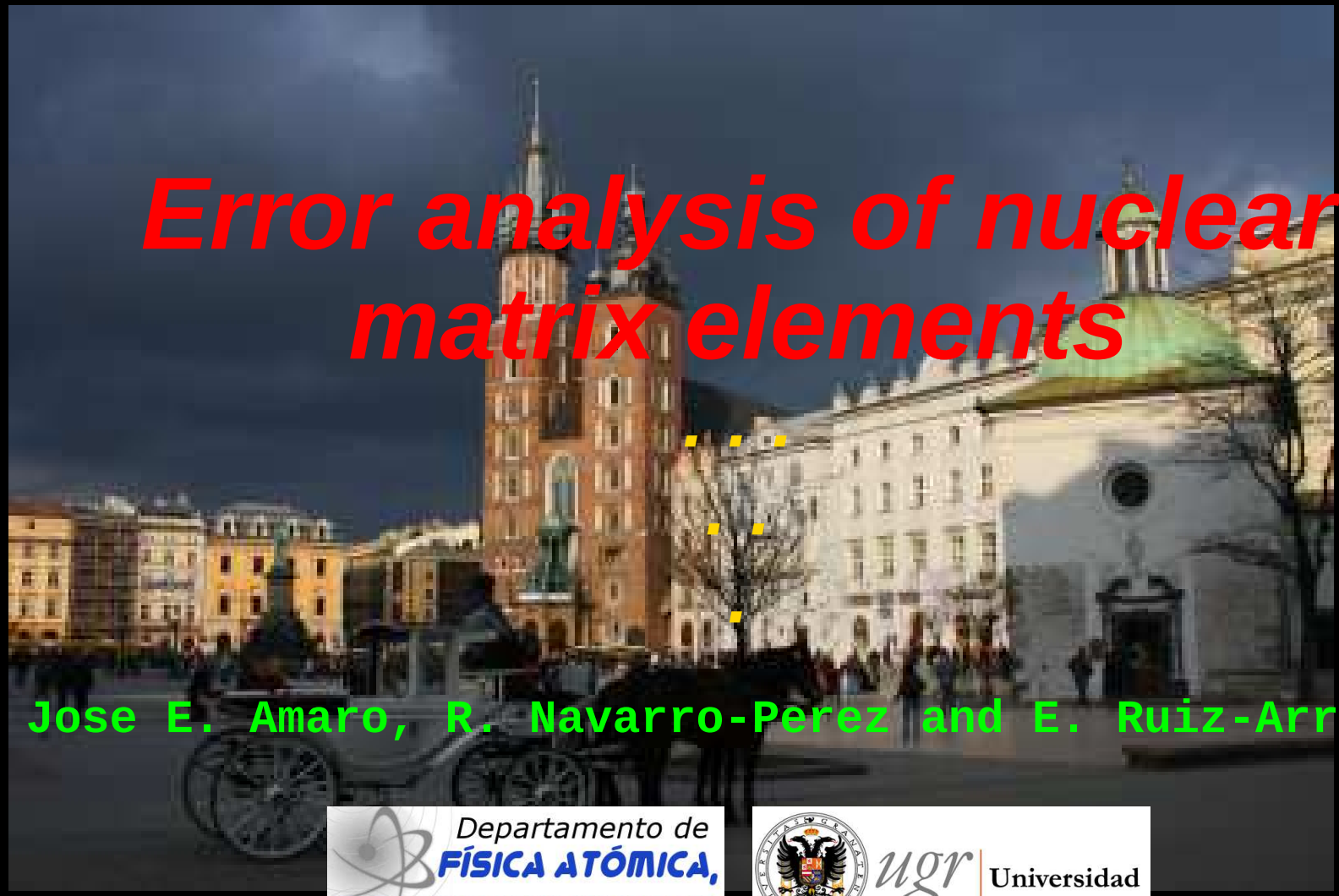

Error analysis of nuclear matrix elements

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Outline

1. Motivation
2. Error analysis of phase-shifts
3. Binding energy uncertainties
4. Coarse GRained potential results
5. Summary

1. Introduction

- The NN interation is fundamental in the description of nuclear properties
- Thousands of np and pp data have been collected along the years
- The impact of NN uncertainties in the Nuclear Many Body problem remains an open chalenge
- It determines a lower bound on the inaccuracy of first principles calculations
- Nuclear binding energies are known to high accuracy $\Delta B = 0.01 - 10$ KeV
- Liquid-drop model mass fit yield accuracy $\Delta B = 0.6$ MeV.

Estimate of binding energy uncertainties

- We compute and propagate two-body systematic errors
- To provide a theoretical *a priori* estimate of binding energy uncertainties
- We use a NN-potential fitting the available np and pp data with $\chi^2/dof \sim 1$
- Simple semi-analytical solutions of the NN scattering problem are needed to simplify the extraction of errors in the fitting parameters
- We use a coarse grained (GR) potential as a sum of δ-shells
- A recent partial wave analysis (PWA) of NN data with the GR potential gives $\chi^2/dof = 1.06$ fitting 46 parameters.

Partial Wave Analysis. Coarse Grained (GR) potential

→ Next talk by Rodrigo Navarro

PHYSICAL REVIEW C **88**, 024002 (2013)

Partial-wave analysis of nucleon-nucleon scattering below the pion-production threshold

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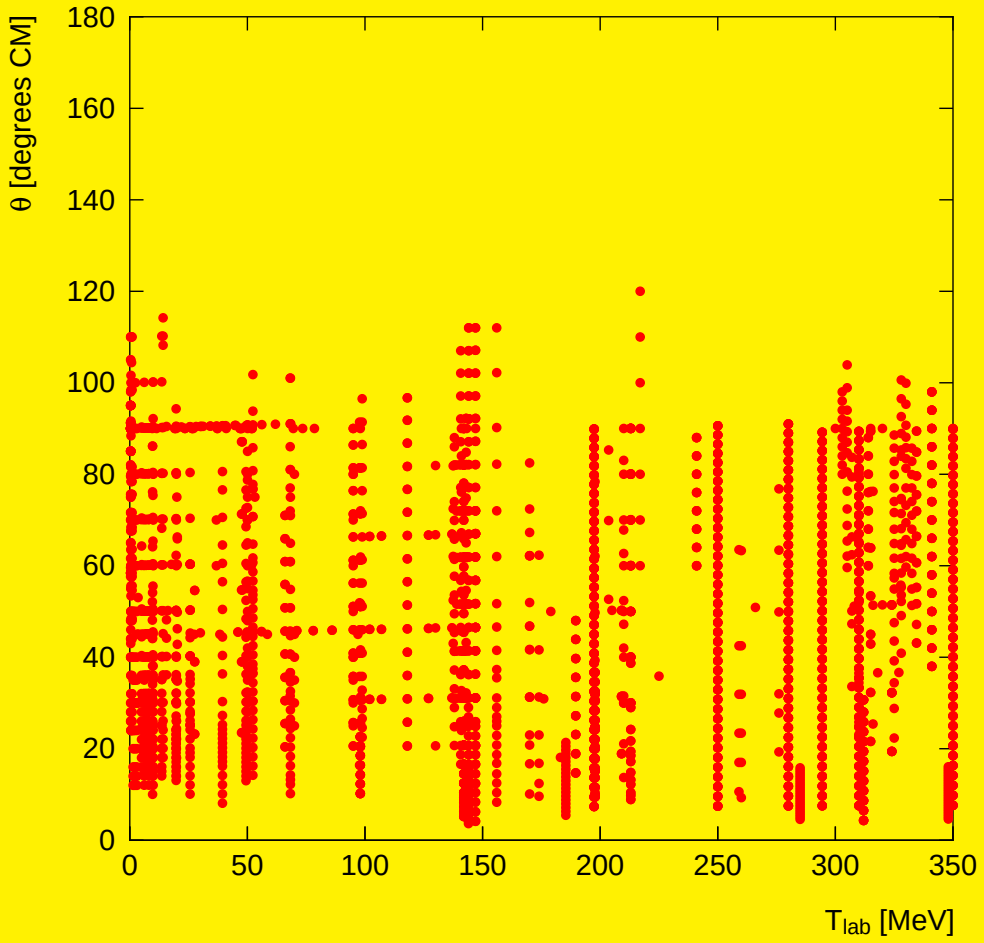
We undertake a simultaneous partial wave analysis of proton-proton and neutron-proton scattering data below the pion production threshold up to laboratory energies of 350 MeV. We represent the interaction as a sum of δ shells in configuration space below 3 fm and a charge dependent one pion exchange potential above 3 fm together with electromagnetic effects. We obtain a chi square value of 2813, for *pp*, and 3985, for *nn*, with a total of 2747 and 3691 *pp* and *nn* data, respectively, obtained till 2013 and a total number of 46 fitting parameters yielding a chi square value by degree of freedom of $\chi^2/\text{d.o.f} = 1.06$. Special attention is payed to estimate the errors of the phenomenological interaction as well as the derived effects on the phase shifts and scattering amplitudes.

