INT Program INT-16-2a
Bayesian Methods in Nuclear Physics
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Optimisation of the shell-model Hamiltonian for heavy nuclei

and the underlying uncertainty

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Göran Gustafsson Stiftelse

Outline

- Introduction (to the black box)
- The shell model effective interaction (the parameters)
- Optimization of the effective Hamiltonian (parameter estimation)
- Problems
- Summary

there are known knowns…

there are known unknowns…

But there are also unknown unknowns – the ones we don't know we don't know
Donald Rumsfeld, 2002

What is the difference between model calibration and parameter estimation? (http://bayesint.github.io/)

Nuclear theory: guiding principles

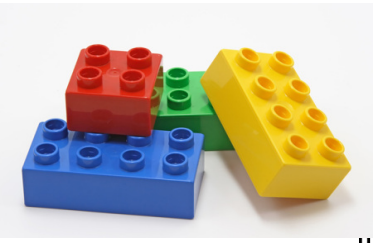
The quest for the mean field

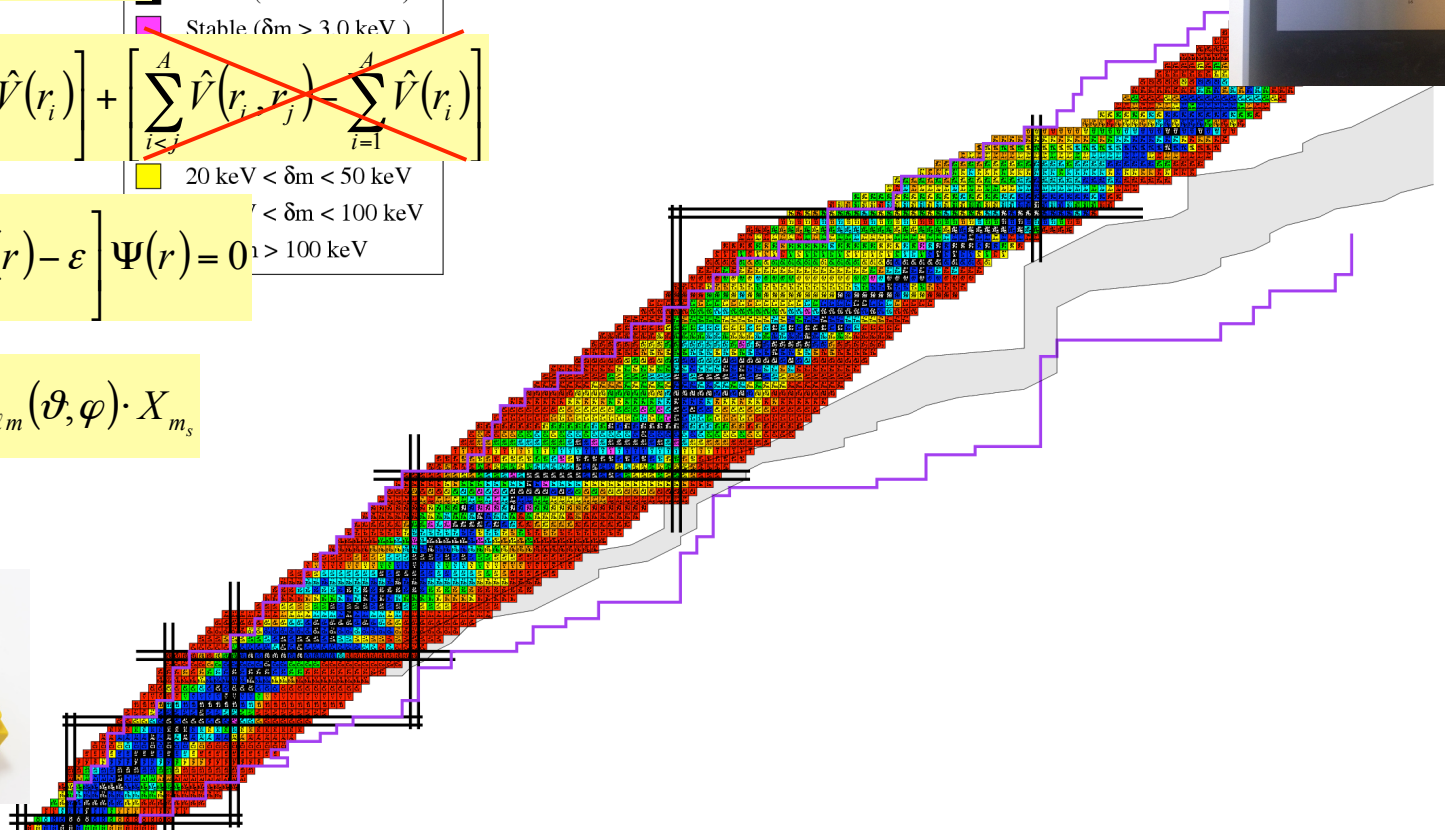
$$\hat{H} = \sum_{i=1}^{A} \frac{\hat{p}_i^2}{2m_i} + \sum_{i<j}^{A} \hat{V}(r_i, r_j)$$

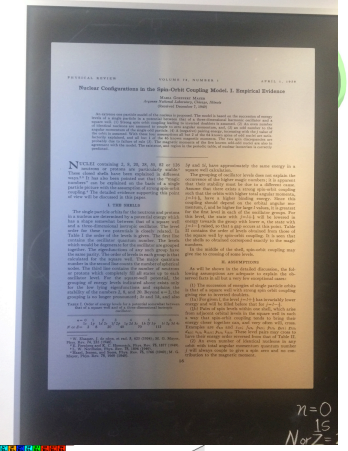
$$\hat{H} = \sum_{i=1}^{A} \left[\frac{\hat{p}_i^2}{2m_i} + \hat{V}(r_i) \right] + \left[\sum_{i<j}^{A} \hat{V}(r_i, r_j) - \sum_{i=1}^{A} \hat{V}(r_i) \right]$$

$$\left[-\frac{\hbar^2}{2 \cdot m} \nabla^2 + V(r) - \varepsilon \right] \Psi(r) = 0$$

$$\Psi(r) = \frac{u_\ell(r)}{r} \cdot Y_{\ell m}(\vartheta, \varphi) \cdot X_{m_s}$$







Building blocks: neutron and protons

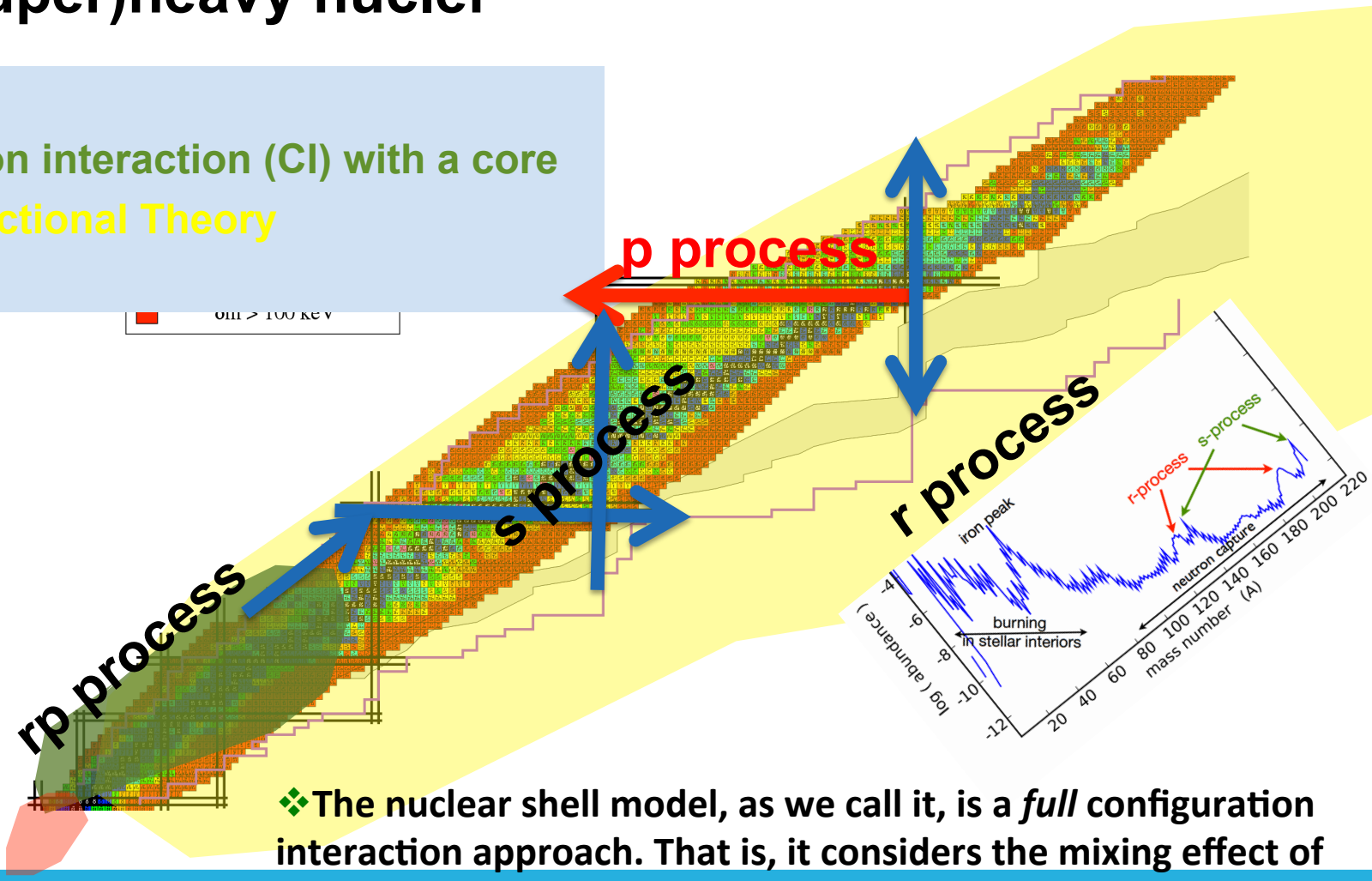
Motivation

microscopic shell-model description of (super)heavy nuclei

Ab initio

Configuration interaction (CI) with a core

Density Functional Theory



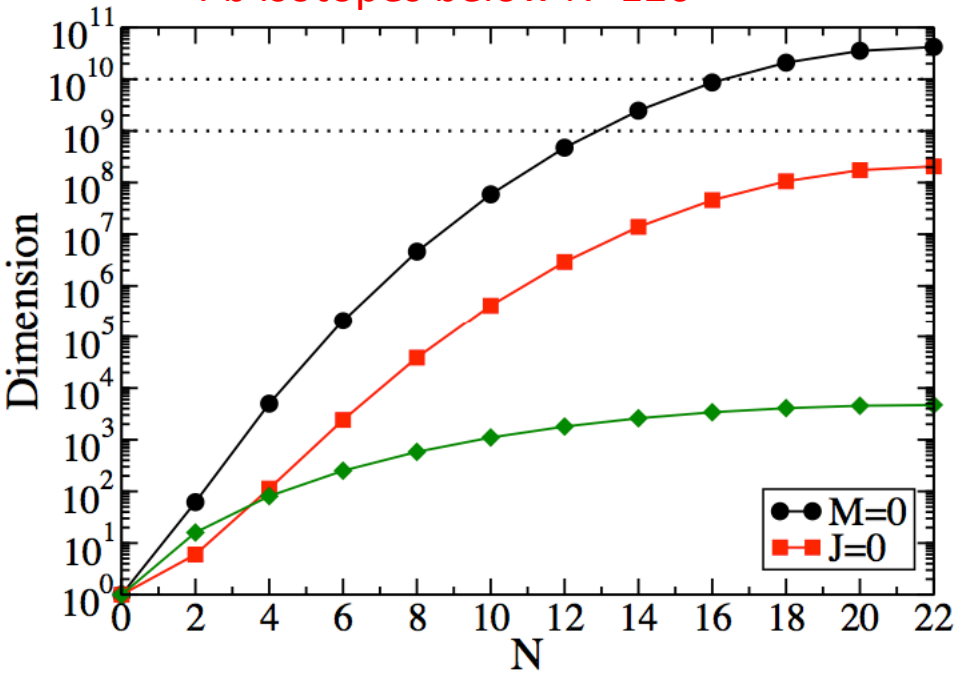
❖The nuclear shell model, as we call it, is a *full* configuration interaction approach. That is, it considers the mixing effect of all possible configurations within a given model space.

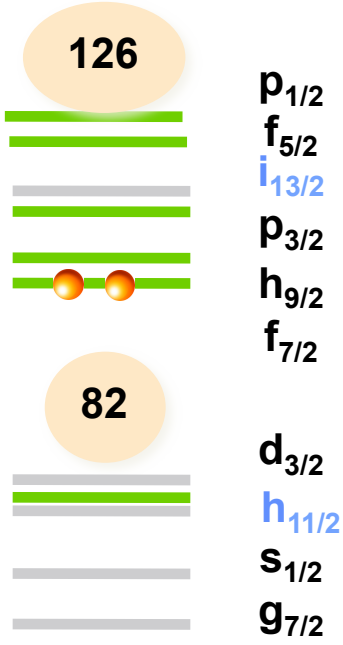
❖The most accurate and precise theory on the market. But there is a price to pay

See also B. Szpak, D. Vretenar's talks last week

Computational challenge

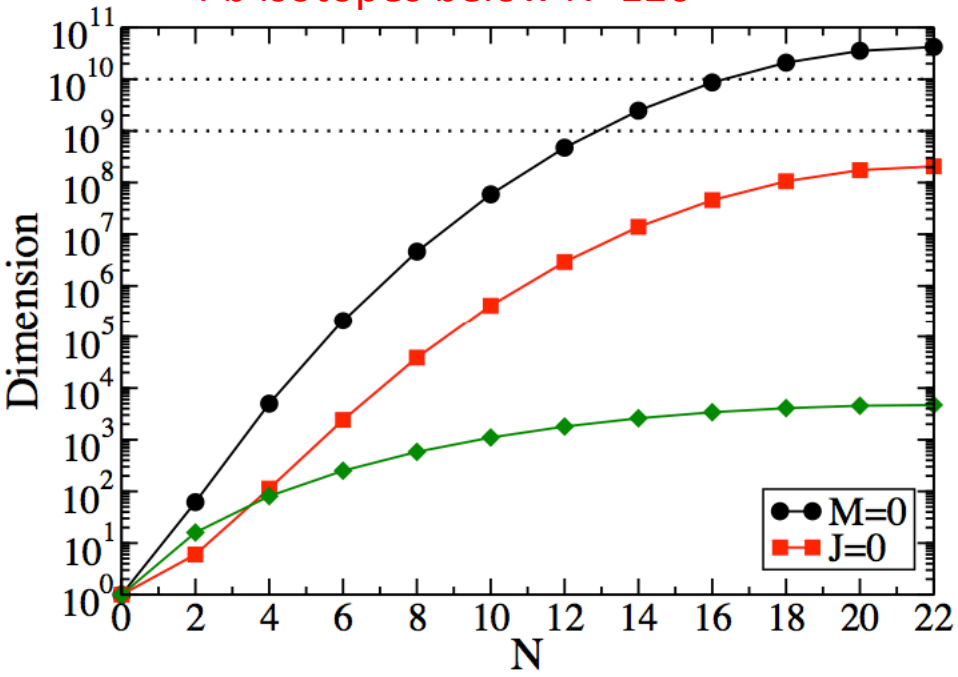
Pb isotopes below N=126

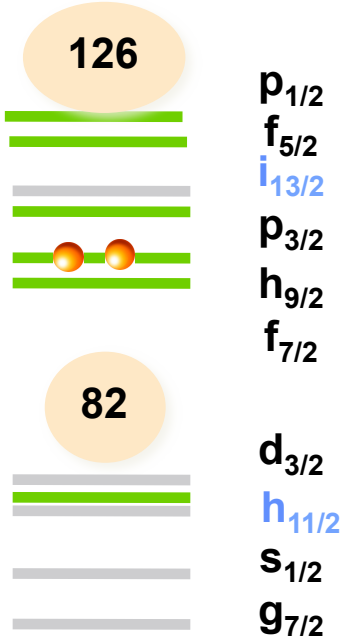




Computational challenge

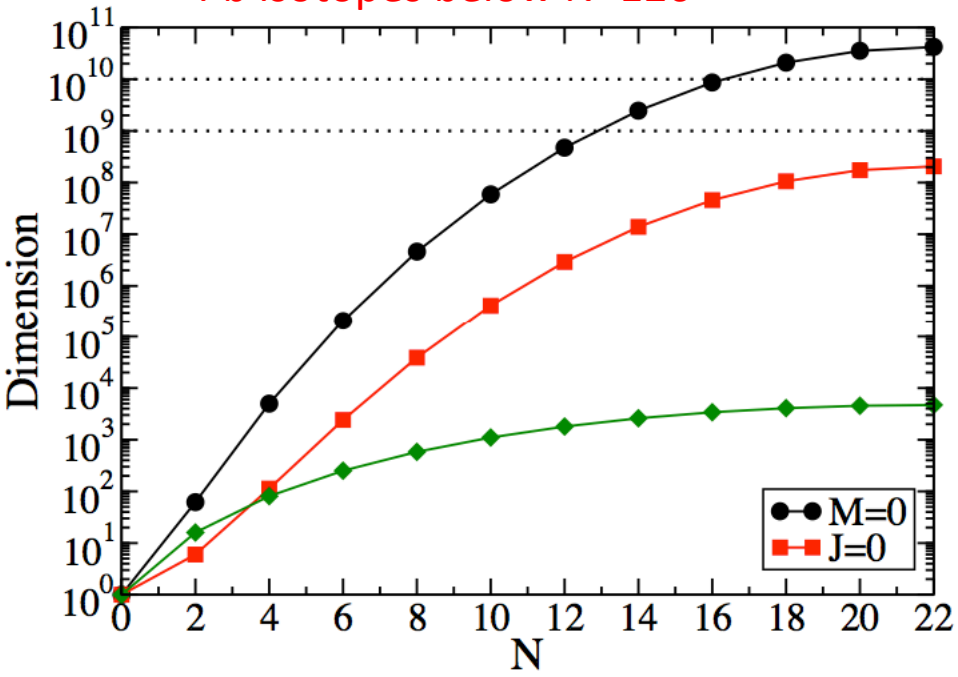
Pb isotopes below N=126

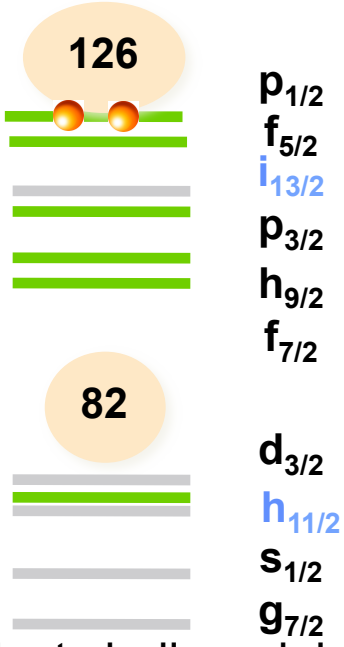




Computational challenge

Pb isotopes below N=126

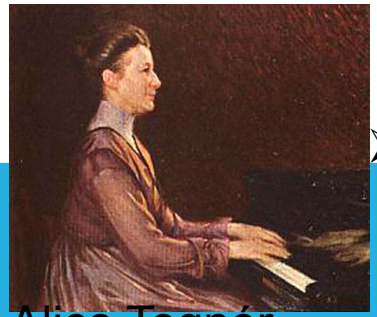




- Most shell-model codes are in M-scheme: Simple algorithm; avoid the complicated angular momentum coupling
- N~Z Systems are relatively easier to solve by applying the so-called factorization technique (as in ANTOINE)
- System with identical particles can be more difficult to treat. Possible factorization under development.[7]

