Some challenges for Nuclear Density Functional Theory

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Outlook

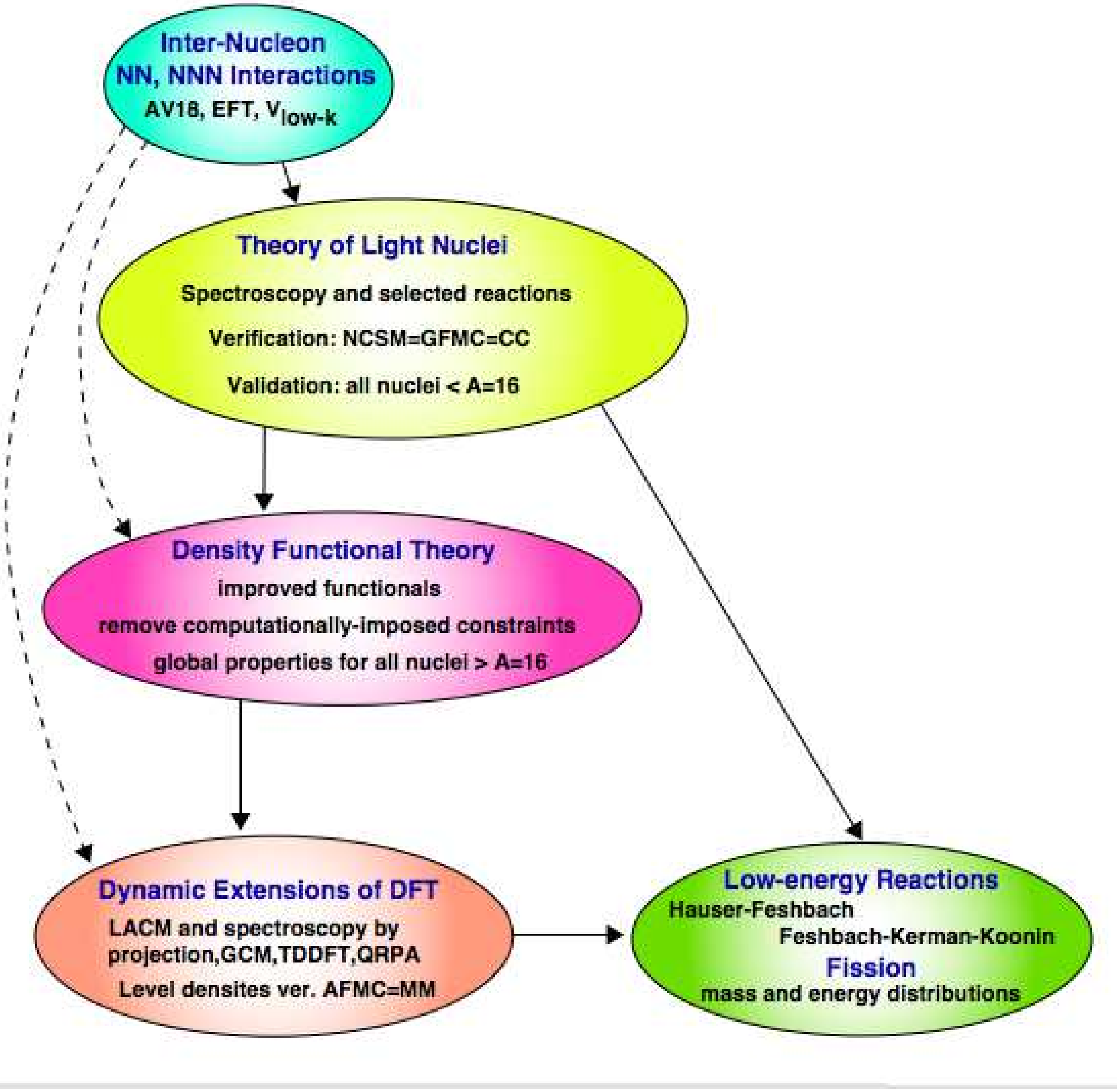
I. A few words about DFT and selected challenges (non exhaustive)

II. First illustration: isovector properties and isovector effective mass

III. Second illustration: ill-defined Particle-Number Projected DFT

IV. Perspectives

Nuclear Structure and Low-Energy Reactions



From George Berstch and others...

Nuclear Density Functional Theory

I. Goal = describe for all nuclei but the lightest

- ♣ Ground-States properties: E, def., radii, s.p. energies (to some extent) drip-lines, pairing
- ♣ Low energy spectroscopy: I, vib., shape isomers, giant resonances
- ♣ Probability transitions: γ, β...
- ♣ EOS of (asymmetric) nuclear matter up to a few ρ_{sat}

II. Basic Ingredients

- ♣ Energy is a functional of one-body density (matrices) $\rho_{ji} = \langle \Phi | a_i^\dagger a_j | \Phi \rangle$ and $\kappa_{ij}^* = \langle \Phi | a_i^\dagger a_j^\dagger | \Phi \rangle$

$$\mathcal{E}\left[\rho, \kappa, \kappa^*\right] = \sum_{ij} t_{ij} \rho_{ji} + \sum_{ikjl} \left[w_{ikjl}^{\rho\rho} \, \rho_{ji} \rho_{lk} + w_{ikjl}^{\kappa\kappa} \, \kappa_{ik}^* \kappa_{jl} \right] \neq \frac{\langle \Phi | H | \Phi \rangle}{\langle \Phi | \Phi \rangle} = E$$

- ♣ $|\Phi\rangle$ is a symmetry breaking product state (HFB functional)
- ♣ Underlying mean-field generated by a Skyrme/Gogny functional
- ♣ Pairing properties (n-n and p-p) generated by a specific part of the functional
- ♣ Direct extensions for excited states (cranking, QRPA)
- ♣ Projected-GCM DFT = Beyond mean-field extension to include long-range correlations
- ♣ Similar for Relativistic DFT

III. Recent milestones and limitations (for now...)

1995	Cranked DFT	$\mathcal{J}^{(2)}$, superdeformation, rotational alignment, Coriolis anti-pairing
2000	Global application of DFT	Mass fits: r.m.s. $\sigma \approx 0.7$ MeV $\Leftrightarrow$ mic-mac models
2000	Spectroscopy by projected GCM	Shape mixing, collective states, Q_s, $M(E0)$ and $B(E2)$ values
2001	DFT at the limits of mass	Predictions for superheavy nuclei: E, lifetimes
2003	Time-dependent DFT	Heavy-ion reactions, low-energy strength functions
2004	Nuclear response in QRPA	Self-consistent QRPA, $dB_\lambda(\omega)/d\omega$ in exotic nuclei, β decay
2004	DFT for fission	Systematics of static fission barriers
2005	Fission dynamics	Mass and kinetic energy distributions in TDGCM-GOA
2005	Correlations in GCM-DFT	Systematics of quadrupole correlations for even-even nuclei

✓ Properties over the known mass table

★ Predictive power in unknown regions $\Longrightarrow$ Witek: "Property of asymptotic freedom of DFT"

