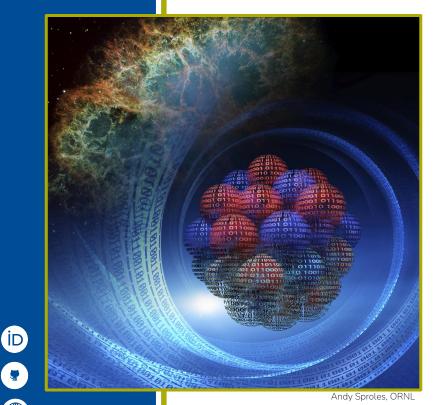
WOUTER RYSSENS



A new generation of Skyrme mass models on a mesh

Wouter Ryssens

22nd of November 2023



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The Brussels state of mind

Extrapolations in

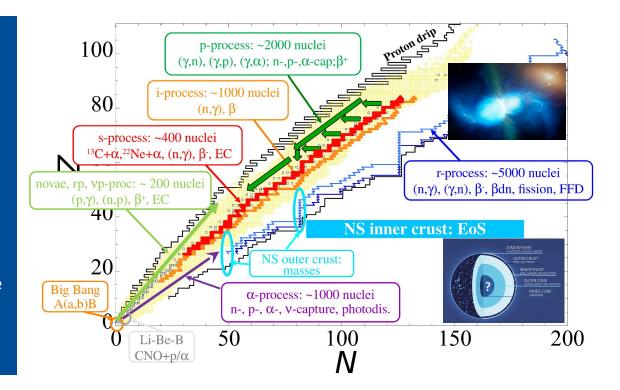
- nucleon number
- energy
- temperature
- density
-

and all of that for

- ~7000 nuclei
- many reactions

what we need is models that should be

- 1. predictive....
- 2. but also **complete**



Brussels-Skyrme-on-a-Grid: BSkG BSkG1 (2021)

- fitted to 2457 masses
- fitted to 884 charge radii
- includes triaxial deformation

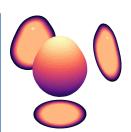
BSkG2 (2022)

- fitted to 45 fission barriers
- includes spins, currents,...

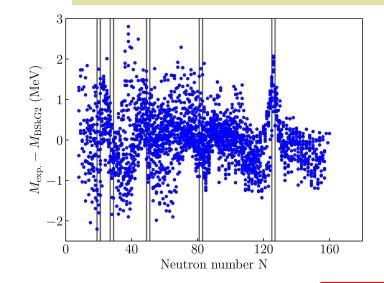


BSkG3 (2023)

- larger max. neutron star mass
- includes octupole deformation

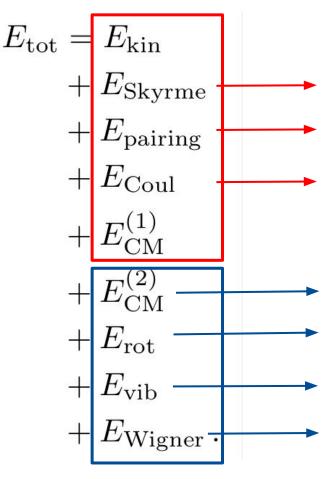


BSkG1: G. Scamps et al., EPJA 57, 333 (2021).
BSkG2: W. Ryssens et al., EPJA 58, 246 (2022). W. Ryssens et al., EPJA 59, 96 (2023).
BSkG3: G. Grams et al., EPJA 59, 270 (2023).



Rms σ	BSkG1	BSkG2	BSkG3
Masses [MeV]	0.741	0.678	0.631
Radii [fm]	0.024	0.027	0.024
L J	0.88	0.44	0.33
Secon. barriers [MeV]	0.87	0.47	0.51
Fission isomers [MeV]		0.49	0.34
Max. NS mass $[M_{\odot}]$	1.8	1.8	2.3

Ingredients: BSkG3



Variationally treated

Skyrme form with additional density dependencies and well-defined time-odd terms (**17** parameters) Mimicking pairing in INM + gradient terms (**3**)

includes finite-size effects of protons and neutrons

Semi-variationally treated

P. Da Costa et al., arXiv:2310.05090

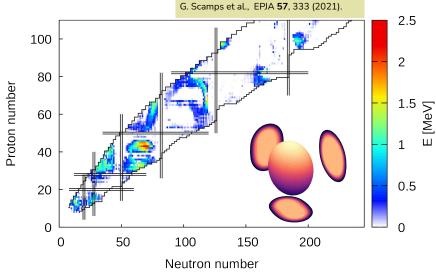
crucial to include for deformation properties

