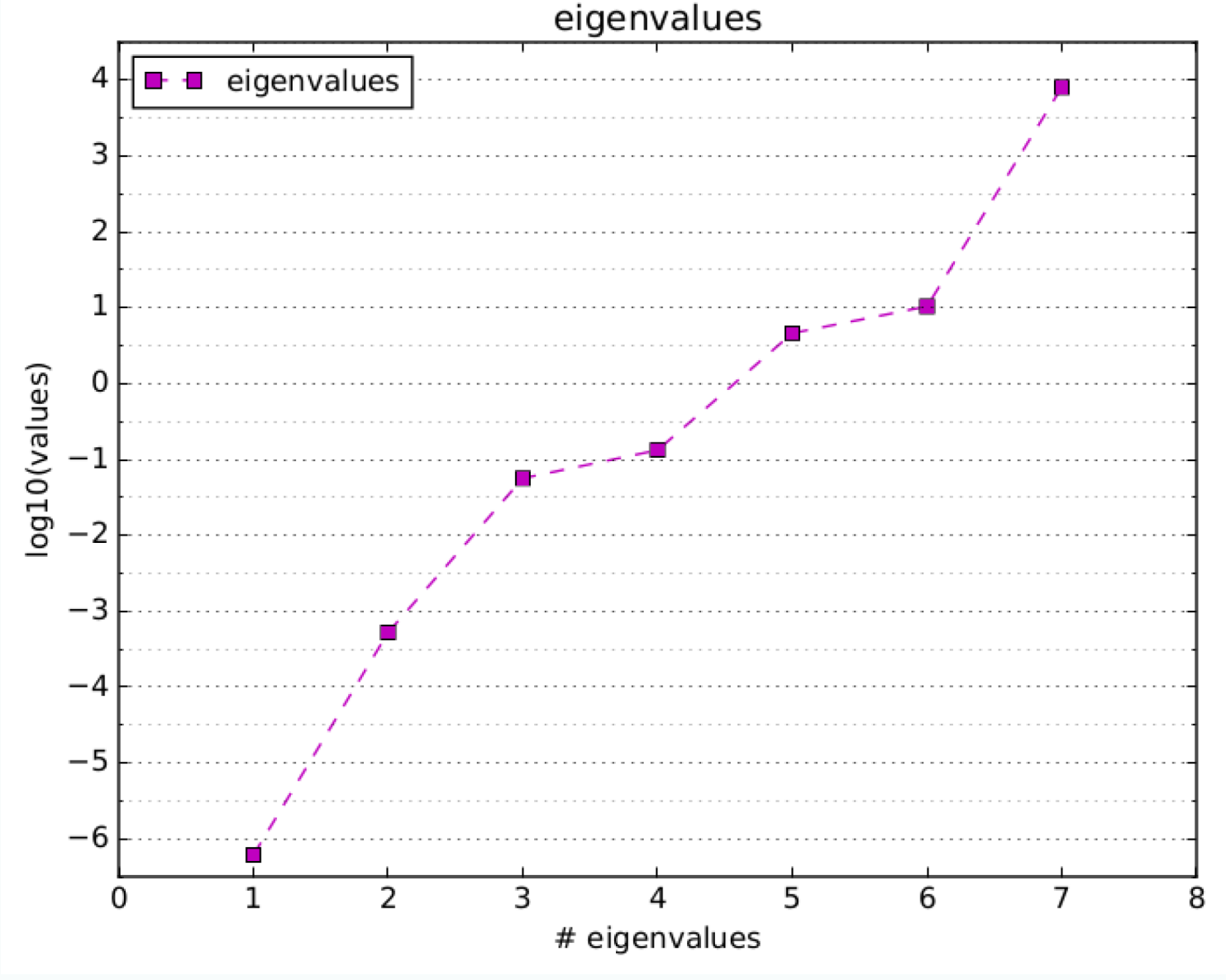
J.D., J. Phys. G: Nucl. Part. Phys. 43, 04LT01 (2016)