★ More specific problems to be addressed but not less important

III. Selection of challenges and crucial inputs from RIA (✓)

Improved phenomenology	✓ Improving single-particle spectra is crucial ⇒ Incorrect spacings spoil low-energy spectroscopy ⇒ RIA = particle/hole states around ^{78}Ni ✓ Tensor force could help (see Jacek's talk on thursday) ✓ Data on superdeformed states, fission isomers/barriers of (exotic) nuclei ✓ Pairing: gradient versus density dependences (isovector, low-density) ⇒ "All" functionals do the job between ^{104}Sn and ^{132}Sn ⇒ RIA = masses up to $^{146/150}Sn$ or ^{81}Ni with $\delta E = 50$ keV ⇒ RIA = reaction cross sections up to ^{85}Ni / $r_n - r_p = 0.5$ fm
Connection to underlying methods	♠ Skyrme/Gogny functionals do not offer enough freedom ★ ⇒ Need guidance beyond a fit on *existing* data ♠ Functional validated through well-defined benchmark ab-initio results★ ♠ Constructive framework from EFT (coherent 2-body/3-body)
Grounding nuclear DFT	♠ No Hohenberg-Kohn theorem for projected-GCM DFT ⇒ Ad-hoc prescription to go from HFB to projected-GCM ♠ Ill-defined Particle-Number Projected DFT ★

Constraining the isovector effective mass m_v^*

T. Lesinski, B. Cochet, K. Bennaceur, T. D. and J. Meyer

I. Why ? Because m_s^* and m_v^* influence

- ♣ Masses and single-particle density of states
- ♣ Shell corrections in superheavy nuclei around the island of stability ($N = 184, Z = 114/126$)
- ♣ Static and dynamical correlations beyond the mean-field level (def., pairing, vibr./rot.)
- ♣ Heavy ion collisions observable to learn about the nuclear OES ; Li *et al.* (2004)

II. How ?

- ♣ $m_s^* (\approx 0.8)$ via the ISGQR in ^{208}Pb ; Reinhard (1999) (consistent with BHF)
- ♣ Constraint on $m_v^* (\approx 0.7 - 0.9)$ via the IVGDR is not strong enough
- ♣ Ab-initio predictions $\Delta m_{n-p}^* = m_n^* - m_p^* \geq 0 \;\Rightarrow\; m_s^* \geq m_v^*$ for $I = (\rho_n - \rho_p)/\rho \geq 0$

  BHF $\Delta m_{n-p}^*|_{I=1} \approx 0.22$ (with/without NNN force) ; Zuo et al. (1999)

  DBHF $\Delta m_{n-p}^*|_{I=1} \approx 0.13$; Ma et al. (2004), van Dalen et al. (2005)

- ♣ Consistent with the energy dependence of the Lane potential; Li (2004)

In DFT

I. Current situation

♣ SLyX forces adjusted on the PNM EOS have $\Delta m^*_{n-p} < 0$; Chabanat et al. (1995)

♣ SkM*/SIII which have an incorrect PNM EOS have the right splitting $\Delta m^*_{n-p} > 0$!

♣ Same with Gogny "old" $D1S$ pamareterization versus new "FT65" ; Girod, private comm.

♣ Relativistic DFT always predict $\Delta m^*_{n-p} < 0$; not trivial to correct for that

Improving global isovector quantities (OES/a_I) seems to deteriorate state-dependent ones (m^*_v)

II. Can we have it all?

♣ Parameterizations (f_3, f_4, f_5) with same fitting protocol (close to SLy5) but different m^*_v

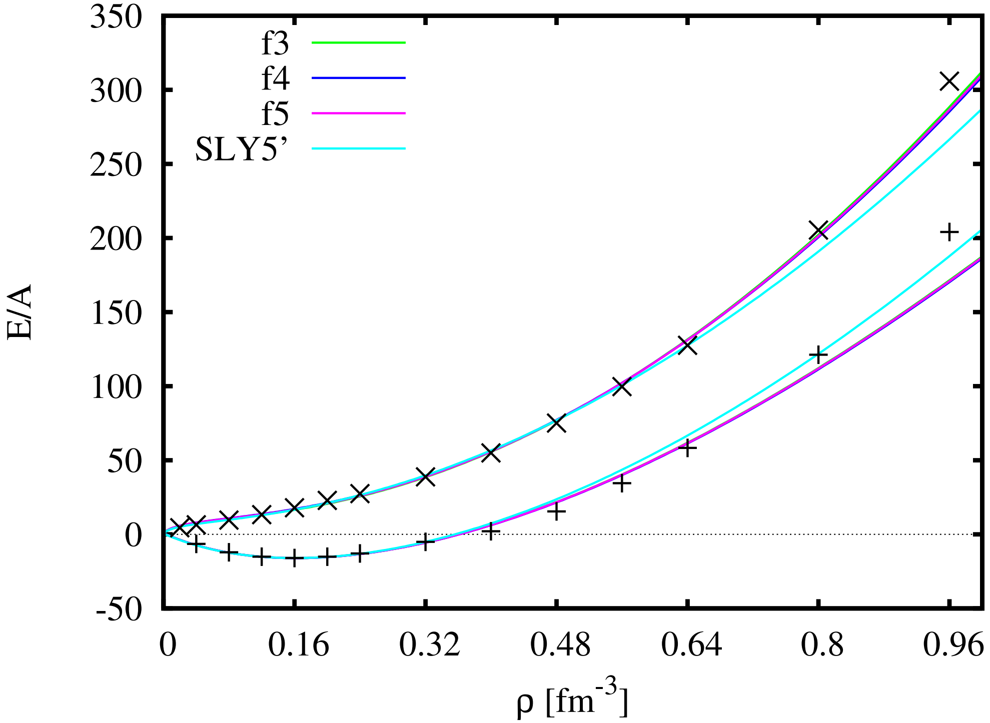
♣ Two density terms $\propto \rho_0^{1/3}; \rho_0^{2/3}$ + no spin-isospin instablities for $\rho < 2\rho_{sat}$ and $I = 0, 1$