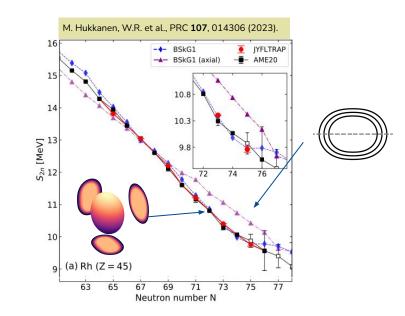
based on simple cranking rotational model (3)

simple rescaling of rotational correction (2)

simple formula; mostly active for light N~Z (4)

Successes: masses

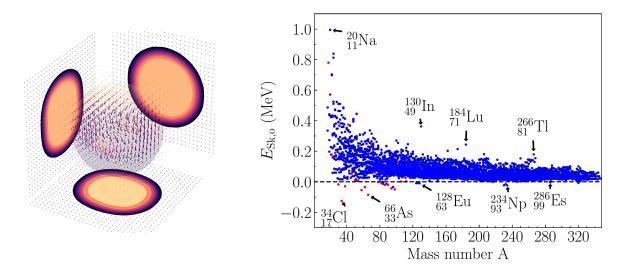




Triaxial deformation

- many nuclei are affected
- effects up to 2.5 MeV near Z~44
- does help reproduce trends, e.g. Rh

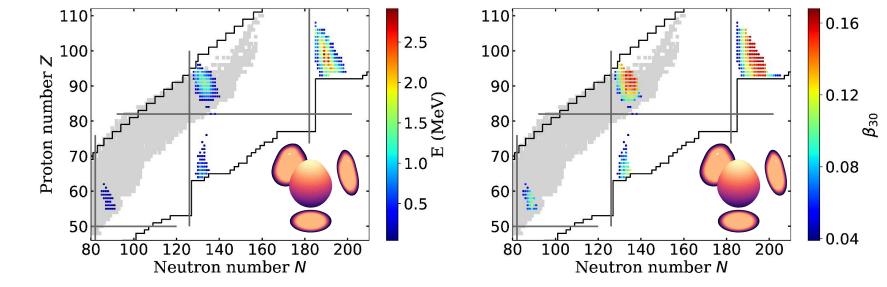
Successes: masses



Time-odd terms

- small impact on the masses
- globally repulsive
- first time checked on this scale!
- first step towards other observables

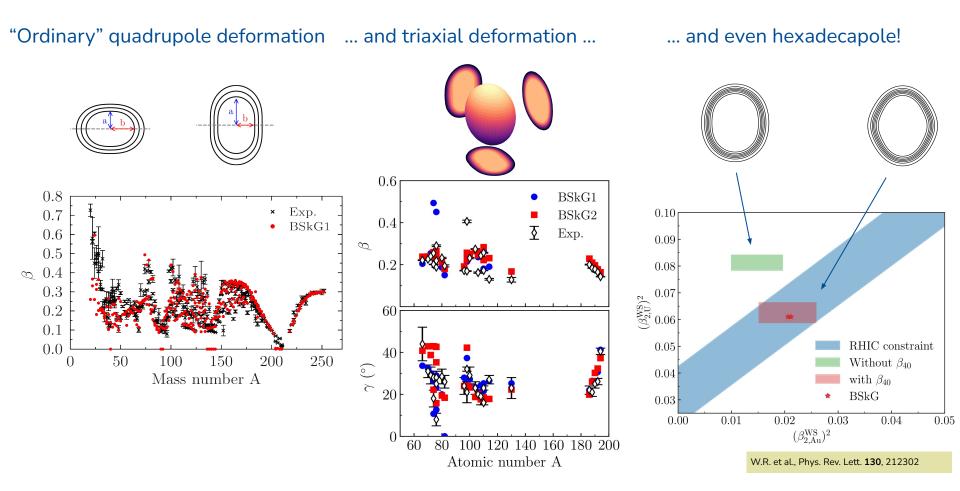
Successes: masses



Reflection asymmetry

- small number of known nuclei affected
- Near N=184:
 - large effect up to 2.5 MeV
 - dripline modified
 - fission properties modified

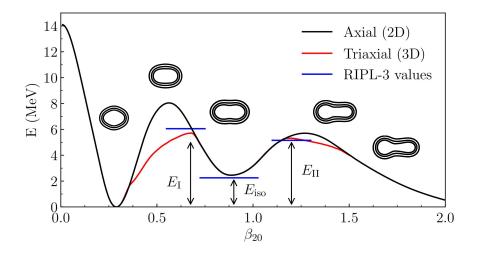
Successes: deformations



Successes: fission $60^{\circ} 50^{\circ}$ 30° 15° 40° 20° $\gamma =$ 10° 0.38 $20.2 \frac{100}{5} \frac{100}{5}$ 5° 0.0 0.21.60 0.40.60.81.01.21.4 β_{20}