Two new computers became available from 2016

PDC's supercomputer Beskow

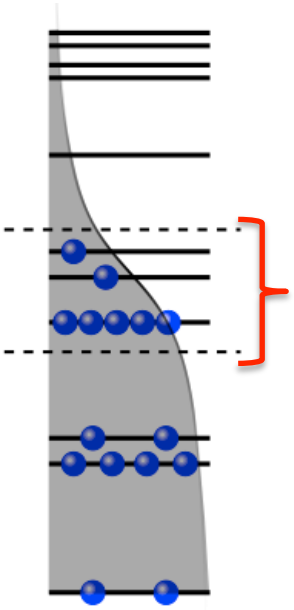


Alice Tegnér

Shell model as a local theory

We are still not able to build a universal Hamiltonian;

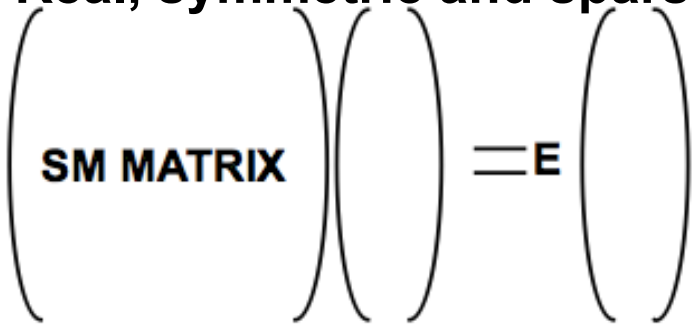
Even if we can, we will not be able to solve it.



Shell model:
Limited number of orbitals
Full configuration

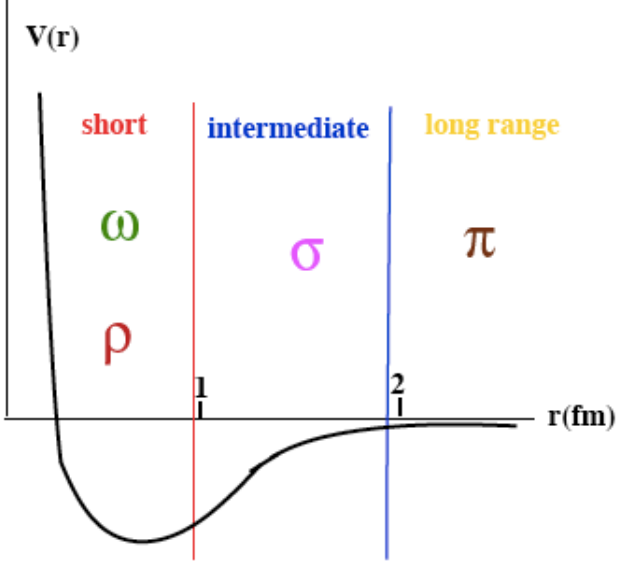
$$\Phi_\alpha(1,2,\ldots,A) \equiv \Phi_{\alpha_1\alpha_2\ldots\alpha_A}(1,2,\ldots,A) = \frac{1}{\sqrt{A!}} \begin{vmatrix} \phi_{\alpha_1}(\vec{r}_1) & \phi_{\alpha_1}(\vec{r}_2) & \ldots & \phi_{\alpha_1}(\vec{r}_A) \\ \phi_{\alpha_2}(\vec{r}_1) & \phi_{\alpha_2}(\vec{r}_2) & \ldots & \phi_{\alpha_2}(\vec{r}_A) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_{\alpha_A}(\vec{r}_1) & \phi_{\alpha_A}(\vec{r}_2) & \ldots & \phi_{\alpha_A}(\vec{r}_A) \end{vmatrix}$$

Real, symmetric and sparse matrix

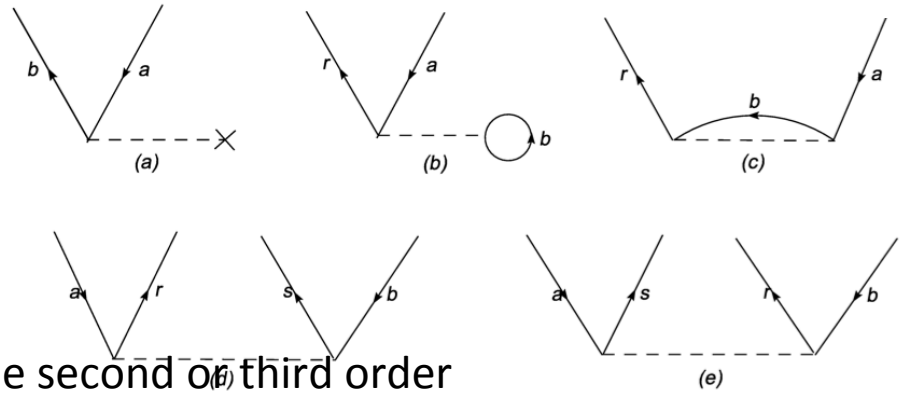


"Bare" Nucleon-Nucleon Potentials:

- Argonne V18: PRC 56, 1720 (1997)
- CD-Bonn 2000: PRC 63, 024001 (2000)
- *N³LO: PRC 68, 041001 (2003)*
- *INOY: PRC 69, 054001 (2004)….*



Perturbation treatment



and many others.
Usually we stop at the second or third order

Can do:

- Reproduce NN scattering data with a high precision (~40 parameters)
- Benchmark calculations for very light nuclei

Cannot do:

- Nuclear saturation (wrong by ~1MeV/A)
- Shell structure (N=14, 28…)
- May be due to the missing three-body force

Quest of the effective interaction

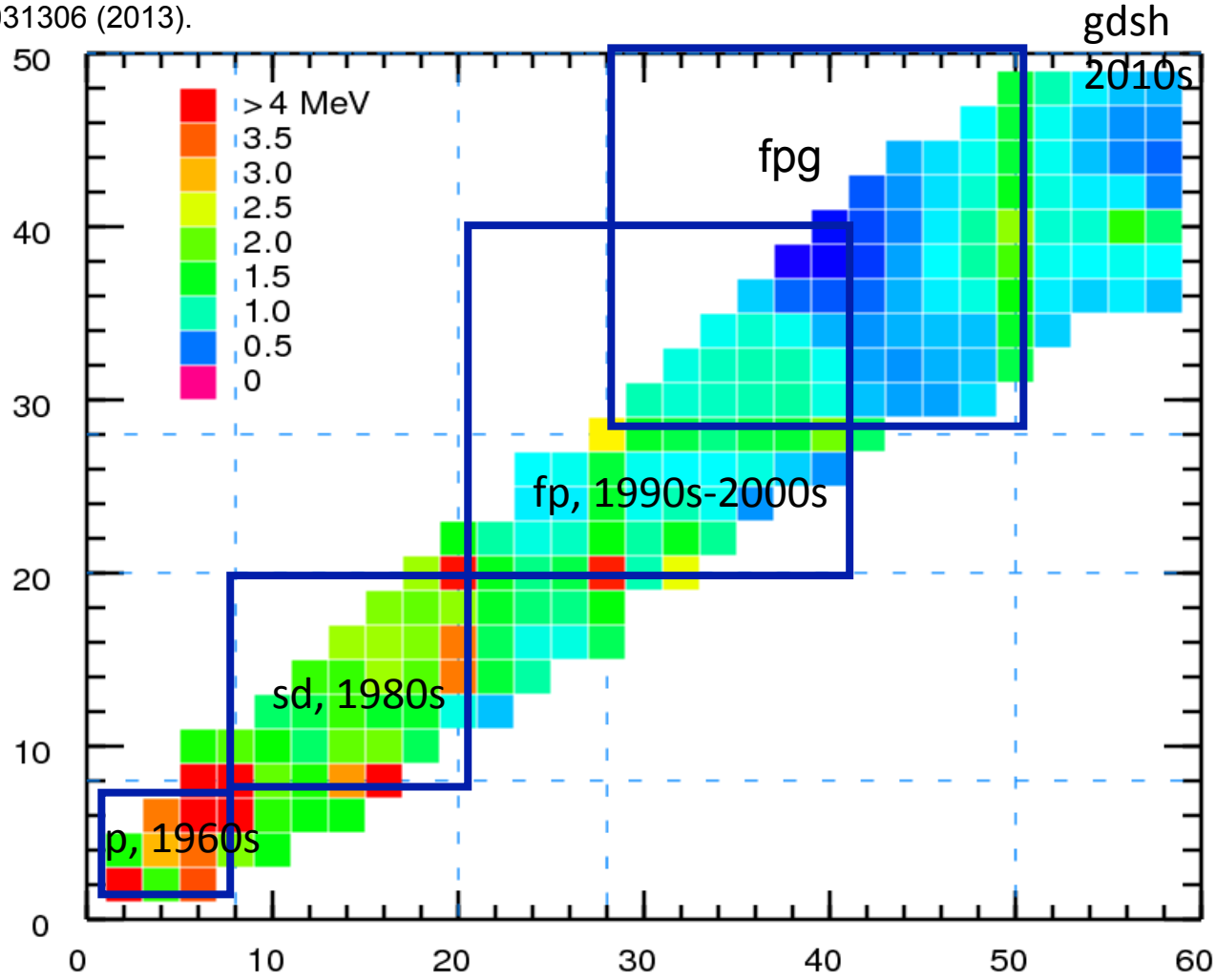
◆Empirical effective interaction

- ❖USD, B. A. Brown and W. A. Richter, Phys. Rev. C 74, 034315 (2006).
- ❖fp (KB3, gxpf), 1990s
- ❖fpg, M. Honma et al., Phys. Rev. C 80, 064323 (2009)
- ❖**gdsh, CQ, Z. Xu, Phys. Rev. C 86, 044323 (2012)**
- ❖**Cross-shell fpg+gdsh to understand the effect of the N=50 shell**

T. Bäck, CQ et al.PRC 87, 031306 (2013).

One has to consider:

- **The core polarization effects induced by the assumed inert core**
- **Optimization of the monopole interaction due to the neglect of three-body and other effects**



Monopole Hamiltonian

Determines average energy of eigenstates in a given configuration.

- Important for binding energies, shell gaps

$$H_m = \sum_a \varepsilon_a n_a + \sum_{a \le b} \frac{1}{1+\delta_{ab}} \left[\frac{3V^1_{ab} + V^0_{ab}}{4} n_a (n_a - \delta_{ab}) + (V^1_{ab} - V^0_{ab})(T_a \cdot T_b - \frac{3}{4} n_a \delta_{ab}) \right]$$

n_a, T_a … number, isospin operators of orbit *a*

Monopole centroids

- Angular-momentum averaged effects of two-body interaction
- **The monopole interaction itself does not induce mixing between different configurations.**
- **Strong mixture of the wave function is mainly induced by the residual J=0 *pairing* and *QQ* np interaction**

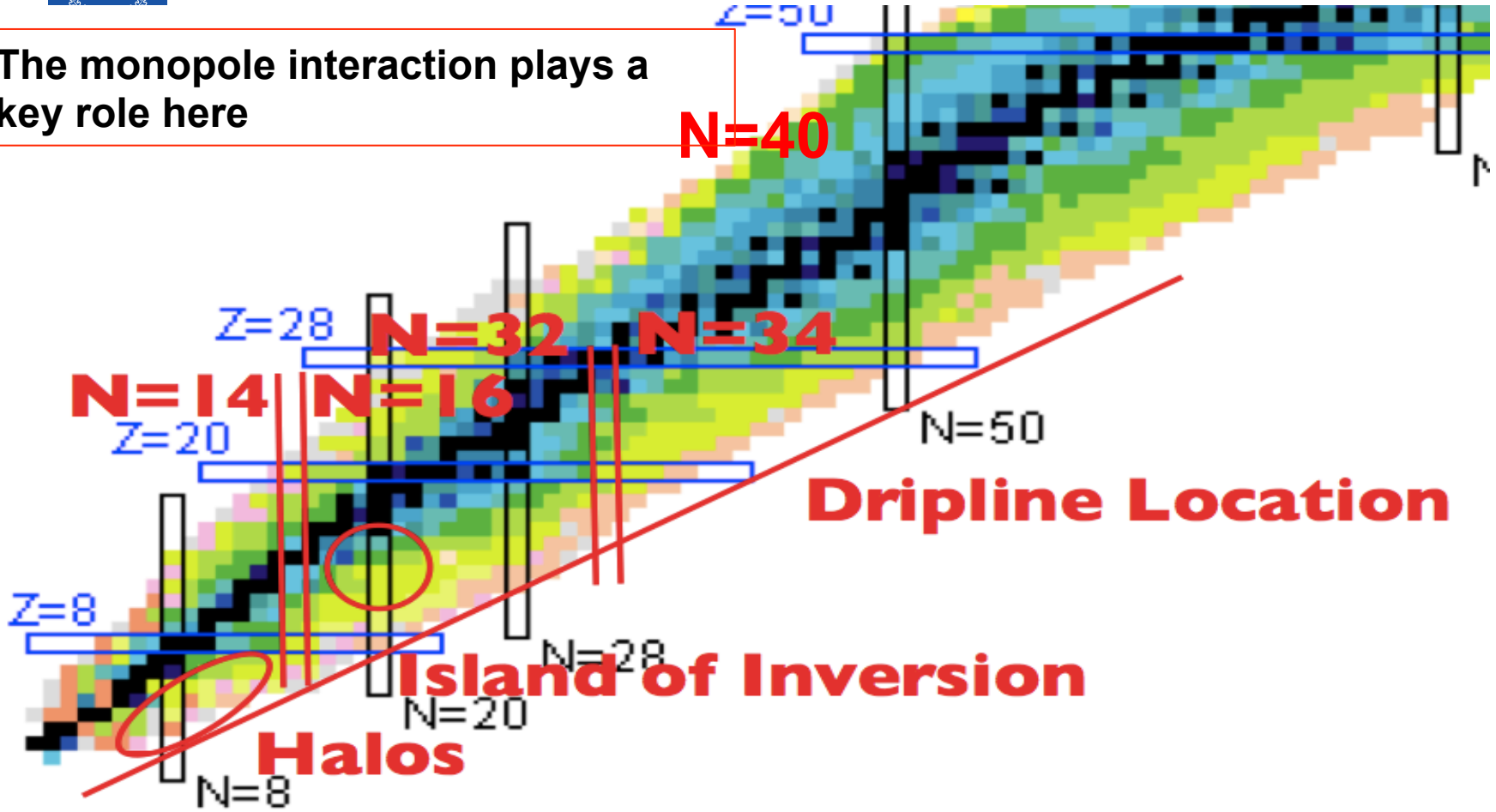
$$V^T_{ab} = \frac{\sum_J (2J+1) V^{JT}_{abab}}{\sum_J (2J+1)}$$

The monopole terms represent only a very small part of the total ‘parameter’ space.