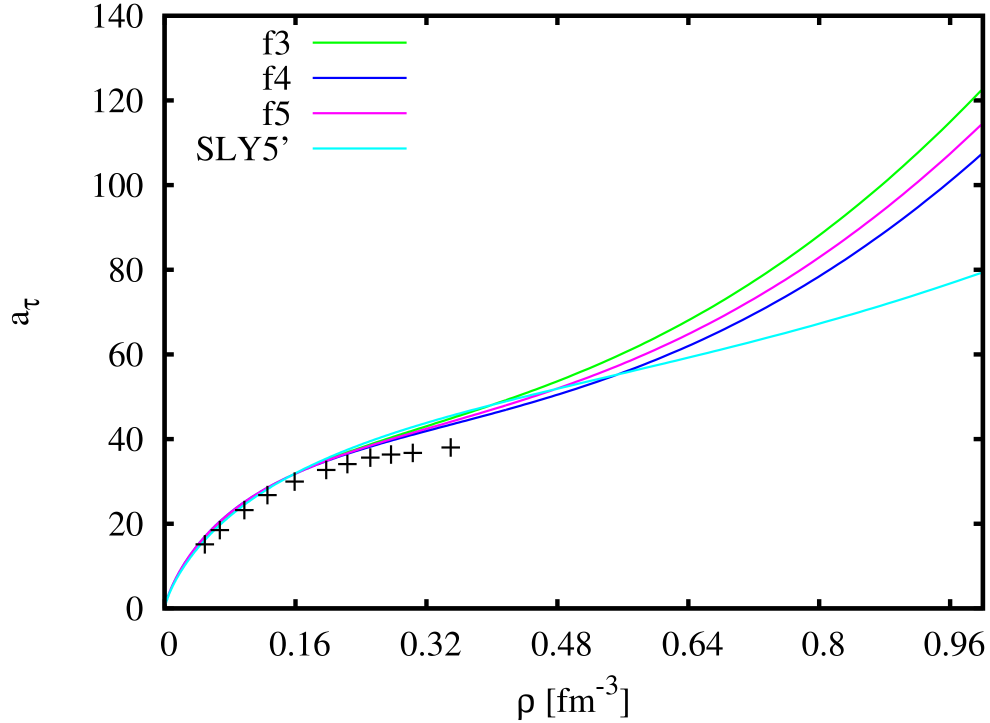
	ρ_{sat}	E/A_{sat}	K_∞	a_I	m^*	$\Delta m^*_{n-p}\|_{I=1}$
SkM*	0.160	-15.770	217	30	0.79	0.356
SkP	0.162	-15.948	201	30	1.00	0.399
SLy5'	0.161	-15.987	230	32	0.70	-0.182
f3	0.162	-16.029	230	32	0.70	-0.284
f4	0.162	-16.036	230	32	0.70	0.170
f5	0.162	-16.035	230	32	0.70	0.001

Results and lessons

I. Global isovector properties

♣ SNM/PNM EOS and a_I versus ab-initio predictions



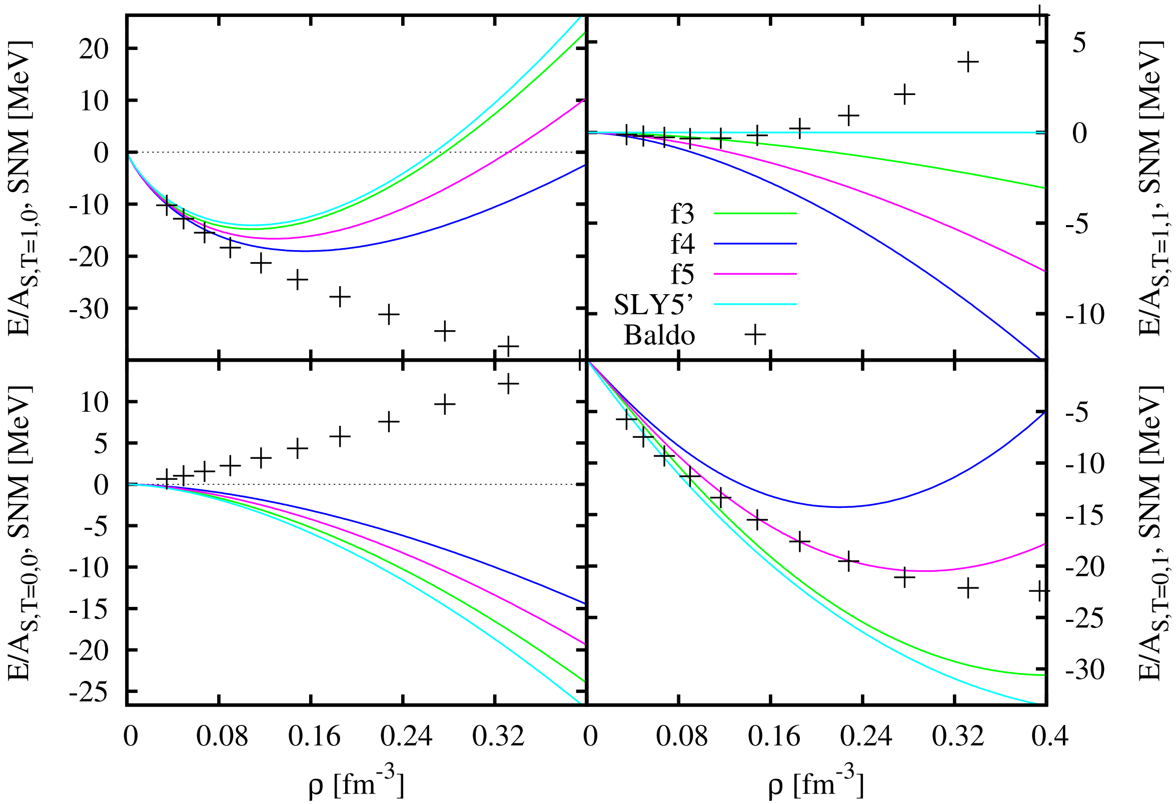


♣ VCS calculations with NN/NNN forces ; $\begin{cases} \text{Akmal } \textit{et al.} \text{ (1998) for EOS} \\ \text{Lagaris and Pandharipande (1981) for } a_I \end{cases}$

♣ Identical properties for (f_3, f_4, f_5) and as good as SLy5'

♣ Is it a good enough test of the quality of isovector properties of the functional ?

♣ Potential energy per (S,T) channel in SNM versus ab-initio predictions



♣ BHF calculations with NN/NNN forces ; Baldo, private comm.

♣ $(S,T) = (0,1); (1,0)$ could be better ; saturation mechanism is not reproduced

♣ $(S,T) = (1,1); (0,0)$ are disastrous $\Leftrightarrow$ density-independent P-wave term ($\propto \vec{k}' \cdot \vec{k}$)

♣ It mainly gets worse as $\Delta m^*_{n-p}|_{I=1}$ is improved !

★ Overall EOS is one thing but good (S,T) properties require more $\Rightarrow$ benchmark ab-initio results

II. Problems encountered

♣ Spin-isospin instability makes it difficult to $\nearrow m^*$ to 0.8

♣ $m^* = 0.7 \Rightarrow$ difficult to lower m^*_v and get PNM OES $\Rightarrow$ Two density terms $\propto \rho_0^{1/3}; \rho_0^{2/3}$

♣ Finite-size isospin instability develops as $\begin{cases} m^*_v \searrow \\ \Delta m^*_{n-p} \nearrow \end{cases} \Leftrightarrow \begin{cases} \rho_n \text{ and } \rho_p \text{ split in finite nuclei} \\ \text{Related to } C_1^{\nabla\rho}\left(\vec{\nabla}\rho_1\right)^2 \text{ in the functional} \\ \text{Already the case of SkP} \end{cases}$

♣ The latter is related to how the energy splits among the four (S,T) channels

	$\Delta m^*_{n-p}\|_{I=1}$	$C_1^{\nabla\rho}$
SkP	0.399	-35.0
SLy5'	-0.182	-16.7
f3	-0.284	-5.4
f4	0.170	-29.4
f5	0.001	-21.4