W. R. et al., EPJA **59**, 96 (2023).

Successes: fission



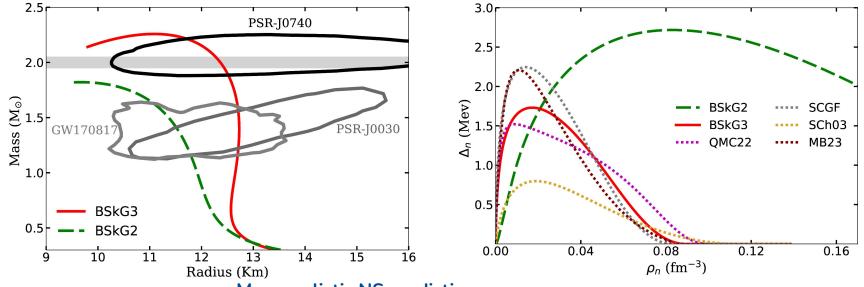
Rms σ	BSkG1	BSkG2	BSkG3
Masses [MeV]	0.741	0.678	0.631
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Fission isomers [MeV]	1.0	0.49	0.34
Max. NS mass $[M_{\odot}]$	1.8	1.8	2.3

Fission properties of 45 actinide nuclei

- includes odd-A and odd-odds
- <u>all</u> inner barriers exploit triaxiality
- <u>all</u> outer barriers exploit
 - octupole deformation
 - triaxial deformation

Successes: neutron stars

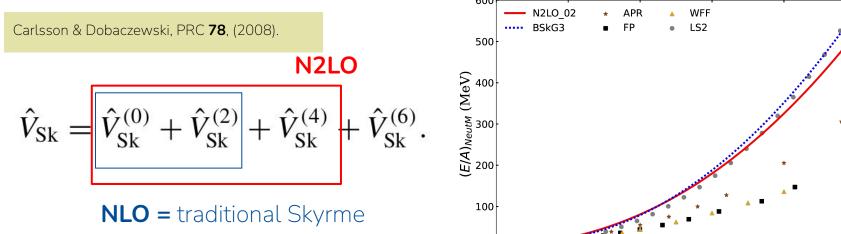
G. Grams et al., EPJA 59, 270 (2023).



More realistic NS predictions:

- higher maximum mass
- realistic pairing properties in INM
 - constrained to advanced calculations
- but not at the cost of finite nuclei!
 - at the cost of extra density dependencies

BSkG4: an N2LO parameterization?



NxLO functional forms

- systematic expansion in gradients....
- but not improvable
- hope for improved spectroscopy
- significant numerical challenges
 => See MB's talk

My (modest) hopes

0.2

8.0

- realistic masses
- sufficiently heavy neutron stars

0.4

 sufficient DoF to get an effective mass more in line with ab initio indications

0.6

0.8

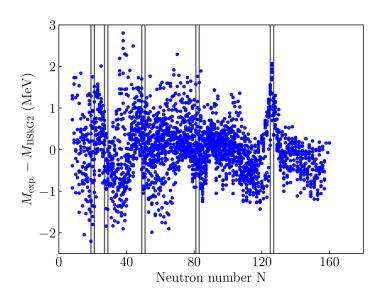
1.0

• ... with LESS density dependencies

 ρ (fm⁻³)

Failures

- 1. Residual structure in mass differences
- 2. Disastrous spectroscopy
- 3. Missing global observables
- 4. Phenomenological treatment of collective motion
- 5. Form of the functional



$$\begin{aligned} \mathcal{E}_{t,e}(\mathbf{r}) &= C_t^{\rho\rho}(\rho_0) \, \rho_t^2(\mathbf{r}) + C_t^{\rho\tau}(\rho_0) \, \rho_t(\mathbf{r}) \, \tau_t(\mathbf{r}) \\ &+ C_t^{\rho\nabla J} \, \rho_t(\mathbf{r}) \, \nabla \cdot \mathbf{J}_t(\mathbf{r}) \\ &+ C_t^{\rho\Delta\rho} \, \rho_t(\mathbf{r}) \, \Delta\rho_t(\mathbf{r}) \\ &+ C_t^{\nabla\rho\nabla\rho}(\rho_0) \, \nabla\rho_t(\mathbf{r}) \cdot \nabla\rho_t(\mathbf{r}) \\ &+ C_t^{\rho\nabla\rho\nabla\rho}(\rho_0) \, \rho_t(\mathbf{r}) \nabla\rho_0(\mathbf{r}) \cdot \nabla\rho_t(\mathbf{r}) \end{aligned}$$