DOI: 10.1103/PhysRevC.88.024002 PACS number(s): 03.65.Nk, 11.10.Gh, 13.75.Cs, 21.30.Fe

2. Error analysis of NN phase-shifts

- Different high quality potentails fitting NN-data with $\chi^2/dof \sim 1$ show discrepancies in the phaseshifts
- Different treatment of the mid and short range interaction
- Different fits agree on kinematical regions where data exist
- They may disagree in other regions where there are not data
- This desagreements propagates to the phase-shifts
- We evaluate the systematic errors as the spreading of the existing high-quality potentials

pp data distribution



High quality potentials

NN potentials fitting a large set of scattering data with $\chi^2/dof \sim 1$:

- CD Bonn: Machleidt, Sammarruca and Song, PRC 53 (1996)
- Nijmegen I and II: Stoks, Klomp, Rentmeester, de Swart, PRC 48 (1993)
- Argonne AV18: Wiringa, Stoks, Schiavilla, PRC 51 (1995)
- Reid 93: Friar, Payne, Stoks, de Swart PLB 311 (1993)
- Covariant spectator model: Gross and Stadler, PRC 78 (2008)
- Coarse grained GR: Navarro-Perez, Amaro, Ruiz-Arriola PRC 88 (2013)

One-Pion exchange (OPE) and Charge-Dependent (CD) tails, electromagnetic effects, etc

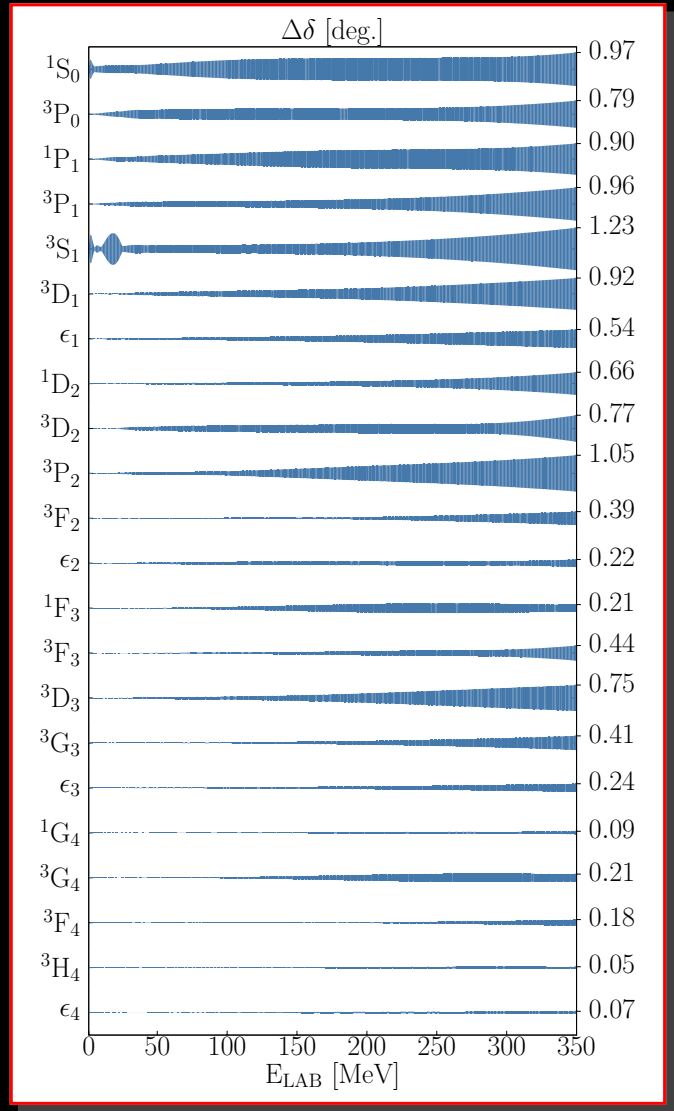
The unknown short-range parts display a variety of shapes, local or non-local, angular momentum, energy or lineal momentum dependence.

Phase-shifts. Systematic error

Absolute systematic error bands.
Standard deviation $|\Delta\delta|$ between the different potentials

$$\Delta\delta = \sqrt{\frac{\sum_{i=1}^{N}(\delta_i - \overline{\delta})^2}{N-1}}$$

N = CD Bonn, Nijm I, Nijm II, AV18, Reid93, CEM, GR

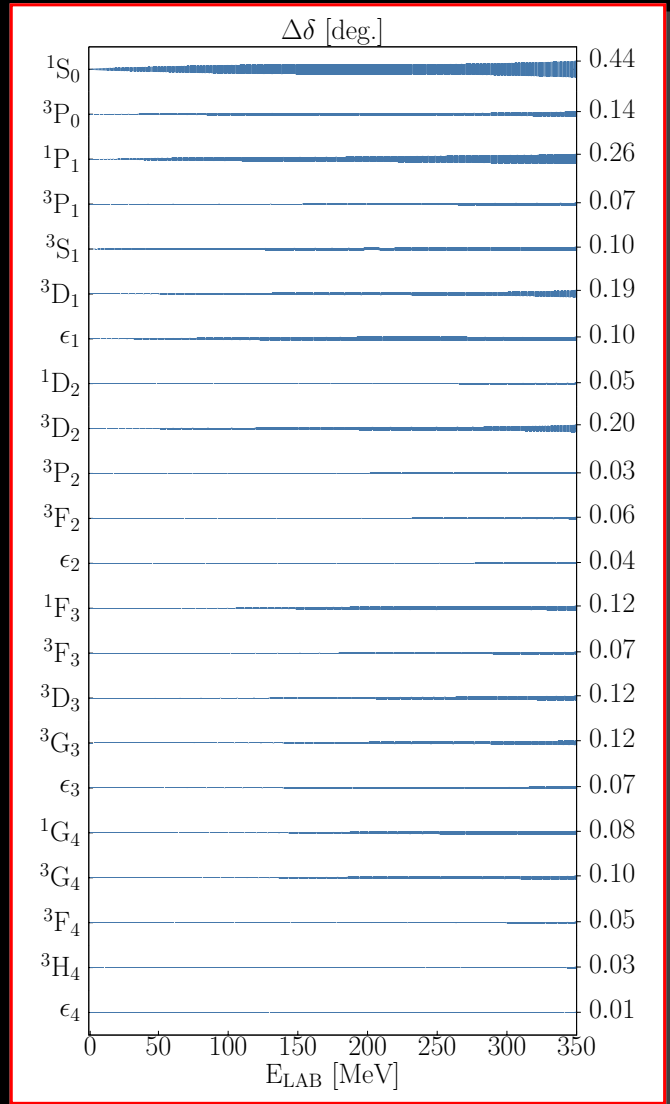


Phase-shifts. Statistical error

Statistical error bands from the partial wave analysis with the GR potential
[see Next talk by Rodrigo Navarro]

