Statistical analysis in nuclear DFT: central depression as example

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Outline

1. Motivation: nuclear bubbles – bubble nuclei
2. Framework: nuclear DFT, calibration& statistical analysis
   - Typical structure of nuclear density functionals
   - Optimization of model parameters (χ^2 fits), statistical analysis
3. Central density $\rho(0)$ and central depression w of nuclear charge density
   - Charge formfactor, charge density and all that
4. Nuclear DFT and central depression: trends, correlations, predictions
   - Averages and variances: trends with size and proton number
   - Correlations (with Coulomb energy, model parameters, groups, ...)
   - Inter-correlations: nuclei in different regions
5. Toward estimating a systematic error
   - Confrontation with data, variation of the model,
6. Conclusions

Acknowledgements (short list)

Bastian Schütrumpf (GSI) & Witek Nazarewicz (MSU) $\leftrightarrow$ central depression [PRC **96** (2017) 024306]

Jochen Erler and Peter Klüpfel $\leftrightarrow$ Skyrme parametrizations [PRC **79** (2009) 034310]

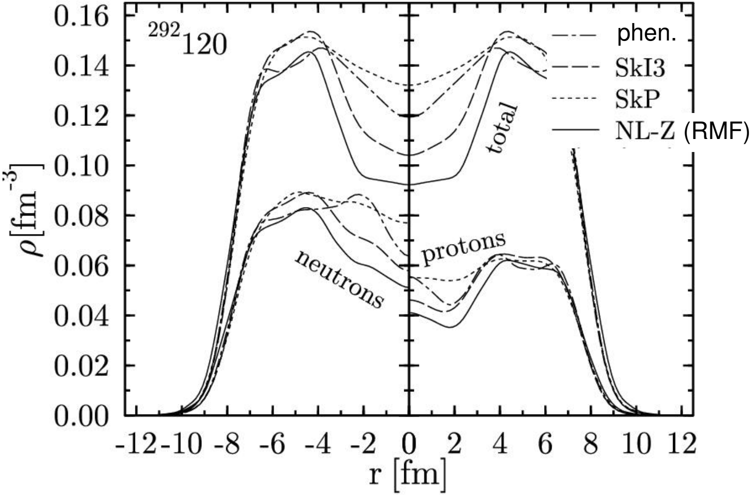
Witek Nazarewicz (MSU) $\leftrightarrow$ Fayans functionals [PRC **95** (2017) 064328]

Jörg Friedrich $\leftrightarrow$ charge formfactors etc [NPA **373** (1982) 192, NPA **459** (1986) 10]

1) Motivation: nuclear bubbles – bubble nuclei

Super-heavy elements (SHE) $\longleftrightarrow$ bubble nuclei ?

example:local density distribution $\rho(r = 0)$ for SHE just above known region



other examples in some light nuclei (^{34}Si, ^{46}Ar)

bubble = dip at $\rho(0)$, central depression ⇒ **develop measure & test with stat. analysis**

2) Framework: nuclear DFT, calibration & statistical analysis

A nuclear density functional – non-relativistic Skyrme-Hartree-Fock

energy: $E = E_{\rm kin} + \int d^3r\,\mathcal{E}_{\rm pot}(\rho_p, \rho_n, \tau_p, \tau_n, J_{ls,p}, J_{ls,n}, \chi_{\rm pair}, \ldots\text{time odd}\ldots) + E_{\rm CoM}$

- $\chi_{\rm pair}$ → pairing density
- $J_{ls,p}$ → spin orbit density
- τ_p → kinetic-energy density
- ρ_p → density

$$\mathcal{E}_{\rm pot} = \sum_{T=0}^{1}\Big[C_T^{(0)}(\rho_0)\,\rho_T^2 + C_T^{\Delta}\,\rho_T\Delta\rho_T + C_T^{(\rm kin)}\,\tau_T\rho_T + C_T^{(\rm ls)}\,\nabla J_T\rho_T\Big] + \sum_{t\in\{p,n\}} C_t^{(\rm pair)}(\rho_0)\chi_t^2$$

density dependence: $C_T^{(0)}(\rho_0) = C_T^{(0)}(0) + C_T^{(\rho)}\rho_0^{\alpha}\;,\; C_t^{(\rm pair)}(\rho_0) = V_t^{(\rm pair)}\left(1 - \frac{\rho_0}{\rho_{\rm pair}}\right)$

isospin recoupling: $\rho_0 = \rho_n + \rho_p \quad , \quad \rho_1 = \rho_n - \rho_p$