SV-like EDF from CD Bonn



G. Salvioni et al., to be published

SV-like EDF from CD Bonn



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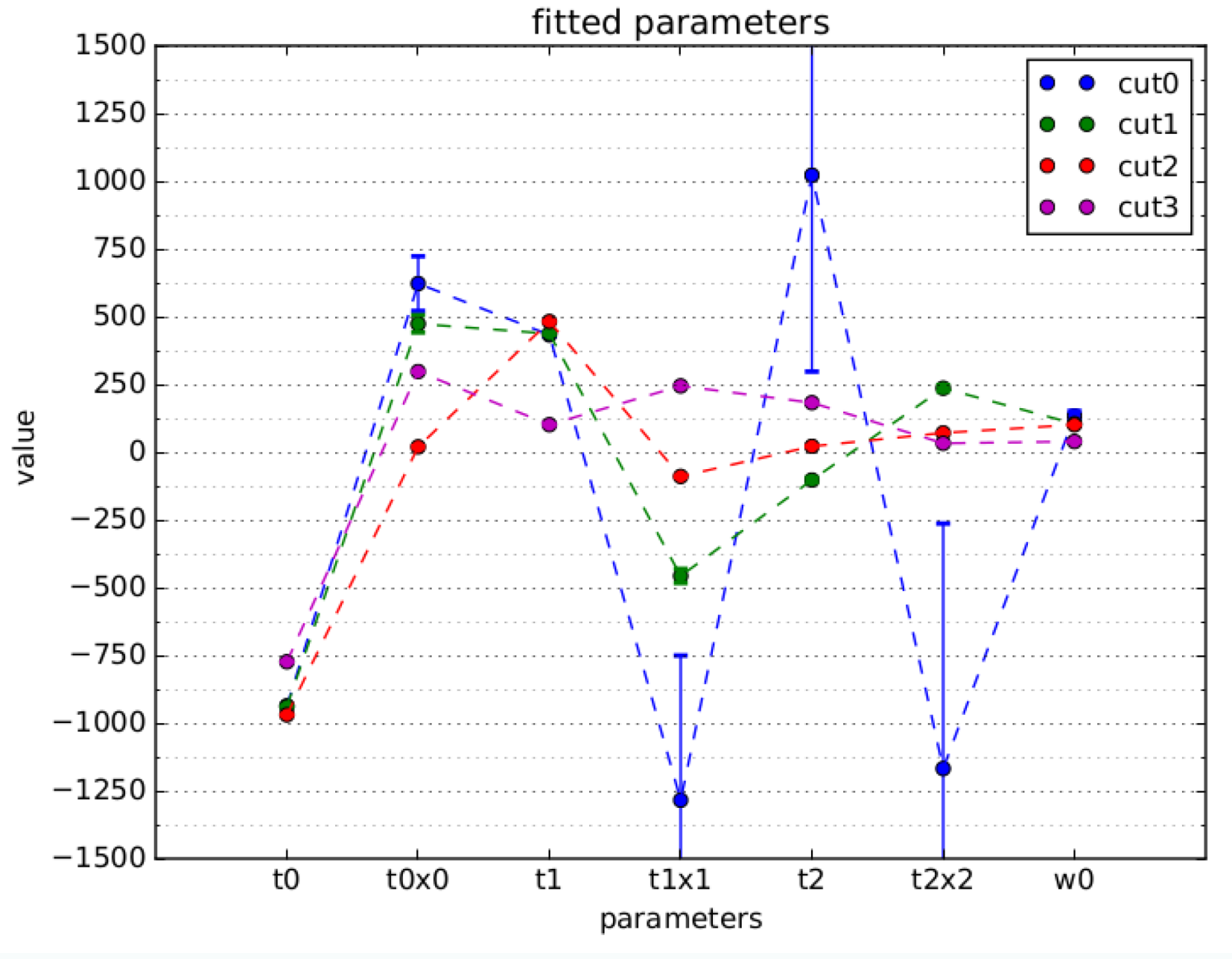
SV-like EDF from CD Bonn



G. Salvioni et al., to be published

Conclusions

- *Ab initio* **derivations of density functionals are progressing.**

Thank you

Collectivity

beyond mean field, ground-state correlations, shape coexistence, symmetry restoration, projection on good quantum numbers, configuration interaction, generator coordinate method, multi-reference DFT, etc….