$$\begin{aligned} \mathcal{E}_{t,o}(\mathbf{r}) &= C_t^{ss}(\rho_0) \, \mathbf{s}_t(\mathbf{r}) \cdot \mathbf{s}_t(\mathbf{r}) + C_t^{jj}(\rho_0) \, \mathbf{j}_t(\mathbf{r}) \cdot \mathbf{j}_t(\mathbf{r}) \\ &+ C_t^{j\nabla s} \, \mathbf{j}_t(\mathbf{r}) \cdot \nabla \times \mathbf{s}_t(\mathbf{r}) \, . \end{aligned}$$

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The pipeline is:

1. incomplete

a. almost nothing is shared (exception: HFB solvers)

b. not all nuclei are even-even

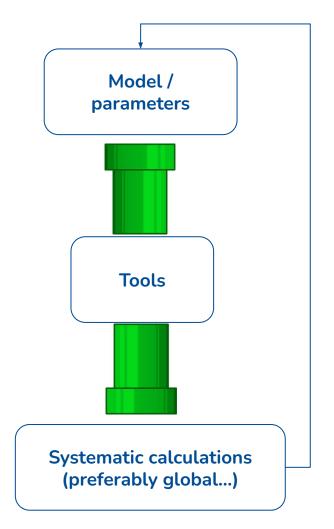
2. fragile

- a. interoperability ~ 0
- b. LOTS of oversight needed
- c. not repeatable

3. slow

- a. "good-enough" algorithms
- b. development takes forever

"How routine are global calculations?" They are absolutely not!

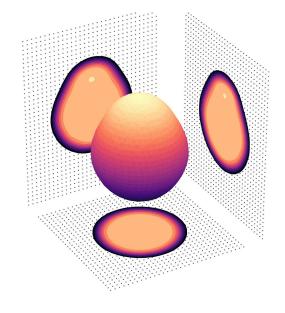


The tools behind: MOCCa

W. R. PhD Thesis, ULB (2016).
W. R. et. al., PRC 92, 064318 (2015).
W. R. et. al., EPJA 55, 93 (2019).
W. R. and M. Herbst, in preparation.
W. R., in preparation.

HFB solver

- successor to EV8/EV4/CR8/...
- flexibility regarding imposed symmetries
- 3D coordinate space representation
- high and easily controllable accuracy

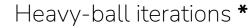


Algorithms

- 1. ... for speed
- 2. for EDF / spacing-agnostic convergence
- 3. ... to automatically estimate numerical parameters
- 4. for automatic implementation of EDFs

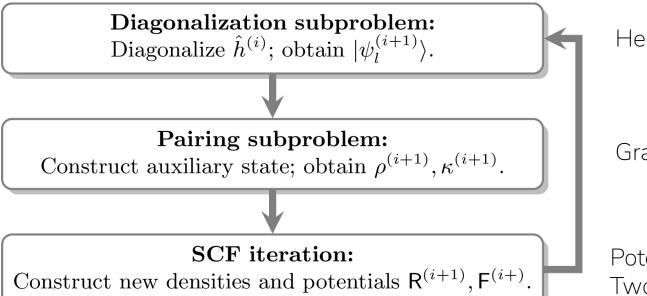
Coming to EPJA in 2024!

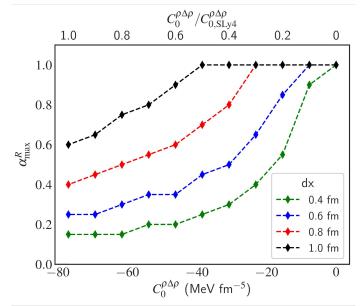
* W. Ryssens et al. EPJA **55** (2019).# W. Ryssens, (forever) in preparation



Gradient-pairing-solver **#**

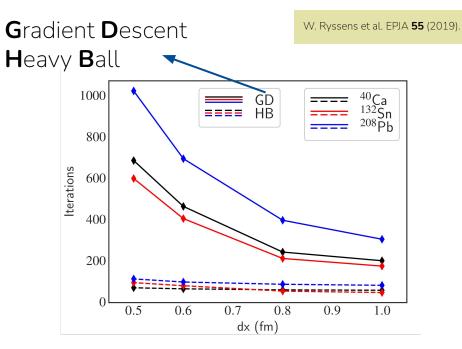
Potential preconditioning * Two-step constraints #