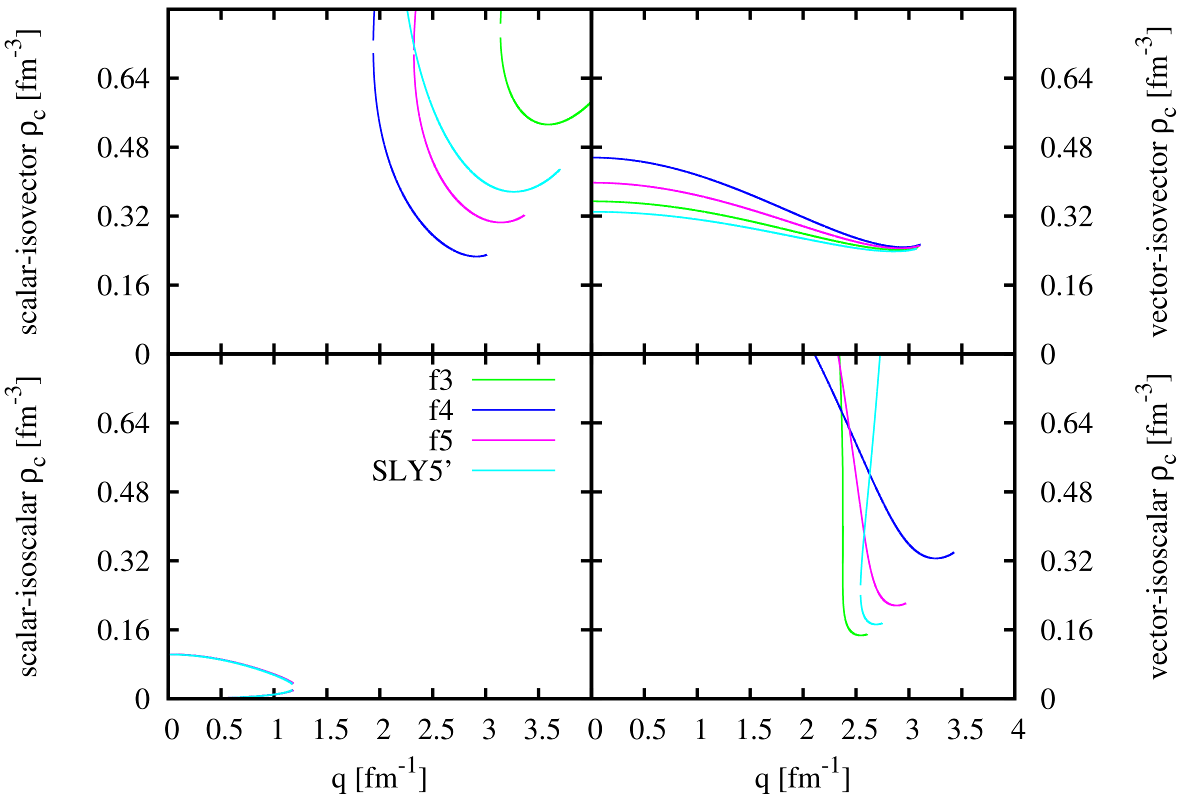
♣ For the Skyrme *force* $C_1^{\nabla\rho}$ is a decreasing function of $\Delta m^*_{n-p}|_{I=1}$

★ Need to be quantified in order to better control the fit/properties of the functional

III. Finite-size instabilities made quantitative : response function (RPA) in SNM

♣ Perturbation $Q^{(\alpha)}(\vec{q}) = \sum_i e^{i\vec{q}\cdot\vec{r}_i}\,\mathcal{O}_i^{(\alpha)}$ with $\mathcal{O}^{(ss)} = 1\,;\mathcal{O}^{(vs)} = \vec{\sigma}\,;\mathcal{O}^{(sv)} = \vec{\tau}\,;\mathcal{O}^{(vv)} = \vec{\sigma}\vec{\tau}$

♣ Poles of $\chi^{(\alpha)}(\omega, q) \Rightarrow \omega(q)$; $\omega(q) = 0$ at density $\rho_c \Leftrightarrow$ Instability of wavelength $\lambda = 2\pi/q$



♣ Spinodal instability for $\rho_0 \leq \rho_c^{ss} \approx 0.1$ fm^{-1} $\Rightarrow$ matter is unstable / compression mode

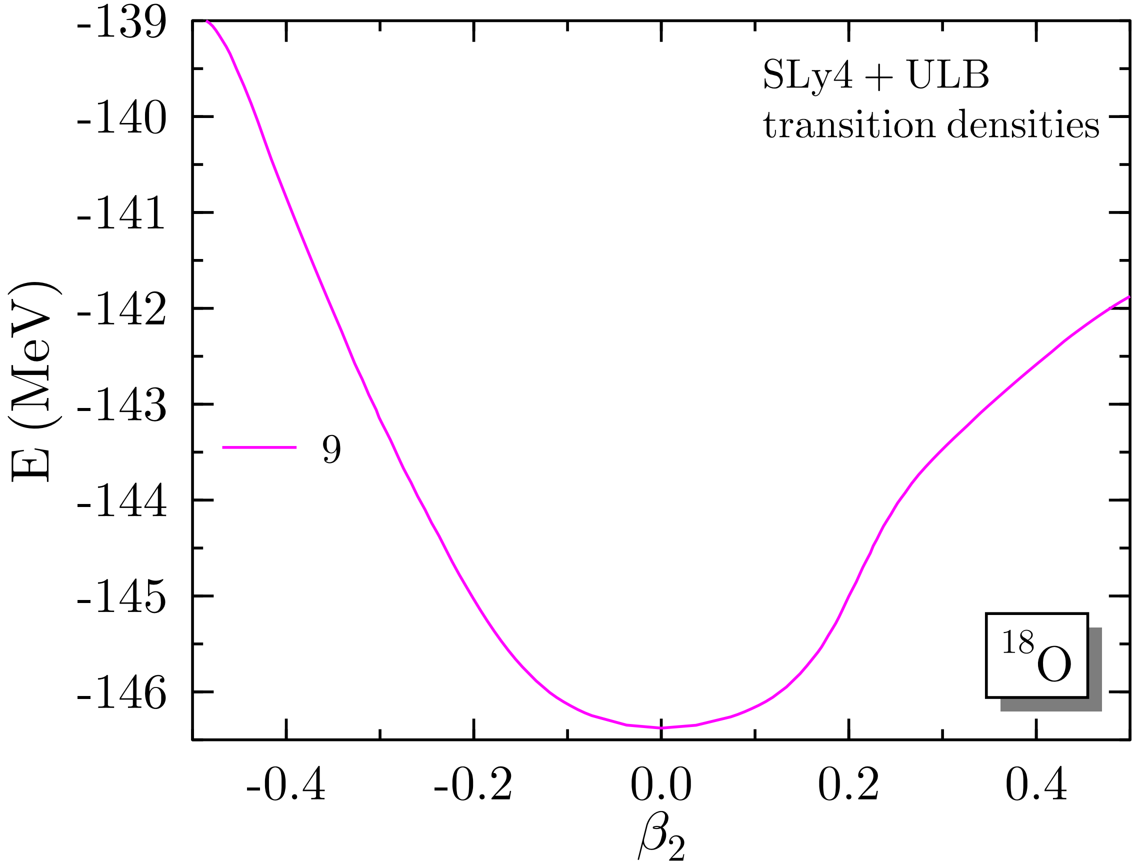
♣ Spin-isospin instabilities (ρ_c^{vv}) are more "dangerous" at finite q than at $q = 0$