$\longleftrightarrow$ universal = same parameters for all systems

$\longleftrightarrow$ insufficient "ab-initio" data $\Rightarrow$ model parameters from χ^2-fit to empirical data

in the following using parametrization **SV-min** from PRC **79** (2009) 034310.

fit data: E, $r_{\rm rms}$, $R_{\rm diffr.}$, $\sigma_{\rm surf}$, ϵ_{ls}, $\Delta^{(3)}_{\rm pair}$ in semi-magic nuclei (255 data points)

Physical model parameters

For the smooth part: liquid-drop model parameters (LDM)

$E/A\|_{\mathrm{eq}}$	volume energy	isoscalar	bulk
ρ_{eq}	equilibrium density	isoscalar	bulk
K	incompressibility	isoscalar	bulk
J	symmetry energy	isovector	bulk
L	slope of symmetry energy	isovector	bulk
a_{surf}	surface energy	isoscalar	surface
$a_{\mathrm{surf,sym}}$	surface symmetry energy	isovector	surface

For shell fluctuations: kinetic and pairing parameters

m^*/m	effective mass	isoscalar	influence on spectra
κ_{TRK}	TRK sum rule enhancement	isovector	influence on spectra
$b_{\mathrm{ls},T=0}$	spin-orbit strength	isoscalar	influence on spectra
$b_{\mathrm{ls},T=1}$	spin-orbit strength	isovector	influence on spectra
$V_{\mathrm{pair},p}$	proton pairing strength		sensitive to spectra
$V_{\mathrm{pair},n}$	neutron pairing strength		sensitive to spectra
ρ_{pair}	pairing density dependence		sensitive to spectra

Optimization of model parameters and statistical analysis

global quality measure: $\chi^2(\mathbf{p}) = \sum_{f=1}^{N_\mathrm{data}} \frac{\left(\mathcal{O}_f(\mathbf{p}) - \mathcal{O}_f^\mathrm{exp}\right)^2}{\Delta\mathcal{O}_f^2}$, $\mathcal{O}_f$ = fit observable,

$\mathbf{p} = (p_1, ..., p_{N_p})$ = model parameters. $\Delta\mathcal{O}_f$ = adopted error

optimal parameters $\mathbf{p}_0$: $\chi^2(\mathbf{p}_0)$ = minimal

statistical interpretation: $W(\mathbf{p}) \propto \exp\left(-\chi^2(\mathbf{p})\right)$ ≡ probability for parameter set **p**

$\Longrightarrow$ average $\equiv \overline{A} = \int d\mathbf{p}\, WA(\mathbf{p})$, variance $\equiv \overline{\Delta^2 A} = \int d\mathbf{p}\, W(A-\overline{A})^2$.

Taylor expansions: Covariance matrix $\equiv \mathcal{C}^{-1}_{p_ip_j} = \partial_{p_i}\partial_{p_j}\chi\Big|_{\mathbf{p}_0}$

$\Longrightarrow$ average $\overline{A} = A(\mathbf{p}_0)$, variance $\overline{\Delta^2 A} = \partial_\mathbf{p}A \cdot \hat{\mathcal{C}} \cdot \partial_\mathbf{p}A$

covariance $\overline{\Delta A \Delta B} = \partial_\mathbf{p}A \cdot \hat{\mathcal{C}} \cdot \partial_\mathbf{p}B$

coefficient of determination (CoD): $r_{AB}^2 = \frac{|\overline{\Delta A \Delta B}|^2}{\overline{\Delta^2 A}\,\overline{\Delta^2 B}}$

multiple correlation coeff. (MCC): $R_{\mathbf{A}B}^2 = \sum_{ij} r_{BA_i}\left(r_{\mathbf{AA}}\right)^{-1}_{ij} r_{A_jB}$

