Optimization and theoretical uncertainties

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Acknowledgements

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Outline

1. Models and observables
2. Optimization of model parameters and estimate of uncertainties
   - Error propagation – covariance analysis
   - Strategies to estimate errors (systematic and statistical)
   - 3 short examples: trends of residuals, compare with data, far extrapolations
3. More detailed results for 3 strategies: comparison of models, trends, covariances
   - Comparison of models
   - Dedicated variation of NMP: example symmetry energy
   - Covariances
4. Conclusions

Models and observables

The four models in the contest

(T= isospin: $T=0 \leftrightarrow$ isoscalar, $T=1 \leftrightarrow$ isovector)

Skyrme Hartree Fock (SHF):

point couplings ($T=0$ density)^2, ($T=0$ kinetic dns.)^2, ($T=0$ l*s dns.)^2, ($T=0$ ∇dns.)^2
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RMF – density-dependent point-coupling (DD-PC):

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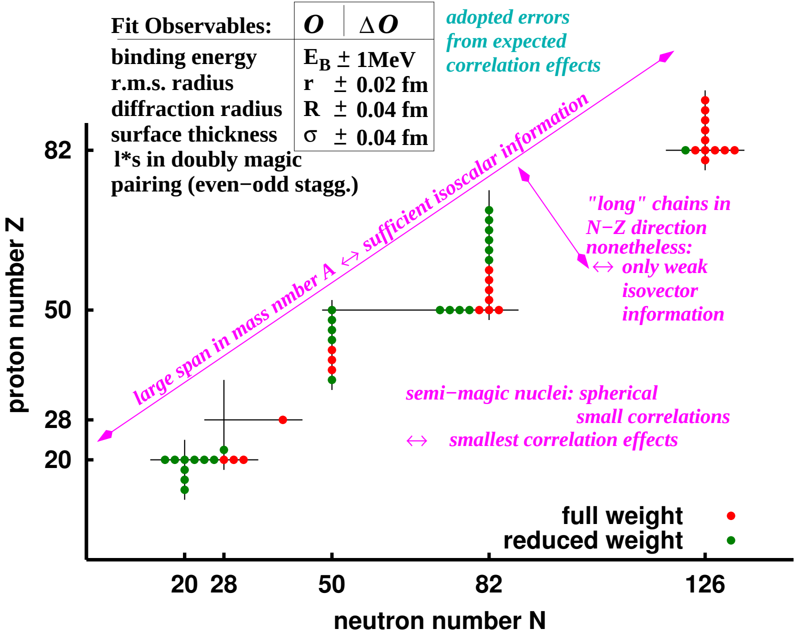
all RMF: l*s couplings automatically included, poor in $T=1$ channel
all models: 6–11 free parameters, to be determined empirically by fit to data

Observables in the pool of fit data



The nuclear matter parameters (NMP)

given $E/A(\rho)$ = energy per particle in symmetric nuclear matter (ρ = total density)
this allows to define basic properties near equilibrium:

$E/A_{\rm eq}$	binding energy per particle at equilibrium point
$\rho_{\rm eq}$	equilibrium density
$K = 9\rho_0^2\partial_\rho^2\dfrac{E}{A}$	incompressibility (isoscalar static response)
$\dfrac{m^*}{m}$	effective mass (isoscalar dynamic response)
$J = a_{\rm sym}$	symmetry energy (isovector static response)
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2 interpretations for NMP: extrapolation to huge systems (matter, neutron stars)
equivalent to part of the model parameters (volume params.)

“Predicted” observables in the forthcoming test cases

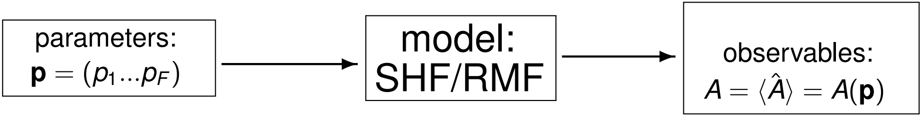
- neutron r.m.s. radius r_n in ^{208}Pb
- neutron skin $r_n - r_p$ in ^{208}Pb
- weak-charge formfactor $F_W(q_{\rm PREX} = 0.475/{\rm fm})$ in ^{208}Pb (related to PREX)
- binding energy E_B for extremely exotic nuclei (super heavy, very neutron rich)
- Q_α value (energy gain in α emission) for super-heavy element
- S_{2n} two-neutron separation energy for Sn chain
- B_f = fission barrier in ^{266}Hs
- dipole polarizability $\alpha_D = \int_0^\infty {\rm d}\omega\, S_D(\omega)\, \omega^{-1}$ in ^{208}Pb
- dipole strength distribution $S_D(\omega) = B(E1,\omega)$ (note: $\sigma_{photoabs}(\omega)) = \omega S_D(\omega))$

Optimization of model parameters and subsequent variation

Optimization of model parameters and exploring its variation

model:
SHF/RMF

Optimization of model parameters and exploring its variation



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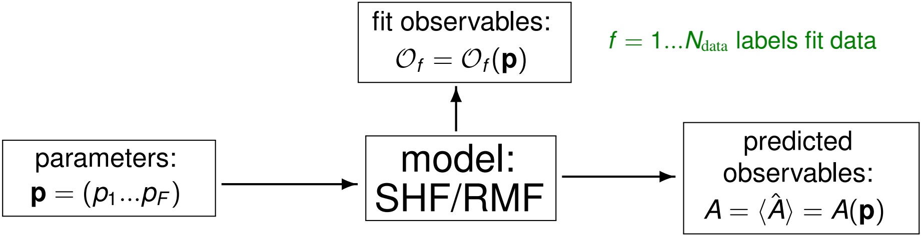

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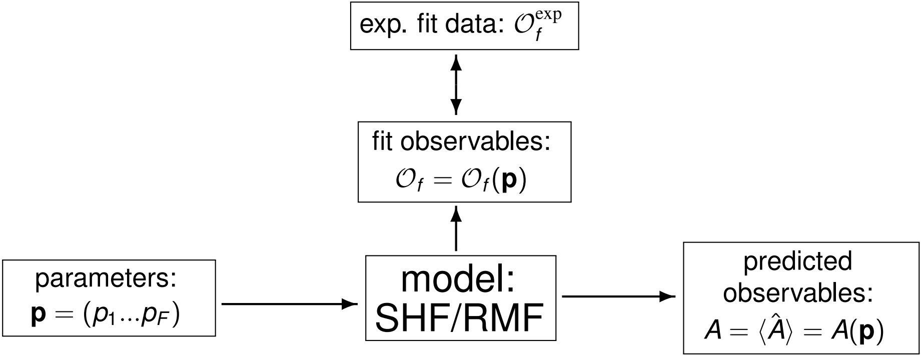

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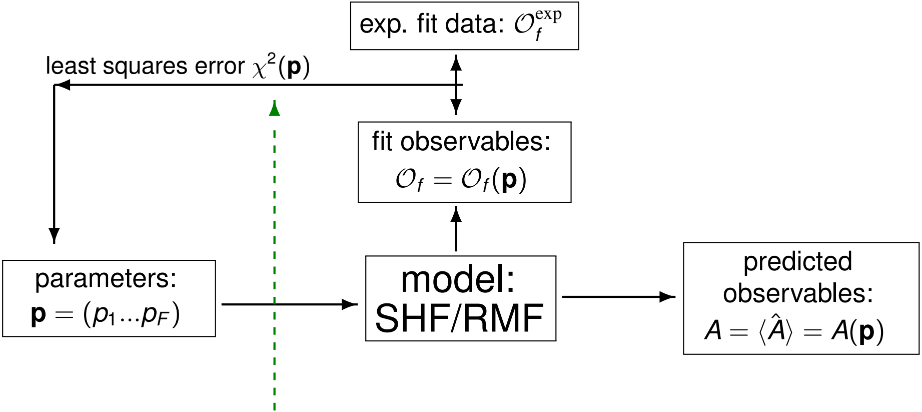

$$\chi^2(\mathbf{p}) = \sum_{f=1}^{N_{\mathrm{data}}} \frac{\left(\mathcal{O}_f(\mathbf{p}) - \mathcal{O}_f^{\mathrm{exp}}\right)^2}{\Delta\mathcal{O}_f^2}$$

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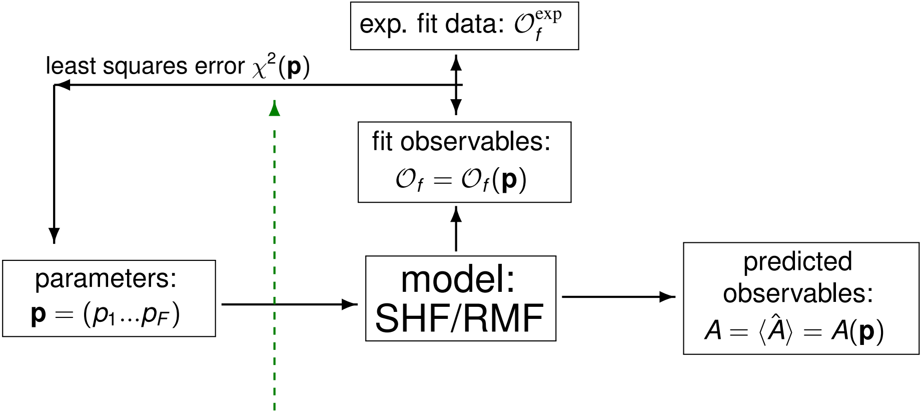