♣ At $q \approx 2.5 fm^{-1}$ $\rho_c^{sv} \searrow \rho_{sat}$ as $\Delta m^*_{n-p} \nearrow$

★ Functional is too constrained ; especially the density-independent P-wave term

Problem with PNP-HFB method I

T. D. and M. Bender



$$|\Psi^N\rangle = \frac{1}{2\pi}\int_0^{2\pi} d\varphi\, e^{-i\varphi N}\,|\Phi(\varphi)\rangle$$

$$\mathcal{E}^N = \int_0^{2\pi} d\varphi\, \frac{e^{-i\varphi N}}{2\pi\,\mathcal{D}_N}\,\mathcal{E}\,[\varphi]\;\mathcal{I}[\varphi]$$

PES: ^{18}O

3D PNP-HFBLN (PAV)

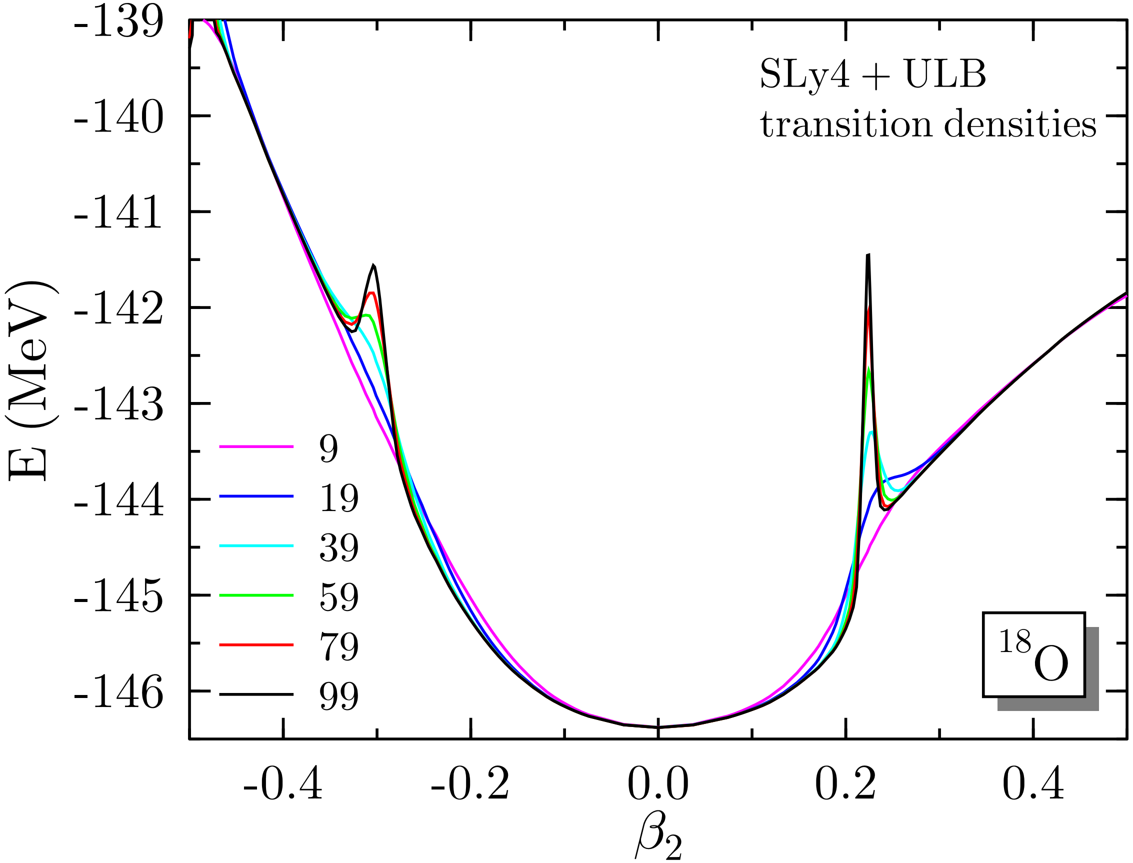
SLy4+ULB

9 φ-integration points

✓Typical of calculations performed so far

✓Results look very reasonable and converged

Problem with PNP-HFB method II



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9/99 φ-integration points

✓Divergence when a pair of states crosses λ, *Anguiano et al. (2001)*

✓Offset in the PES before and after the crossing, *Dobaczewski et al. priv. comm.*

✓More dramatic consequences for VAP calculations

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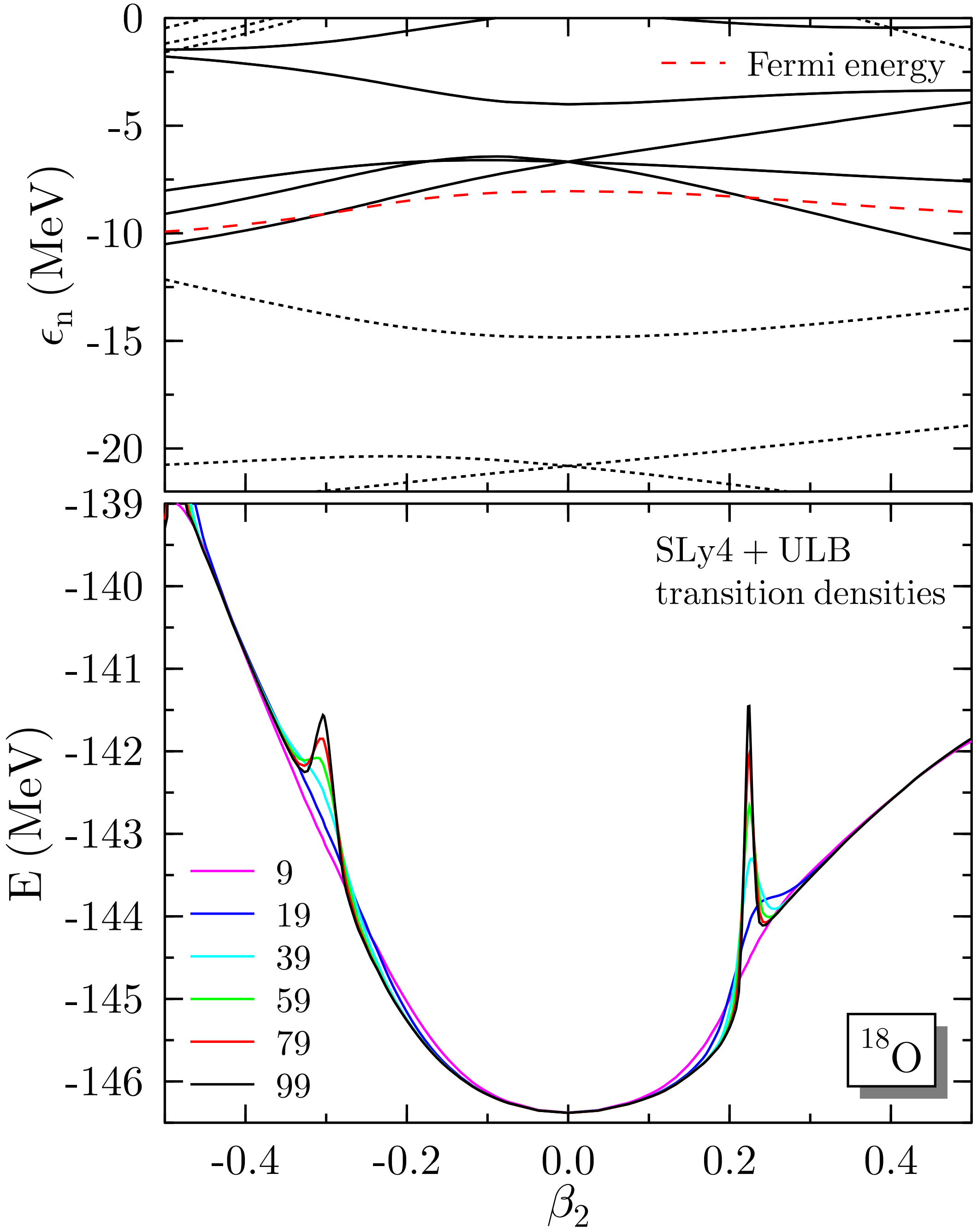