$$E = \frac{\langle\Psi|\hat{H}|\Psi\rangle}{\langle\Psi|\Psi\rangle} \simeq \int\int \mathrm{d}\vec{r}\mathrm{d}\vec{r}\,' \mathcal{H}(\rho(\vec{r},\vec{r}\,'))$$

True for interaction

$$\text{for} \quad \rho(\vec{r},\vec{r}\,') = \frac{\langle\Psi|a^{+}(\vec{r}\,')a(\vec{r}\,')|\Psi\rangle}{\langle\Psi|\Psi\rangle}$$

$$\frac{\langle\Psi_1|\hat{H}|\Psi_2\rangle}{\langle\Psi_1|\Psi_2\rangle} \simeq \int\int \mathrm{d}\vec{r}\mathrm{d}\vec{r}\,' \mathcal{H}(\rho_{12}(\vec{r},\vec{r}\,'))$$

$$\text{for} \quad \rho_{12}(\vec{r},\vec{r}\,') = \frac{\langle\Psi_1|a^{+}(\vec{r}\,')a(\vec{r}\,')|\Psi_2\rangle}{\langle\Psi_1|\Psi_2\rangle}$$

The density dependence causes havoc

Particle-number projection impossible

Strong self interaction present

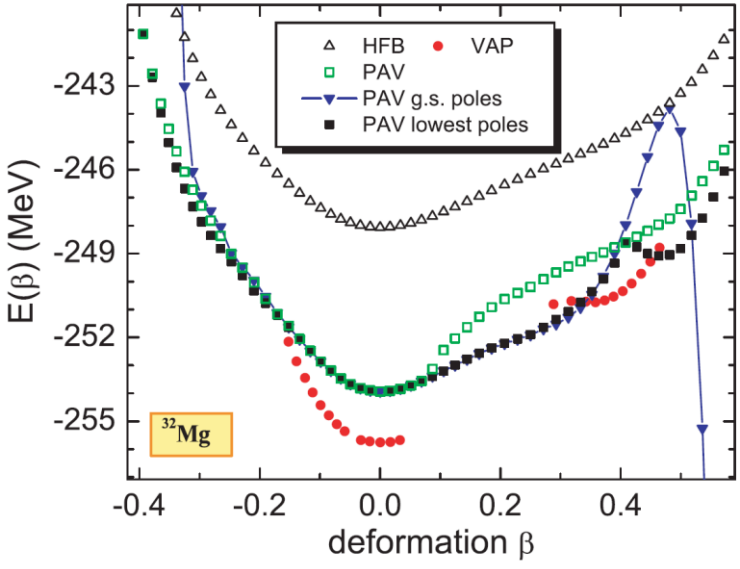


FIG. 11. (Color online) Deformation energy $E(\beta)$ as a functio quadrupole deformation β calculated for ^{32}Mg with the SIII force volume pairing interaction. Results of the PAV HFB+LN calculati (squares and triangles) are compared with the VAP PNP results (d The standard HFB result is shown by open triangles.