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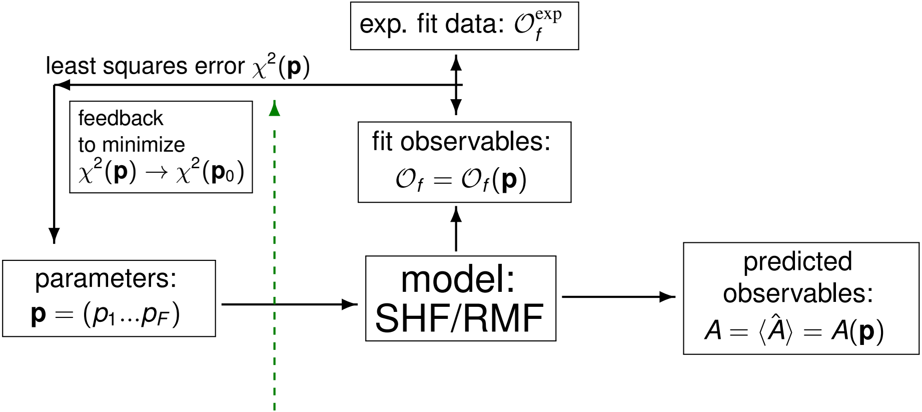

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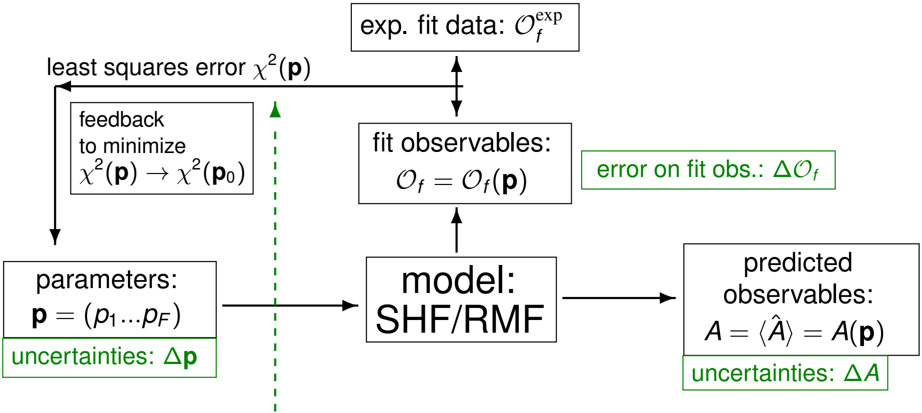

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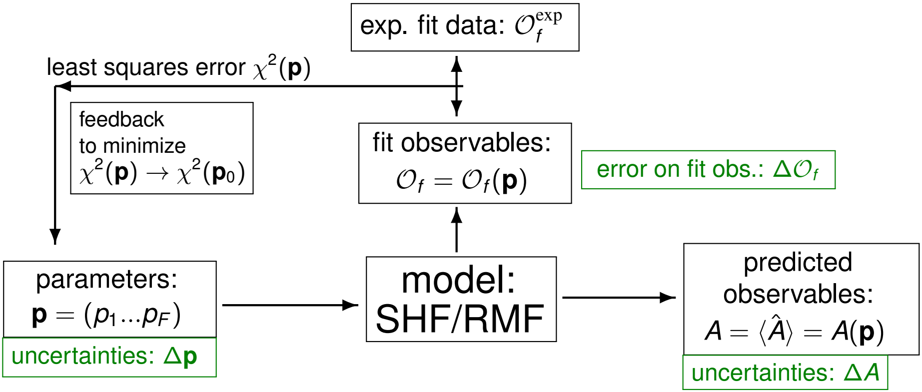

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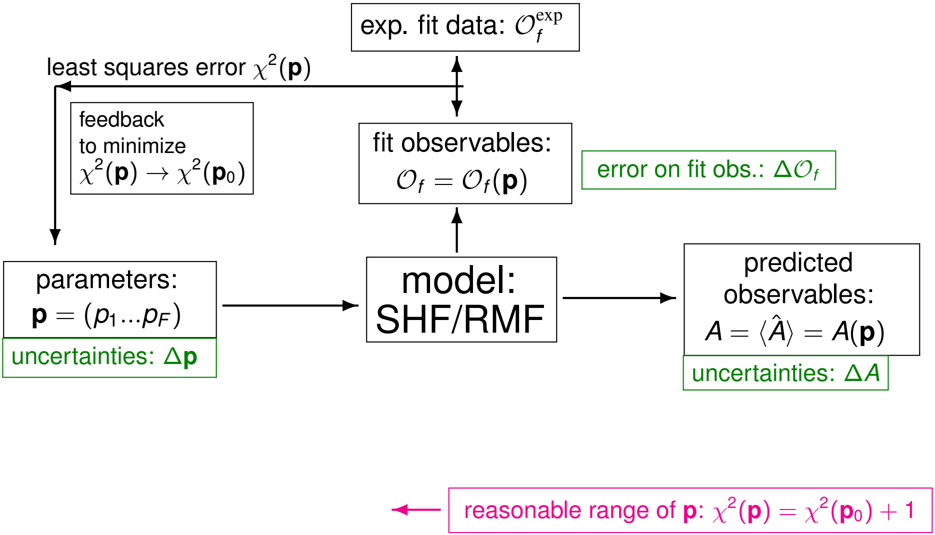

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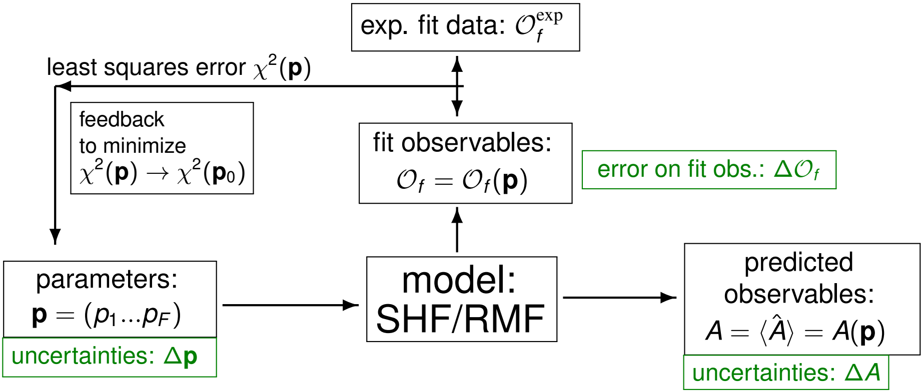

key: covariance matrix $\hat{\mathcal{C}} = \hat{\mathcal{M}}^{-1}$
$\mathcal{M}_{ij} = \partial_{p_i}\partial_{p_j}\chi^2$

← reasonable range of $\mathbf{p}$: $\chi^2(\mathbf{p}) = \chi^2(\mathbf{p}_0) + 1$

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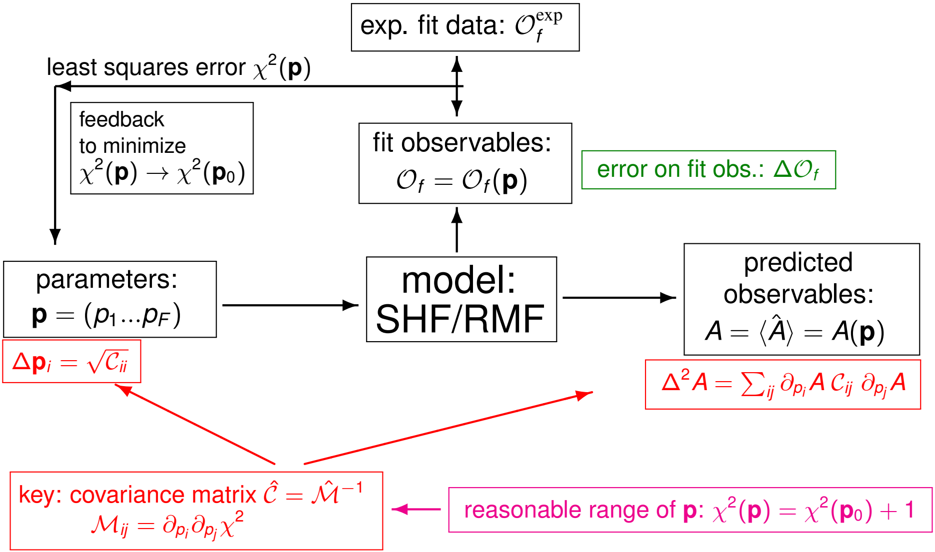