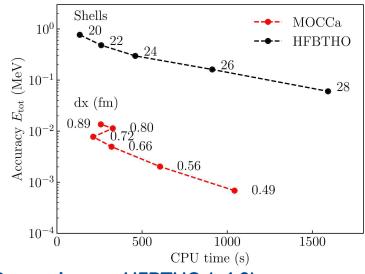
Convergence depends on many things

- details of representation
- balance of coupling constants
- nasty surprises in complicated EDF forms



Compared to EV8

- one order of magnitude speed-up
- with minimal coding
- ENTIRELY fire-and-forget
- [also algorithms for constraints)



Comparison vs HFBTHO (v4.0)

- <u>2D</u> HO versus <u>3D</u> r-space
- HF minimum of ²⁴⁰Pu for SLy4
- reference: 30 shells, dx = 0.43 fm

$$\begin{array}{c} \mathcal{H}(\mathcal{R})\mathcal{W} = E^{\mathrm{qp}}\mathcal{W}, \\ \mathcal{R} = \mathcal{W}^{\dagger}\mathcal{C}\mathcal{W}, \end{array} \end{array}$$

$$\mathcal{W} \to e^{-i\mathcal{Z}}\mathcal{W}$$

 $\approx [1 - i\mathcal{Z}]\mathcal{W}$

$$\mathcal{Z} = \alpha \begin{pmatrix} 0 & H^{20} \\ H^{02} & 0 \end{pmatrix}$$

$$\delta R_{xy} \sim \sum_{\alpha \kappa ab} \frac{C_{\kappa} - C_{\alpha}}{E_{\kappa} - E_{\alpha}} W_{\alpha a} W_{b\kappa}^{\dagger} \mathcal{W}_{x\alpha}^{\dagger} \mathcal{W}_{\kappa y} \delta \mathcal{H}_{ab} \,.$$

Direct diagonalisation

- easiest to code
- the choice of blocked qp is crucial
- doomed to fail in systematic calculations
- particularly with time-odd terms

Gradient solver

- based on Thouless theorem
- can also be accelerated by HB!

 $\delta \mathcal{R} = -i[\mathcal{Z}, \mathcal{R}].$

- almost unconditionally stable
- only lowest state accessible (for now...)

The tools behind: Hephaestos

Many different Skyrme EDF extensions:

N2LO/N3LO

B.G. Carlsson et al., PRC 78, 044326 (2008) B. G. Carlsson, PRL 105, 122501 (2010). D. Davesne et al. PRC 91, 064303. (2015).

• Tensor terms

F. Tondeur , PLB 123, 139 (1983). T. Lesinski et al., PRC 76, 014312 (2007). G. Colò et al., PLB 646, 227 (2007).

• multi-reference J. Dobaczewski et al., NPA 422, 103 (1984)

J. Dobaczewski et al., NPA 422, 103 (1984). J. Dobaczewski, J. Phys. G 43, 04LT01 (2016). J.Sadoudi et al., Phys. Scripta, T154, 014013 (2013).

density dependencies S.A. Fayans et al., NPA 676, 49–119 (2000). N. Chamel et al., PRC 80, 065804 (2009).

A. Bulgac et al., PRC 80, 065804 (2009).
 A. Bulgac et al., PRC 97,044313 (2018).
 P.-G. Reinhard et al., PRC 95, 064328 (2017).

• ab initio

[too many to list]

All of these forms are <u>complicated</u>... ... and none explored at scale!