$\Longrightarrow$

Statistical errors are smaller than systematic errors

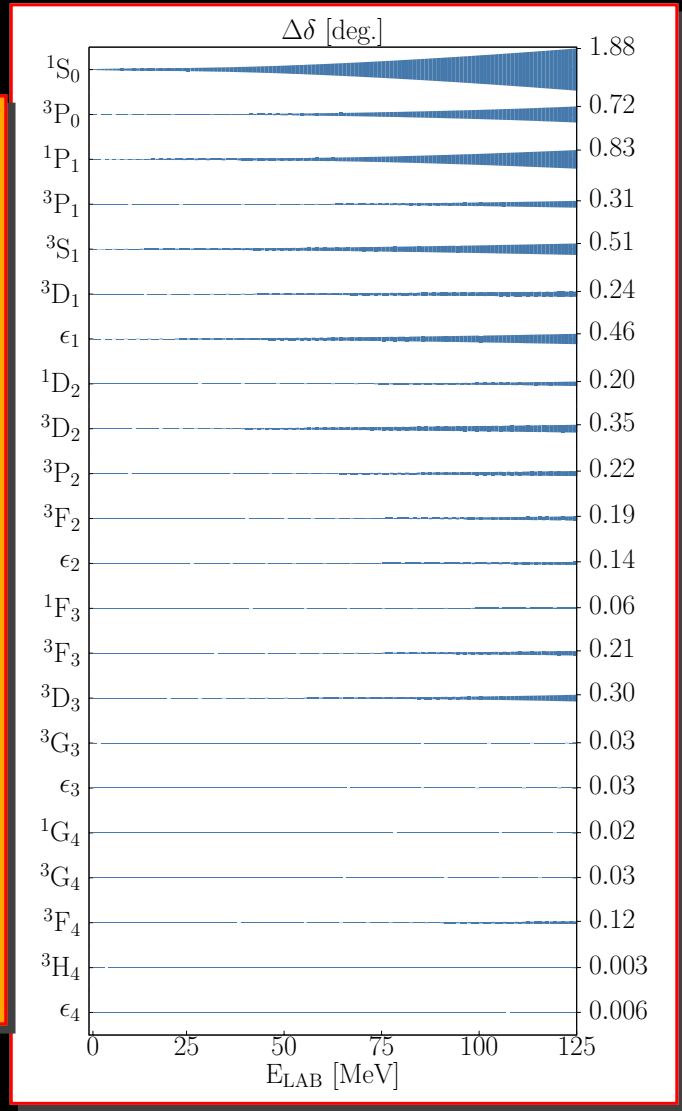


Uncertainty with chiral forces.

Theoretical uncertainty in a fit with chiral interaction.
Statistical error obtained in a second PWA.
Fit to data below $E < 125$ MeV.
The GR potential is fixed for $r > 1.8$ fm

$$V(r) = V_{OPE}(r) + V_{TPE}(r) + V_{em}(r)$$

V_{OPE}: one-pion exchange
V_{TPE}: chiral two-pion exchange
[Rentmeester, Timmermans, Friar, de Swart, PRL 82 (1999)]
V_{em}: electromagnetic potential

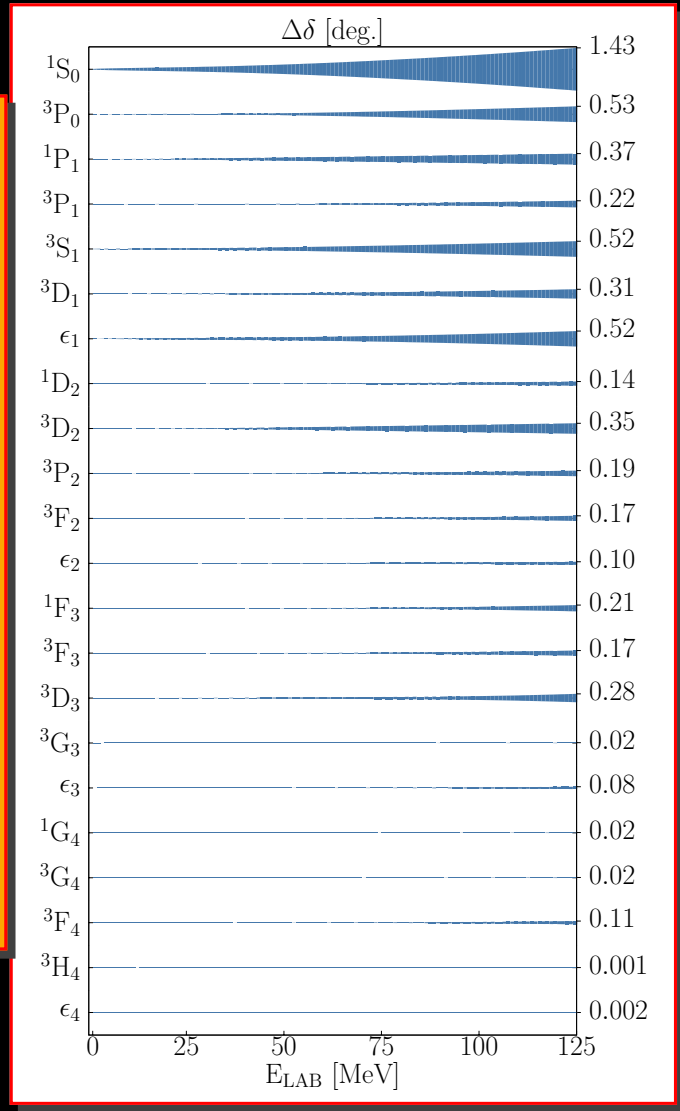


Uncertainty with OPE

Theoretical uncertainty in a fit with OPE.
Statistical error obtained in a third PWA.
Fit to data below $E < 125$ MeV.
The GR potential is fixed for $r > 1.8$ fm

$$V(r) = V_{OPE}(r) + V_{em}(r)$$

V_{OPE}: one-pion exchange
V_{em}: electromagnetic potential
The uncertainties are smaller than in the fit with Chiral force



3. Binding energy uncertainties

Way of analyzing binding energy uncertainties from systematic errors:

- Ab initio calculation with different two-body potentials $V_2^{(1)}$, $V_2^{(2)}$,... yielding nuclear binding energy $B^{(1)}(A)$, $B^{(2)}(A)$, ...
- Compute the mean

$$\overline{B}(A) = \sum_1^N B^{(i)}(A),$$

- Compute the standard deviation

$$\Delta B(A) = \sqrt{\frac{1}{N-1}\sum_1^N (B^{(i)}(A) - \overline{B}(A))^2}$$

Example: ^3H theoretical uncertainty

- Triton theoretical energy in MeV. Fadeev calculations:

CD Bonn	Nijm I and II	Reid93	AV18	Covariant spectator model
8.00	7.62	7.63	7.72	8.50

- Experimental $B_{exp}(3) = 8.4820(1)$ MeV
- Theoretical average and dispersion:

$$\overline{B}(3) = 7.85 MeV \qquad \Delta B(3) = 0.34 MeV$$

- Theoretical ucertainty per nucleon: $\Delta B(3)/3 = 0.11$ MeV

Three-body force

- A three-body interaction V_3 is needed to account for the missing energy
  ~ 1 MeV for ^{3}H
  ~ 4 MeV for ^{4}He
- the definition of V_3 depends on V_2
- Any uncertainty in the two-body interaction will carry over to the three body interaction
- It can be shown that if correlations between two and three body forces are ignored

$$\Delta B(A)^2 = \Delta V_2^2 + \Delta V_3^2 + \cdots$$

- Thus, estimating the two-body uncertainty provides a lower bound of the total uncertainty

$$\Delta B > \Delta V_2$$

Estimating the ucertainty for $A > 4$

- Difficult due to computational and theoretical problems
- Only Monte Carlo calculations may go up to $A = 10$ with Argonne-type potentials (AV18)
- The question of the systematic errors remain
- Short distance core of the AV18 potential demands short-range correlations
- How to avoid the short-range correlations?
  Schematically, for a closed-shell nucleus,

$$\langle V_2 \rangle = \frac{A(A-1)}{2} \int d^3r P_2(r) V_C(r)$$

- $P_2(r)$: probability of finding two particles at a distance r.
- The contribution of $P_2(r)V_C(r)$ from the core $r < a_{core}$ is small
- We use a coarse grained potential where $V_C = 0$ for $r < a_{core}$

The Afnan and Tang argument

- Suggested by Afnan and Tang, Physical Review 175 (1968)
- For $A = 3, 4$ nuclei
- They realized that the relevant NN interaction energies inside a nucleus do not probe the core explicitly.
- Soft core potentials, fitted to NN low partial waves up to $E = 100$ MeV provided reasonable binding eneergies
- This is the physics behind the V_{lowk} potentials: effective truncated Hilbert space below a cut-off $\Lambda \sim \sqrt{M_N m_\pi}$

4. Coarse Grained potential results

- A potential averaged over a given space resolution

$$\Delta r \sim b_{min} \sim 1/\Lambda = 1/\sqrt{M_N m_\pi} \sim 0.5 fm$$

- Fiting data below pion production theshold
- The information can be encoded in a finite number of points without any specyfic form of the potential
- Calculations become simple by taking δ-shells below $r_c = 3$ fm.
- Potential for the partial wave $^{2S+1}(l,l')_J$