1D to 2D shell structure

Shell evolution at drip lines

The monopole interaction plays a key role here

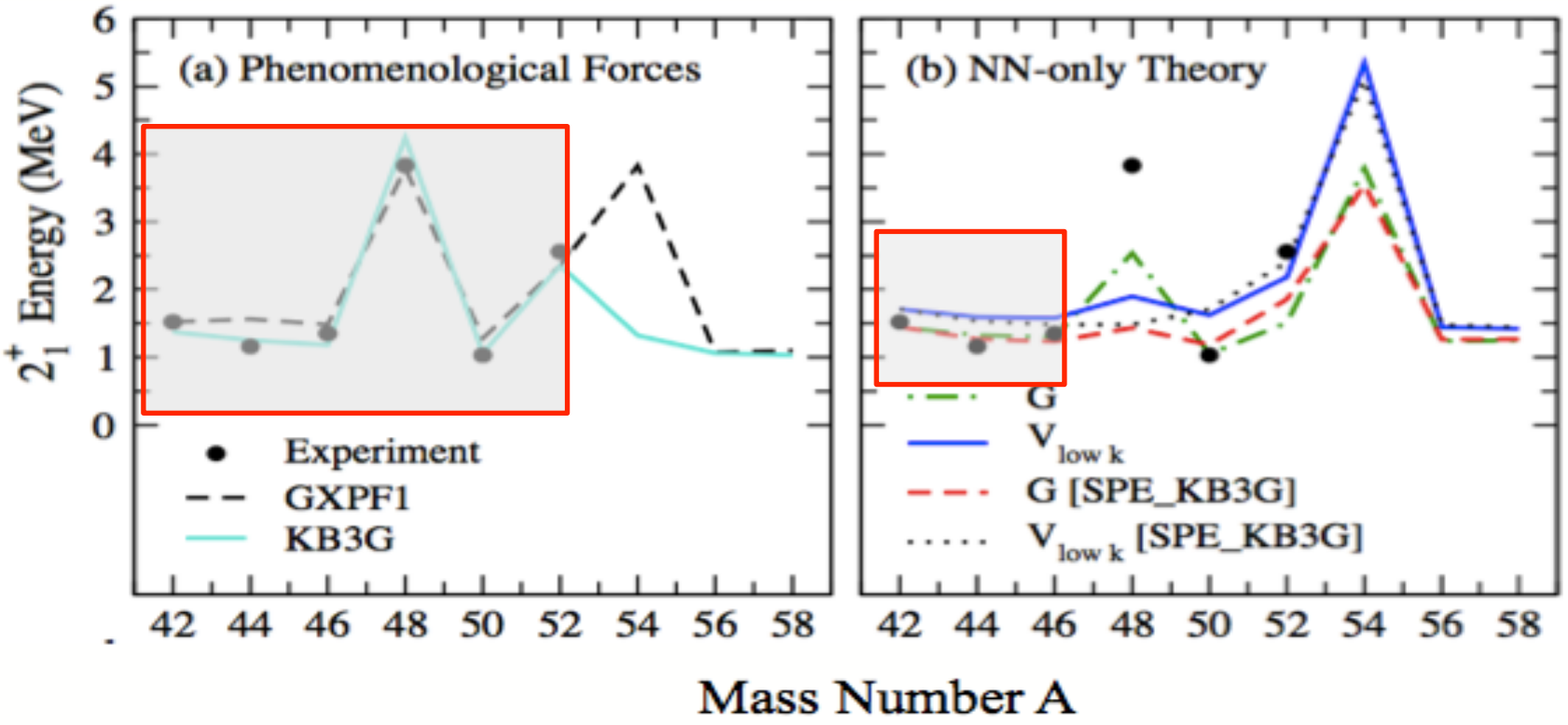


O. Sorlin, M.-G. Porquet, Prog. Part. Nucl. Phys. 61, 602 (2008).

Z. Xu, CQ, Phys. Lett. B (2013)

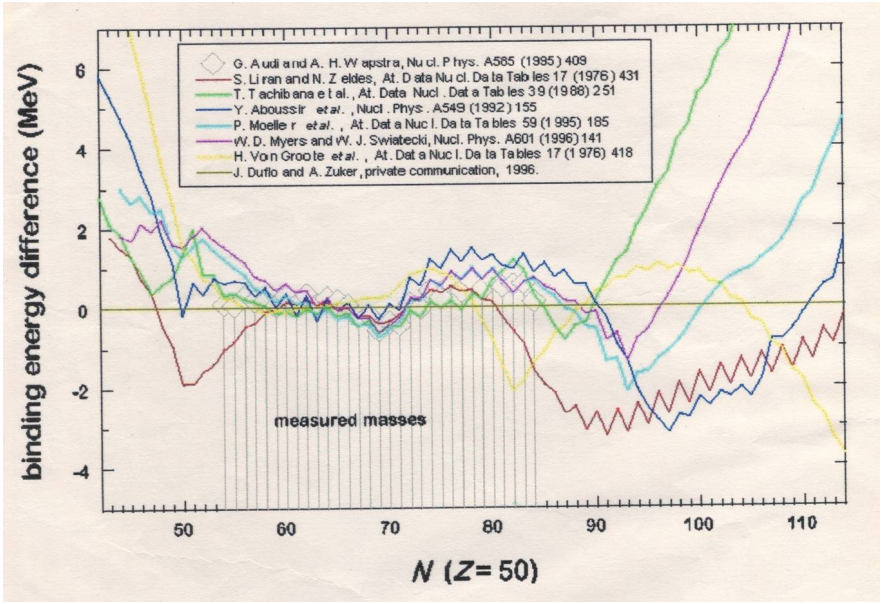
Large uncertainties
Shell model predictions for the 2+ energies,

which are one of the key quantities for determining the shell gap



"Just because it's correct, doesn't mean it's right"

Model predictions diverges when extrapolated to unknown regions: Other examples



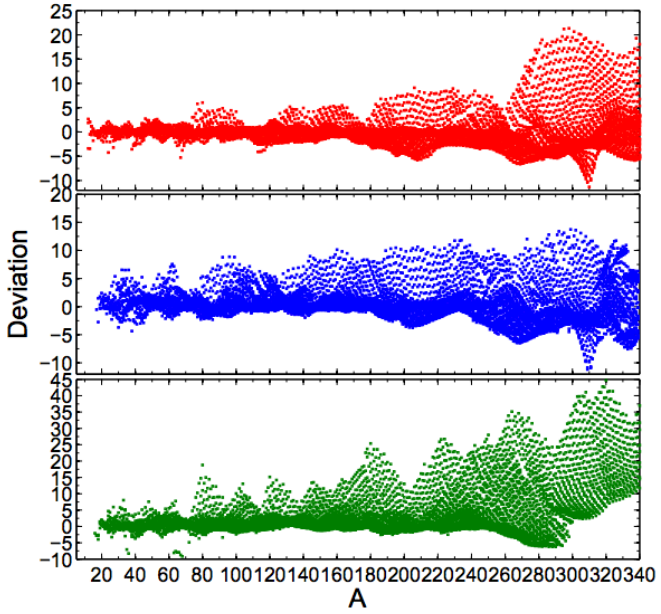
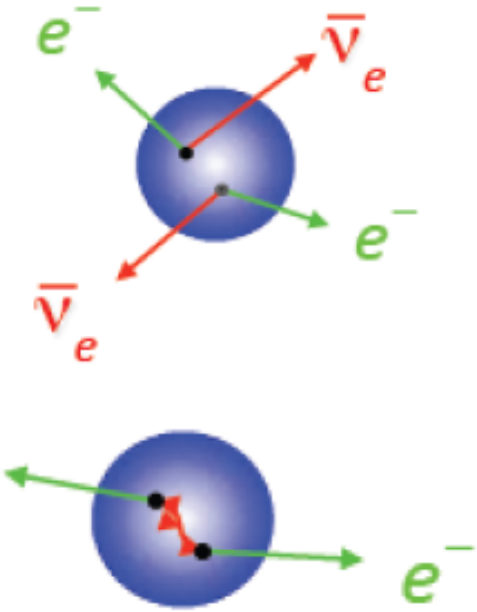


FIG. 2. (Color online) Differences (in MeV) between DZ10 mass model calculations with the parameter set II from Table I and the macroscopic-microscopic liquid drop model calculation of Ref. [20] (upper), the finite-range droplet model [26] (middle) and the HFB-21 model [32] (bottom).

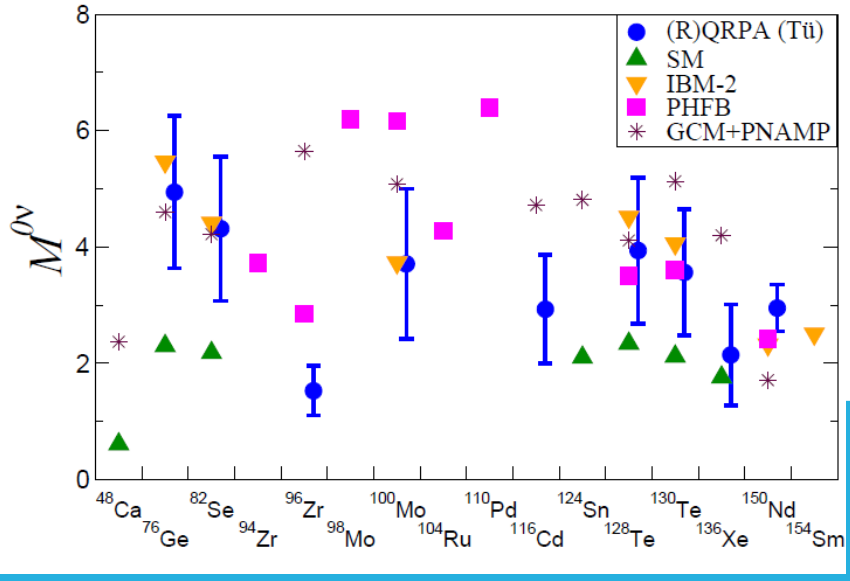
Two neutrino and neutrinoless double beta decay

Experiment	Isotope	Mass	Technique	Present Status	Location
AMoRE[89,90]	^{100}Mo	50 kg	$CaMoO_4$ scint. bolometer crystals	Development	Yangyang
CANDLES[91]	^{48}Ca	0.35 kg	CaF_2 scint. crystals	Prototype	Kamioka
CARVEL[92]	^{48}Ca	1 ton	CaF_2 scint. crystals	Development	Solotvina
COBRA[93]	^{116}Cd	183 kg	^{enr}Cd CZT semicond. det.	Prototype	Gran Sasso
CUORE-0[69]	^{130}Te	11 kg	TeO_2 bolometers	Construction - 2012	Gran Sasso
CUORE[69]	^{130}Te	203 kg	TeO_2 bolometers	Construction - 2013	Gran Sasso
DCBA[94]	^{150}Ne	20 kg	^{enr}Nd foils and tracking	Development	Kamioka
EXO-200[57]	^{136}Xe	160 kg	Liq. ^{enr}Xe TPC/scint.	Operating - 2011	WIPP
EXO[70]	^{136}Xe	1-10 t	Liq. ^{enr}Xe TPC/scint.	Proposal	SURF
GERDA[71]	^{76}Ge	≈35 kg	^{enr}Ge semicond. det.	Operating - 2011	Gran Sasso
GSO[95]	^{160}Gd	2 ton	Gd_2SiO_5:Ce crys. scint. in liq. scint.	Development	
KamLAND-Zen[96]	^{136}Xe	400 kg	^{enr}Xe disolved in liq. scint.	Operating - 2011	Kamioka
LUCIFER[97,98]	^{82}Se	18 kg	ZnSe scint. bolometer crystals	Development	Gran Sasso
MAJORANA[77,78,79]	^{76}Ge	26 kg	^{enr}Ge semicond. det.	Construction - 2013	SURF
MOON [99]	^{100}Mo	1 t	^{enr}Mofoils/scint.	Development	
SuperNEMO-Dem[87]	^{82}Se	7 kg	^{enr}Se foils/tracking	Construction - 2014	Fréjus
SuperNEMO[87]	^{82}Se	100 kg	^{enr}Se foils/tracking	Proposal - 2019	Fréjus
NEXT [82,83]	^{136}Xe	100 kg	gas TPC	Development - 2014	Canfranc
SNO+[84,85]	^{150}Nd	55 kg	Nd loaded liq. scint.	Construction - 2013	SNOLab

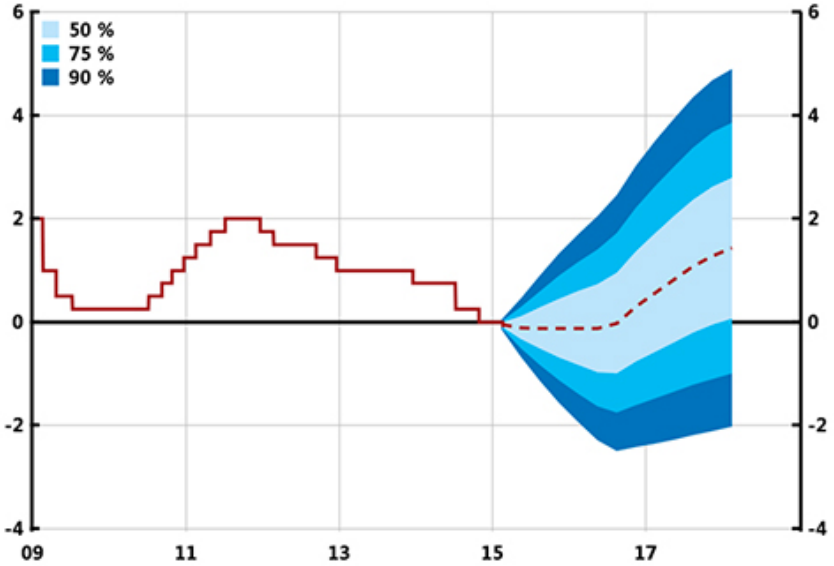


$$[T^{0\nu}_{1/2}]^{-1} = G^{0\nu} \, |M^{0\nu}|^2 \, |\langle m_\nu \rangle|^2 / m_e^2$$

The nightmare of matrix elements



Uncertainties

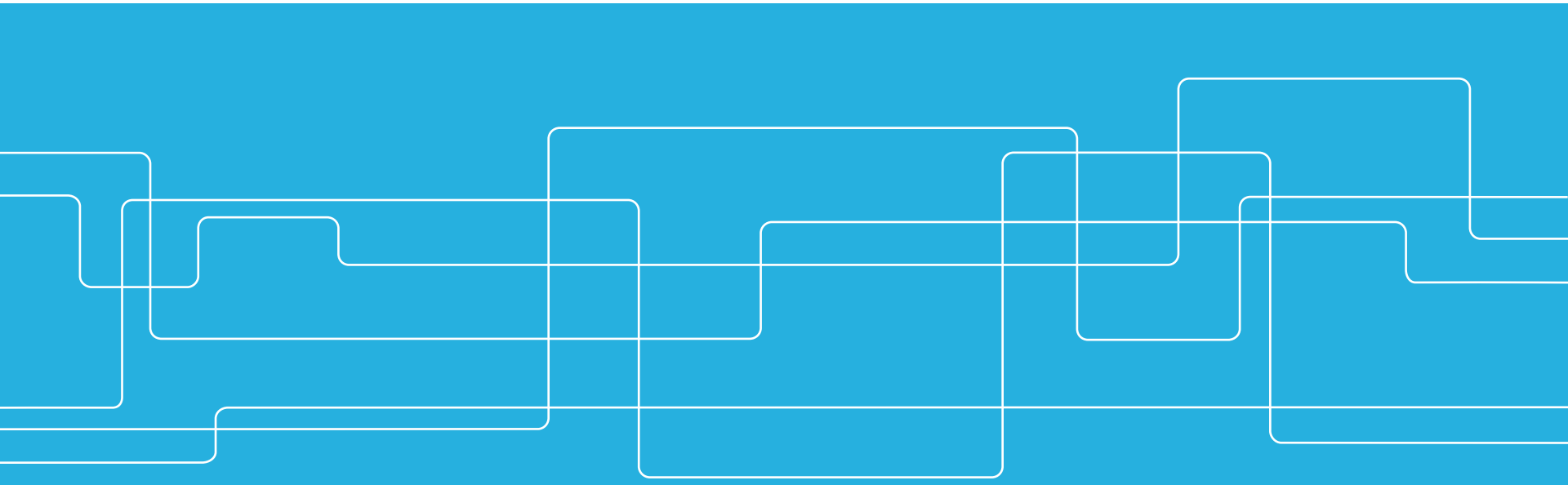


"Remember that all models are wrong; the practical question is how wrong do they have to be to not be useful"
Box G E P and Draper N R 1987 Empirical Model Building and Response Surfaces (New York: Wiley)

"The difference between the right ~~word~~ and the almost right ~~word~~ is the difference between lightning and a lightning bug"
Mark Twain

http://www.riksbank.se/sv/Penningpolitik/Prognoser-och-rantebeslut/Aktuell-prognos-for-reporanta-inflation-och-BNP/

Optimization of the effective interaction



Optimization of the effective interaction

The experimental (negative) binding energy of a given state i is given by

$$E_i^{\rm exp} = {\rm BE}_{\rm gs}^{\rm exp}(N) + {\rm Ex}(i), \qquad (2)$$

where BE and Ex denote the binding energy of the nucleus (with N valence nucleons) and the corresponding excitation energy of the state relative to the ground state,

$$E_i^{\rm cal} = \left[C + N\varepsilon_0 + \frac{N(N-1)}{2} V_m \right] + \langle \Psi_I | H | \Psi_I \rangle,$$

CORE,eg,^{100}Sn

$$E^{\rm SM} = \langle \Psi_I | H | \Psi_I \rangle$$
$$= \sum_\alpha \varepsilon_\alpha < \hat{N}_\alpha > + \sum_{\alpha \le \beta} V_{m;\alpha\beta} \left\langle \frac{\hat{N}_\alpha (\hat{N}_\beta - \delta_{\alpha\beta})}{1+\delta_{\alpha\beta}} \right\rangle$$
$$+ \langle \Psi_I | H_M | \Psi_I \rangle, \qquad (4)$$

where $\sum_\alpha < \hat{N}_\alpha >= N$ and

Monopole interaction

$$\sum_{\alpha \le \beta} \left\langle \frac{\hat{N}_\alpha (\hat{N}_\beta - \delta_{\alpha\beta})}{1+\delta_{\alpha\beta}} \right\rangle = \frac{N(N-1)}{2}. \qquad (5)$$

Optimization of the effective interaction

least mean square criterion

We optimize the single-particle energies and monopole terms of the realistic effective interaction by minimizing the quantity

$$\chi^2 = \sum_i^D \left[E_i^{\rm cal} - E_i^{\rm exp}\right]^2, \qquad (6)$$

$$E_i^{\rm Cal.} = \sum_k^P V_k x_k + \varepsilon_{1d_{5/2}} \langle N_{1d_{5/2}} \rangle + \langle H_M \rangle,$$

Linear approximation

$\langle \Psi_I(n) | \Psi_I'(n) \rangle \sim 1$. One has

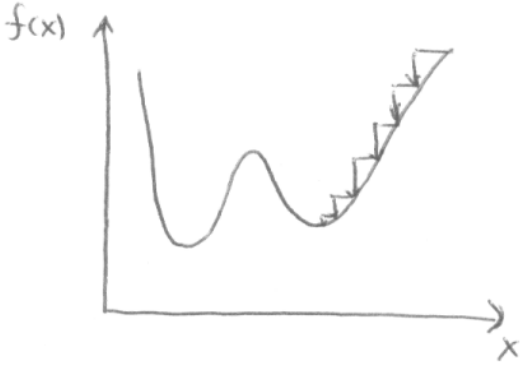
$$E_i^{\rm Cal.}(n)' - E_i^{\rm Cal.}(n) \approx \sum_k^P [V_k'(n) - V_k(n)] x_k,$$

That is, I assume the wave function does not change between two iterations

Monte Carlo/Simulated annealing Optimization

To find the optimal solution of an algorithmically hard problem.