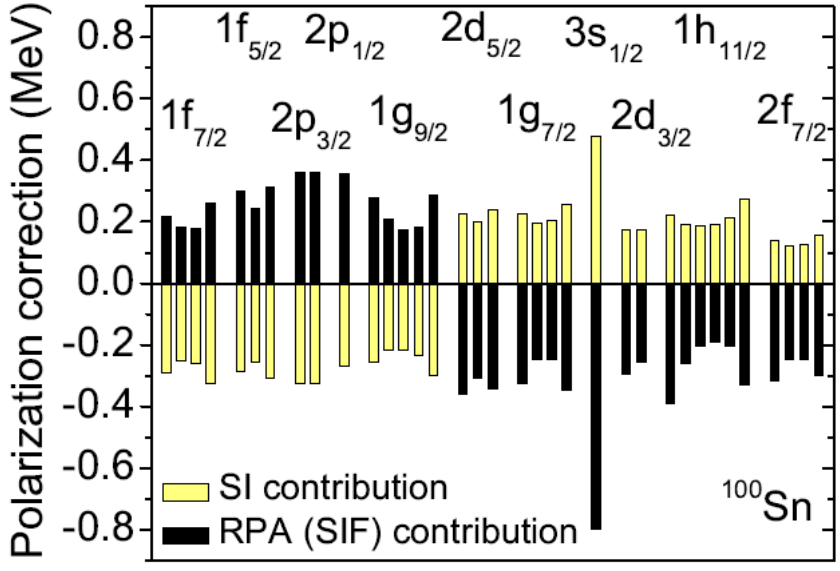
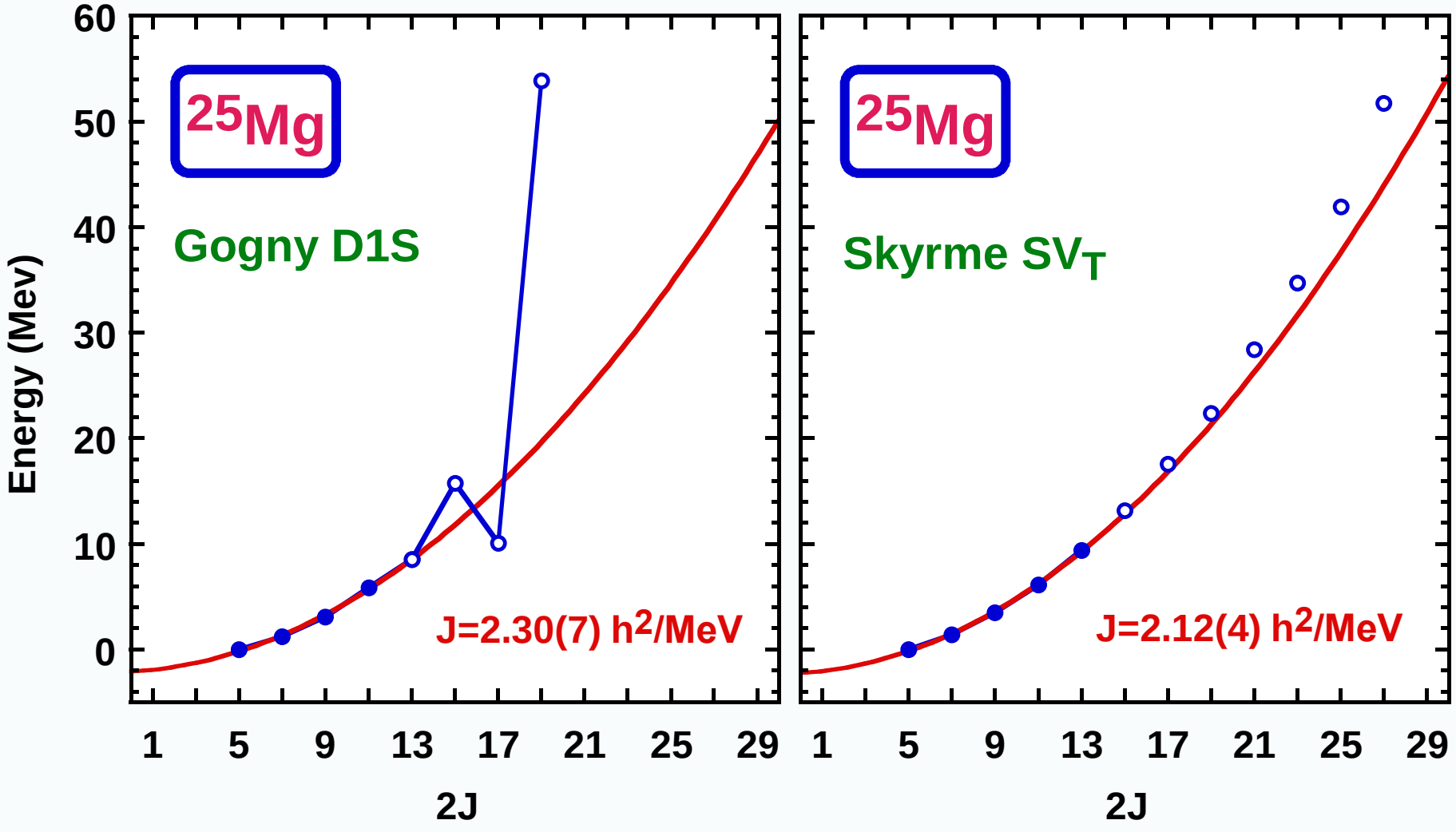


FIG. 6: (Color online) The SIF and SI contributions to the polarization corrections of Eq. (46), calculated in ^{100}Sn for the Skyrme EDF SLy5.