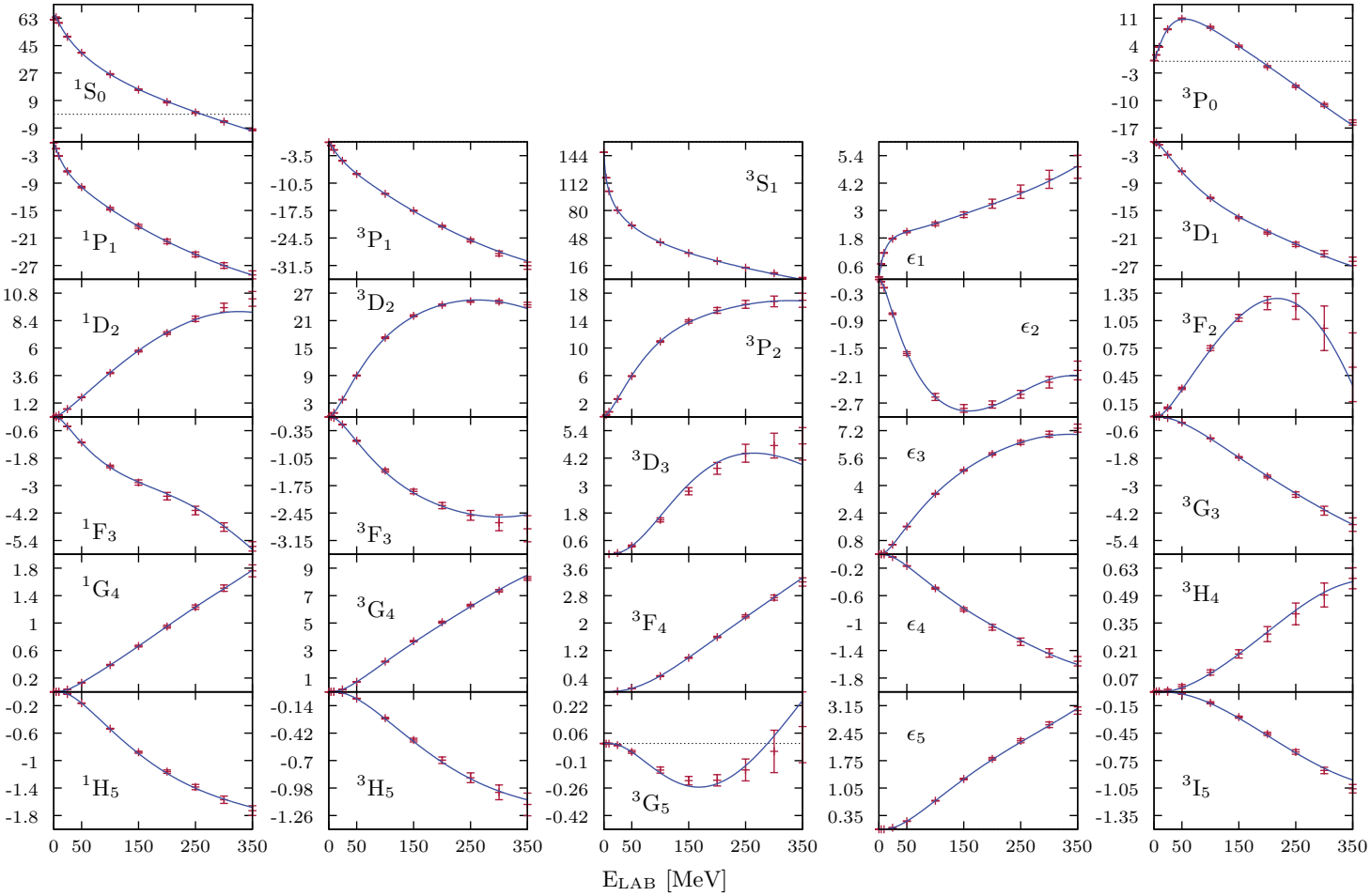
$$V^{JS}_{l,l'}(r) = \frac{1}{2\mu}\sum_{n=1}^{N}(\lambda_n)^{JS}_{l,l'}\delta(r-r_n), \qquad r \leq r_c$$

- For $r > 3$ fm we use the Charge-dependent OPE + electromagnetic interactions.

Potential parameters and systematic errors

- Navarro-Perez, Amaro, and Ruiz-Arriola, PLB 724 (2013) 138
- We fit theoretical phase-shifts as “pseudodata”
- Choose a discrete set or energies $E_1, E_2, \ldots, E_n$
- For each partial wave ${}^{2S+1}L_J$
- We extract the theoretical phase-shifts from the several PWA
- Taking the mean value and dispersion over the different models we obtain a set of “pseudodata” and “pseudoerrors”
- We fit the parameters of the GR potentail by minimizing the χ^2 to the pseudata for each partial wave
- Performing variations of the pseudata within their error interval and repeating the fit we obtain the systematic error of the potential parameters.

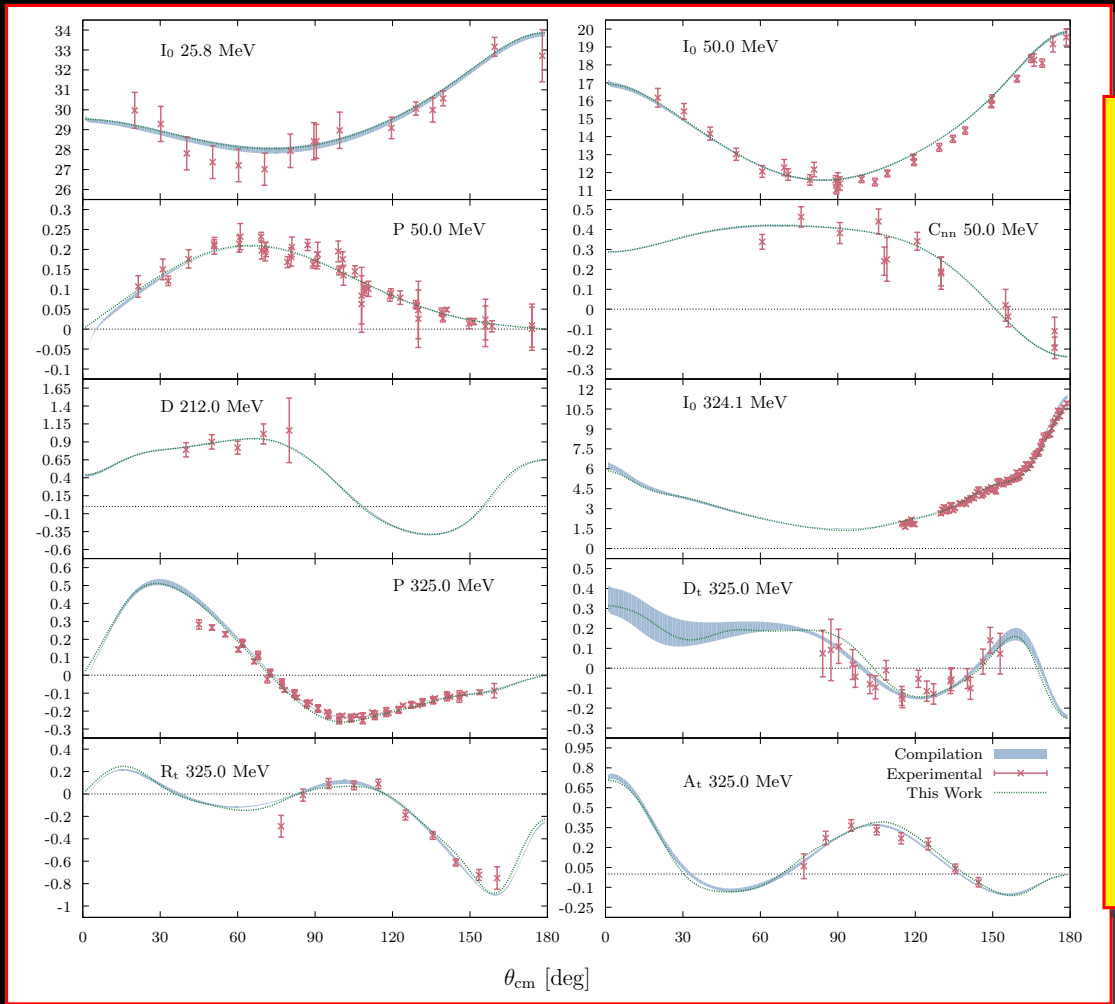
Phase-shifts. Fit to pseudodata.