Need to move in wrong directions sometimes to escape local minima (traps).



Algorithm:

- Choose a $\delta > 0.$
- Start at $\vec{x}_i.$ Propose a Move to $\vec{x}_t \ni \ 0 < \left|\vec{x}_t - \vec{x}_i\right| < \delta.$
- If $f\left(\vec{x}_t\right) \leq f\left(\vec{x}_i\right)$, let $\vec{x}_{i+1} = \vec{x}_t\,.$
- If $f\left(\vec{x}_t\right) > f\left(\vec{x}_i\right)$, let $\vec{x}_{i+1} = \vec{x}_t$ with probability $g\left(f\left(\vec{x}_t\right) - f\left(\vec{x}_i\right)\right),$

Where g is a decreasing function.

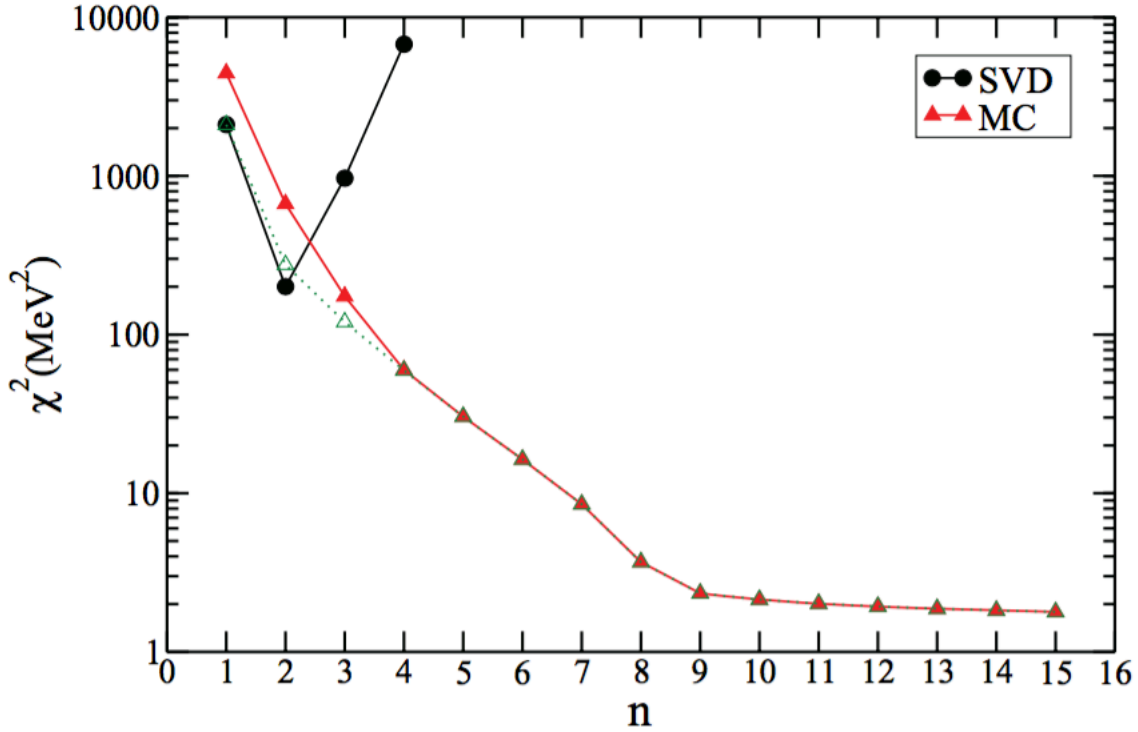


FIG. 2. (Color online) The convergence of the mean-square deviations χ^2 as a function of iteration number within the singular value decomposition (SVD) and Monte Carlo global optimization (MC) approaches starting from a random monopole Hamiltonian.

Convergence (is astonishing fast)

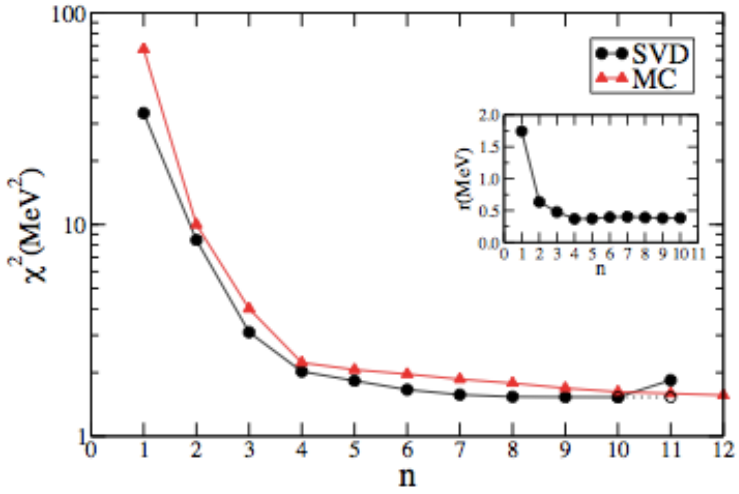


FIG. 3. (Color Online) The convergence of the mean-square deviations χ^2 as a function of iteration number for fittings that are started from the realistic CD-Bonn interaction. The insert shows the maximal deviation $r = \max|E_i^{\rm cal} - E_i^{\rm exp}|$ in each step.

Deviations from experimental data

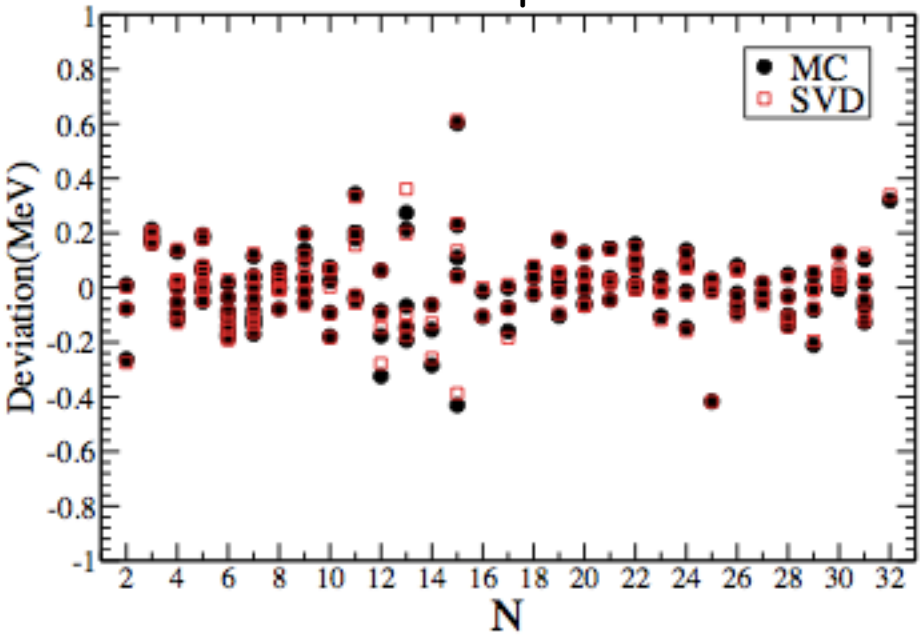


FIG. 4. (Color Online) Differences between experimental and calculated binding energies, $E_i^{\rm exp} - E_i^{\rm cal}$, as a function of valence neutron number.

The binding energies of 157 states in tin isotopes can be reproduced within an average deviation **~130 keV.**

Controllable calculations with error bars

Understanding the uncertainties and limitations of the theory. Otherwise large-scale calculations can be very misleading.

TABLE II. The final mean square deviation χ^2 (in MeV^2) given by the SVD and MC fittings and the predicted values of the variables C, ε_0 and V_m and their uncertainties (in MeV).

	χ^2	C	ε_0	V_m
MC	2.697	-825.5 ± 0.288	-10.666 ± 0.0410	0.167 ± 0.00249
SVD	2.686	-825.5 ± 0.288	-10.669 ± 0.0410	0.172 ± 0.00249

data new: -824.9+-0.5606
data old: -824.8+-0.7054

The largest uncertainties of the optimized monopole Hamiltonian are related to the single-particle energies. The values predicted by the MC approach are $\varepsilon_{1d_{3/2}} = 5.013 \pm 3.10$, $\varepsilon_{2s_{1/2}} = 0.369 \pm 2.63$ and $\varepsilon_{0h_{11/2}} = 3.249 \pm 0.83$ MeV. The single-particle energies given by the SVD

How to choose the criterion?

The object of the minimax fit is to find the minimum of the Chebyshev norm as

$$\varepsilon = \arg\min_{\mathbf{x}} \max_{A} |\mathrm{BE}^{\mathrm{Expt.}}(A) - \mathrm{BE}^{\mathrm{Calc.}}(A, \mathbf{x})|, \qquad (10)$$

where $\mathbf{x}$ denote the coefficients to be determined. arg min (arg max) stand for the argument of the minimum (maximum) for which the value of the given expression attains its minimum (maximum) value within a given set of values for argument $\mathbf{x}$.

A mass model

Term	I	IV
Coulomb	0.705 ± 0.001	0.710
Symmetry	149.033 ± 0.468	149.087
Surface symmetry	202.642 ± 1.848	204.424
Pairing	5.167 ± 0.138	5.143
$\mathcal{M} + \mathcal{T}$	18.552 ± 0.037	18.834
$(\mathcal{M} + \mathcal{T})/\rho$	15.120 ± 0.125	15.626
FS	1.069 ± 0.040	1.186
fs−	4.414 ± 0.259	5.416
fc+	−10.353 ± 0.753	−10.074
PM+	−0.498 ± 0.011	−0.552
PS+	−0.082 ± 0.008	−0.077
S3	0.515 ± 0.015	0.413
s3	2.381 ± 0.069	2.001
SQ−	0.393 ± 0.022	0.441
sq−	1.581 ± 0.120	1.841
d3+QQ+	7.204 ± 0.169	5.969
D0	−21.533 ± 0.699	−26.463
d0	−89.904 ± 3.220	−115.392
SS	0.431 ± 0.050	0.064
χ(I)	0.425	0.712

- if the fitting has N adjustable parameters, there will be N + 1 critical members of the data set that have a residual equal to ε. These N + 1 critical cases are the ones being used in determining the parameters.
- ultimate criterion for a perfect model?

RMS deviation

Differential evolution

- DE optimizes a problem by maintaining a population of candidate solutions (N) and creating new candidate solutions, and then keeping whichever candidate solution has the best fitness.
- The optimization problem is again treated as a black box.
- Easy to parallelize

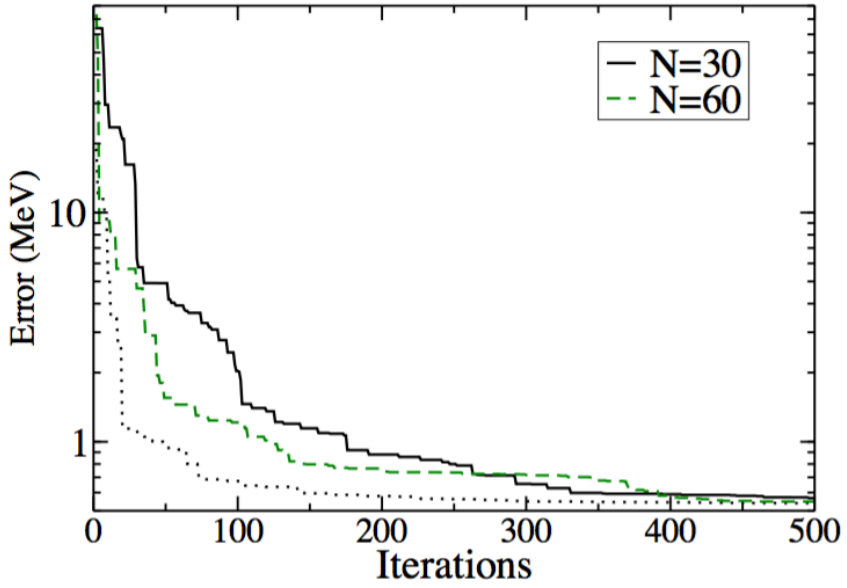
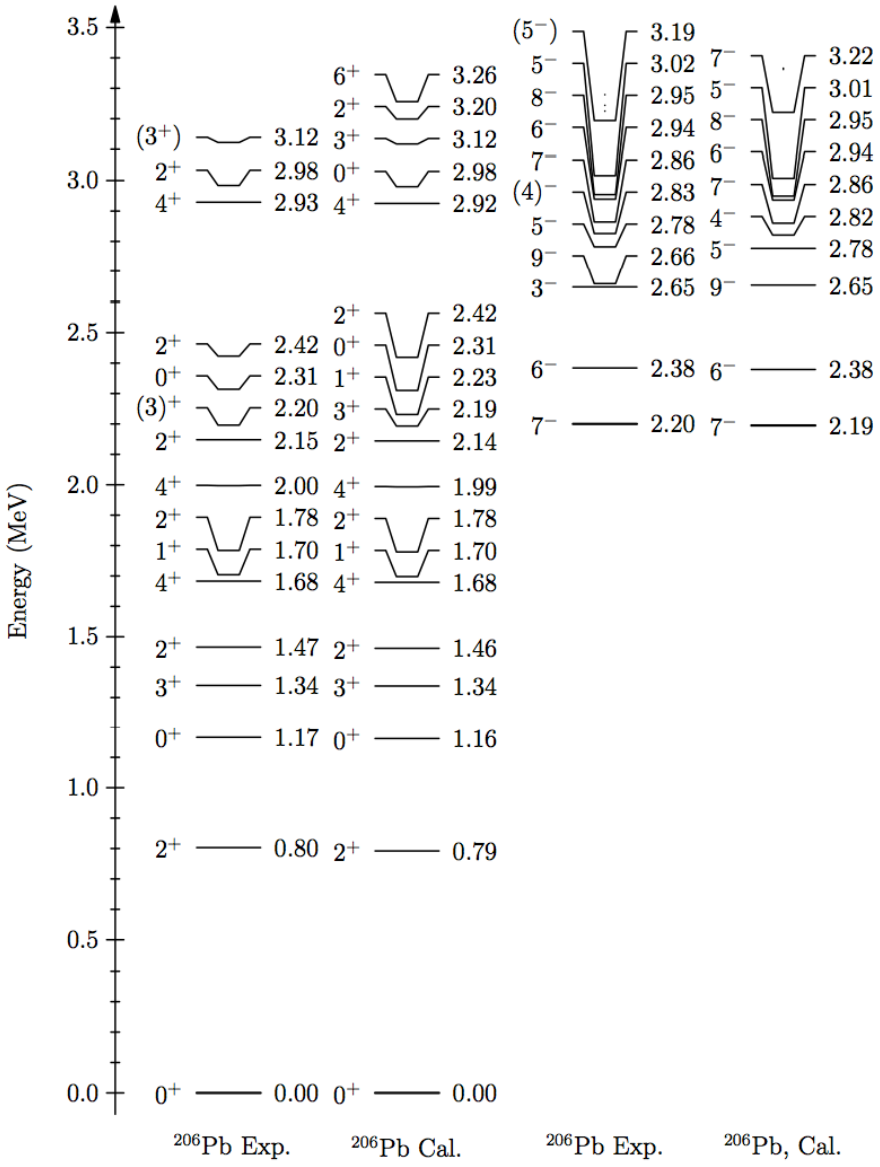