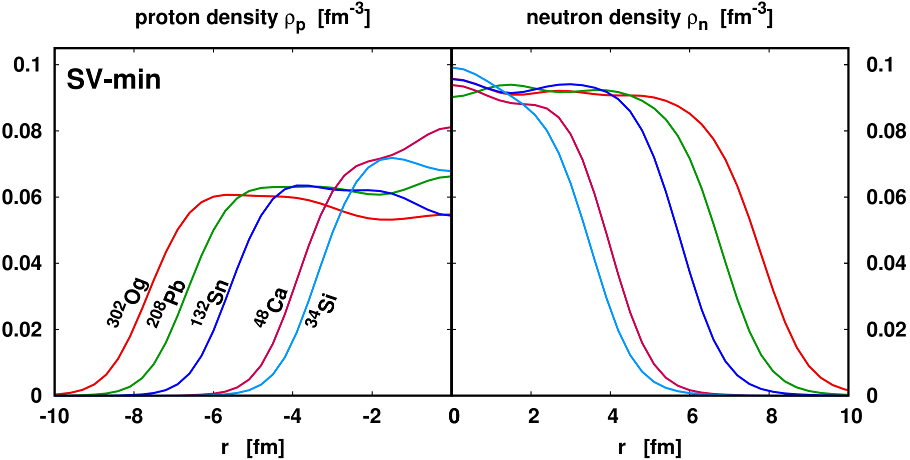
$\leftrightarrow$ CoD $R_{\mathbf{A}B}^2$ of a group of obs. $\mathbf{A} = (A_1, ..., A_g)$ with obs. B

Stages of model development

	model	observable
physics explorations		
modeling	range of applicability (RoA)	observable in RoA
data	fit observables in RoA	direct or model dep. ?
statistical analysis		
averages	unresolved trends in fit obs.	predictions, extrapolations
		comparison with data ?
variances	strong vs. soft model params.	extrapolation errors
CoD, MCC	sensitivity analysis	(in-)dependent obs./params.
	superflous parameters	redundant or useful data ?
	$\Rightarrow$ directions for extensions	
systematic errors	no systematic way $\rightarrow$ trial and error, variations of model	
	$\Longrightarrow$ back to physics	

3) Central density $\rho(0)$ and central depression *w*

Density profiles for various nuclear sizes

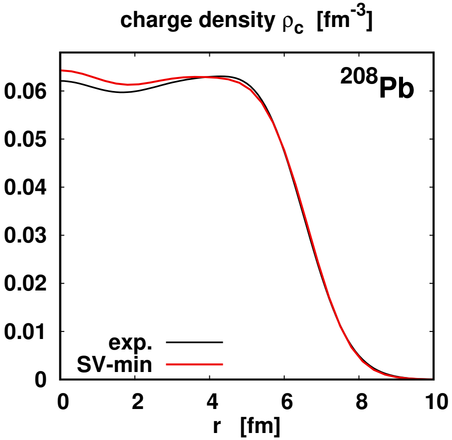


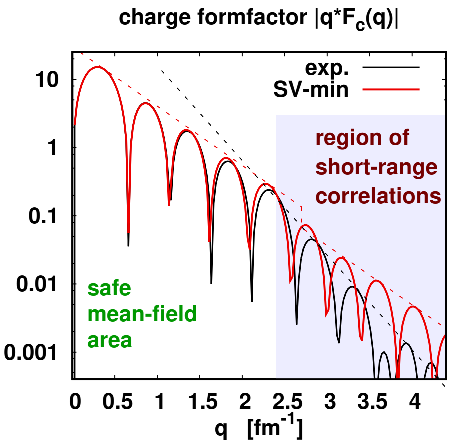
develop closely around average density ↔ nuclear saturation

central density $\rho_{p/n}(0)$ fluctuates $\pm$ about average ↔ shell effects

$\Longrightarrow$ $\rho_{p/n}(0)$ contains info on both: bulk properties (LDM) & shell effects

Safe and unsafe regions of formfactor $F(\mathbf{q}) = \int d^3r\, e^{\mathrm{i}\mathbf{q}\cdot\mathbf{r}} \rho(\mathbf{r})$





systematic deviation for $F(q)$ above $q > 2.5/\mathrm{fm} \leftrightarrow$ suppressed by short-range correl.

$r \approx 0$ sensitive to large $q \overset{?}{\Rightarrow}$ central density $\rho(0)$ not a perfect mean-field observable

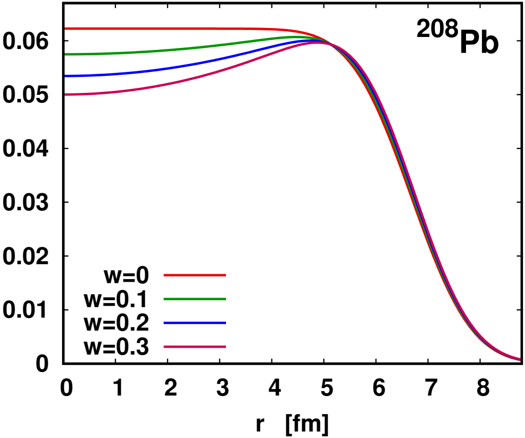
$\Longrightarrow$ try alternative measure for central depression $\leftrightarrow$ from $F(q)$ in $q < 2.5/\mathrm{fm}$