Coarse grained potential and systematic errors

Wave	λ_1	λ_2	λ_3	λ_4	λ_5	χ^2/D.o.F
$^1S_0$	2.12(7)	-0.987(7)	–	-0.087(2)	–	0.3476
$^3P_0$	–	1.26(4)	-0.43(1)	–	-0.037(2)	0.6589
$^1P_1$	–	1.23(2)	–	0.079(4)	–	0.0088
$^3P_1$	–	1.33(2)	–	0.053(2)	–	0.4323
$^1D_2$	–	–	-0.252(3)	–	-0.0163(9)	0.6946
$^3D_2$	–	–	-0.596(8)	-0.08(1)	-0.050(4)	0.6144
$^1F_3$	–	–	0.34(1)	–	0.010(2)	0.3812
$^3F_3$	–	–	–	0.060(2)	–	0.4177
$^1G_4$	–	–	-0.22(2)	–	-0.0137(9)	0.8090
$^3G_4$	–	–	–	-0.267(3)	–	1.8670
$^1H_5$	–	–	–	0.071(8)	–	0.6577
$^3H_5$	–	–	–	0.04(1)	–	0.4193
$^3S_1$	1.57(4)	-0.40(1)	–	-0.064(3)	–	
ε_1	–	-1.69(1)	-0.379(4)	-0.216(5)	-0.027(3)	
$^3D_1$	–	–	0.52(2)	–	0.041(3)	0.4313
$^3P_2$	–	-0.415(6)	–	-0.0384(9)	–	
ε_2	–	0.65(1)	–	0.106(2)	–	
$^3F_2$	–	–	0.14(3)	-0.076(6)	–	0.3881
$^3D_3$	–	–	–	–	–	
ε_3	–	–	-0.47(3)	-0.24(1)	-0.020(4)	
$^3G_3$	–	–	–	0.101(6)	–	0.6806
$^3F_4$	–	–	-0.163(4)	–	-0.0101(4)	
ε_4	–	–	–	0.108(3)	–	
$^3H_4$	–	–	–	–	-0.010(1)	0.2659
$^3G_5$	–	–	–	0.025(4)	–	
ε_5	–	–	–	-0.35(1)	–	
$^3I_5$	–	–	–	–	–	0.5354

NN observables

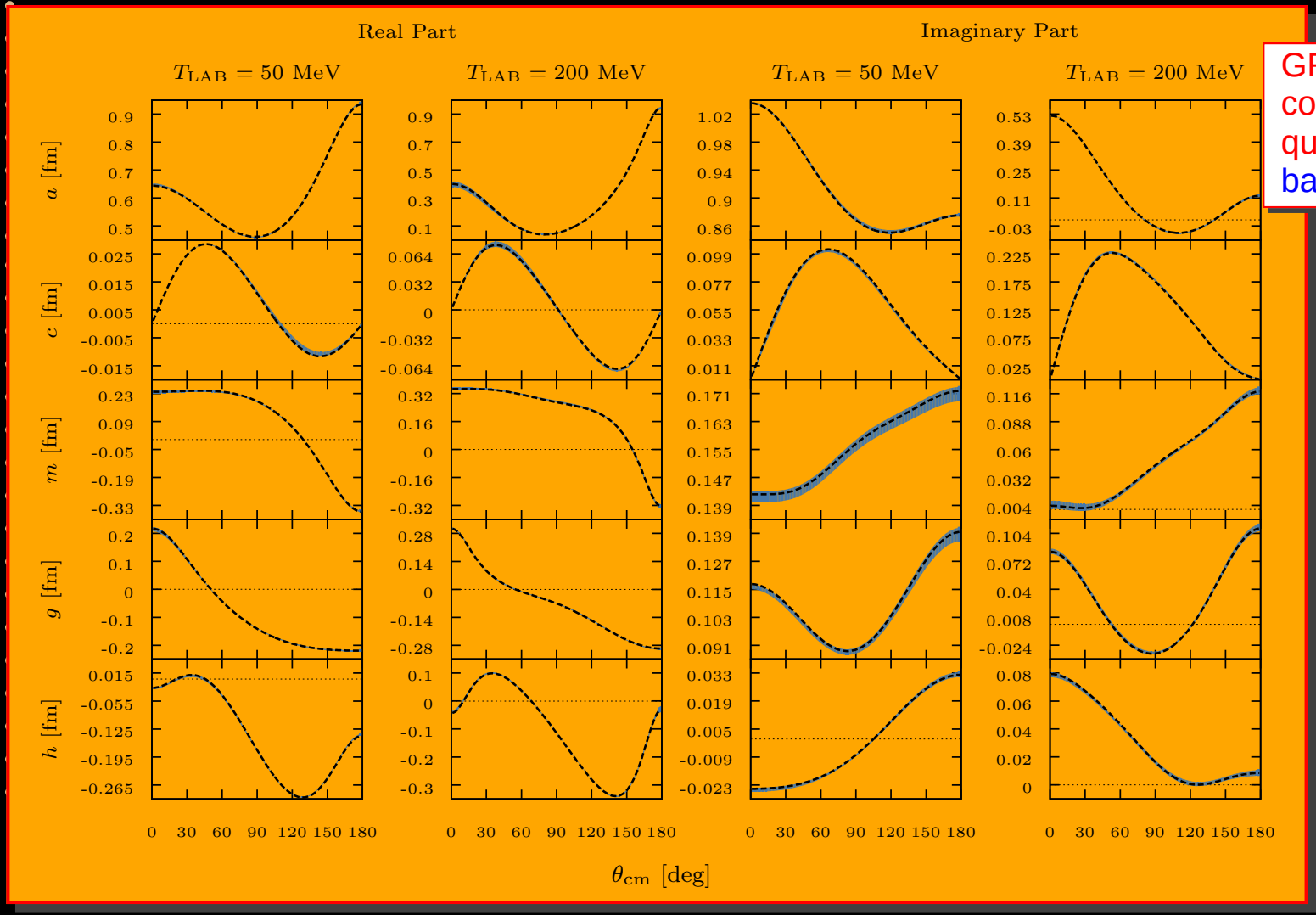


- Since the pseudodata have been extracted from PWA, the GR potential is a faithful representation of the experimental data
- $\chi^2/dof = 1.12$ to experimental data
- Readjusting the parameters in a PWA the GR potential gives $\chi^2/dof = 1.06$