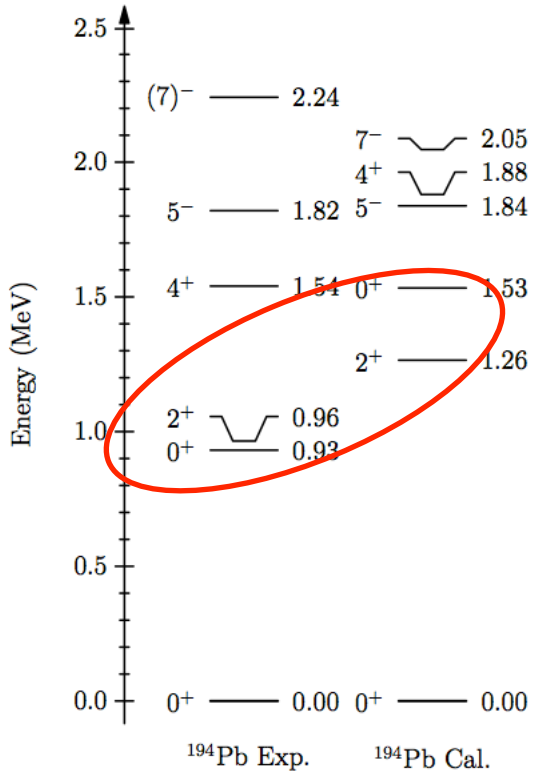
FIG. 2. Convergence of the root-mean-square deviation between the shell-model mass formula and experimental binding energies as a function of the iteration. The dotted line corresponds to calculation within a smaller uncertainty range.

http://www1.icsi.berkeley.edu/~storn/code.html

https://en.wikipedia.org/wiki/Differential_evolution

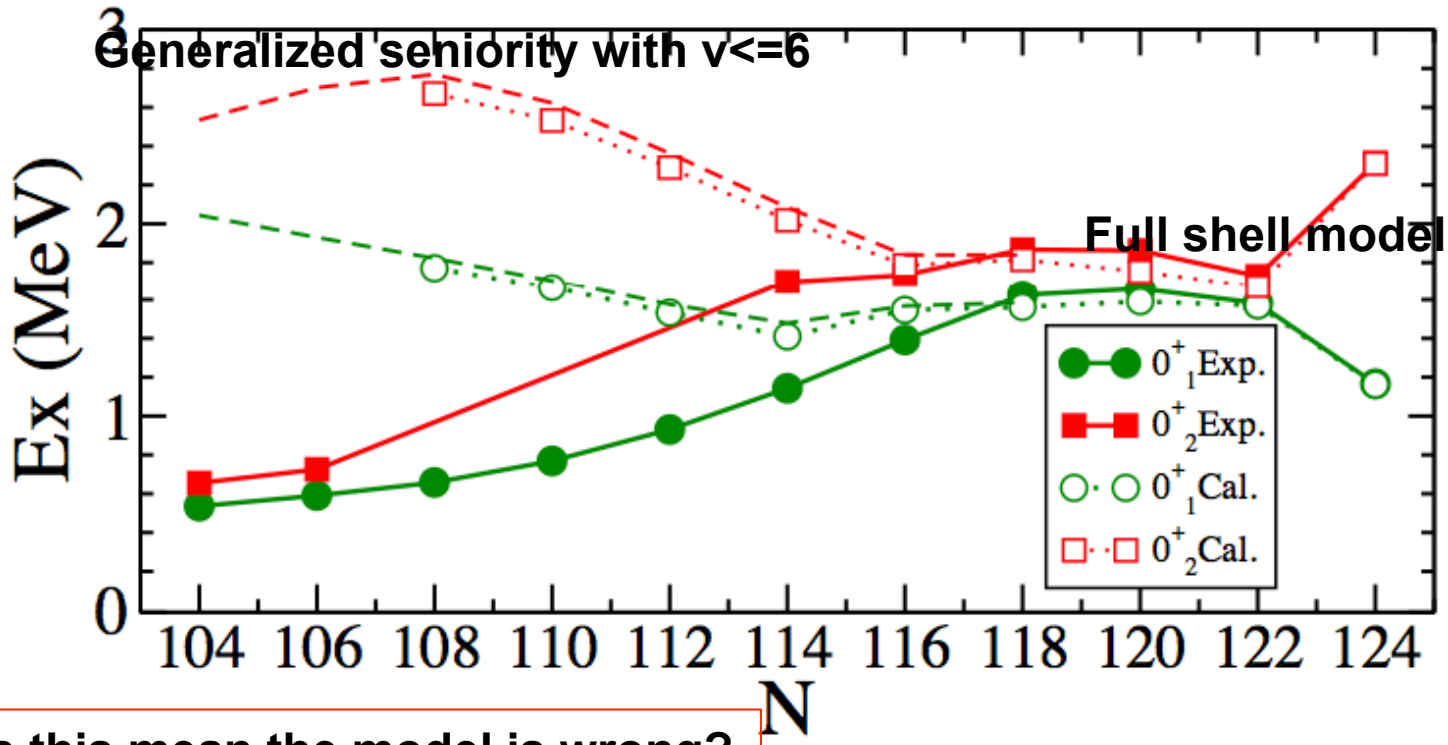
Level schemes of Pb isotopes





- We have six 0+ states for 206Pb within the model space
- 3- state in 206Pb is understood to be a core excited collective state.
- 194Pb is the lighest system we solved in the full model space

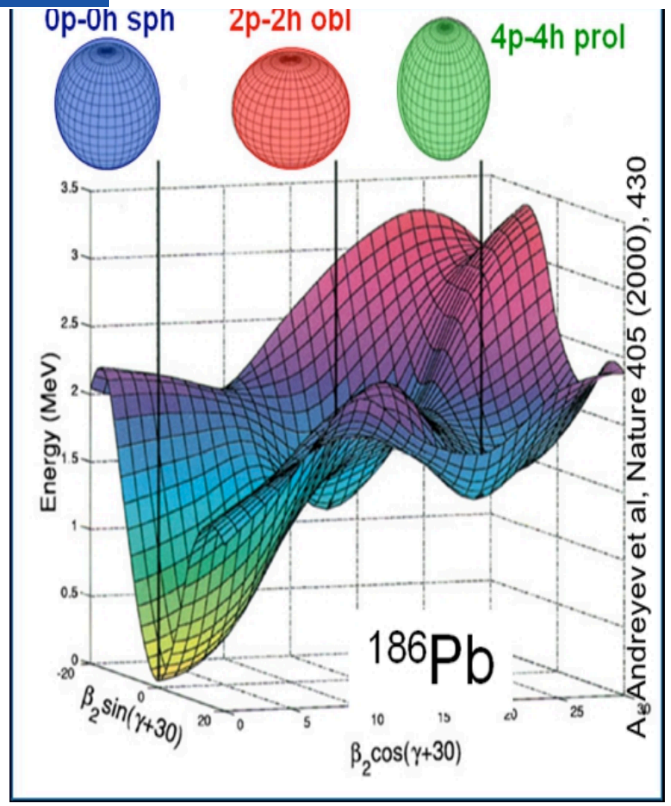
The excited 0^+ states



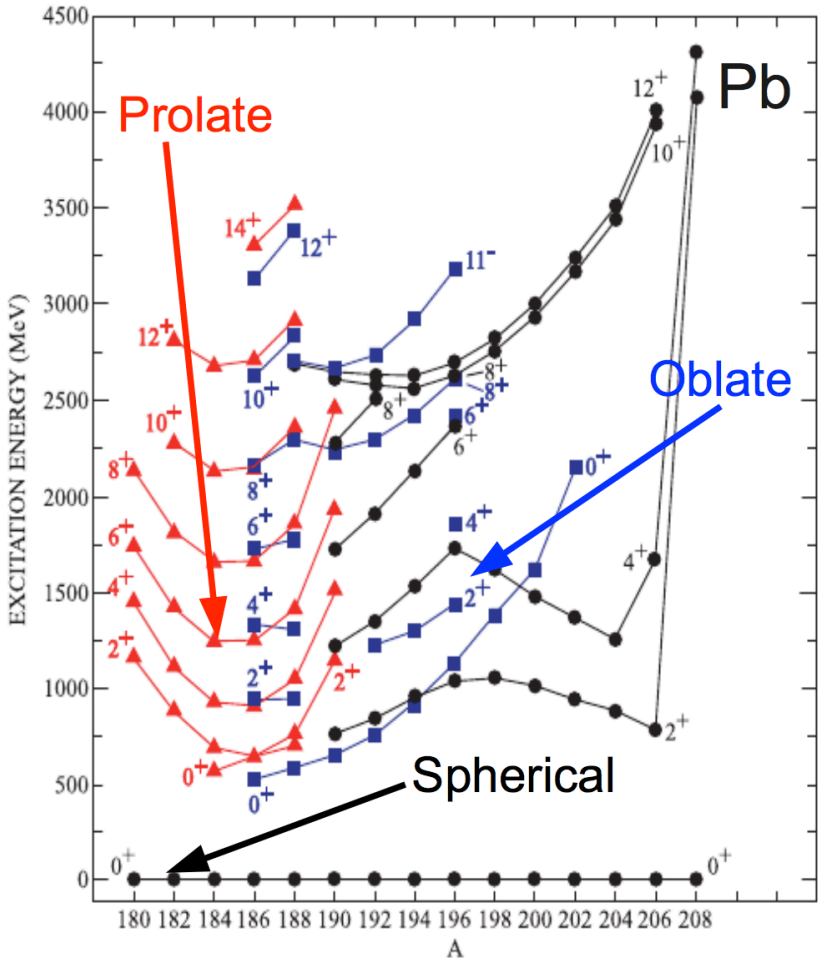
Does this mean the model is wrong?

To how much extent those spherical components contribute to the observed excited 0+ states?

Physics beyond the model



A. N. Andreyev et al., Nature 405, 430 (2000).



Shell-model calculations of Pb may provide

- Better description of the (spherical) low-lying levels which may be beyond the scope of symmetry truncated models like IBM
- Critical test of the effective interaction
- Benchmarks for approximation/truncation methods
- Further constraint on the role of (coexisting) deformed shapes

Binding energy and odd-even staggering in Sn and Pb isotopes

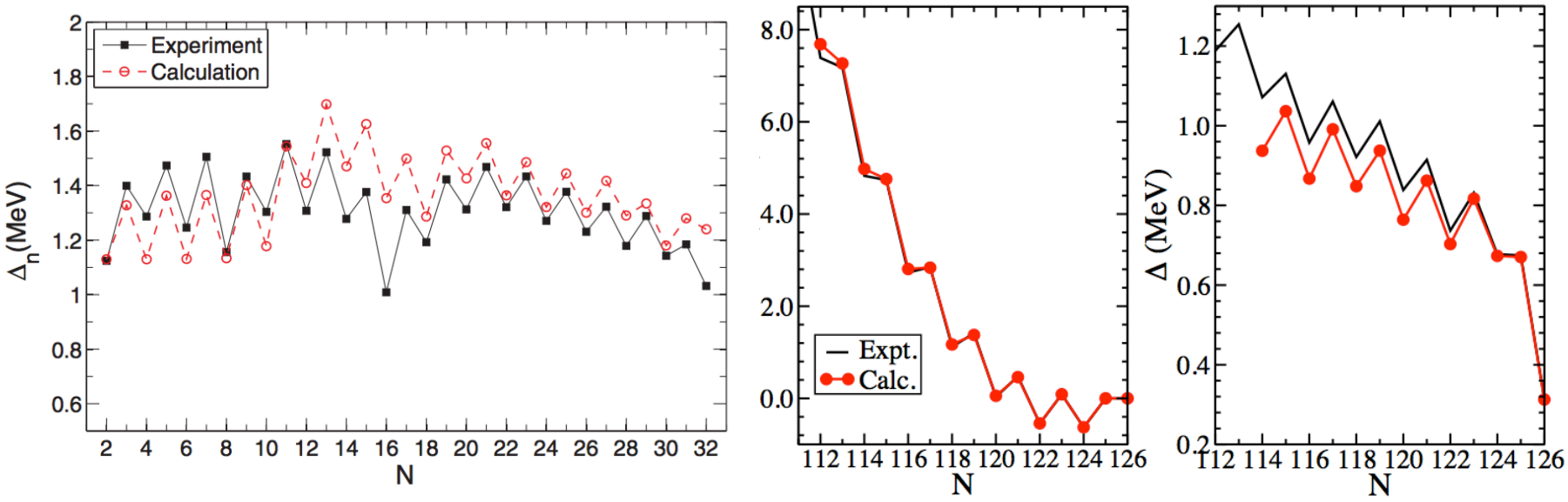


FIG. 9. (Color online) Neutron pairing gaps in Sn isotopes extracted from the experimental and calculated binding energies.

FIG. 9. (color online) Left: Experimental [80] and calculated shell-model correlation energies as a function of neutron number; Right: The empirical pairing gaps as extracted according to Eq. (5).

$$E_i^{\rm cal} = C + N\varepsilon_0 + \frac{N(N-1)}{2}V_m + \langle\Psi_I|H|\Psi_I\rangle,$$

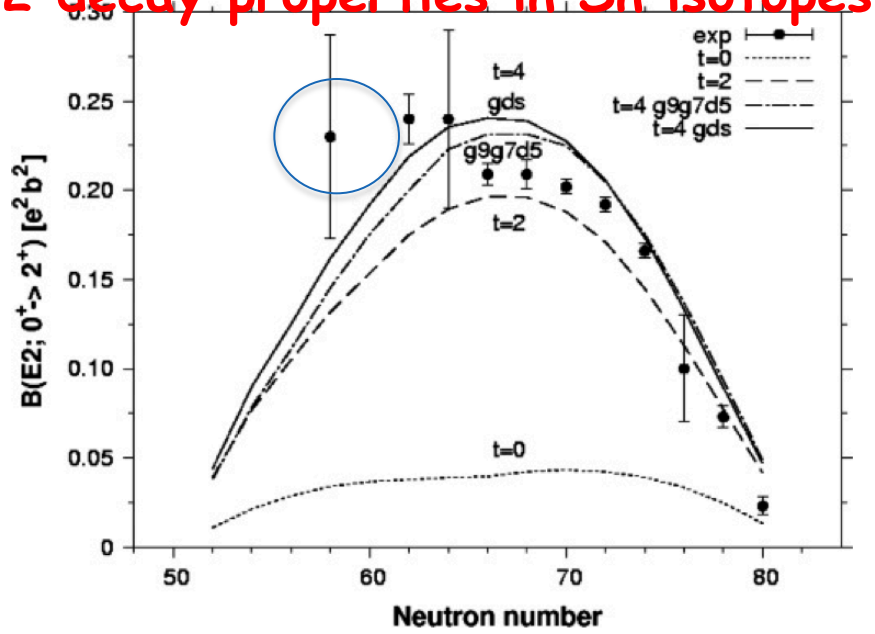
Experience can lead to wrong

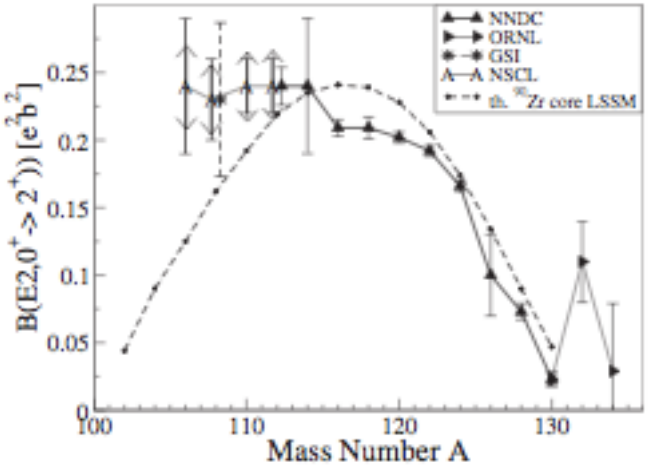
PHYSICAL REVIEW C 72, 061305(R) (2005)

^{108}Sn studied with intermediate-energy Coulomb excitation

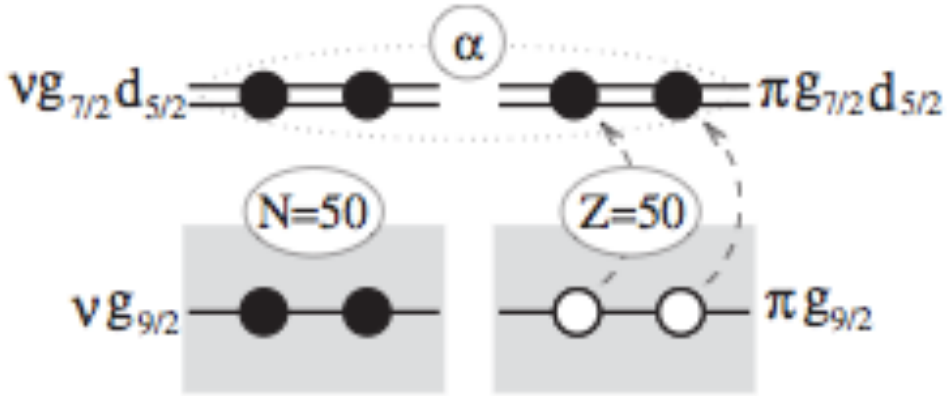
A. Banu,[1,2,*] J. Gerl,[1] C. Fahlander,[3] M. Górska,[1] H. Grawe,[1] T. R. Saito,[1] H.-J. Wollersheim,[1] E. Caurier,[4] T. Engeland,[5] A. Gniady,[4] M. Hjorth-Jensen,[5] F. Nowacki,[4] T. Beck,[1] F. Becker,[1] P. Bednarczyk,[1,6] M. A. Bentley,[7] A. Bürger,[8] F. Cristancho,[3,†] G. de Angelis,[9] Zs. Dombrádi,[10] P. Doornenbal,[1,11] H. Geissel,[1] J. Grębosz,[1,6] G. Hammond,[12,‡] M. Hellström,[1,§] J. Jolie,[11] I. Kojouharov,[1] N. Kurz,[1] R. Lozeva,[1,||] S. Mandal,[1,¶] N. Mărginean,[9] S. Muralithar,[1,**] J. Nyberg,[13] J. Pochodzalla,[2] W. Prokopowicz,[1,6] P. Reiter,[11] D. Rudolph,[3] C. Rusu,[9] N. Saito,[1] H. Schaffner,[1] D. Sohler,[10] H. Weick,[1] C. Wheldon,[1,††] and M. Winkler[1]