This complexity stops both

- 1. initial exploration
- 2. sharing of EDF forms

$$\begin{split} \mathcal{E}_{\mathrm{Sk},\mathrm{e}}^{(0)} &= \sum_{t=0,1} \left[A_{\mathrm{t},\mathrm{e}}^{(0,1)} \left(D_{t}^{1,1} \right)^{2} + A_{\mathrm{t},\mathrm{e}}^{(0,2)} \left(D_{0}^{1,1} \right)^{\alpha} \left(D_{t}^{1,1} \right)^{2} \right], \\ \mathcal{E}_{\mathrm{Sk},\mathrm{e}}^{(2)} &= \sum_{t=0,1} \left[A_{\mathrm{t},\mathrm{e}}^{(2,1)} D_{t}^{1,1} \left(\Delta D_{t}^{1,1} \right) + A_{\mathrm{t},\mathrm{e}}^{(2,2)} D_{t}^{1,1} D_{t}^{(\nabla,\nabla)} + A_{\mathrm{t},\mathrm{e}}^{(2,3)} \sum_{\mu\nu} C_{t,\mu\nu}^{1,\nabla\sigma} C_{t,\mu\nu}^{1,\nabla\sigma} + A_{\mathrm{t},\mathrm{e}}^{(2,4)} D_{t}^{1,1} \left(\nabla \cdot C_{t}^{1,\nabla\times\sigma} \right) \right], \\ \mathcal{E}_{\mathrm{Sk},\mathrm{e}}^{(4)} &= \sum_{t=0,1} \left[A_{\mathrm{t},\mathrm{e}}^{(4,1)} \left(\Delta D_{t}^{1,1} \right) \left(\Delta D_{t}^{1,1} \right) + A_{\mathrm{t},\mathrm{e}}^{(4,2)} D_{t}^{1,1} D_{t}^{\Delta,\Delta} + A_{\mathrm{t},\mathrm{e}}^{(4,3)} D_{t}^{(\nabla,\nabla)} D_{t}^{(\nabla,\nabla)} \\ &\quad + A_{\mathrm{t},\mathrm{e}}^{(4,4)} \sum_{\mu\nu} D_{\tau,\mu\nu}^{\nabla,\nabla} D_{\tau,\mu\nu}^{\nabla,\nabla} + A_{\mathrm{t},\mathrm{e}}^{(4,5)} \sum_{\mu\nu\nu} D_{\tau,\mu\nu}^{\nabla,\nabla} \left(\nabla_{\mu} \nabla_{\nu} D_{t}^{1,1} \right) \\ &\quad + A_{\mathrm{t},\mathrm{e}}^{(4,6)} \sum_{\mu\nu} C_{t,\mu\nu}^{1,\nabla\sigma} \left(\Delta C_{t,\mu\nu}^{1,\nabla\sigma} \right) + A_{\mathrm{t},\mathrm{e}}^{(4,7)} \sum_{\mu\nu\kappa} \left(\nabla_{\mu} C_{t,\mu\kappa}^{1,\nabla\sigma} \right) \left(\nabla_{\nu} C_{t,\nu\kappa}^{1,\nabla\sigma} \right) + A_{\mathrm{t},\mathrm{e}}^{(4,8)} \sum_{\mu\nu} C_{t,\mu\nu}^{1,\nabla\sigma} C_{t,\mu\nu}^{\Delta,\nabla\sigma} \right], \\ \mathcal{E}_{\mathrm{Sk},0}^{(0)} &= \sum_{t=0,1} \left[A_{\mathrm{t},0}^{(0,1)} \tilde{p}_{1}^{1,\sigma} \cdot \tilde{p}_{1}^{1,\sigma} + A_{\mathrm{t},0}^{(0,2)} D_{0}^{1,1} \sigma \tilde{p}_{1}^{1,\sigma} \cdot \tilde{p}_{1}^{1,\sigma} \cdot \tilde{p}_{1}^{1,\sigma} + A_{\mathrm{t},0}^{(2,3)} \tilde{p}_{1}^{1,\sigma} \cdot \tilde{c}_{t}^{1,\nabla} + A_{\mathrm{t},0}^{(2,4)} \tilde{p}_{t}^{1,\sigma} \cdot \left(\nabla \times \tilde{c}_{t}^{1,\nabla} \right) \right], \\ \mathcal{E}_{\mathrm{Sk},0}^{(1)} &= \sum_{t=0,1} \left[A_{\mathrm{t},0}^{(4,1)} \left(\Delta \tilde{p}_{1}^{1,\sigma} \right) \left(\Delta \tilde{p}_{t}^{1,\sigma} \right) + A_{\mathrm{t},0}^{(2,2)} \tilde{p}_{1}^{1,\sigma} \cdot \tilde{p}_{t}^{1,\sigma} \cdot \tilde{p}_{t}^{\Delta,\Delta\sigma} + A_{\mathrm{t},0}^{(4,3)} \tilde{p}_{t}^{(\nabla,\nabla)\sigma} \cdot \tilde{p}_{t}^{(\nabla,\nabla)\sigma} \right. \\ + A_{\mathrm{t},0}^{(4,4)} \sum_{\mu\nu\kappa} D_{\mu\nu\kappa}^{\nabla,\nabla\sigma} D_{\mu\nu\kappa}^{\nabla,\nabla\sigma} + A_{\mathrm{t},0}^{(4,5)} \sum_{\mu\nu\kappa} D_{\mu\nu\kappa}^{\nabla,\nabla\sigma} \left(\nabla_{\mu}\nabla_{\nu} D_{\sigma} \right) , \\ + A_{\mathrm{t},0}^{(4,4)} \sum_{\mu\nu\kappa} D_{\mu\nu\kappa}^{\nabla,\nabla\sigma} D_{\mu\nu\kappa\sigma}^{\nabla,\nabla\sigma} + A_{\mathrm{t},0}^{(4,5)} \sum_{\mu\nu\kappa} D_{\mu\nu\kappa}^{\nabla,\nabla\sigma} \left(\nabla_{\mu}\nabla_{\nu} D_{\sigma} \right) \right. \\ + A_{\mathrm{t},0}^{(4,4)} \sum_{\mu\nu\kappa} D_{\mu\nu\kappa}^{\nabla,\nabla\sigma} D_{\mu\nu\kappa\sigma}^{\nabla,\nabla\sigma} + A_{\mathrm{t},0}^{(4,5)} \sum_{\mu\nu\kappa} D_{\mu\nu\kappa}^{\nabla,\nabla\sigma} \left(\nabla_{\mu}\nabla_{\nu} D_{\sigma} \right) \right], \\ \left. + A_{\mathrm{t},0}^{(4,0)} \tilde{c}_{t}^{1,\nabla} \cdot \left(\Delta \tilde{c}_{t}^{1,\nabla} \right) + A_{\mathrm{t},0}^{(4,5)} \sum_{\mu\nu\kappa} D_{\mu\nu\kappa}^{\nabla,\nabla\sigma}$$