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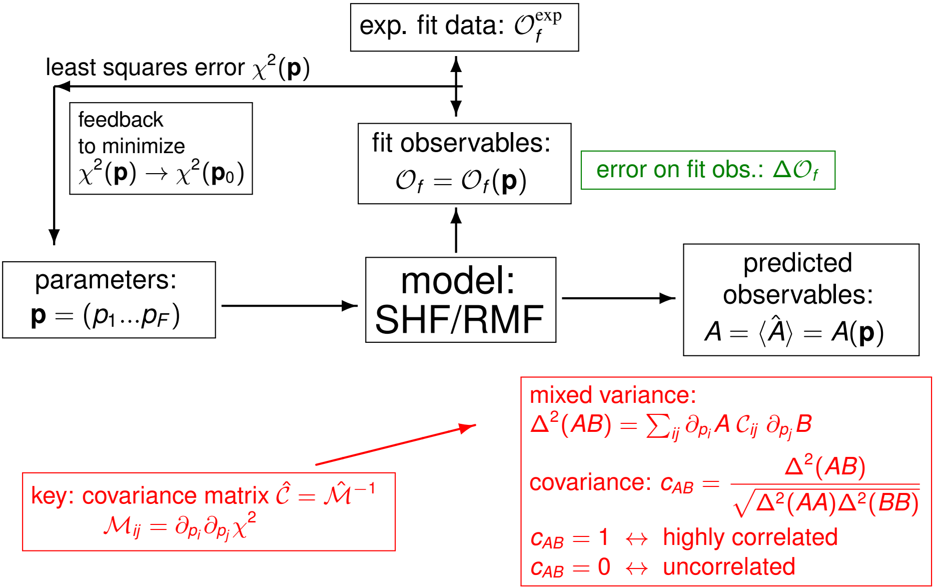

Error propagation – "resonable parametrizations" and uncertainties

probability distribution of "reasonable" parameters:

$$W(\mathbf{p}) \propto e^{-\chi^2(\mathbf{p})} \approx \exp\left(-\frac{1}{2}(\mathbf{p}-\mathbf{p}_0)\hat{\mathcal{M}}(\mathbf{p}-\mathbf{p}_0)\right)\ ,\ \mathcal{M}_{ij} = \partial_{p_i}\partial_{p_j}\chi^2$$

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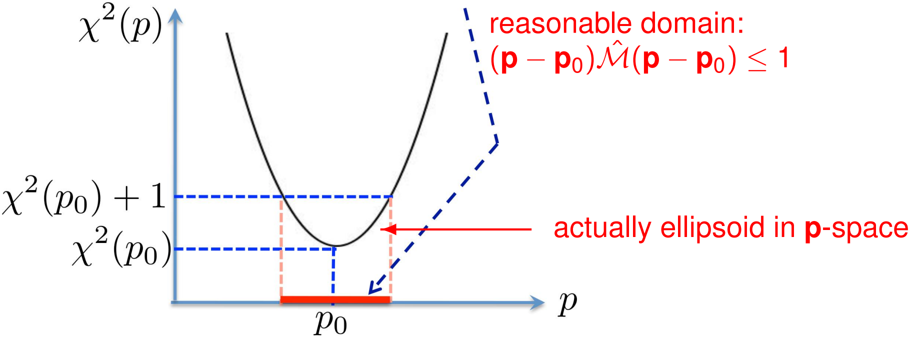

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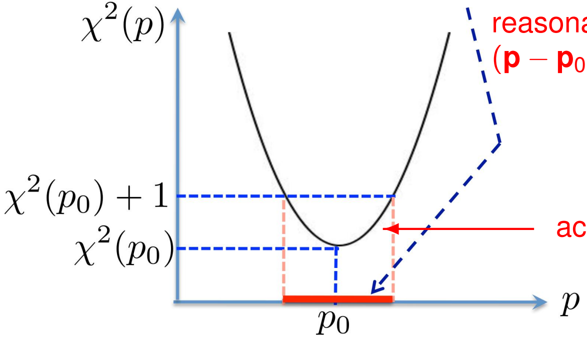


reasonable domain:
$(\mathbf{p}-\mathbf{p}_0)\hat{\mathcal{M}}(\mathbf{p}-\mathbf{p}_0) \leq 1$

actually ellipsoid in **p**-space

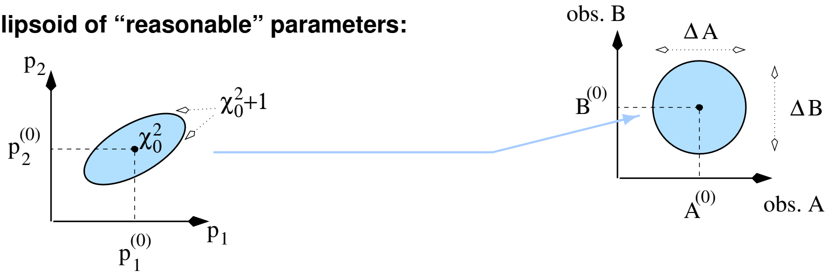
mean values and variances as probability averages (statistical):

$$\overline{A} = \int \mathrm{d}\mathbf{p}\, W(\mathbf{p})\, A(\mathbf{p}) \approx \int \mathrm{d}\mathbf{p}\, W(\mathbf{p})\, \left(A(\mathbf{p}_0) + (\mathbf{p}-\mathbf{p}_0)\cdot\nabla A\right) = A(\mathbf{p}_0)$$

$$\overline{AB} = \int \mathrm{d}\mathbf{p}\, W(\mathbf{p})\, A(\mathbf{p}) B(\mathbf{p}) \approx= \nabla A \cdot \hat{\mathcal{M}}^{-1} \cdot \nabla B$$

Error propagation – covariance analysis

ellipsoid of "reasonable" parameters:



given by: $\Delta\mathbf{p}\cdot(\nabla\otimes\nabla\chi^2)\cdot\Delta\mathbf{p}=1$

observables: $A=A(\mathbf{p})$, $B=B(\mathbf{p})$

$$\Longrightarrow \quad \boxed{\overline{\Delta A\,\Delta B}=\nabla A\cdot(\nabla\otimes\nabla\chi^2)^{-1}\cdot\nabla B}$$

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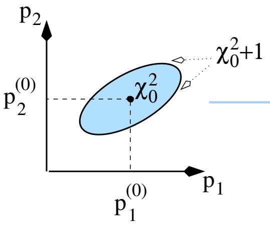

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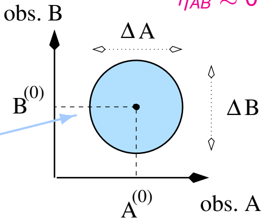
uncertainty: $\quad \Delta A=\sqrt{\overline{\Delta A\,\Delta A}}$

correlation: $\quad \eta_{AB}=\dfrac{\overline{\Delta A\,\Delta B}}{\sqrt{\overline{\Delta^2 A}\;\overline{\Delta^2 B}}}$

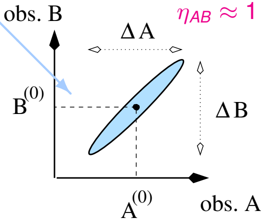
uncorrelated observables:

$\eta_{AB}\approx 0$



highly correlated observables:

$\eta_{AB}\approx 1$



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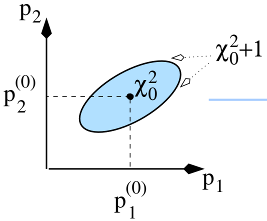

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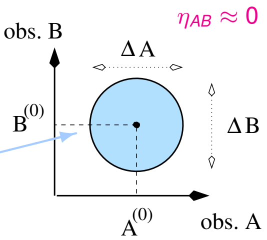

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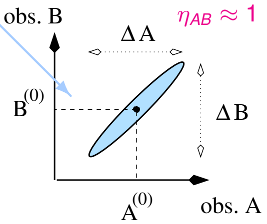
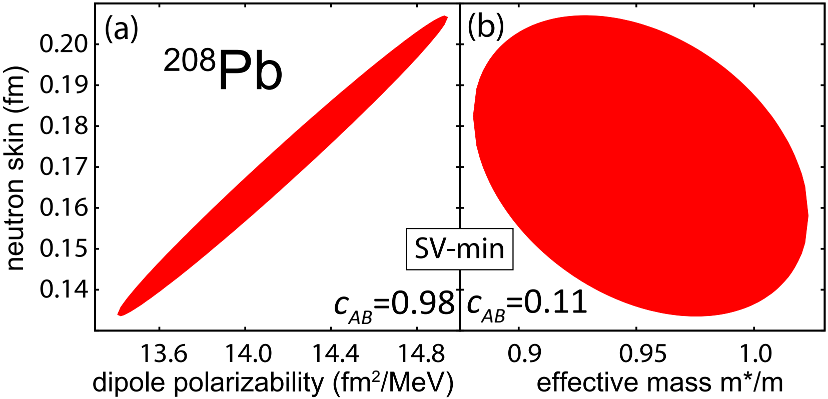


correlations $\longleftrightarrow$ underlying nuclear model $\Longrightarrow$ “reasonable model” required