E2 decay properties in Sn isotopes

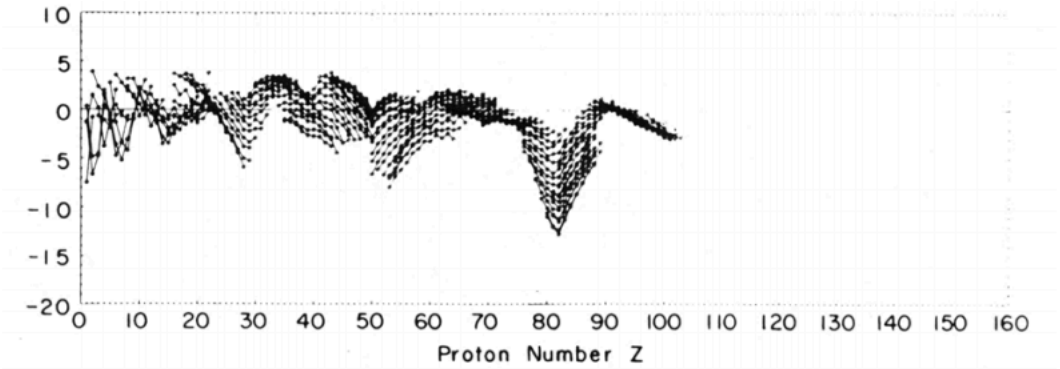




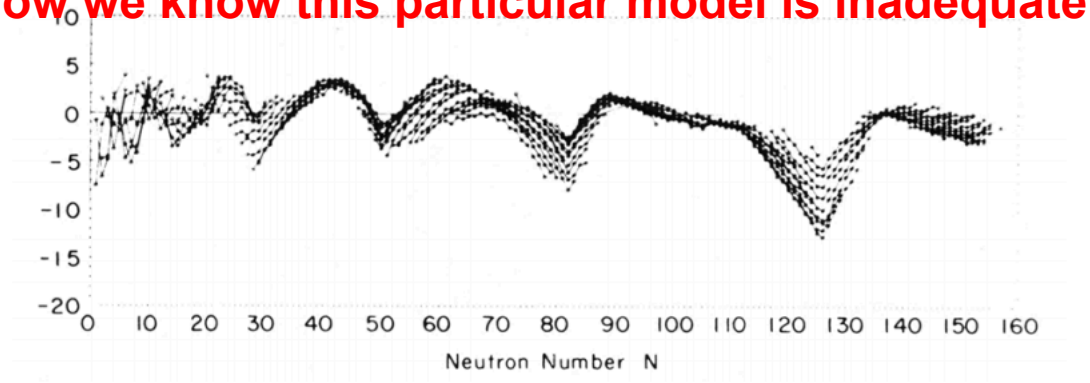
PRL 99, 162501 (2007)
PRL 101, 012502 (2008)



Systematical error underfitting

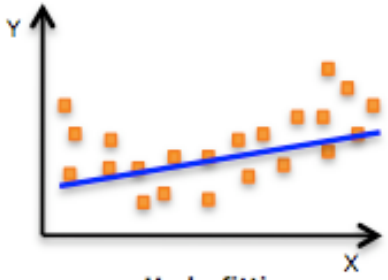


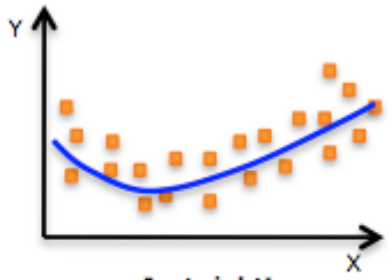
Now we know this particular model is inadequate.

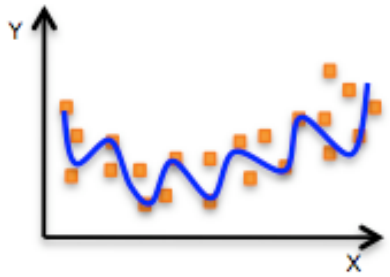


From W.D. Meyers and W.J. Swiatecki, Nucl. Phys. **81**, 1 (1966).

How to identify the limitations of a model in general?







Alpha formation probability from experiments

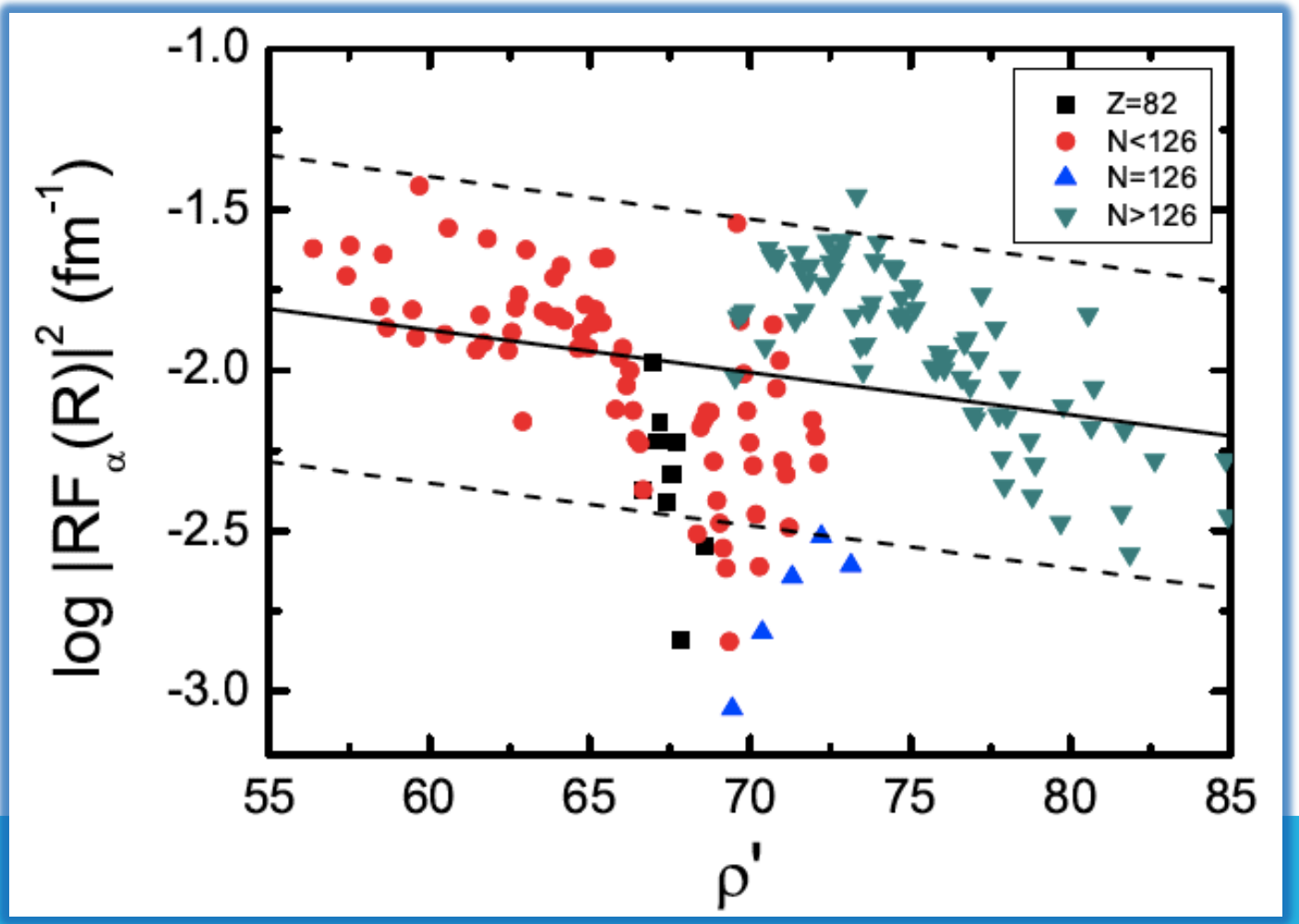
$$\log |RF(R)|^{-2} = \log T_{1/2}^{\text{Expt.}} - \log \left[\frac{\ln 2}{\nu} |H_0^+(\chi, \rho)|^2 \right],$$

R should be large enough that the nuclear interaction is negligible, i.e., at the nuclear surface.

$R=1.2(A_d^{1/3}+A_c^{1/3})$

$$\chi' = \frac{\hbar}{e^2\sqrt{2M}}\chi = Z_c Z_d \sqrt{\frac{A}{Q_c}},$$

$$\rho' = \frac{\hbar}{\sqrt{2MR_0e^2}}(\rho\chi)^{1/2} = \sqrt{AZ_cZ_d(A_d^{1/3}+A_c^{1/3})},$$

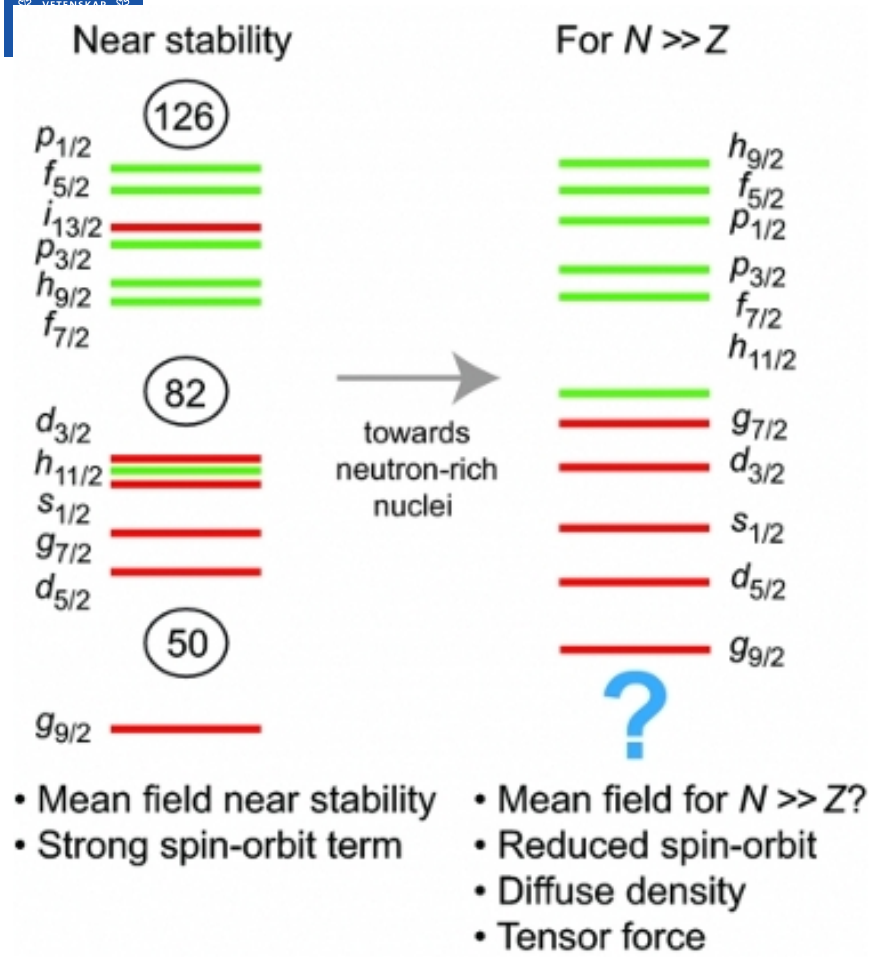


CQ et al, Phys.Rev.C80,044326 (2009); 81,064319 (2010).PLB B 734, 203-206 (2014)

What happens if the model is/was overcomplete?

It ain't what you don’t know that gets you into trouble. It's what you know for sure that just ain’t so.
Mark Twain

Shell structure at the drip lines



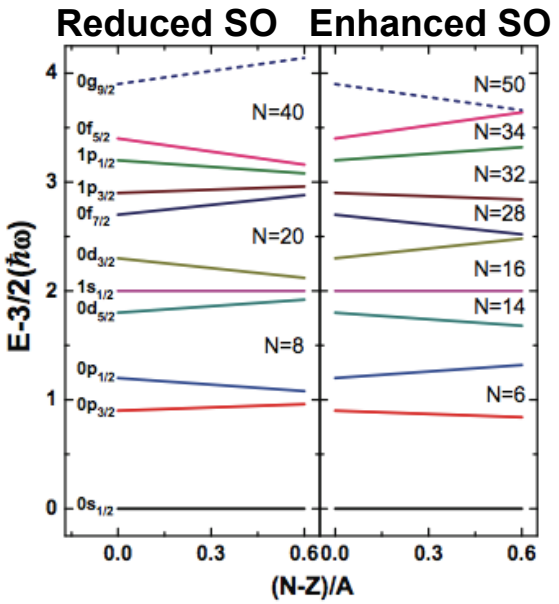


FIG. 1. (Color online) The evolution of the shell structure as a function of $(N-Z)/A$ with the HO potential plus SO coupling of the form $\lambda(1+\kappa_{SO}\frac{N-Z}{A})\hbar\omega\mathbf{l}\cdot\mathbf{s}$. We take $\lambda = 0.2$ and $\kappa_{SO} = -1$ (left) and 1 (right). The $0g_{9/2}$ orbital is shifted upwards by $0.3\hbar\omega$ for a clearer presentation.

- N=8, 20 shells disappear in neutron-rich nuclei
- N=14,16, 32 emerge as new magic numbers
- Role played by tensor force and three body force
- A comprehensive review can be found in: O. Sorlin, M.-G. Porquet, Prog. Part. Nucl. Phys. 61, 602 (2008).

Mean-field for dripline nuclei

➢Orbitals with higher *l* loses its energy faster when going towards the dripline I. Hamamoto, Phys. Rev. C 85, 064329 (2012).

This naturally explains the disappearing of N=14 subshell in C and N isotopes [It is due to a complicated interplay between NN and NP interactions from a shell-model point of view, C.X. Yuan, C. Qi, F.R. Xu, Nucl. Phys. A 883, 25 (2012).].

➢Choice of the Central and SO potential

$$V = V_0(1 + \frac{4\kappa}{A}\mathbf{t} \cdot \mathbf{T}_d),$$

and

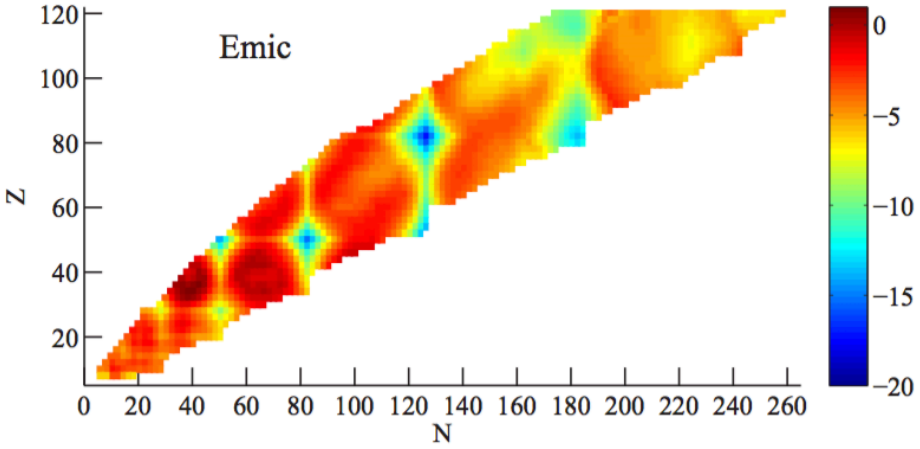
$$V_{SO} = \lambda V_0(1 + \frac{4\kappa_{SO}}{A}\mathbf{t} \cdot \mathbf{T}_d),$$

The standard WS potential

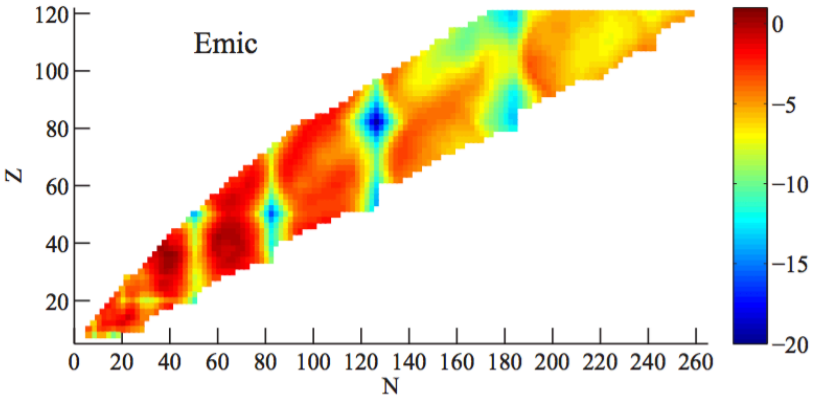
A. Bohr and B.R. Mottelson, Nuclear Structure (Benjamin, New York, 1969), Vol. I.