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3D PNP-HFBLN (PAV)

SLy4+ULB+Trans. Dens.

9/99 φ-integration points

λ crosses $\nu d_{5/2}$ orbits

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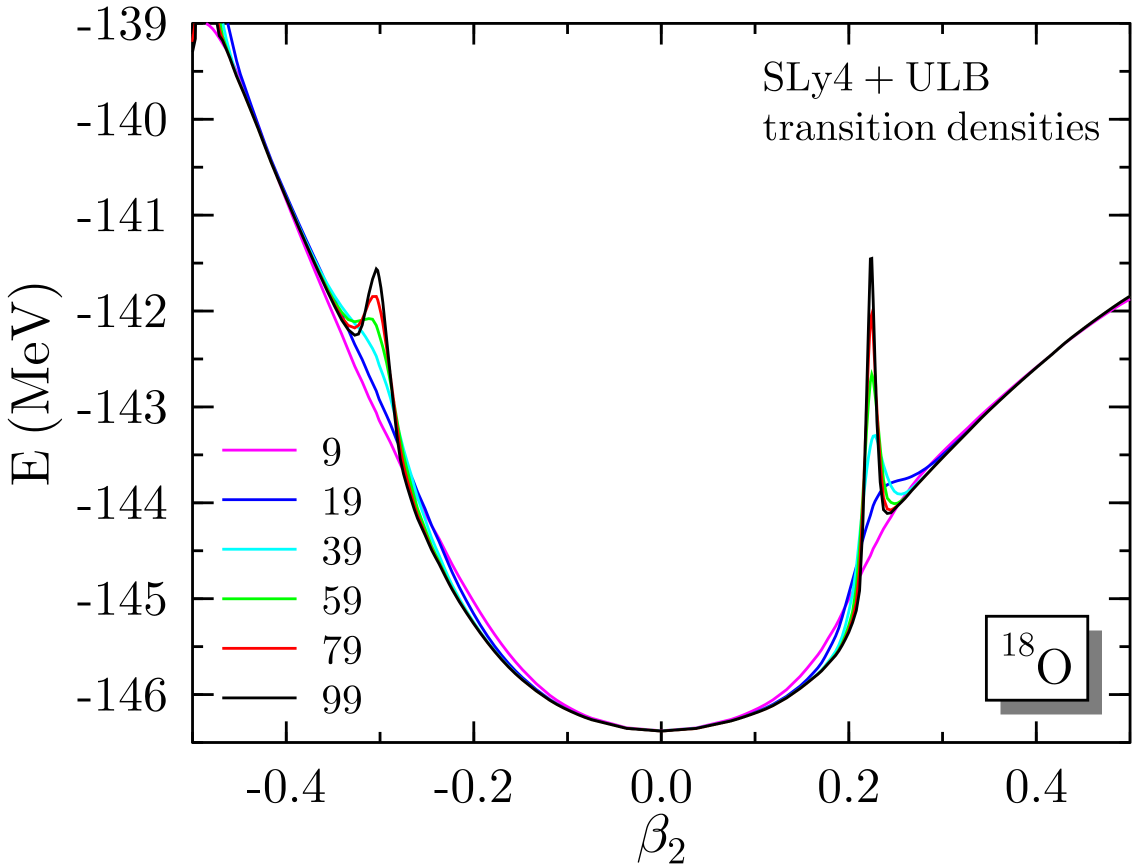

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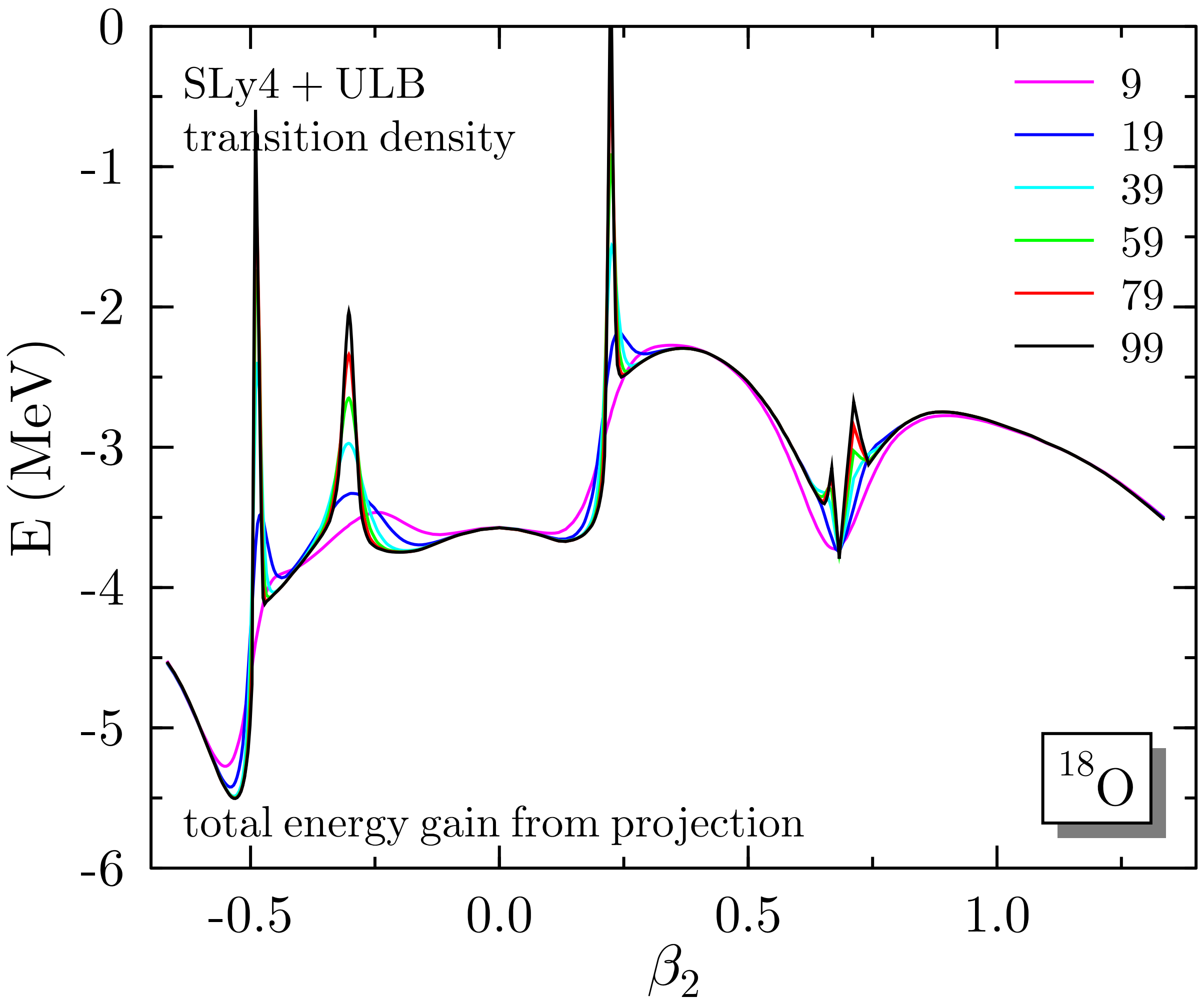
Substracting the HFB energy = gain from projection