Covariance analysis: example r_n, α_D, and m^*/m in ^{208}Pb

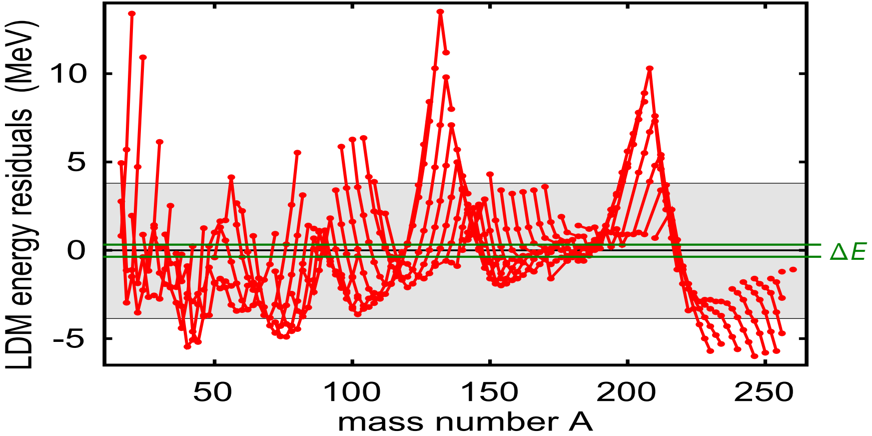


highly correlated: polarizability α_D $\leftrightarrow$ neutron skin $r_n - r_p$
almost uncorrelated: isoscalar effective mass m^*/m $\leftrightarrow$ neutron skin $r_n - r_p$

Strategies to estimate errors (systematic and statistical)

1. **Dedicated variations of parameters (NMP):** **(statistical)**
   perform χ^2 with fixed $\mathcal{O}_{\mathrm{NMP}}$, watch the trend of $A(\mathbf{p})$ when varying $\mathcal{O}_{\mathrm{NMP}}$
2. **Extrapolation uncertainties from statistical analysis (statistical):**
   $\chi^2(\mathbf{p})$ & observable $A(\mathbf{p}) \quad \Longrightarrow \quad$ uncertainty ΔA
3. **Correlations between observables from statistical analysis (statistical):**
   $\chi^2(\mathbf{p})$ & two observables $A(\mathbf{p}), B(\mathbf{p}) \quad \Longrightarrow \quad$ covariance c_{AB}
4. **Sensitivity analysis for the model parameters p (statistical):**
   Take a model parameter p_α as "observable" ($p_\alpha \equiv B$), look at covariance c_{Ap_α}
5. **Variations of fit data:** **(statistical/systematic)**
   switch on/off groups of fit observables $\hat{\mathcal{O}}_i$, energy, radius, ...
6. **Trends of residual errors:** **(systematic)**
   is distribution of residuals $\mathcal{O}_i(\mathbf{p}) - \mathcal{O}_i^{\mathrm{exp}}$ stochastic? $\leftrightarrow$ trends signal insufficiencies
7. **Comparison with predicted data:** **(systematic)**
   actual deviation should fulfill $A(\mathbf{p}_0) - A^{(\mathrm{exp})} \leq \Delta A$, larger deviations indicate problems
8. **Variations of the model:** **(systematic)**
   compare different models (RMF $\leftrightarrow$ SHF), extend a model by new terms

Trends of residual errors: example LDM and energy systematics

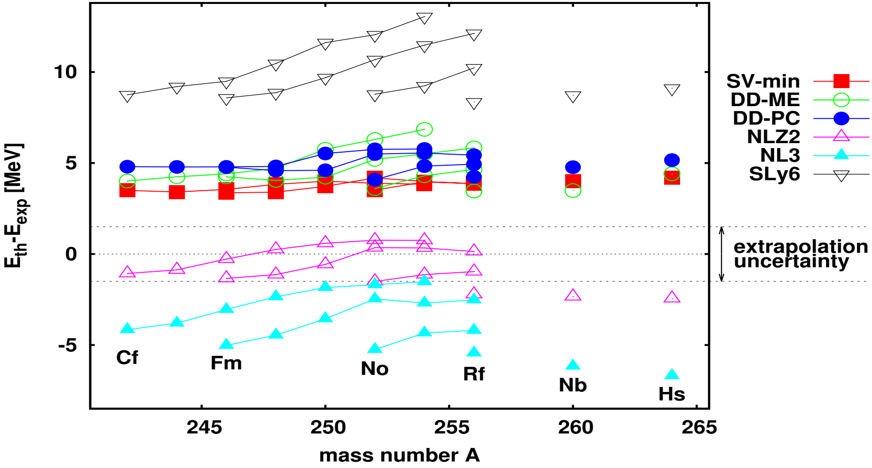


LDM misses quantum shell effects $\leftrightarrow$ can describe only average trends of $E_B(N, Z)$

residual errors on E_B not stochastically distributed $\leftrightarrow$ trends reflect shell effects

actual average error (grey area) $\gg$ extrapolation error from χ^2 analysis (ΔE)

Comparison with predicted data: example known super-heavy elements



residual errors on E_B stay $\leq \pm 1$ MeV for $A < 220$ for all parametrizations

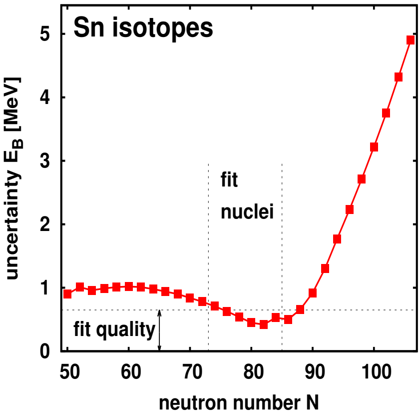
deviations of E_B grow systematically with $A \Leftrightarrow$ something missing in all models

deviations have different sign for RMF vs. SHF $\Leftrightarrow$ something different is missing

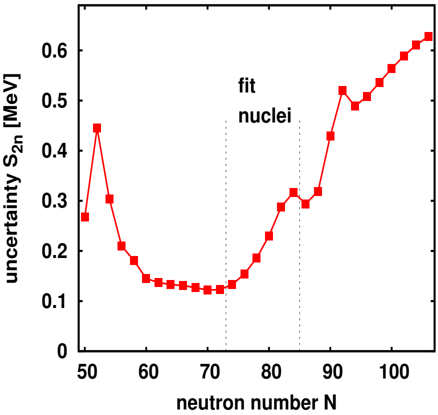
good performance of (RMF) NL-Z irrelevant $\leftrightarrow$ NL-ME has poor quality else wise

Extrapolation uncertainties: example chain of Sn isotopes

binding energies



2-neutron separation energies



uncertainty E_B grows quickly with $N \nearrow$, far beyond ΔE_B in fit
$\leftrightarrow$ extrapolations deteriorate with distance to fit data

but uncertainty S_{2n} generally smaller & not dramatically growin(factor < 2)
$\rightarrow$ differences E_B often more reliable than E_B as such

$\Longrightarrow$: uncertainties ΔA from statistical analysis very useful indicators

Comparison SHF $\leftrightarrow$ 3$\times$RMF

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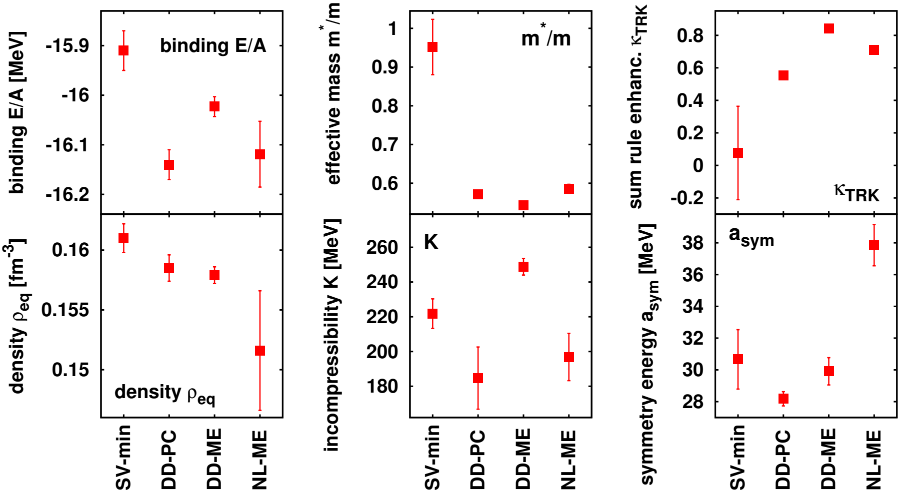
Goal: large differences in predictions indicate intrinsic differences of models
and give an idea about possible systematic errors