J.D. et *al.*, Phys. Rev. C 76, 054315 (2007)

D. Tarpanov. et *al.*, Phys. Rev. C 89, 014307 (2014)

Rotational symmetry restoration in odd nuclei



M. Bender & J.D., to be published

1) **"Remember that all models are wrong; the practical question is how wrong do they have to be to not be useful"**
G.E.P. Box and N.R. Draper
Empirical Model Building and Response Surfaces
(John Wiley & Sons, New York, 1987)

- **Error Estimates of Theoretical Models: a Guide:**
  J. Dobaczewski, W. Nazarewicz, P.-G. Reinhard,
  J. Phys. G: Nucl. Part. Phys. 41 (2014) 074001
- **Enhancing the interaction between nuclear experiment and theory through information and statistics**
  D.G. Ireland and W. Nazarewicz
  J. Phys. G: Nucl. Part. Phys. 42 (2015) 030301

Zero-range vs. regularized finite-range pseudopotentials and functionals

Zero range:

B.G. Carlsson *et al.*, Phys. Rev. C 78, 044326 (2008)
F. Raimondi et al., Phys. Rev. C 83, 054311 (2011)

$$\hat{V}^{\tilde{n}'\tilde{L}'}_{\tilde{n}\tilde{L},v_{12}S} = \tfrac{1}{2} i^{v_{12}} \left(\left[\left[K'_{\tilde{n}'\tilde{L}'} K_{\tilde{n}\tilde{L}} \right]_S \hat{S}_{v_{12}S} \right]_0 + (-1)^{v_{12}+S} \left[\left[K'_{\tilde{n}\tilde{L}} K_{\tilde{n}'\tilde{L}'} \right]_S \hat{S}_{v_{12}S} \right]_0 \right) \times \left(1 - \hat{P}^M \hat{P}^\sigma \hat{P}^\tau \right) \delta(\vec{r}\,'_1 - \vec{r}_1) \delta(\vec{r}\,'_2 - \vec{r}_2) \delta(\vec{r}_1 - \vec{r}_2).$$

Finite range:

F. Raimondi *et al.*, J. Phys. G 41, 055112 (2014)

$$\hat{V}^{\tilde{n}'\tilde{L}',\bar{t}}_{\tilde{n}\tilde{L},v_{12}S} = \tfrac{1}{2} i^{v_{12}} \left(\left[\left[K'_{\tilde{n}'\tilde{L}'} K_{\tilde{n}\tilde{L}} \right]_S \hat{S}_{v_{12}S} \right]_0 + (-1)^{v_{12}+S} \left[\left[K'_{\tilde{n}\tilde{L}} K_{\tilde{n}'\tilde{L}'} \right]_S \hat{S}_{v_{12}S} \right]_0 \right) \times \left(\hat{P}^\tau \right)^{\bar{t}} \left(1 - \hat{P}^M \hat{P}^\sigma \hat{P}^\tau \right) \delta(\vec{r}\,'_1 - \vec{r}_1) \delta(\vec{r}\,'_2 - \vec{r}_2) g_a(\vec{r}_1 - \vec{r}_2).$$

Numbers of terms of the finite-range pseudopotential at different orders up to N^{3}LO. In the second, third, and fourth column, numbers of central ($\tilde{S} = 0$), SO ($\tilde{S} = 1$), and tensor ($\tilde{S} = 2$) terms, respectively, are displayed.

Order	$\tilde{S} = 0$	$\tilde{S} = 1$	$\tilde{S} = 2$	Total
0	4	0	0	4
2	8	2	4	14
4	16	4	10	30
6	24	8	20	52
N^{3}LO	52	14	34	100