$$\kappa = \kappa_{SO} = -\frac{33}{51},$$

The binding energies for known nuclei are not sensitive to the sign of Kso



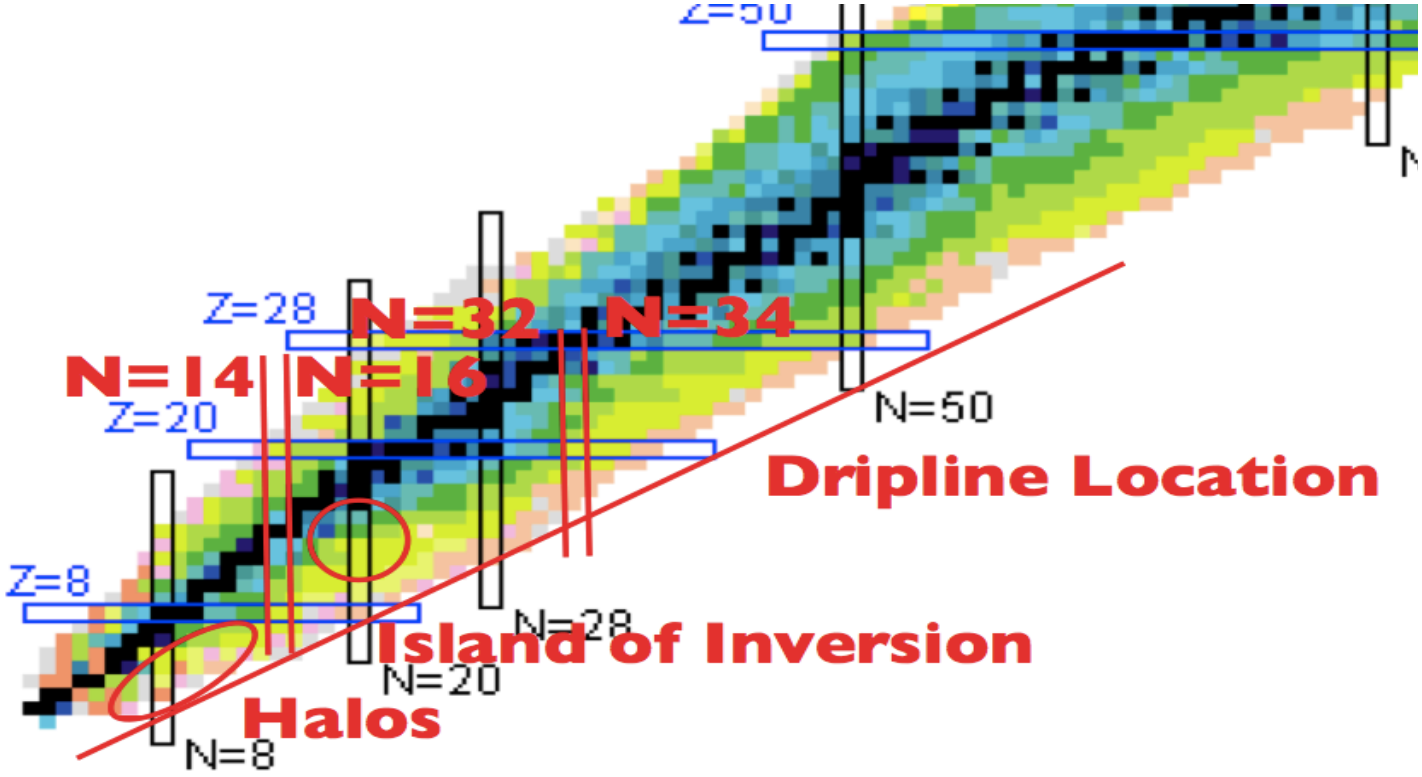
Standard



$$\kappa_{SO} = -\kappa,$$

PHYSICAL REVIEW C **92**, 024306 (2015)

The model fails to predict new shell closures



Why not a opposite value?

$$\kappa_{SO} = -\kappa,$$

We assume

- Orbitals with higher *l* loses its energy faster;
- The SO coupling is 'relatively' enhanced at the neutron drip line

TABLE I. Woods-Saxon potential parameters obtained by fitting to single-particle and single-hole states around doubly-magic nuclei with the restriction $\kappa_{SO} = -\kappa$ and comparison with some existing parameters.

	V_0 (MeV)	r_0 (fm)	r_{SO} (fm)	a, a_{SO} (fm)	λ	κ	
	50.92	1.285	1.146	0.691	24.07	0.644	$\kappa_{SO} = -\kappa$
Refs. [5, 12]	51	1.27	1.27	0.67	32.13	0.647	$\kappa_{SO} = \kappa$
Ref. [14]	49.6	1.347(n)/1.275(p)	1.31(n)/1.32(p)	0.7	35(n)/36(p)	0.86	$\kappa_{SO} = \kappa$
Ref. [15]	52.06	1.260	1.16	0.662	24.1	0.639	$\kappa_{SO} = 0$

[5]A. Bohr and B.R. Mottelson, Nuclear Structure (Benjamin, New York, 1969), Vol. I.
[12]J. Blomqvist and S. Wahlborn, Ark. Fys. 16 543 (1960).
[14] J. Dudek, Z. Szymanski, T. Werner, A. Faessler and C. Lima, Phys. Rev. C26 1712 (1982).
[15] N. Schwierz, I. Wiedenho ̈ver, and A. Volya, arXiv:0709.3523 (2007).

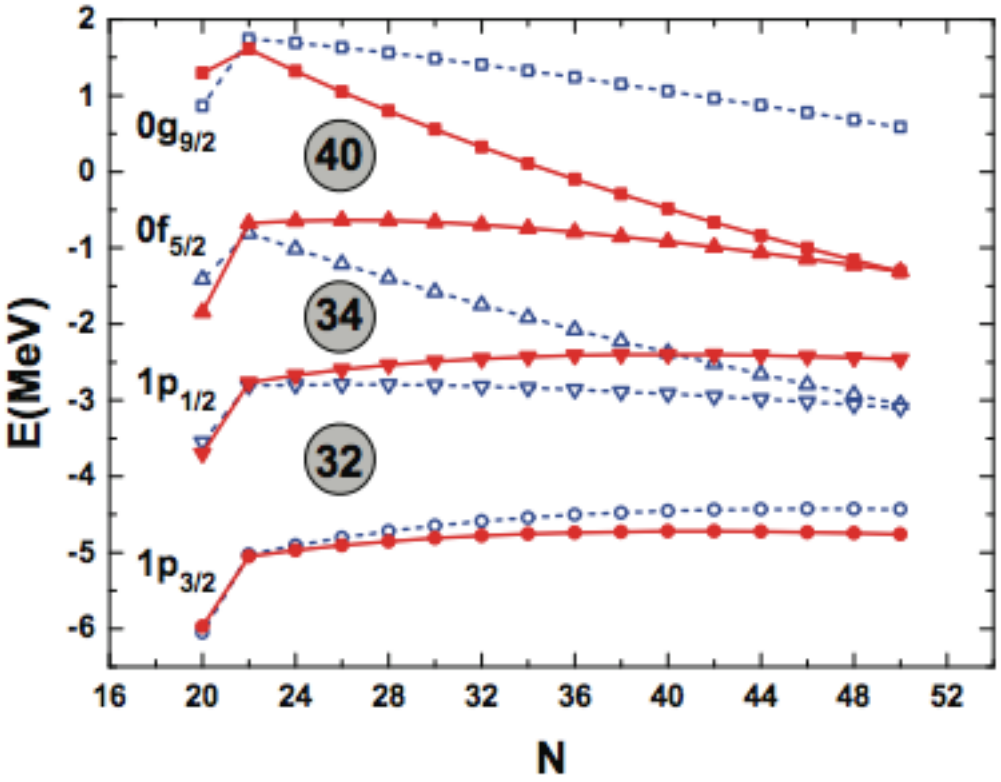
Such a simple picture can explain all known data
Simple rules of shell evolution

- HO magic numbers like N=8, 20 disappear;
- New SO magic numbers like N = 6, 14, 16, 32 and 34 will appear;
- The traditional SO magic numbers N = 28 and 50 and the magic number N = 14 will be eroded somehow but are more robust than the HO magic numbers;
- Pseudospin symmetry breaks, resulting in new shell closures like N = 56 and 90;
- HO shell closures like N = 40 and 70 will not emerge.

Z. Xu, C. Qi, Phys. Lett. B 724, 247 (2013)

Single-particle structure of Ca isotopes

- HO shell closures like N = 40 and 70 will not emerge.



Binding energies of Ca isotopes

WS + constant pairing

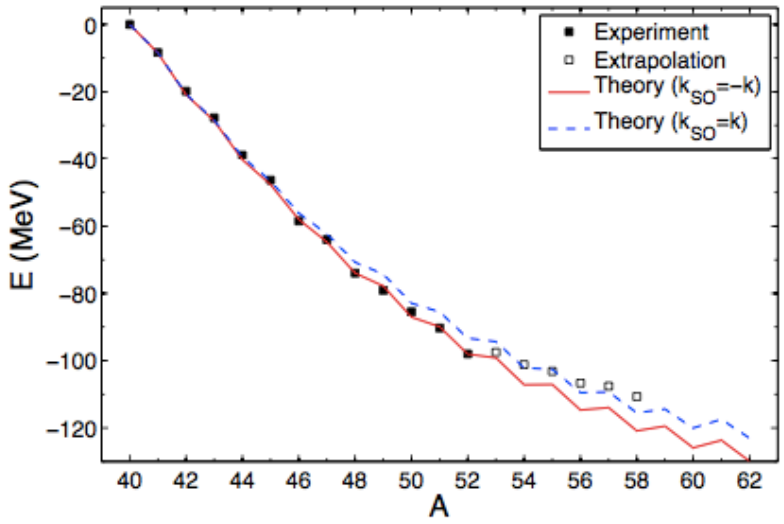
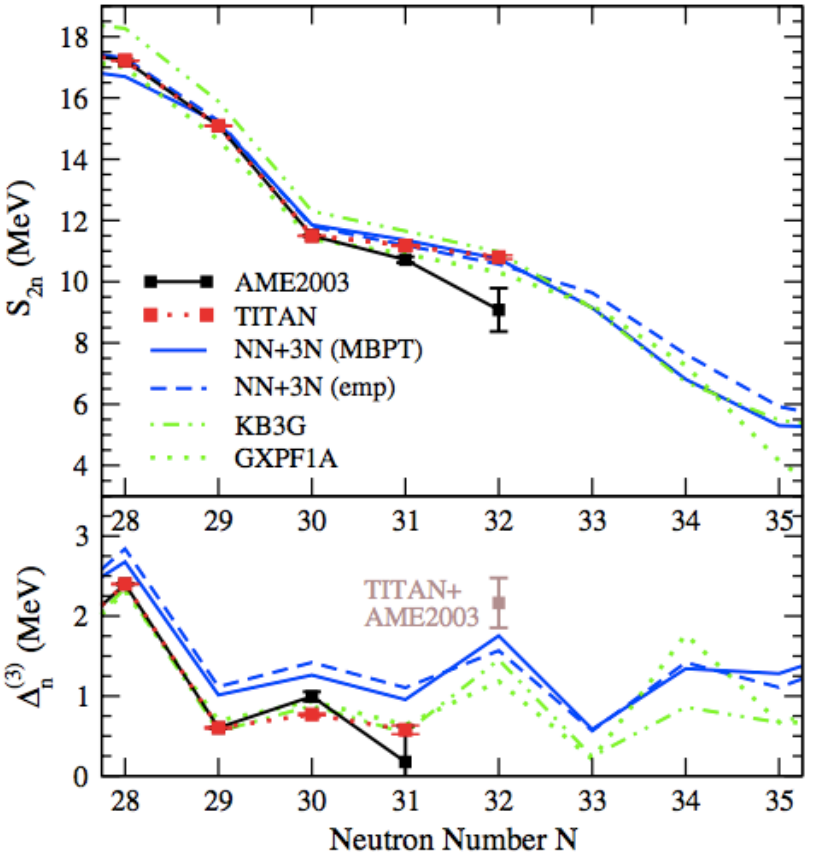


FIG. 6. (Color online) Experimental [34, 37] and calculated ground-state energies of Ca isotopes, relative to that of ^{40}Ca, as a function of mass number A.



A. T. Gallant et al., PRL 109, 032506 (2012)

Calculations with three-body interaction

J.D. Holt, T. Otsuka, A. Schwenk, and T. Suzuki, J. Phys. G 39, 085111 (2012).

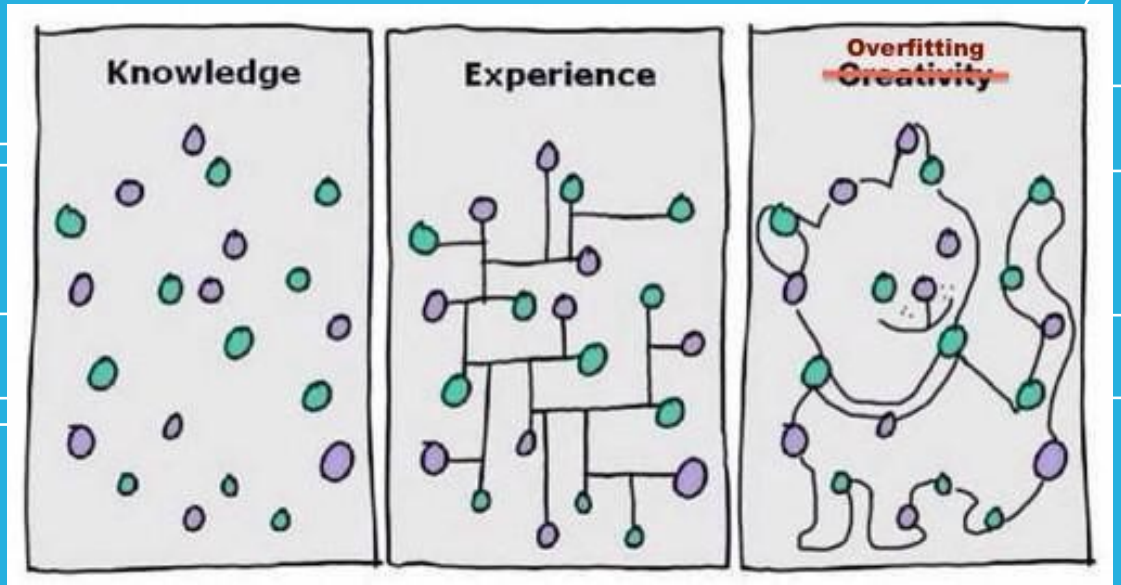
G. Hagen, M. Hjorth-Jensen, G.R. Jansen, R. Machleidt,
T. Papenbrock, Phys.Rev.Lett. 109, 032502 (2012).

Unknown unknown?

Overfitting?

With four parameters I can fit an elephant, and with five I can make him wiggle his trunk.

--John von Neumann



How to identify parameters that can not be controlled by available data?