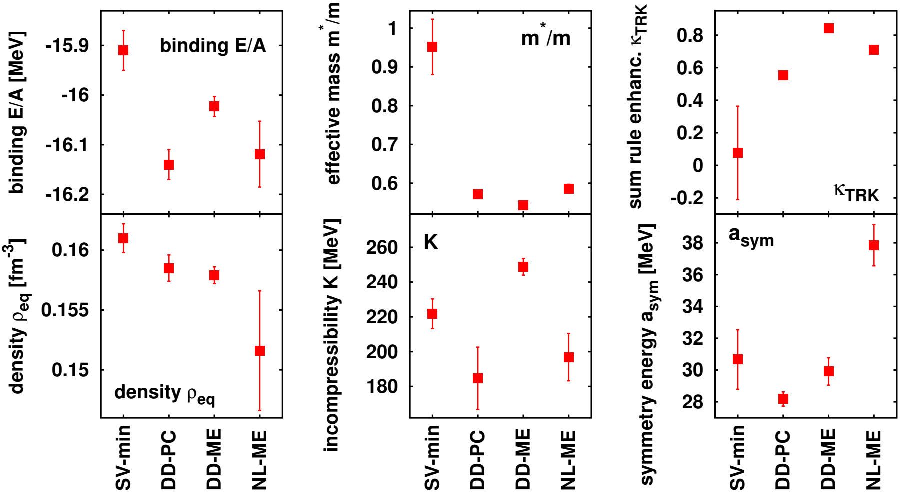
SHF $\leftrightarrow$ 3×RMF: predictions for NMP



uncertainties $\Delta\mathcal{O}$: very different $\leftrightarrow$ specific structure of models

m^*/m, κ_{TRK} fixed in RMF; a_{sym} larger in SHF; NL-ME generally weak

SHF $\leftrightarrow$ 3×RMF: predictions for NMP

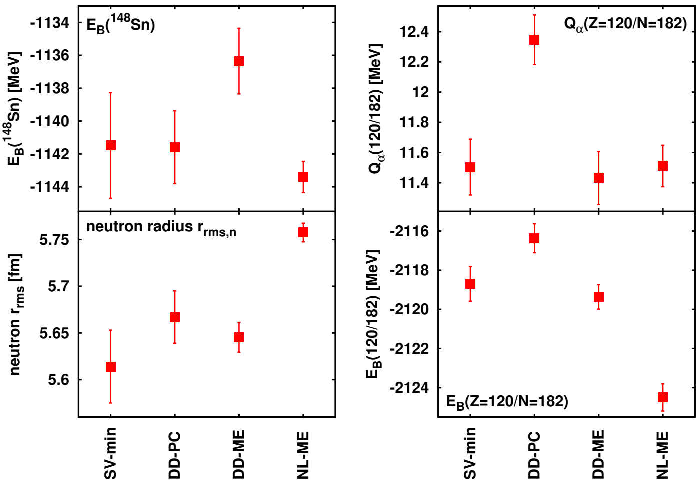


uncertainties $\Delta\mathcal{O}$: very different $\leftrightarrow$ specific structure of models

m^*/m, $\kappa_{\rm TRK}$ fixed in RMF; $a_{\rm sym}$ larger in SHF; NL-ME generally weak

deviations between models: often larger than $\Delta\mathcal{O}$ $\leftrightarrow$ systematic differences of models

SHF $\leftrightarrow$ 3$\times$RMF: predictions for observables in (super-)heavy nuclei



T=1 obs. (left panels): SHF larger $\Delta\mathcal{O} \leftrightarrow$ isovector freedom
NL-ME: smallest $\Delta\mathcal{O} \leftrightarrow$ predictive power? – too rigid model!
deviations $> \Delta\mathcal{O}$: not as dramatic as for NMP

Dedicated variation: example trends with symmetry energy a_{sym} (J)

strategy: produce parametrizations with constraint on a_{sym}
$\Longrightarrow$ a set of parametrizations with systematically varied a_{sym}
and else wise similar properties

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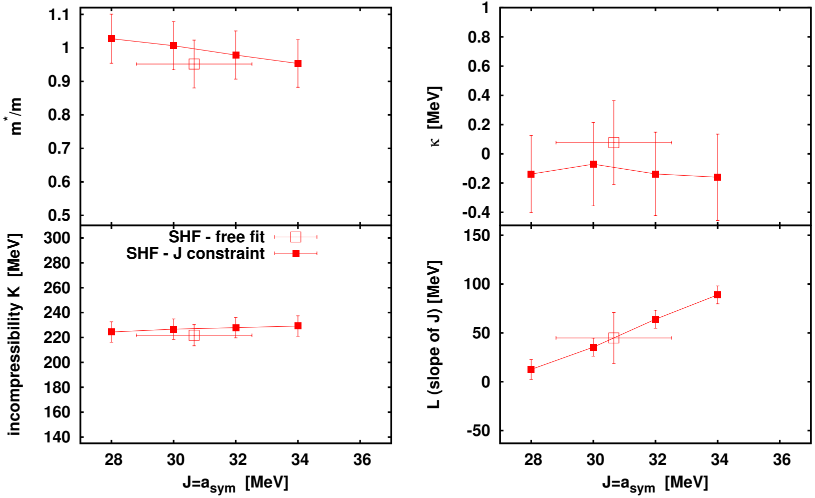
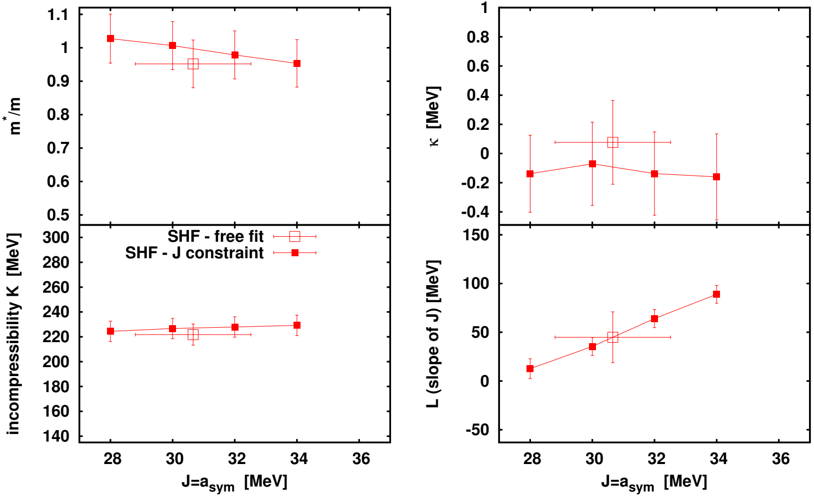
combined with comparison of models – SHF & 3×RMF

Trends of nuclear matter properties (NMP) with a_{sym} for the case of SHF



ΔJ of free fit = reasonable range $J \leftrightarrow \Delta\mathcal{O}$ of free fit complies with slope of constr. fits

Trends of nuclear matter properties (NMP) with $a_{\rm sym}$ for the case of SHF

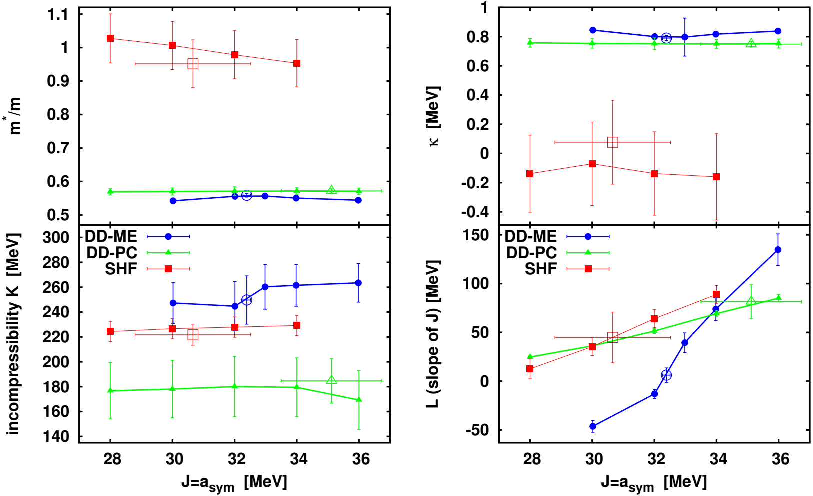


ΔJ of free fit = reasonable range $J \leftrightarrow \Delta\mathcal{O}$ of free fit complies with slope of constr. fits

K, m^*/m, κ independent of J $(= a_{\rm sym})$ $\Longrightarrow$ four independent model parameters

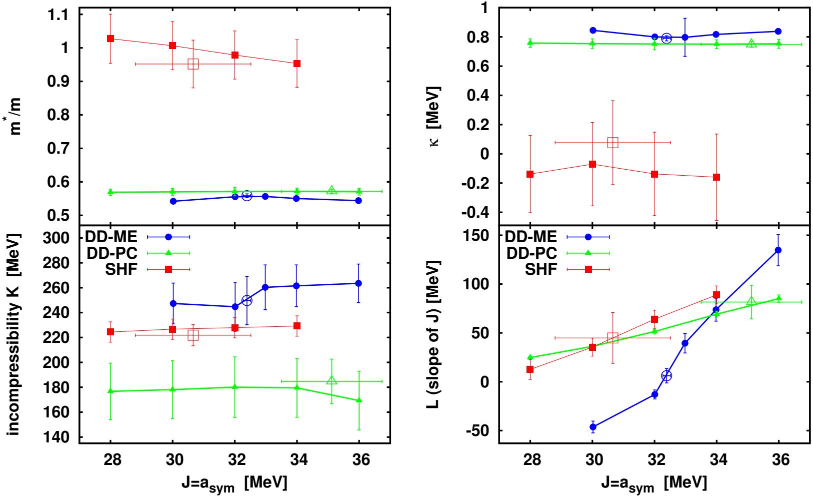
L = slope of J strongly linked with J $\longleftrightarrow$ hidden correlation in data (and model)

Trends of nuclear matter properties (NMP) with a_{sym} – SHF & RMF



for all cases: K, m^*/m, κ independent of a_{sym}, and L strongly linked with J
but $L(J)$ differs between models $\leftrightarrow$ density dependent T=1 terms?