A safe (?) measure: central depression parameter w

liquid drop model (LDM) for density distribution:

$$\rho_{\rm model}(\mathbf{r}) \propto \mathcal{G}_\sigma \star \left(1 + \overline{w}\frac{\mathbf{r}^2}{\langle r^2\rangle}\right)\theta(R_{\rm d,1} - |\mathbf{r}|) \quad ,$$

$\mathcal{G}_\sigma \equiv$ Gaussian folding, surface width σ
$R_{d,1} \equiv$ 1. diffraction radius
from 1. zero in $F(q)$
$\equiv$ box-equivalent radius



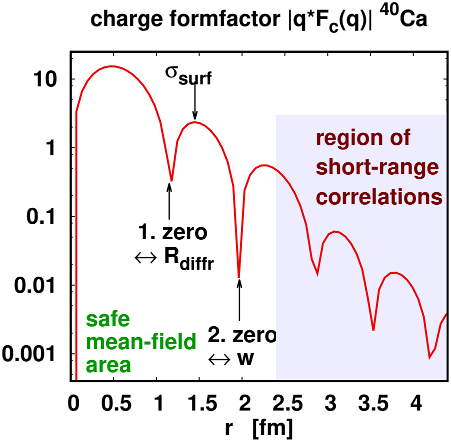
compare systematics
$\Longrightarrow$

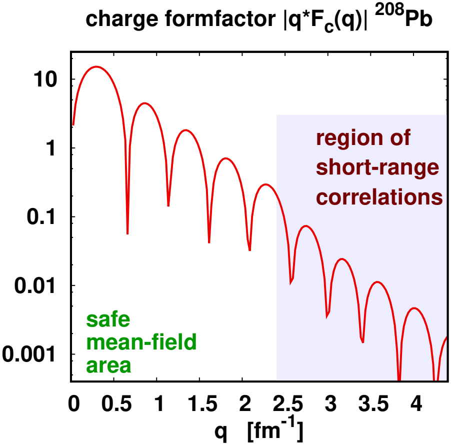
$$\overline{w} \approx w = 15.3\left(\frac{R_{\rm d,1}}{R_{\rm d,2}} - 1\right)$$

$R_{\rm d,2} \equiv$ 2. diffraction radius
from 2. zero in $F(q)$

$\Longrightarrow$ **task: what is the more robust observable $\rho(0)$ or w?**

Formfactor zeroes and critical region





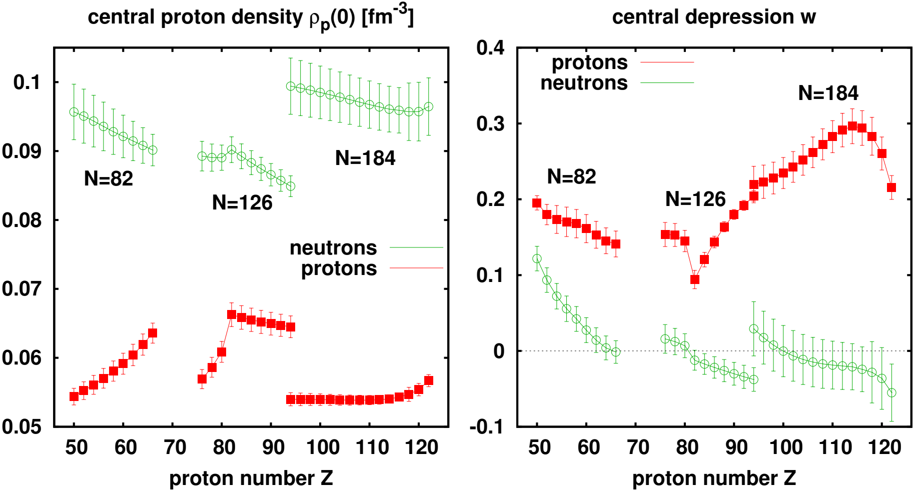
1.&2. zero, 1. maximum $\leftrightarrow$ diffraction radius $R_{\rm diffr}$, surface thickn. $\sigma_{\rm surf}$, central depr. w