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SLy4+ULB+Trans. Dens.

9/99 φ-integration points

Depends on discretization

Divergences and steps

Origin: self-interaction and self-pairing in DFT

I. Self-interaction

A single nucleon in a state φ_μ cannot interact with itself

✓Approximate functionals are usually not self-interaction free

✓Well known issue in Kohn-Sham DFT, *Perdew and Zunger (1981)*

✓Violation of the Pauli principle at the two-body level

✓Exists in Nuclear DFT (Skyrme, Gogny, RMF) but has never been addressed

II.

✓

✓

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II. *Self-pairing*

Two fermions in a pair of conjugated states $(\varphi_\mu, \varphi_{\bar{\mu}})$ cannot get additional binding through a pairing process by scattering onto themselves

✓Exists at the level of HFB $\Rightarrow$ spurious contributions to the energy

✓Pair additive problem

Both are responsible for the dramatic problems at the level of PNP-HFB

Spurious contribution to $\mathcal{E}^N$ in realistic PNP-HFB

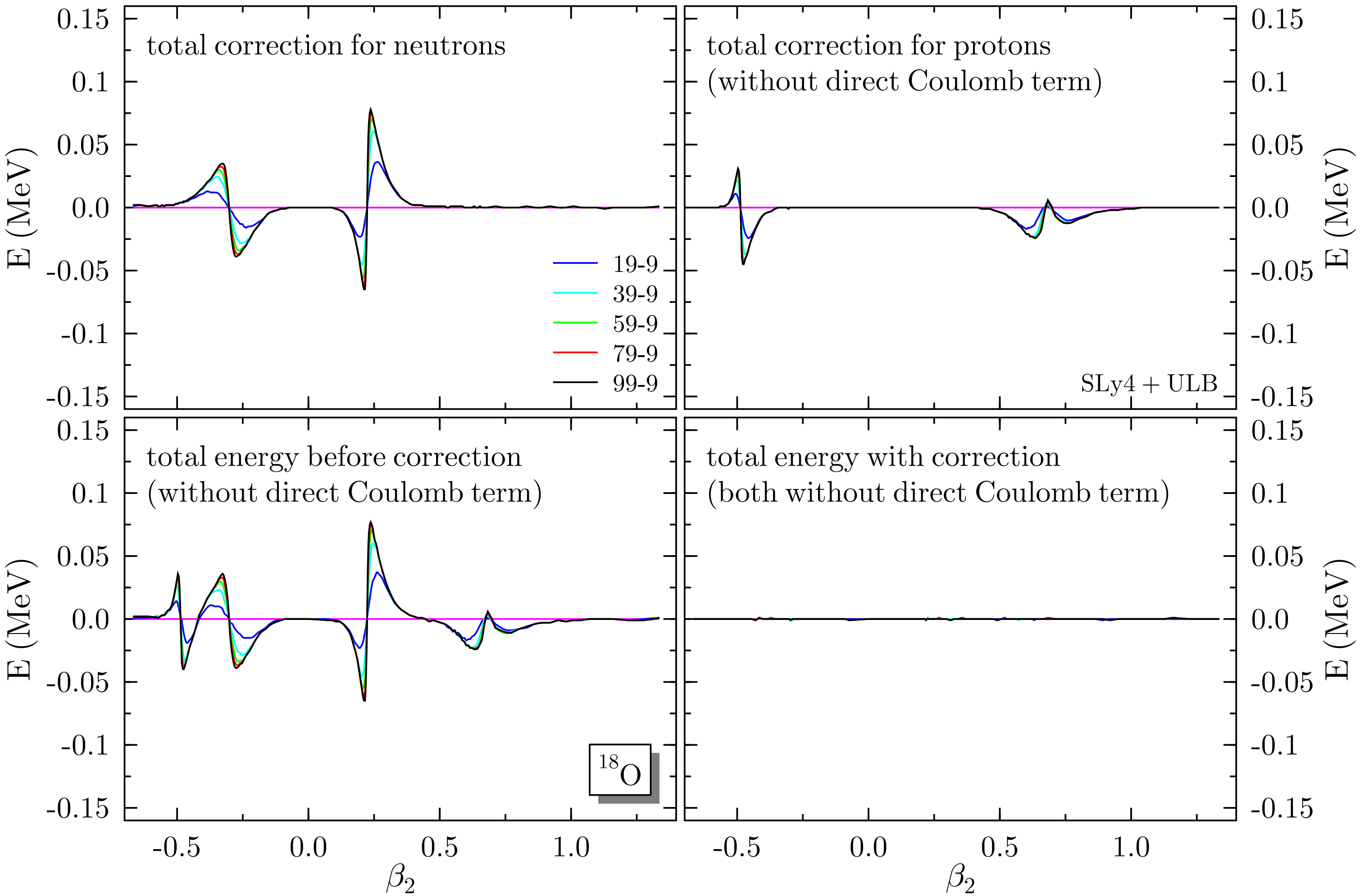
$$\mathcal{E}^N_{spu.} = \sum_{\mu>0} \left[\left(w^{\rho\rho}_{\mu\mu\mu\mu} + w^{\rho\rho}_{\bar{\mu}\bar{\mu}\bar{\mu}\bar{\mu}} + w^{\rho\rho}_{\mu\bar{\mu}\mu\bar{\mu}} + w^{\rho\rho}_{\bar{\mu}\mu\bar{\mu}\mu} \right) - 4\, w^{\kappa\kappa}_{\mu\bar{\mu}\mu\bar{\mu}} \right] \, u^2_\mu v^4_{\bar{\mu}} \int_0^{2\pi} d\varphi \, \frac{e^{-i\varphi N}}{2\pi\, \mathcal{D}_N} \, \frac{e^{2i\varphi} \left(e^{2i\varphi} - 1 \right)}{\left(u^2_\mu + v^2_{\bar{\mu}}\, e^{2i\varphi} \right)^2} \prod_{\nu>0} (u^2_\nu + v^2_{\bar{\nu}}\, e^{2i\varphi})$$