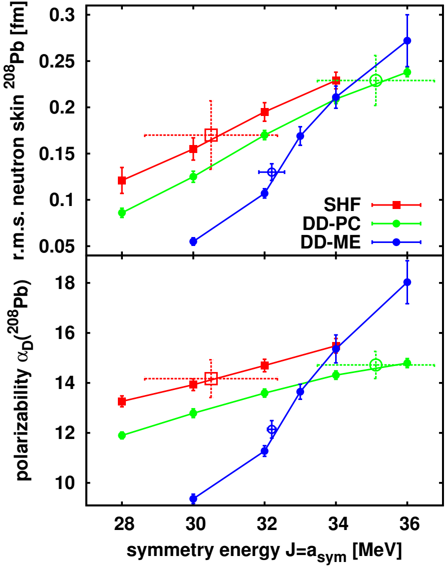
Trends of nuclear matter properties (NMP) with $a_{\rm sym}$ – SHF & RMF



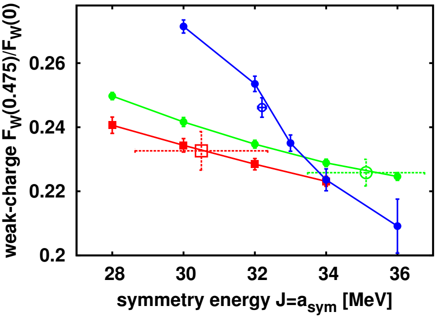
for all cases: K, m^*/m, κ independent of $a_{\rm sym}$, and L strongly linked with J
but $L(J)$ differs between models $\leftrightarrow$ density dependent T=1 terms?

large differences SHF $\leftrightarrow$ RMF: mass parameters m^*/m and κ (already seen before)

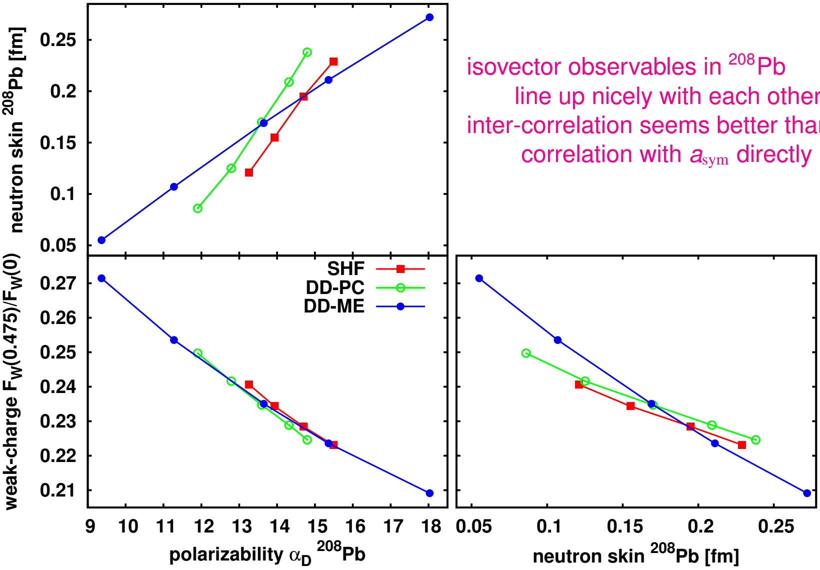
Trends of isovector observables in ^{208}Pb with a_{sym}



for each model: clear trends with a_{sym}
SHF $\leftrightarrow$ DD-PC: same slope,
different offset
DD-ME: even different slope
$\leftrightarrow$ different ρ-dependence
(but small variance of a_{sym})



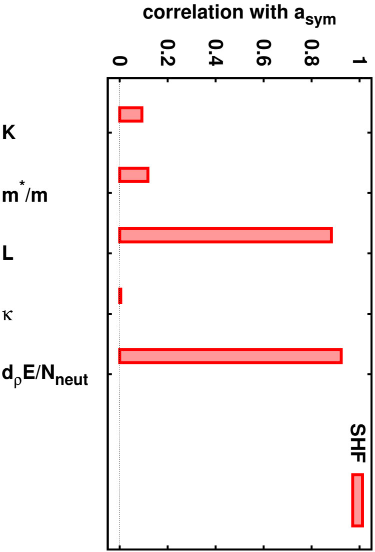
Trends of isovector observables in ^{208}Pb – drawn against each other



isovector observables in ^{208}Pb
line up nicely with each other
inter-correlation seems better than
correlation with a_{sym} directly

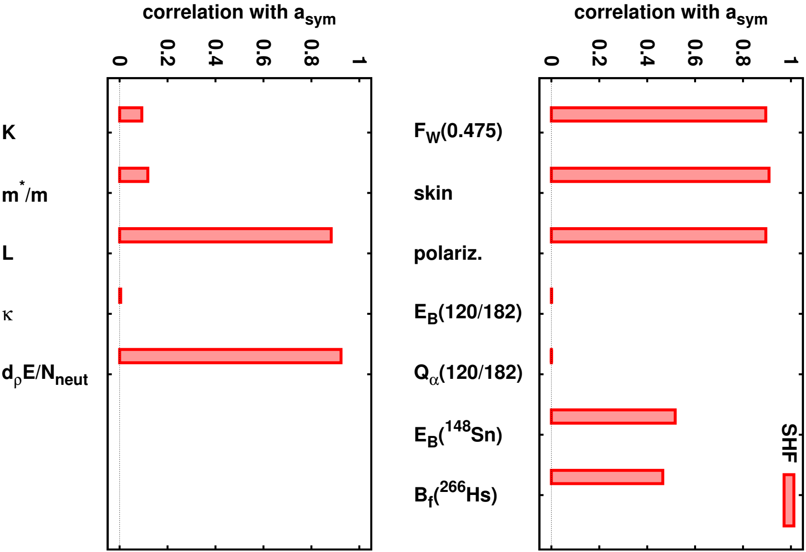
Examples from covariance analysis

Correlations of $a_{\rm sym}$ with NMP, for the case of SHF



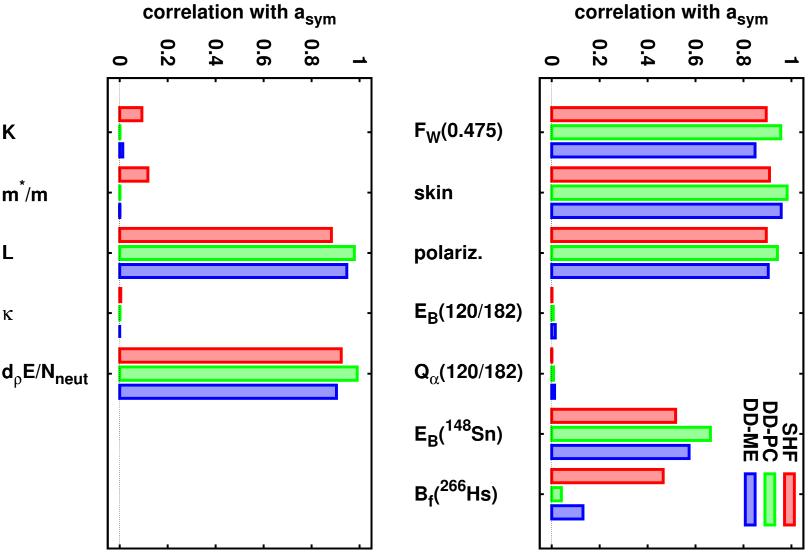
Again: K, m^*/m, κ perfectly independent; but strong correlation with L, $\partial_\rho E_{\rm neut}/N$
surface properties $a_{\rm surf}$, $a_{\rm surf,sym}$ show a mixed picture