<u>small nuclei</u> closer to critical $q \approx 2.5$/fm $\Longrightarrow$ definition of <u>w less robust</u>

4) Nuclear DFT and central depression: trends, correlations, predictions

testing set: 3 isotonic chains, fixed neutron number N & varied proton number Z
$N = 82, 126$ examples from normal nuclei and $N = 184$ chain of SHE

Trends & variances for central depression w_t & central density $\rho_t(0)$

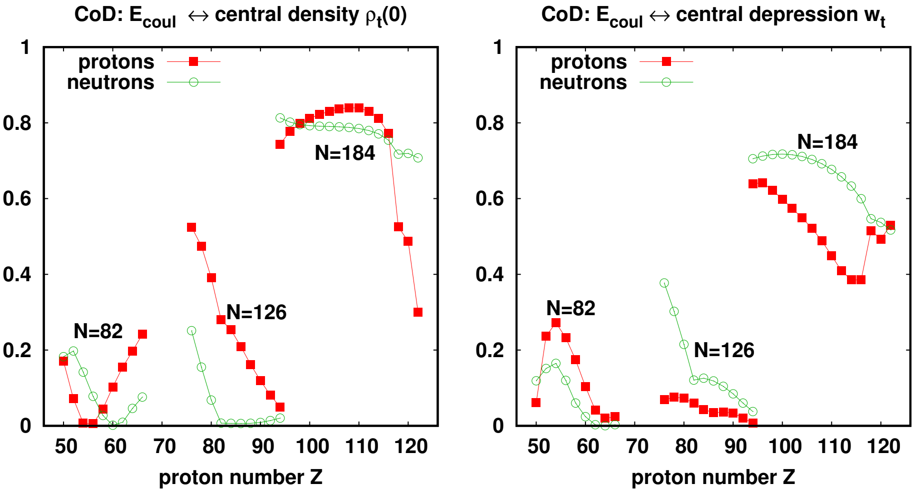


central depression systematically larger for protons $\longleftrightarrow$ Coulomb pressure (?)

kink at magic proton number $Z = 82 \longleftrightarrow$ shell effect (in both observables!)

no unique trend with proton number; extrapolation errors small

Correlations with Coulomb energy

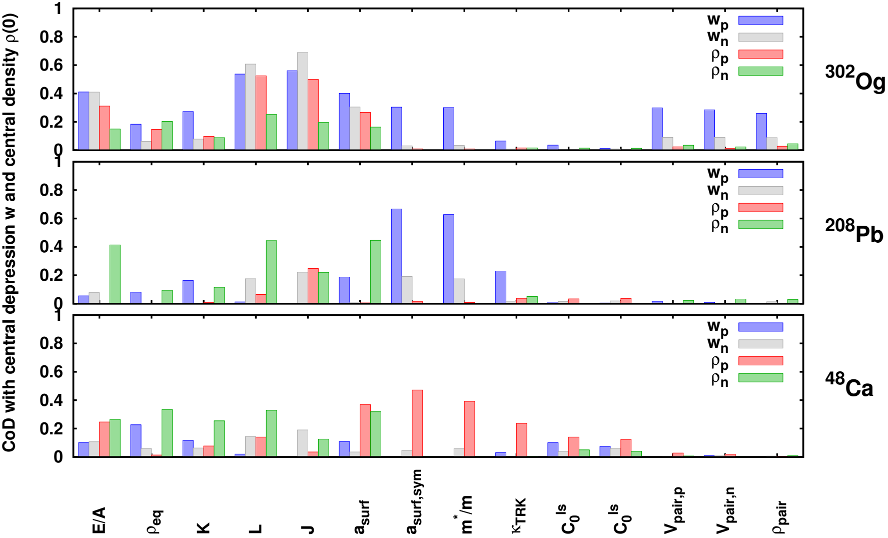


impact of Coulomb energy increases dramatically for SHE

surprisingly little correlation with Coulomb energy for “normal” nuclei

proton and neutron observables show similar correlations

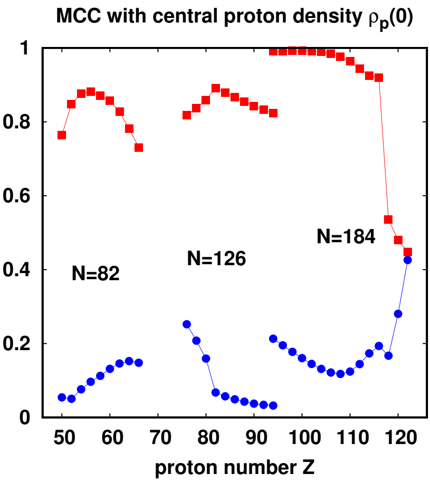
Coefficients of determination (CoD) of $\rho_t(0)$ and w_t with model params.