✓Removes the spurious contribution to $\mathcal{E}^N$ = divergences *and* steps

✓Does not modify the HFB functional (= functional at $\varphi = 0$)

✓Correct "only" the most dramatic self-interaction/-pairing effects

Removing divergences

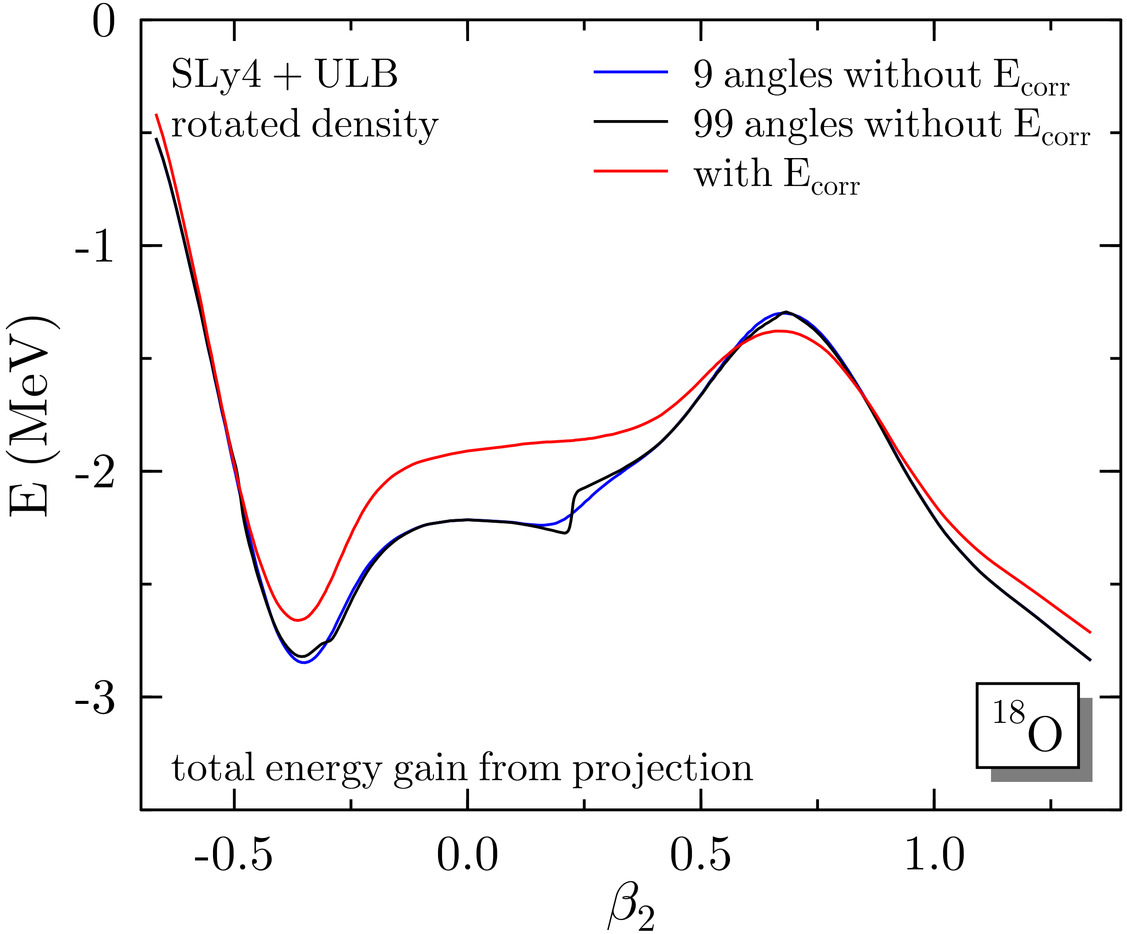


✓S-shape corrections right when neutrons/protons levels cross λ

✓Add up to reproduce the profile of spurious divergences

✓Eliminate perfectly the divergences (numerically stable)

Removing divergences AND steps



✓The projected PES is significantly modified when removing the spurious poles

✓$\mathcal{E}^{N}_{corr.}$ is independent on the number of integration points on a scale of 1 keV

✓Sign of the correction can change ; sum rule $\sum_N \mathcal{D}_N \, \mathcal{E}^{N}_{spu.} = 0$

Conclusions and perspectives

I. Skyrme phenomenology

✓Need to select and reproduce more benchmark ab-initio results.

Ex: potential energy in (S, T) channels. Need to be validated as a benchmark

✓Need to understand over-constraints from covariant analysis of parameters

✓Need to go beyond the standard Skyrme functional

II. Particle Number Projected DFT

✓Solution to the problem of divergences **and jumps** in Particle Number Projected DFT

✓Solution exists for higher-order density dependences

✓Works for Relativistic DFT, *T. Niksic, D. Vretenar, P. Ring, priv. comm.*

✓More systematic study: order of magnitude, stability, impact on GCM mixing ...

✓Self-interaction and self-pairing processes must be corrected for systematically in DFT

✓Projected DFT needs to be properly motivated/constructed

Improved phenomenology	✓ Improving single-particle spectra is crucial ✓ Tensor force could help (see Jacek's talk on thursday) ✓ Data on superdeformed states, fission isomers/barriers of (exotic) nuclei ✓ Constrain time-odd terms (odd nuclei? high-spin states? spin modes?) ✓ Pairing: gradient versus density dependences (isovector, low-density)
Connection to underlying methods	♠ Skyrme/Gogny functionals do not offer enough freedom ★ ⇒ Need guidance beyond a fit on *existing* data ♠ Functional validated through well-defined benchmark ab-initio results ★ ♠ Constructive framework from EFT (coherent 2-body/3-body) ♠ EFT + renormalization group ≡ V_{lowk}+ MBPT ♠ Gradient versus density dependences through DME
Long term strategy	♠ Avoid a "re-invent the wheel" approach ♠ Perdew in Coulomb DFT: "Jacob's ladder" of DFT ♠ Covariant analysis of parameters ; error estimate ; relevance of new data ♠ Improved fitting schemes
Grounding nuclear DFT	♠ No Hohenberg-Kohn theorem for projected-GCM DFT ⇒ Ad-hoc prescription to go from HFB to projected-GCM ♠ Ill-defined Particle-Number Projected DFT ★ ♠ Study spurious self-interaction/-pairing processes and correct for them ★
Multidimensional projected GCM	♠ Breaking more spatial symmetries ♠ Combine quadrupole, octupole, and pairing vibrations ♠ Approximate schemes to reduce computional cost ♠ Inclusion of correlations in the fit of the functional

Constraining the isovector effective mass m_v^*

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I. Why ? Because m_s^* and m_v^* influence

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