Correlations of $a_{\rm sym}$ with NMP and observables in finite nuclei – SHF



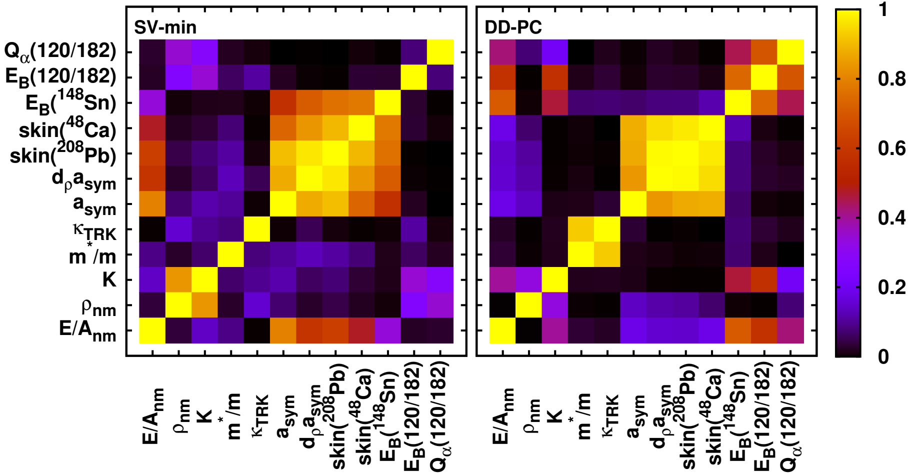
Good isovector observables (in ^{208}Pb): weak-charge formfactor F_W, neutron skin $r_n - r_p$, p
superheavy elements uncorrelated, neutron rich nuclei & fission somewhat correlated

Correlations of a_{sym} with NMP and obs. in finite nuclei – SHF & RMF



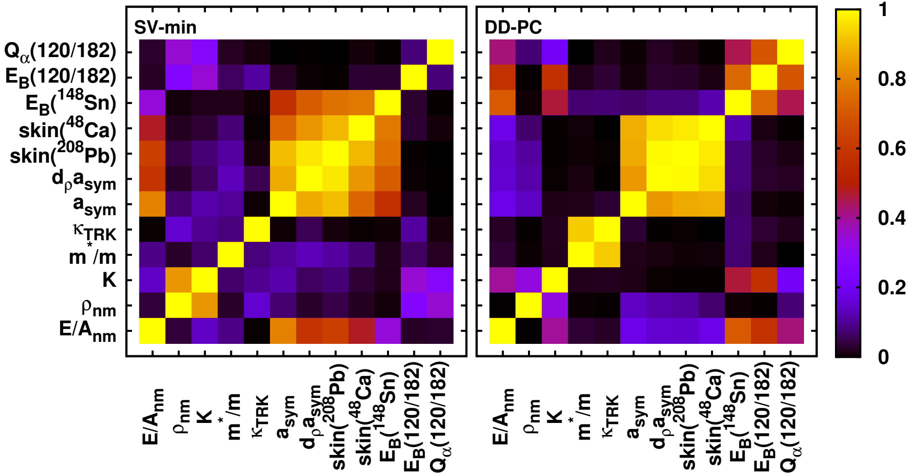
RMF models shows nearly the same correlations as SHF
except for surface properties and fission

Correlations of a_{sym} with NMP and obs. in finite nuclei – SHF & RMF



DD-PC ↔ SHF show at first glance similar correlations

Correlations of a_{sym} with NMP and obs. in finite nuclei – SHF & RMF



DD-PC $\leftrightarrow$ SHF show at first glance similar correlations

differences: $\kappa_{\mathrm{TRK}} \leftrightarrow m^*/m$ – due to “frozen mass” in RMF

$K \leftrightarrow \rho_{\mathrm{nm}}$ – due to different modeling of density dependence

exotic nuclei – density dep. & isovector terms & shell structure (m^*/m)

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powerful tool: extrapolation errors, covariances, trends $\leftrightarrow$ insight into model

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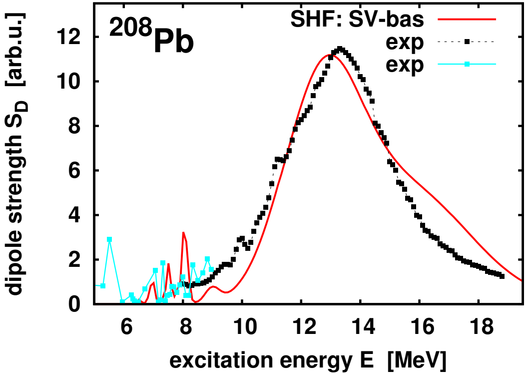
several different tools: comparison models, trend residuals, data, ...
no ultimate solution: there is no systematic way to evaluate systematic errors

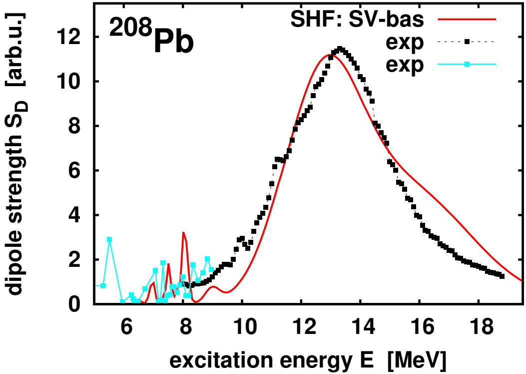
Correlations with dipole strength

Dipole strength and related oobservables



integrated strength: $\mathcal{I}_D^{(n)}(E) = \int_0^E \mathrm{d}E'\, S_D(E')\, E'^n$

Dipole strength and related oobservables



polarizability:

$$\alpha_D = \mathcal{I}_D^{(-1)}(\infty)$$
$$= \int_0^\infty \mathrm{d}E\, S_D(E)\; E^{-1}$$

TRK sum-rule enhancement:

$$\kappa_{\mathrm{TRK}} = \mathcal{I}_D^{(1)}(\infty)$$
$$= \int_0^\infty \mathrm{d}E\, S_D(E)\; E^{+1}$$

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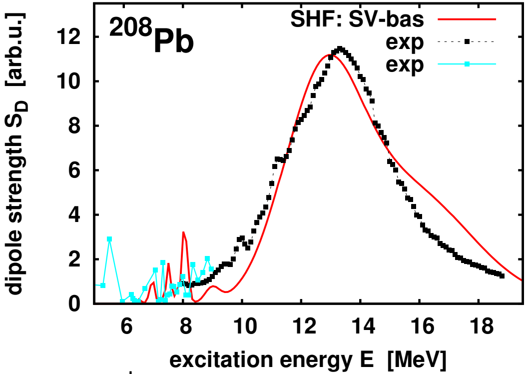
Dipole strength and related oobservables



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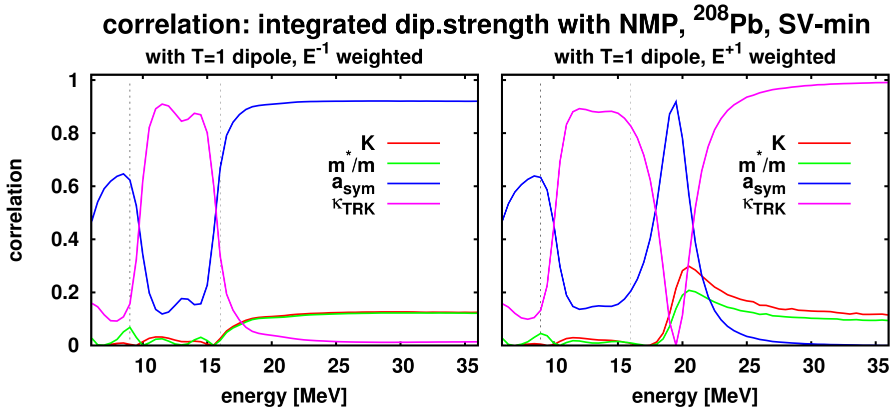
low-lying dip.strength ("pygmy"): $\mathcal{I}_D^{(n)}(9\,\mathrm{MeV})$ $\leftrightarrow$ signal for α_D, κ_{TRK} ?