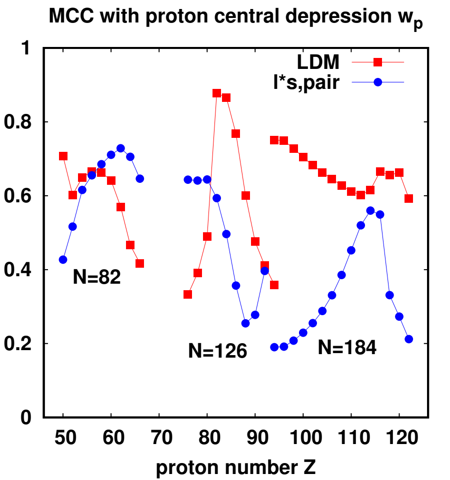


no clearly dominant contributor, influences are spread over many model parameters

$\Longrightarrow$ look for impact of groups of parameters (LDM versus shell)

Trends of multiple correlation coefficients (MCC)



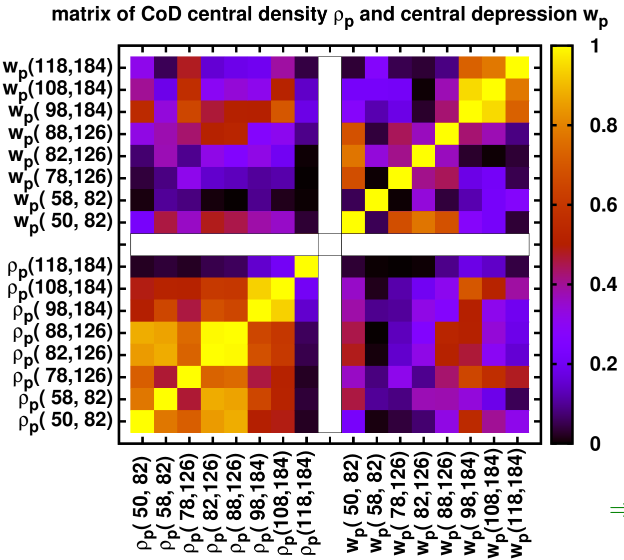


$\rho_p(0)$: "LDM"(=E/A, $\rho_{\rm eq}$, K, J, L,surf) dominates clearly over "shell"(=kinetic,ls,pair)
$\longleftrightarrow$ $\rho(0)$ contains shell effects - but you have little influence on them

w_p: "shell"-group is as important as "LDM" (surprise!)

Correlations between nuclei in different regions

Can one improve extrapolations by $\rho(0)$&w in existing nuclei?



$\rho_p(^{302}\mathrm{Og})$ uncorrelated from all other ρ, w

other $\rho_p(0)$ more or less inter-correlated

w_p show generally less inter-correlation

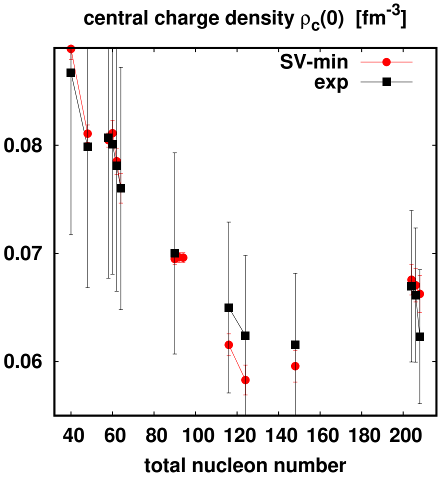
$\rho_p(0) \leftrightarrow w_p$ weakly correl.