Wolfenstein parameters

On-shell np scattering amplitude contains five independent complex quantities,

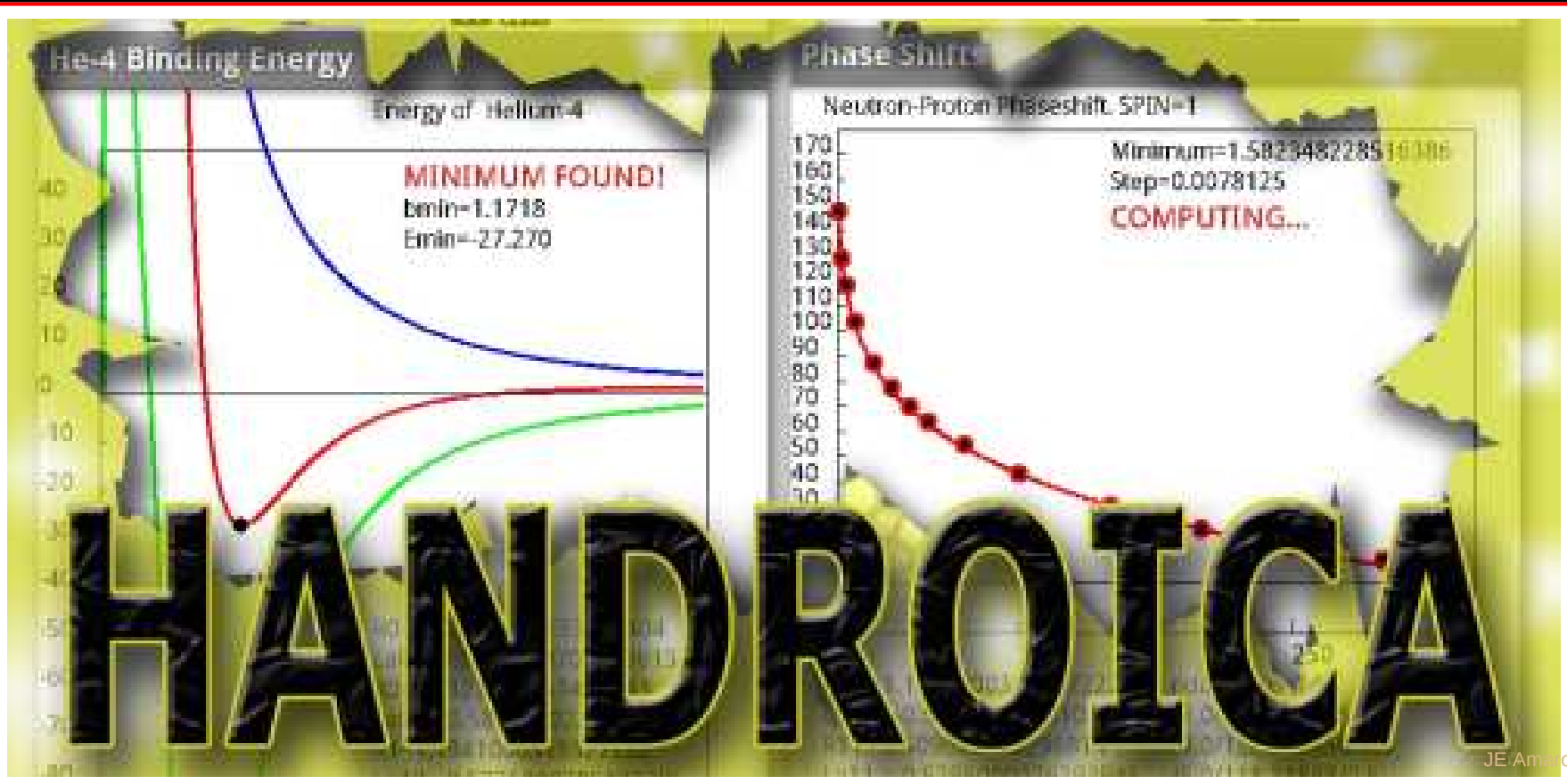
$$M(\mathbf{k}_f, \mathbf{k}_i) = a + m(\sigma_1, \mathbf{n})(\sigma_2, \mathbf{n}) + (g - h)(\sigma_1, \mathbf{m})(\sigma_2, \mathbf{m}) + (g + h)(\sigma_1, \mathbf{l})(\sigma_2, \mathbf{l}) + c(\sigma_1 + \sigma_2, n)$$



GR potential is compared to six high-quality potentials (blue band)

HANDROICA

Educational Android app.
For smartphones and tablets with android 2.1 or above



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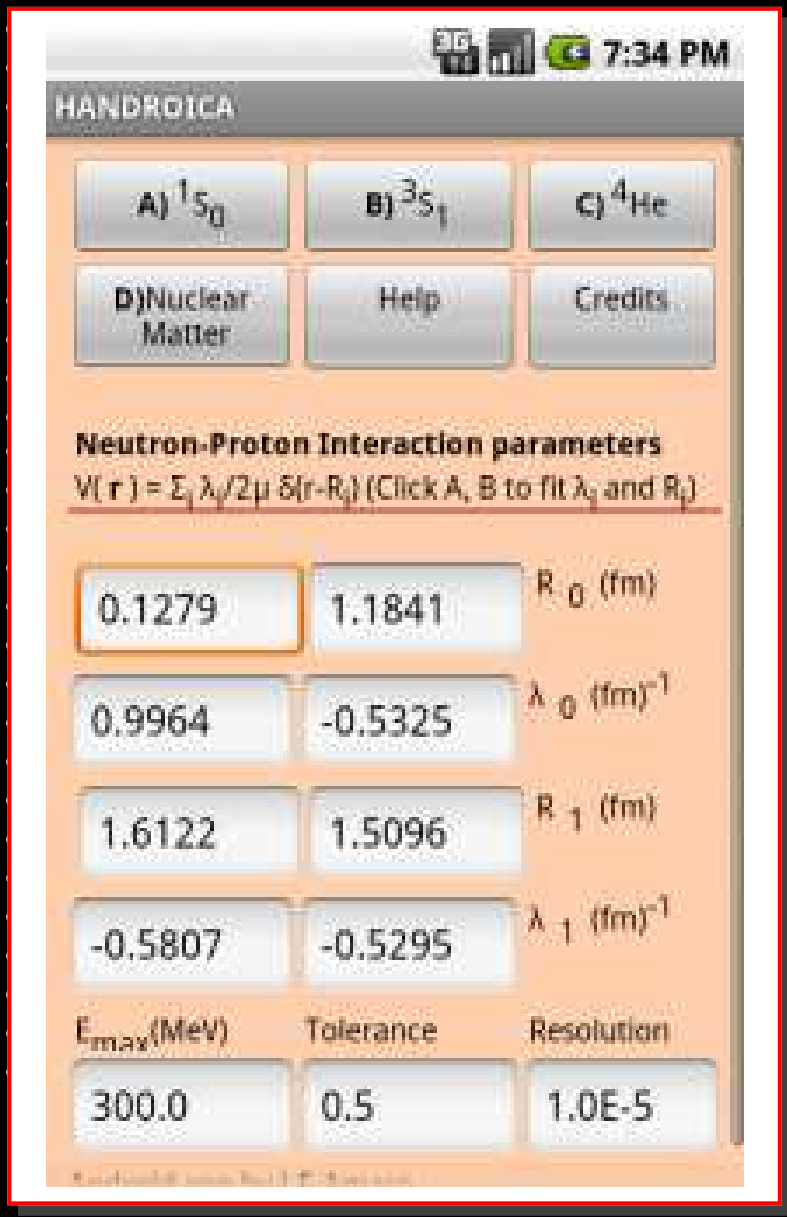
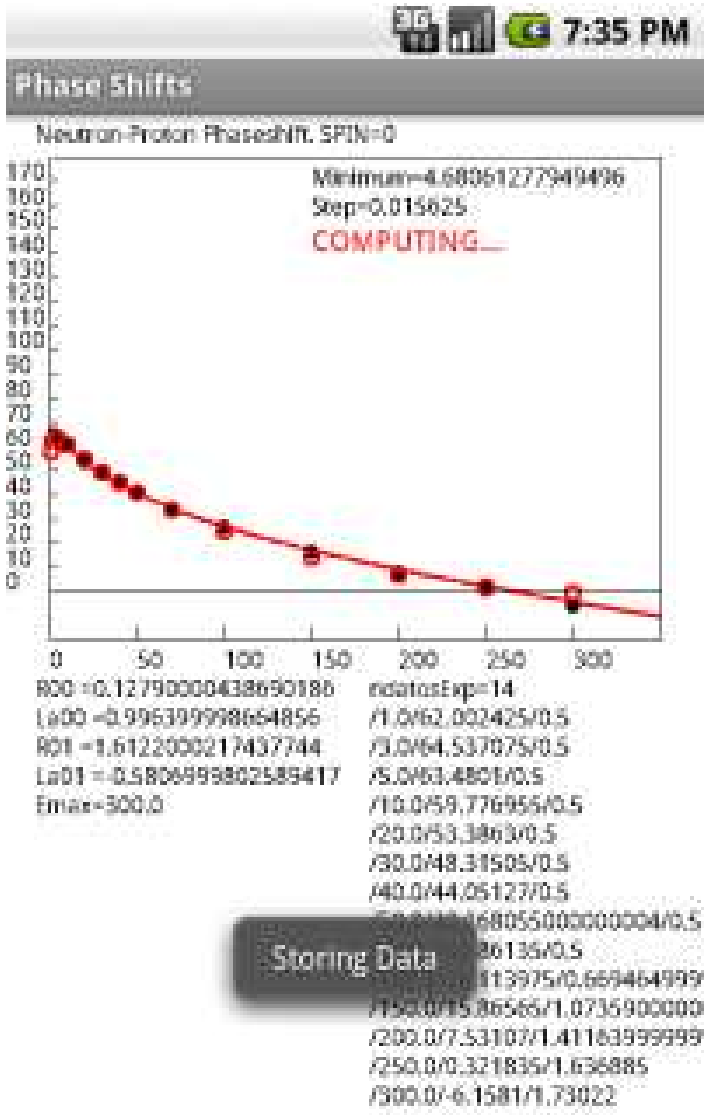
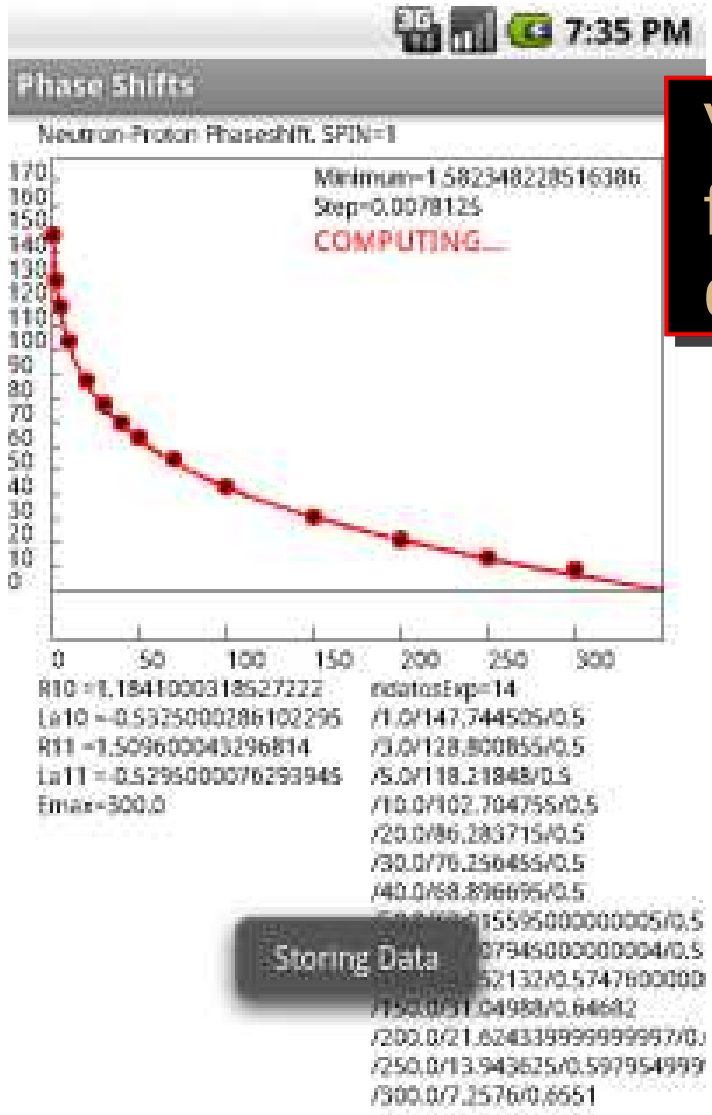
HANDROICA main screen