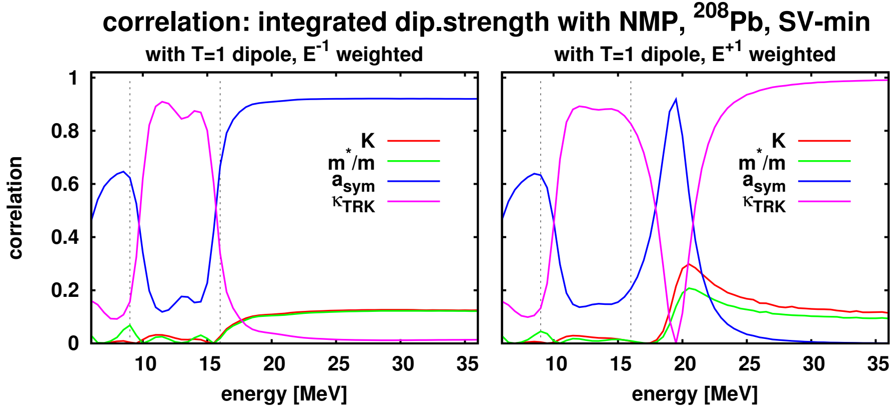
Correlation of $\int_0^E dE' \, \sigma(E') \, E'^n$ with nuclear matter parameters



E^{-1} weight favors $a_{\rm sym}$ for $E \to \infty$

E^{1} weight favors κ for $E \to \infty$

Correlation of $\int_0^E dE' \, \sigma(E') \, E'^n$ with nuclear matter parameters



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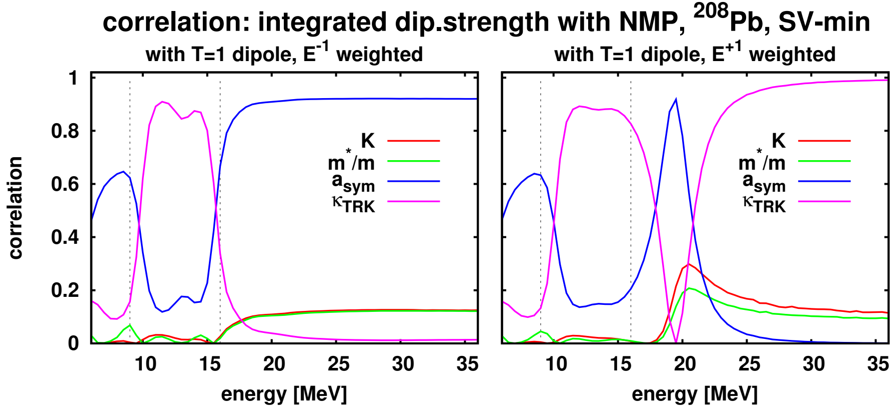

E^{-1} weight favors $a_{\rm sym}$ for $E \to \infty$ E^{1} weight favors κ for $E \to \infty$

GDR region favors κ for all E weights

pygmy region yields mixed info about $a_{\rm sym}$ and κ $\Longrightarrow$ useful data in combined analysis
(open problem: robust choice of cutoff energy $E_{\rm cut}$)

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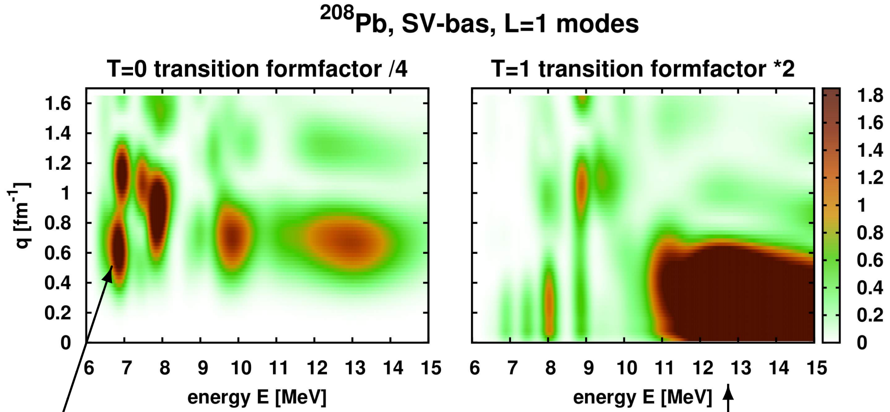
Transition formfactor $f_{\mathrm{trans}}(q, E)$ for $L = 1$ modes in ^{208}Pb



GDR

strong $T = 0$ modes, $q \approx 0.6$
($q = 0$ occupied by c.m. mode)

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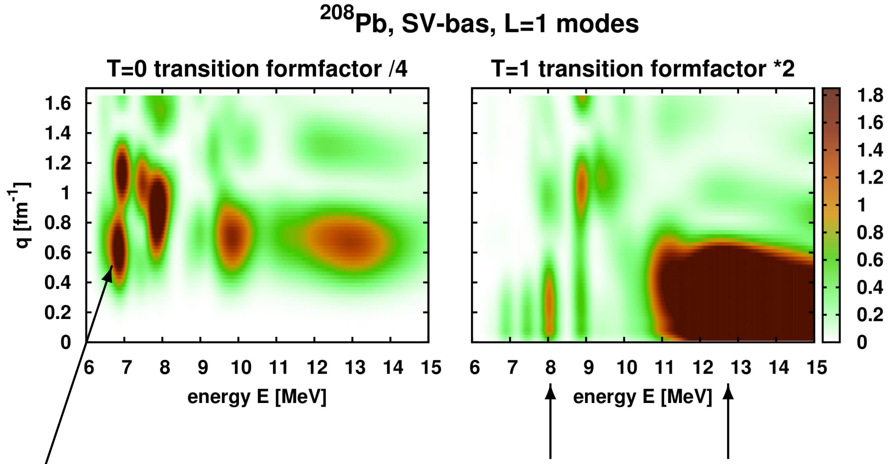

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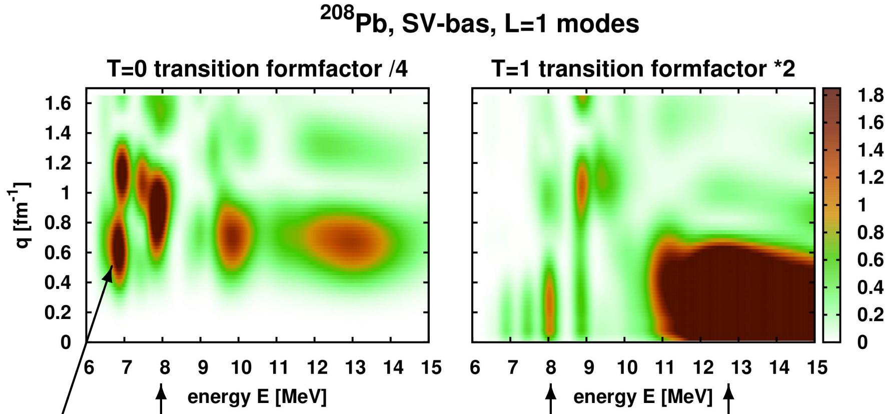

related to strong $T = 0$ mode $\leftarrow$ low E dip.str.

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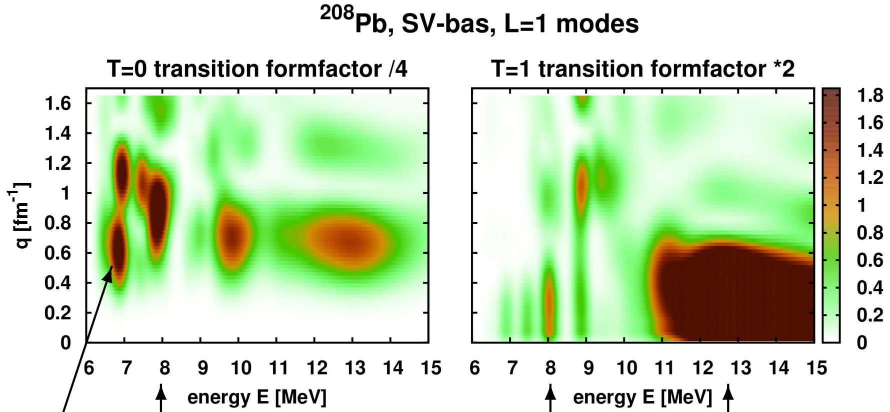

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pure L=1, $q \approx 0.6$

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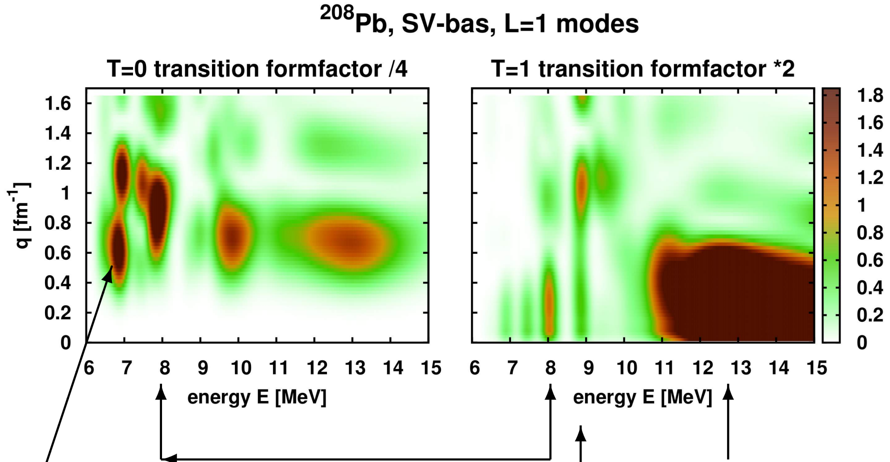

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strong $T = 0$ modes, $q \approx 0.6$

($q = 0$ occupied by c.m. mode)

pure L=1, $q \approx 0.6$

low E dipoles: mixed modes, predominantly isoscalar, nonetheless useful info on NMP