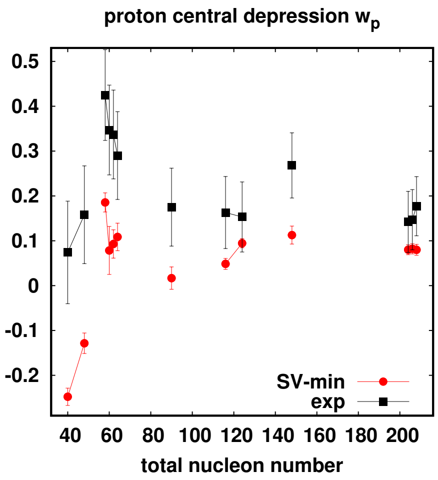
$\Rightarrow$ too small inter-correlations

5) Toward estimating a systematic error

test set for comparison with data: stable, spherical nuclei where $F(q)$-data exist

Comparison with experimental data from $\rho_{\rm charge}(r)$ for stable nuclei





$\rho_c(0)$: agrees with data

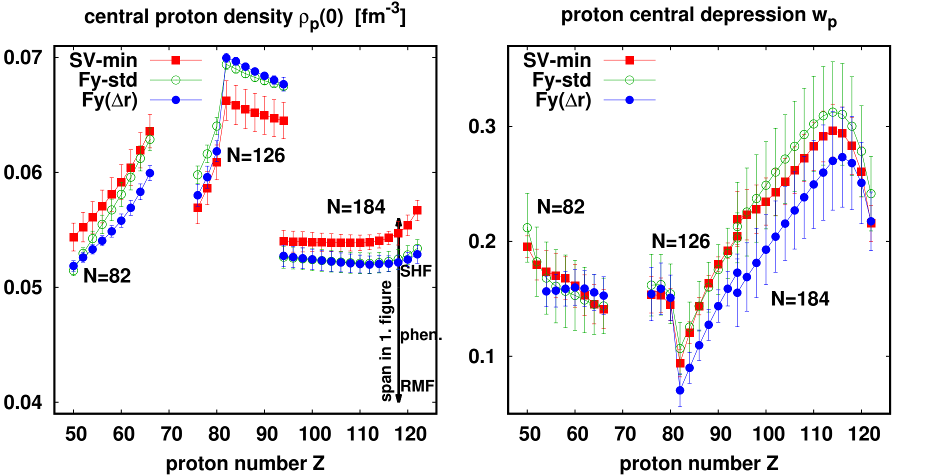
w_c: mean-field theory differs from data, situation improves for heavy nuclei
$\leftrightarrow$ in spite of LDM motivation some impact from short-range correlations

SHE: mean-field predictions increasingly reliable with increasing system size A

Variation of model – add Fayans functionals

Fayans functional:	very similar to Skyrem-Hartree-Fock
	slighlty different density dependence (rational fct. instead of ρ_0^α)
major news:	additional $\nabla\rho_0$ terms in surface parameter $C_T^{\Delta\rho}$ and pairing $C_t^{(\mathrm{pair})}$
	$\Longrightarrow$ more flexible modeling of surface

Variation of model – add Fayans functionals



$\rho_p(0)$: error bars even smaller for Fy functional - in spite of more surface terms
predictions significantly different (outside error bars) – no clear trend

w_p: differences insignificant (inside error bars) – trends different from $\rho_p(0)$

difference Fy↔SV-min smaller than for other (& older) models (RMF,folded Yukawa)

4) Conclusions

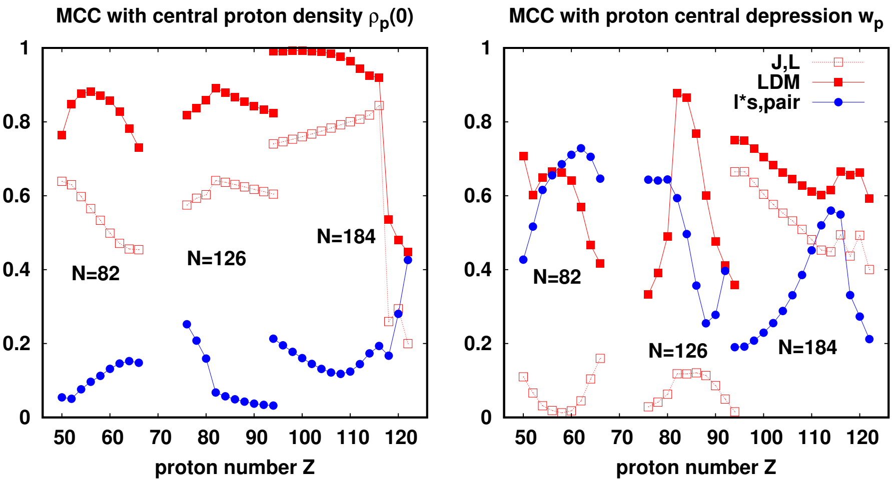
central density $\rho(0)$ & central depression w:
from formfactor $F(q)$, unclear impact of high q (short-range correl., shell fluct.)
$\Rightarrow$ risky observable $\leftrightarrow$ testing ground for statistical analysis