Perform a fit of GR potential with 4 parameters to S-wave phase-shifts up to some energy E_{max}, with some tolerance and resolution.

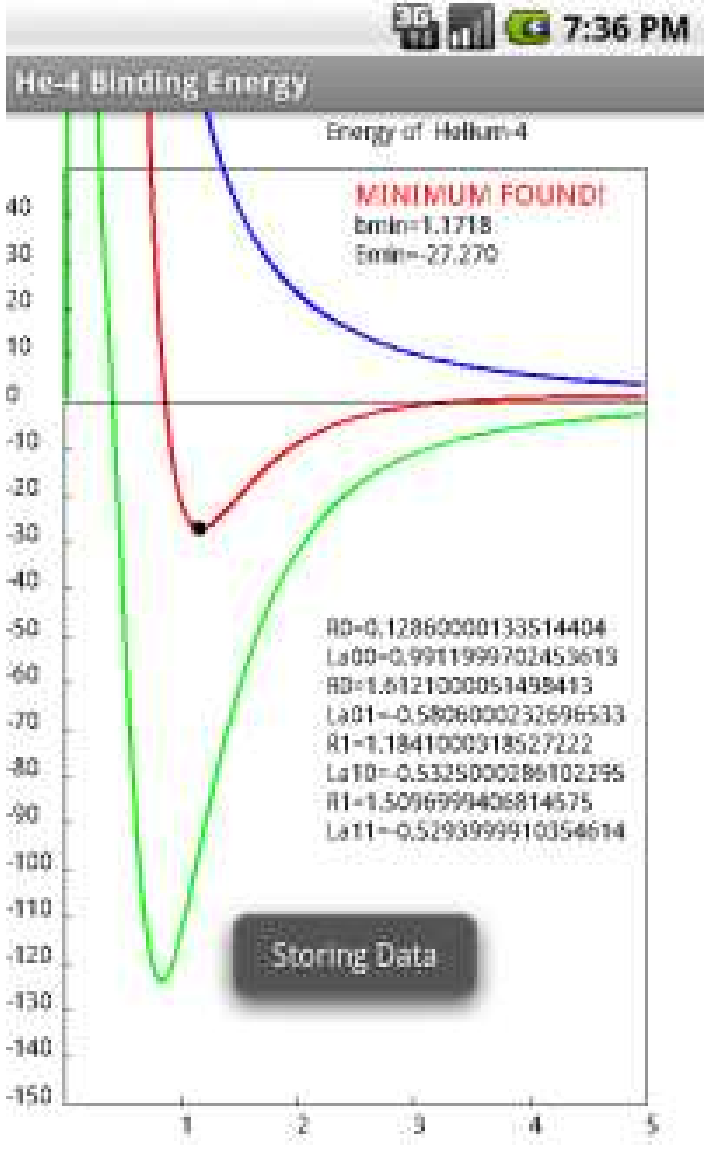
HANDROICA Fitting screens

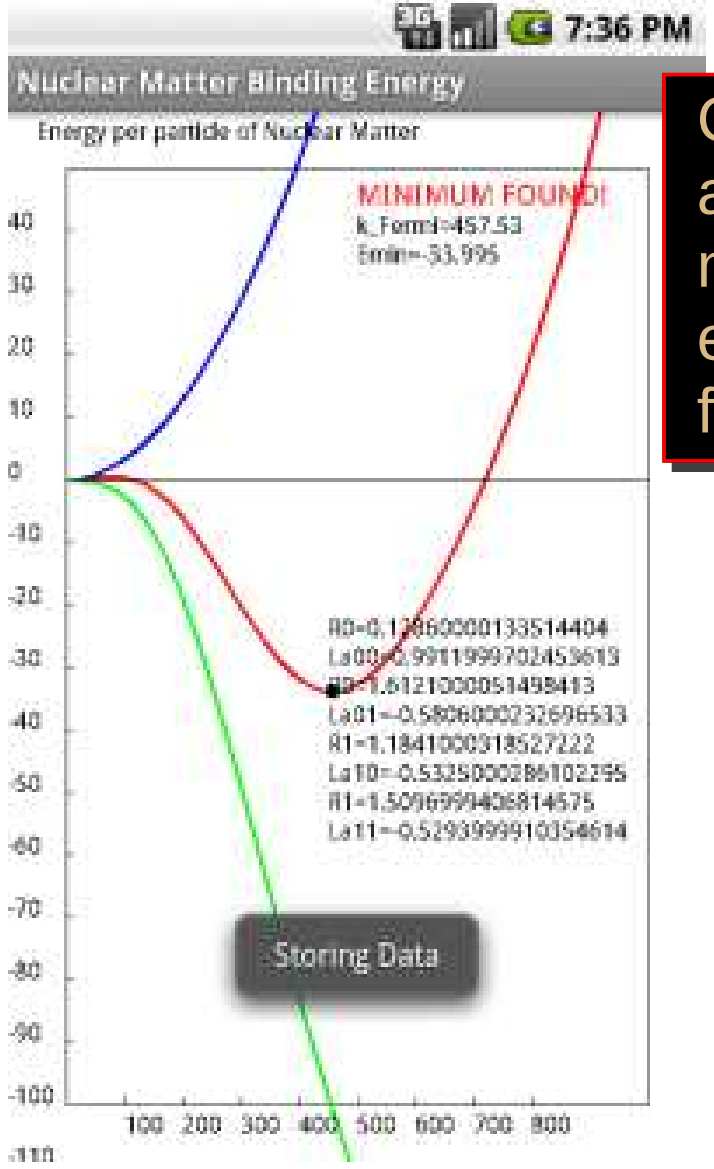




Variational χ^2 fit to pseudo-data

HANDROICA Energy screens





Computes ^{4}He and nuclear matter binding energies with fitted potential

Nuclear binding energy error

- Deuteron static properties compared with empirical values and high-quality potentials calculations