W. Ryssens & M. Bender, PRC 104 044308 (2021).

The tools behind: Hephaestos

$$\begin{split} D^{L,R}(\mathbf{r}) &= \operatorname{Re}\left\{ \hat{L}(\mathbf{r}')\hat{R}(\mathbf{r})\rho(\mathbf{r},\mathbf{r}')\right\} \Big|_{\mathbf{r}=\mathbf{r}'} ,\\ C^{L,R}(\mathbf{r}) &= \operatorname{Im}\left\{ \hat{L}(\mathbf{r}')\hat{R}(\mathbf{r})\rho(\mathbf{r},\mathbf{r}')\right\} \Big|_{\mathbf{r}=\mathbf{r}'} ,\\ \rho(\mathbf{r}) &\rightarrow \quad D^{1,1}(\mathbf{r}) = \mathsf{D}_{-}\mathsf{I}_{-}\mathsf{I} \quad , \end{split}$$

$$\begin{split} \mathbf{j}(\mathbf{r}) &\to \mathbf{C}^{1,\nabla}(\mathbf{r}) = \mathtt{C}_{-}\mathtt{I}_{-}\mathtt{N} \quad , \\ \tau(\mathbf{r}) &\to D^{(\nabla,\nabla)}(\mathbf{r}) = \mathtt{D}_{-}\mathtt{N}\mathtt{m}_{-}\mathtt{N}\mathtt{m} \, , \end{split}$$

Automating EDFs

A HFB solver <u>only</u> depends on the EDF-type via:

- 1. construction of densities
- 2. construction of mean-fields (ph and pp)

Formulas for all relevant quantities obtained through many applications of simple rules.

Complex for humans, but easy for computers!

$$\mathsf{R}_{q} = \left(D_{q}^{1,1}, D_{q,\mu}^{1,\sigma}, D_{q,\mu\nu}^{\nabla,\nabla}, C_{q,\mu\nu}^{1,\nabla\sigma}, C_{q,\mu}^{1,\nabla}, D_{q,\mu\nu\kappa}^{\nabla,\nabla\sigma}, \right. \\ \left. D_{q}^{\Delta,\Delta}, C_{q,\mu\nu}^{\Delta,\nabla\sigma}, D_{q,\mu}^{\Delta,\Delta\sigma}, C_{q,\mu}^{\Delta,\nabla} \right).$$

$$\mathsf{F}_{q,a}(\mathbf{r}) \equiv \frac{\delta E_{\text{tot}}(\mathsf{R})}{\delta \mathsf{R}_{q,a}(\mathbf{r})}.$$

$$\rho\tau \rightarrow \texttt{D_I_J}.\texttt{Mm}.\texttt{Nm}$$

$$\begin{split} F_{\rho}(\mathbf{r}) &\to \frac{\partial E}{\partial \rho} \sim \mathrm{D}_{\mathrm{Nm}} \mathrm{Nm} \,, \\ F_{\tau}(\mathbf{r}) &\to \frac{\partial E}{\partial \rho} \sim \mathrm{D}_{\mathrm{I}} \mathrm{I}_{\mathrm{I}} \,, \end{split}$$

The tools behind: Hephaestos

Hephaestos automates EDF implementation!