impact of model parameters and Coulomb pressure:
$E_{\rm coul}$ only relevant in SHE
influences spread over many model parameters – no dominant influencer
“LDM group”: decisive for $\rho(0)$, still important for w
“shell group”: considerable impact on w, only weak impact on $\rho(0)$

correlations between different A, model depedence, data:
$\rho(0)$&w in SHE independent from normal nuclei
variation of model (Fayans funct.) yields only small differences
theory compatible with data on $\rho_{\rm c}(0)$, systematic deviations for $w_{\rm c}$ in small nuclei

$\Longrightarrow$**:** at variance with expectation: $\rho(0)$ is a better mean-field observable than w
both observables can be safely extrapolated to SHE

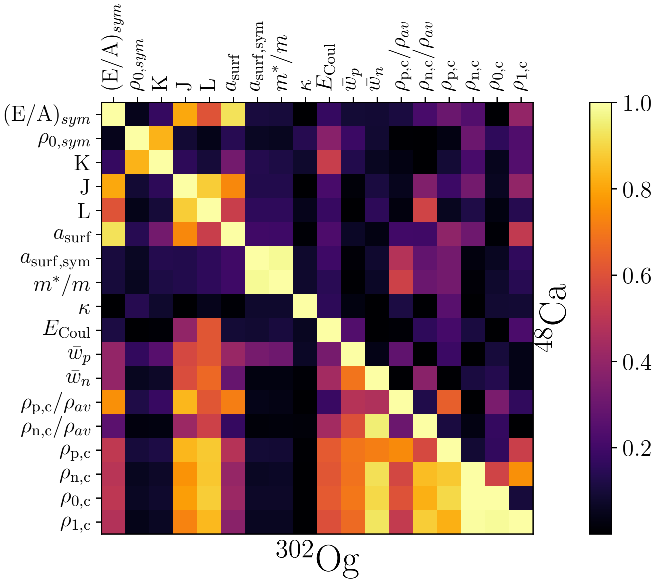
Trends of multiple correlation coefficients (MCC)



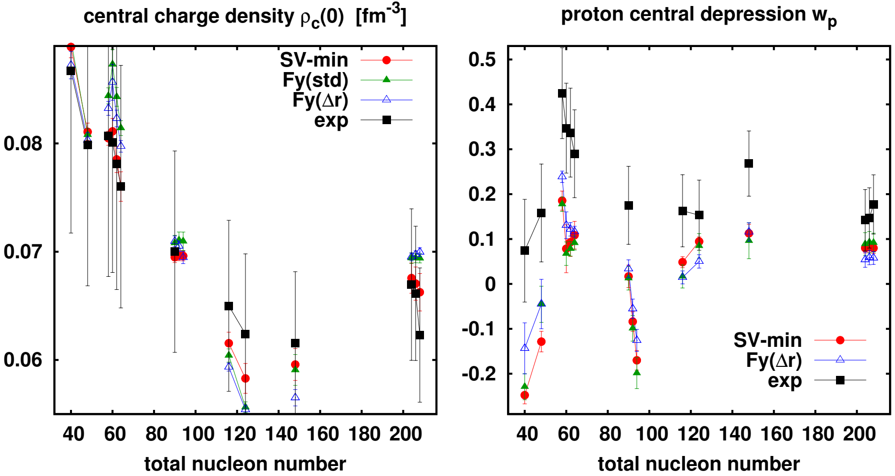
$\rho_p(0)$: "LDM"(=E/A, $\rho_{\rm eq}$, K, J, L,surf) dominates clearly over "shell"(=kinetic,ls,pair)
already "isovector LDM"(=J,L) determines a large fraction

w_p: "shell"-group is as important as "LDM", "J,L" has much less impact

Matrix of CoD for ^{48}Ca and ^{302}Og



Comparison with experimental data from $\rho_{\mathrm{charge}}(r)$ for stable nuclei



$\rho_c(0)$: agrees with data, SV-min generally closest (but insignificant effect)
deviations change sign $\leftrightarrow$ shell fluctuations in mean-field results

w_c: mean-field theory differs from data, situation improves for heavy nuclei
$\leftrightarrow$ in spite of LDM motivation some impact from high *q* (short-range correl.?)

SHE: mean-field predictions increasingly reliable with increasing system size *A*