Mass model: 33 terms vs 19 terms

Term	I
Coulomb	0.702 ± 0.002
Symmetry	149.744 ± 0.721
Surface symmetry	209.351 ± 2.731
Pairing (I)	6.195 ± 0.162
Pairing (II)	9.741 ± 3.594
$\mathcal{M}+\mathcal{T}$	18.382 ± 0.183
$(\mathcal{M}+\mathcal{T})/\rho$	14.965 ± 0.911
FS+	5.160 ± 0.456
fs+	23.679 ± 2.429
FS−	1.692 ± 0.152
fs−	7.708 ± 0.726
FC+	−4.900 ± 1.518
fc+	−41.955 ± 4.159
PM+	−0.453 ± 0.081
pm+	−0.116 ± 0.400
PS+	−0.842 ± 0.084
ps+	−4.264 ± 0.469
PS−	−0.106 ± 0.025
ps−	−0.562 ± 0.121
S3	0.427 ± 0.024
s3	1.964 ± 0.115
SQ−	0.334 ± 0.040
sq−	1.320 ± 0.221
D3	−0.081 ± 2.514
d3	8.205 ± 14.560
QQ+	6.150 ± 6.190
qq+	5.322 ± 33.201
D0	−33.197 ± 2.131
d0	−158.619 ± 10.380
QQ−	−2.777 ± 6.405
qq−	−24.519 ± 34.650
SS	1.152 ± 0.215
ss	3.728 ± 0.919
χ(I)	0.356

Term	I
Coulomb	0.705 ± 0.001
Symmetry	149.033 ± 0.468
Surface symmetry	202.642 ± 1.848
Pairing	5.167 ± 0.138
$\mathcal{M}+\mathcal{T}$	18.552 ± 0.037
$(\mathcal{M}+\mathcal{T})/\rho$	15.120 ± 0.125
FS	1.069 ± 0.040
fs−	4.414 ± 0.259
fc+	−10.353 ± 0.753
PM+	−0.498 ± 0.011
PS+	−0.082 ± 0.008
S3	0.515 ± 0.015
s3	2.381 ± 0.069
SQ−	0.393 ± 0.022
sq−	1.581 ± 0.120
d3+QQ+	7.204 ± 0.169
D0	−21.533 ± 0.699
d0	−89.904 ± 3.220
SS	0.431 ± 0.050
χ(I)	0.425

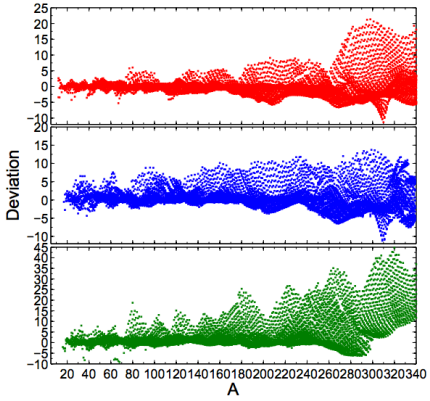
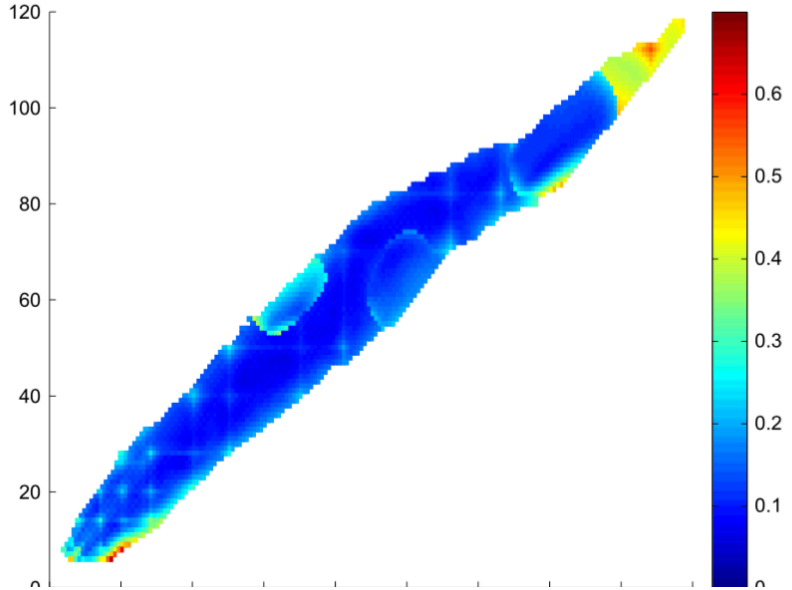
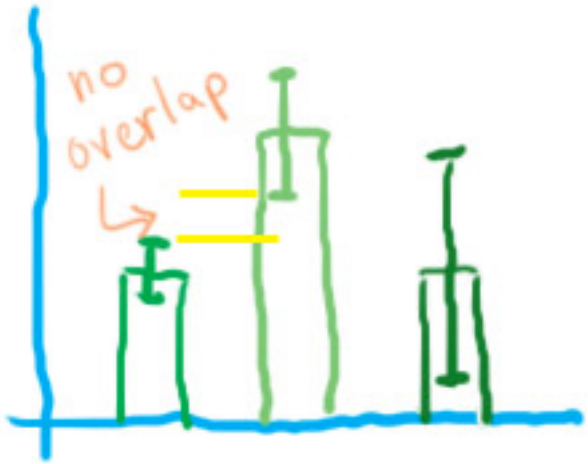


FIG. 2. (Color online) Differences (in MeV) between DZ10 mass model calculations with the parameter set II from Table I and the macroscopic-microscopic liquid drop model calculation of Ref. [20] (upper), the finite-range droplet model [26] (middle) and the HFB-21 model [32] (bottom).

The uncertainty propagation
The statistical error is usually small





http://mathbench.umd.edu/modules/prob-stat_bargraph/page08.htm

$$\sigma^2(\mathrm{BE}) = \sum_{i,j}^{N} \mathrm{Cov}(x_i, x_j) \frac{\partial \mathrm{BE}}{\partial x_i} \frac{\partial \mathrm{BE}}{\partial x_j}, \qquad (11)$$

where BE denotes the binding energy, x_i is the parameter and N denotes the total number of parameters. $\mathrm{Cov}(x_i, x_j)$ is the covariance matrix

CQ, J. Phys. G 42 (4), 045104 (2015)

How do we propagate theoretical uncertainties?
http://bayesint.github.io/index.html

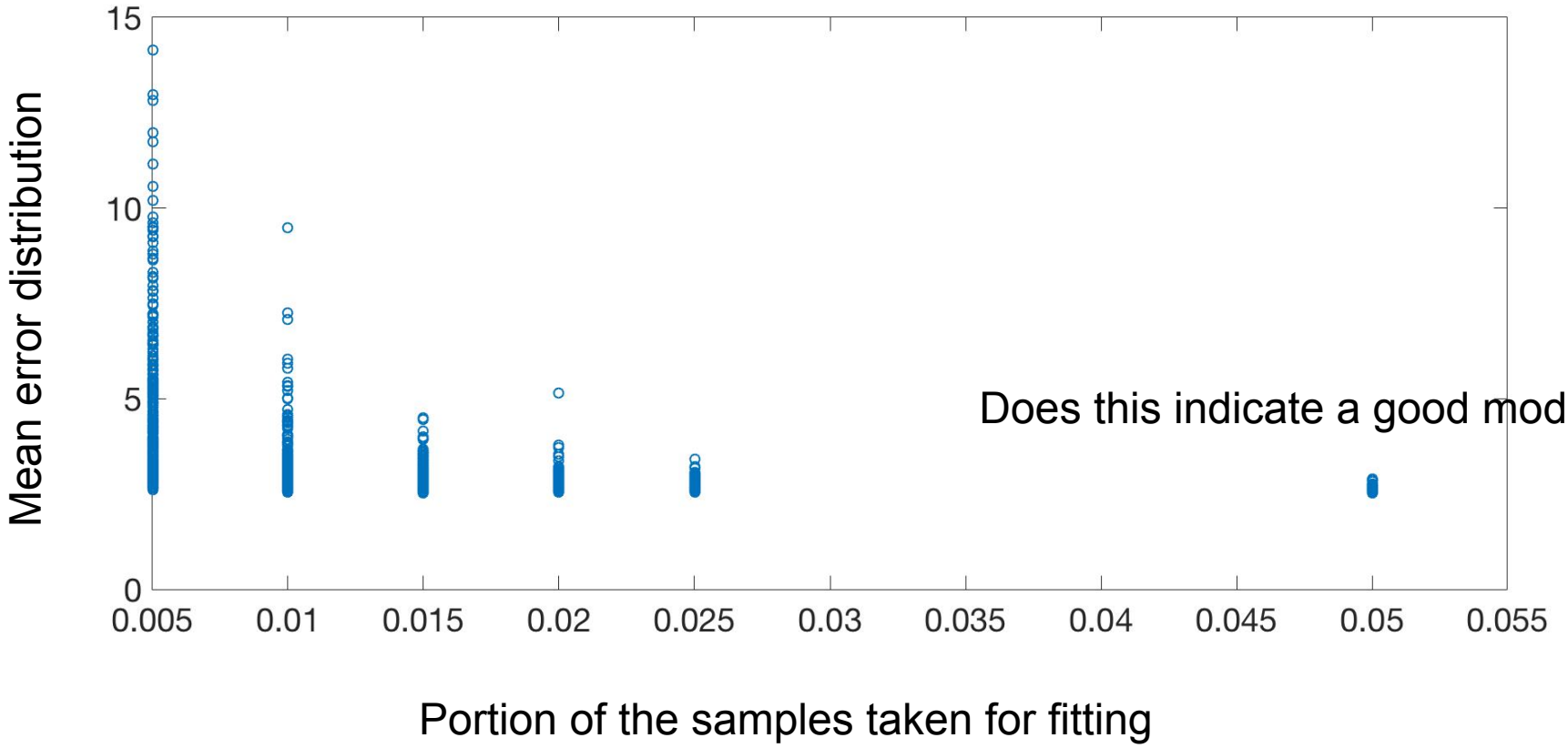
Mini-Minimax Uncertainty Quantification for Emulators

Jeffrey C. Regier† and Philip B. Stark†

Abstract. Consider approximating a "black box" function f by an *emulator* $\hat{f}$ based on n noiseless observations of f. Let w be a point in the domain of f. How big might the error $|\hat{f}(w) - f(w)|$ be? If f could be arbitrarily rough, this error could be arbitrarily large: we need some constraint on f besides the data. Suppose f is Lipschitz with known constant. We find a lower bound on the number of observations required to ensure that for the best emulator $\hat{f}$ based on the n data, $|\hat{f}(w) - f(w)| \leq \epsilon$. But in general, we will not know whether f is Lipschitz, much less know its Lipschitz constant. Assume optimistically that f is Lipschitz-continuous with the smallest constant consistent with the n data. We find the maximum (over such regular f) of $|\hat{f}(w) - f(w)|$ for the best possible emulator $\hat{f}$; we call this the "mini-minimax uncertainty" at w. In reality, f might not be Lipschitz or—if it is—it might not attain its Lipschitz constant on the data. Hence, the mini-minimax uncertainty at w could be much smaller than $|\hat{f}(w) - f(w)|$. But if the mini-minimax uncertainty is large, then—even if f satisfies the optimistic regularity assumption—$|\hat{f}(w) - f(w)|$ could be large, no matter how cleverly we choose $\hat{f}$. For the Community Atmosphere Model, the maximum (over w) of the mini-minimax uncertainty based on a set of 1154 observations of f is no smaller than it would be for a single observation of f at the centroid of the 21-dimensional parameter space. We also find lower confidence bounds for quantiles of the mini-minimax uncertainty and its mean over the domain of f. For the Community Atmosphere Model, these lower confidence bounds are an appreciable fraction of the maximum. To know that the emulator estimates f accurately would require evidence that f is typically more regular than it is across the n sample values.

http://arxiv.org/pdf/1303.3079v4.pdf

We take liquid drop model as an example to test the extrapolation property of a constraint model



Does this indicate a good model?

Model truncation

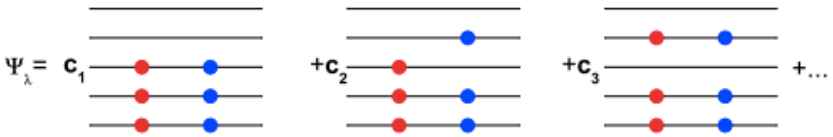
$$H = H_m + H_M$$

$$E^{\mathrm{SM}} = \langle \Psi_I | H | \Psi_I \rangle$$

$$= \sum_{\alpha} \varepsilon_{\alpha} < \hat{N}_{\alpha} > + \sum_{\alpha \leq \beta} V_{m;\alpha\beta} \left\langle \frac{\hat{N}_{\alpha}(\hat{N}_{\beta} - \delta_{\alpha\beta})}{1 + \delta_{\alpha\beta}} \right\rangle$$

$$+ \langle \Psi_I | H_M | \Psi_I \rangle, \qquad (4)$$

‘Monopole’ truncation



- The idea behind is that the Hamiltonian is dominated by the diagonal monopole channel. The monopole interaction can change significantly the (effective) mean field and drive the evolution of the shell structure.
- Easy to implement and keeps the simplicity of the M-scheme algorithm
- Possibility to include certain intruder configurations

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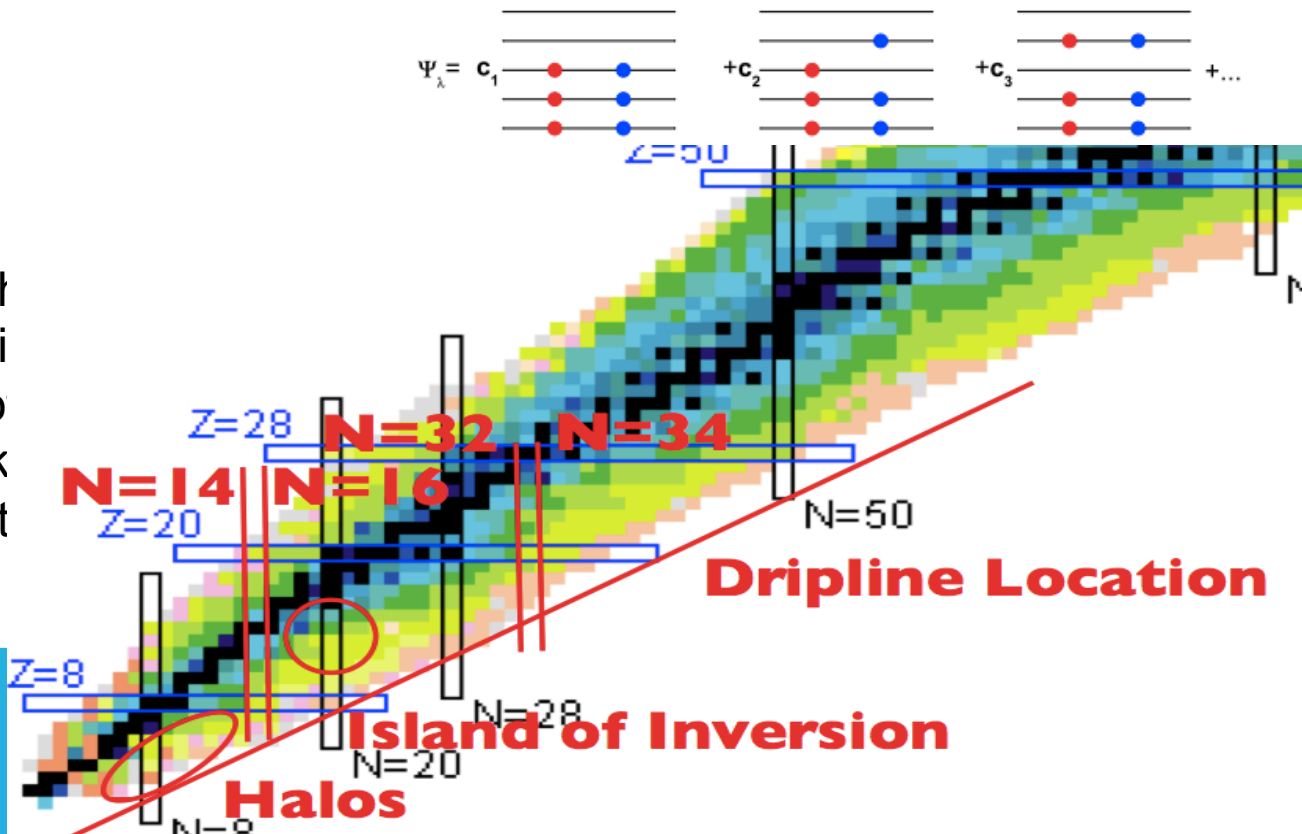
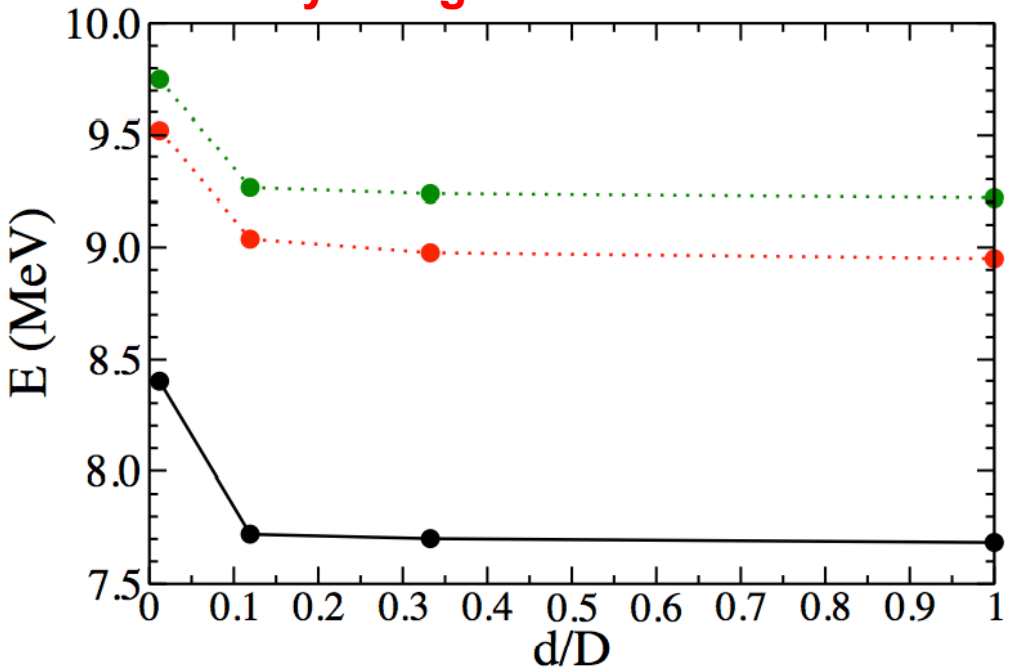


Convergence for ^{194}Pb

When does the calculation converge?
How to quantify the uncertainty at a given truncation?



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CQ, LY Jia, GJ Fu, to appear in PRC

Summary

- **Introduction to the nuclear shell model/full configuration interaction approach**
  - ❖Properties of the effective interaction
  - ❖Applications in Sn, Pb and neighboring isotopes
  - ❖(Empirical) shell model can be a reliable tool for simulating the spectroscopy of intermediate mass and heavy nuclei
- **How to quantify the uncertainty related to the effective interaction and model space truncation**

How many terms do I need?
Whether *f* is adequate?

$$y = f(A_i, x_i) + e$$

How should one do basic regression analysis? (http://bayesint.github.io/index.html)

Thank you

Fitting criterion

- Least-square is based on the assumption that the likelihood is characterized ***by Gaussian*** distribution;
- Systematic deviations may not following Gaussian.

Mini-max

$$\varepsilon = \arg\min_{\mathbf{x}} \max_{A} |\mathrm{BE}^{\mathrm{Expt.}}(A) - \mathrm{BE}^{\mathrm{Calc.}}(A, \mathbf{x})|,$$

Does this criterion make sense?
What are the risks behind?

Maximum likelihood (by assuming student's t distribution)

coincide with Bayesian estimator for uniform prior distribution