	Coarse Grained (δ shell)	Empirical	Nijm I	Nijm II	Reid93	AV18	CD-Bonn
B(MeV)	2.2(2)	2.224575(9)	Input	Input	Input	Input	Input
η	0.025(2)	0.0256(5)	0.02534	0.02521	0.02514	0.0250	0.0256
$A_S(\mathrm{fm}^{1/2})$	0.88(3)	0.8781(44)	0.8841	0.8845	0.8853	0.8850	0.8846
$r_m(\mathrm{fm})$	1.97(8)	1.953(3)	1.9666	1.9675	1.9686	1.967	1.966
$Q_D(\mathrm{fm}^2)$	0.272(9)	0.2859(3)	0.2719	0.2707	0.2703	0.270	0.270
P_D	5.7(2)	5.67(4)	5.664	5.635	5.699	5.76	4.85
$\langle r^{-1}\rangle(\mathrm{fm}^{-1})$	0.45(1)			0.4502	0.4515		

- Errors in the potential parameteres propagated to compute the error in computed binding enegies.
- Binding error per particle:

$$\frac{\Delta B}{2} = 0.1\mathrm{MeV}$$

Shell model

- We computed the ground energy of ^{4}He, ^{16}O and ^{40}Ca by using oscillator wave functions
  [Navarro Perez, Amaro and Ruiz Arriola, Prog. Part. Nucl. Phys. 67 (2012)]
- The experimental energies are reproduced at the 20% – 30% level using a GR potential fitting the pseudodata (phase-shifts) up to $E < 100$ MeV
- 30% is a tolerable accuracy for a first estimate of systematic uncertainties computing **changes** in binding energy

^3H and ^4He energy uncertainty

$$\Delta B(^3\mathrm{H}) = \langle \Delta V_2 \rangle_{^3\mathrm{H}} = 3\langle 1s | \frac{1}{2} \left(\Delta V_{^1S_0} + \Delta V_{^3S_1} \right) | 1s \rangle \,,$$

$$\Delta B(^4\mathrm{He}) = \langle \Delta V_2 \rangle_{^4\mathrm{He}} = 6\langle 1s | \frac{1}{2} \left(\Delta V_{^1S_0} + \Delta V_{^3S_1} \right) | 1s \rangle \,,$$

$|1s\rangle$ is the Harmonic oscillator relative wave function with oscillator parameter b fixed to reproduce the charge radius.

- The factors in front of the matrix elements are Talmi-Moshinsky coefficients.
- Errors in the potential ΔV are computed by adding the individual contributions $(\Delta\lambda_n)^{JS}_{l,l'}$ squared.

^{16}O and ^{40}Ca energy uncertainty

Uncertainty in the potential matrix elements in terms of the uncertainties of the 2-body potential.
For double-closed shell nuclei

$$\Delta B(A) = \sum_{nlSJ} g_{nlJS} \langle nl|\Delta V^{JST}|nl\rangle \qquad (1)$$

where g_{nlJS} depens on the Talmi-Moshinsky brackets.

Explicit formulas for ^{16}O and ^{40}Ca, in the harmonic oscillator basis.

$$\Delta B(^{16}\mathrm{O}) = 21\langle\Delta V_S\rangle_{1s} + \frac{3}{2}\langle\Delta V_S\rangle_{2s} + 6\langle\Delta V_P\rangle_{1p} + \frac{15}{2}\langle\Delta V_D\rangle_{1d}$$

$$\begin{aligned}\Delta B(^{40}\mathrm{Ca}) &= \frac{555}{8}\langle\Delta V_S\rangle_{1s} + \frac{105}{8}\langle\Delta V_S\rangle_{2s} + \frac{9}{8}\langle\Delta V_S\rangle_{3s} \\ &+ 30\langle\Delta V_P\rangle_{1p} + \frac{9}{2}\langle\Delta V_P\rangle_{2p} + \frac{525}{8}\langle\Delta V_D\rangle_{1d} \\ &+ \frac{45}{8}\langle\Delta V_D\rangle_{2d} + \frac{21}{2}\langle\Delta V_F\rangle_{1f} + \frac{81}{8}\langle\Delta V_G\rangle_{1g}\end{aligned}$$

We use the definitions

$$\begin{aligned} V_S &= V_{^1S_0} + V_{^3S_1} \\ V_P &= V_{^1P_1} + 9V_{^3P} \\ V_D &= V_{^1D_2} + V_{^3D} \\ V_F &= V_{^1F_3} + 9V_{^3F} \\ V_G &= V_{^1G_4} + V_{^3G} \end{aligned}$$

and

$$\begin{aligned} V_{^3P} &= \frac{1}{9}\left(V_{^3P_0} + 3V_{^3P_1} + 5V_{^3P_2}\right), \\ V_{^3D} &= \frac{1}{15}\left(3V_{^3D_1} + 5V_{^3D_2} + 7V_{^3D_3}\right), \\ V_{^3F} &= \frac{1}{21}\left(5V_{^3F_2} + 7V_{^3F_3} + 9V_{^3F_4}\right), \\ V_{^3G} &= \frac{1}{27}\left(7V_{^3G_3} + 9V_{^3G_4} + 11V_{^3G_5}\right). \end{aligned}$$

Binding energy error estimates. Systematic

- Systematic error per particle.
- From pseudodata fit $E < 350$ MeV

	^{3}H	^{4}He	^{16}O	^{40}Ca
$\frac{\Delta B(A)}{A}$ [MeV]	0.085	0.13	0.26	0.32

- For ^{3}H the shell model error estimate is in good agreement with the Faddeev estimates
- Oscillator parameter fixed to reproduce the nuclear m.s.r.

Binding energy error estimates. Statistical

From our partial wave analysis (see next talk by Rodrigo Navarro) with GR potential.
Three calculations:

- OPE350: Fitting data up to 350 MeV, using OPE from 3 fm
- OPE125: Fitting data up to 125 MeV, using OPE from 1.8 fm
- TPE125: Fitting data up to 125 MeV, using OPE+ Chiral Two-pion-exchange from 1.8 fm

$B(A)/A$ [MeV]

	^{3}H	^{4}He	^{16}O	^{40}Ca
OPE350	0.04	0.13	0.15	0.21
OPE125	0.63	2.40	2.50	3.51
TPE125	0.98	3.74	10.37	18.17

Skyrme model. Systematic errors

- Skyrme effective interactions approach

$$\frac{\Delta B}{A} = \frac{3}{8A}\Delta t_0 \int d^3x\, \rho(x)^2, \qquad t_0 = \frac{1}{2}\int d^3x (V_{^1S_0} + V_{^3S_1}).$$

- Propagating errors we obtain $\Delta t_0|_{\rm systematic} = 10\ {\rm MeV\,fm}^3$.
- Nuclear matter: $\rho_0 = 0.17{\rm fm}^{-3}$,

$$\frac{\Delta B}{A} = \frac{3}{8}\Delta t_0 \rho_0 = 0.6{\rm MeV}\,.$$

- Finite nuclei: $\rho(r) = C/(1+e^{(r-R)/a})$, We get values in the range

$$\Delta B(A)/A = 0.1 - 0.4{\rm MeV}\,,$$

  depending on the value of A for $4 \leq A \leq 208$.
- Of the same order to the errors obtained in the shell model.

Skyrme model. Statistical errors

- Estimates for the statistical error in the Skyrme parameter t_0 computed propagating the errors of our PWA with the GR potential,
- Three calculations:
  - OPE350: Fitting data up to 350 MeV, using OPE from 3 fm
  - OPE125: Fitting data up to 350 MeV, using OPE from 1.8 fm
  - TPE125: Fitting data up to 125 MeV, using OPE+ Chiral Two-pion-exchange from 1.8 fm

	OPE350	TPE125	OPE125
$\Delta t_0[\mathrm{MeV\,fm^2}]$	5.85	142.26	65.91

- Fitting low-energy data only increases the binding-energy uncertainty more than one order of magnitude.

Summary

- Nuclear force uncertainties may have an impact on first principles calculations
- Nuclear binding energy systematic estimates are in the range $\Delta B(A)/A \sim 0.1$ to 0.4 MeV
- The error exceeds the available precision of ab initio Monte Carlo calculations
- The estatistical errors are smaller by about one half
- Trying to find an optimal NN potential including chiral TPE forces by fitting only the low energy data increases the errors by more than one order of magnitude