Current state:

- arbitrary densities up to N3LO
- no limit on the densities in a term
- (almost) arbitrary density dependencies
- writes quite efficient code
- functional file writing remains a bit complex

Long-term goals:

- extend applications (INM, QRPA, MR, ...)
- starting from a LaTeX expression
- make things solver-agnostic!

This is the tool behind:

- BSkG3: time-to-start-fitting ~ <u>1 week</u>
- BSkG4: time-to-start-fitting ~ <u>1 day</u>

CT0;R-CT1-;R-CSDS0;R-CSI Particle-particle param	<pre><1.;R.t2;R.x2.;R.t3;R.x3;R.t4.;R.t5;R. DS1;R.wsoq</pre>	x4 ;R-x5;R-wso;R-sigma;R-beta-	;Rganna-
Microscopic pairing opt: ptype ;I intertype ERMS	lons		
Central. LO terms		******	
Central, LO terms Time-even			
Term	!.Coupling constant	!.DD pow! i:	sospin indices
DIIDII	; Cc(t0,x0,+1,0,0)		; 0
	:; Cc(t0,x0,+1,0,1) :.+1.0/6.0*Cc(t3,x3,+1,0,0)		
DIIDIIDII	:+1.0/6.0*Cc(t3,x3,+1,0,1)	; signa ; e	. 1 . 1
Time-odd .			
D I Sm D I Sm	; Cc(t0,x0,+1,1,0)	;	;-0
	; Cc(t0,x0,+1,1,1) ; +1.0/6.0*Cc(t3,x3,+1,1,0)		
DIIDISm DISm	:+1.0/6.0*Cc(t3.x3.+1.1.1)	: sigma : 0	1.1.1.1
Central, NLO terms			
Time-even	!.Coupling.constant	L DD parkt in	corpin indicor
DIIDNm Nm	::+1.0/2.0*Cc(t1,x1,+1,0,0)+1.0/2.	0*Cc(t2,x2,-1,0,0) .: 1; 0	-;-0
	; +1.0/2.0*Cc(t1,x1,+1,0,1)+1.0/2.		
	;3.0/8.0*Cc(t1,x1,+1,0,0)+1.0/8		
D I I Lap D I I	; -3.0/8.0*Cc(t1,x1,+1,0,1)+1.0/8.	0*Cc(t2,x2,-1,0,1) ;1; 1	
	-CT1		
Time-odd	,		, -
	;1.0/2.0*Cc(t1,x1,+1,0,0)-1.0/2.		
CINTCINT.	; -1.0/2.0*Cc(t1,x1,+1,0,1)-1.0/2.	0*Cc(t2,x2,-1,0,1)-;1;-1	; 1
D T Sm Lap D T Sm	+CSDS0		. 1
D I Sm D Nk NkSm			: 0
D_I_Sm_D_Nk_NkSm	·····; +CT1······		; . 1
C		••••••	
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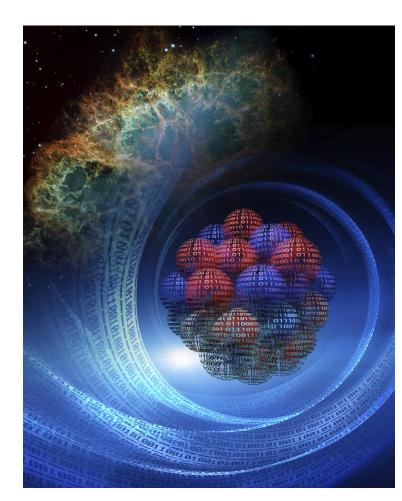
Conclusion

BSkG-models

- symmetry breaking to the max
- excellent bulk properties
- exploitation ongoing
- N2LO version in the works

<u>Numerics</u>

- our tools deserve attention...
- ... automation will be key.
- MOCCa is robust and fast....
- ... and will go open-source in 2024!



What I will be working on:

Improving the BSkG-models:

- 1. towards H's with (ab initio?) inspiration which form to start with?
- 2. larger reach in terms of observables FAM-QRPA, large-scale fission, ...
- 3. treatment of collective motion towards VAP but first through FAM-QRPA

One step at a time!

Crucial in this will be "fixing" the pipeline:

- 1. completeness
- 2. robustness
- 3. speed



Thank you for...

..... all the wonderful work!



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..... the computing time!

SEIT 1386



..... the funding!





G. Scamps

F. Verstraelen

P. Van Duppen

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Thank **you** for...

... your attention! ... a decade of support!