Chiral EFT from a data perspective

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MARIE CURIE ACTIONS

Vetenskapsrådet

Progress in Ab Initio Techniques in Nuclear Physics, TRIUMF, Feb 28 - March 3, 2017.

Overview

- Multiple minima
- Uncertainty quantification
- Summary

Optimization strategies

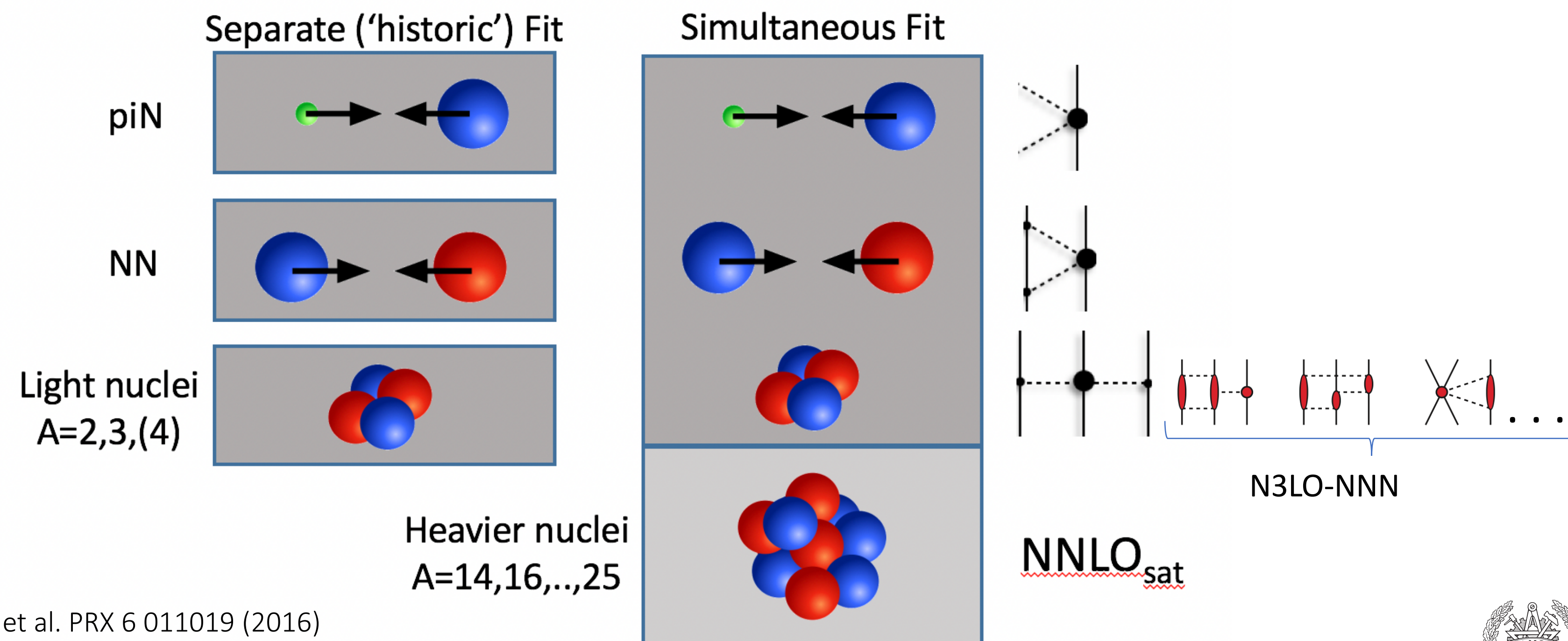
*LECs **p** to be extracted/optimized from data.*

Hinges on Gaussian likelihood and flat prior

$$\chi^2(\mathbf{p}) = \sum_i \left(\frac{\mathcal{O}_{i,\text{theo}}(\mathbf{p}) - \mathcal{O}_{i,\text{exp}}}{\sigma_{i,\text{tot}}} \right)^2$$

$$\begin{aligned}\sigma^2_{i,\text{tot}} &= \sigma^2_{i,\text{exp}} + \sigma^2_{i,\text{theo}} \\ &= \sigma^2_{i,\text{exp}} + \sigma^2_{i,\text{numerical}} + \sigma^2_{i,\text{method}} + \sigma^2_{i,\text{model}}\end{aligned}$$

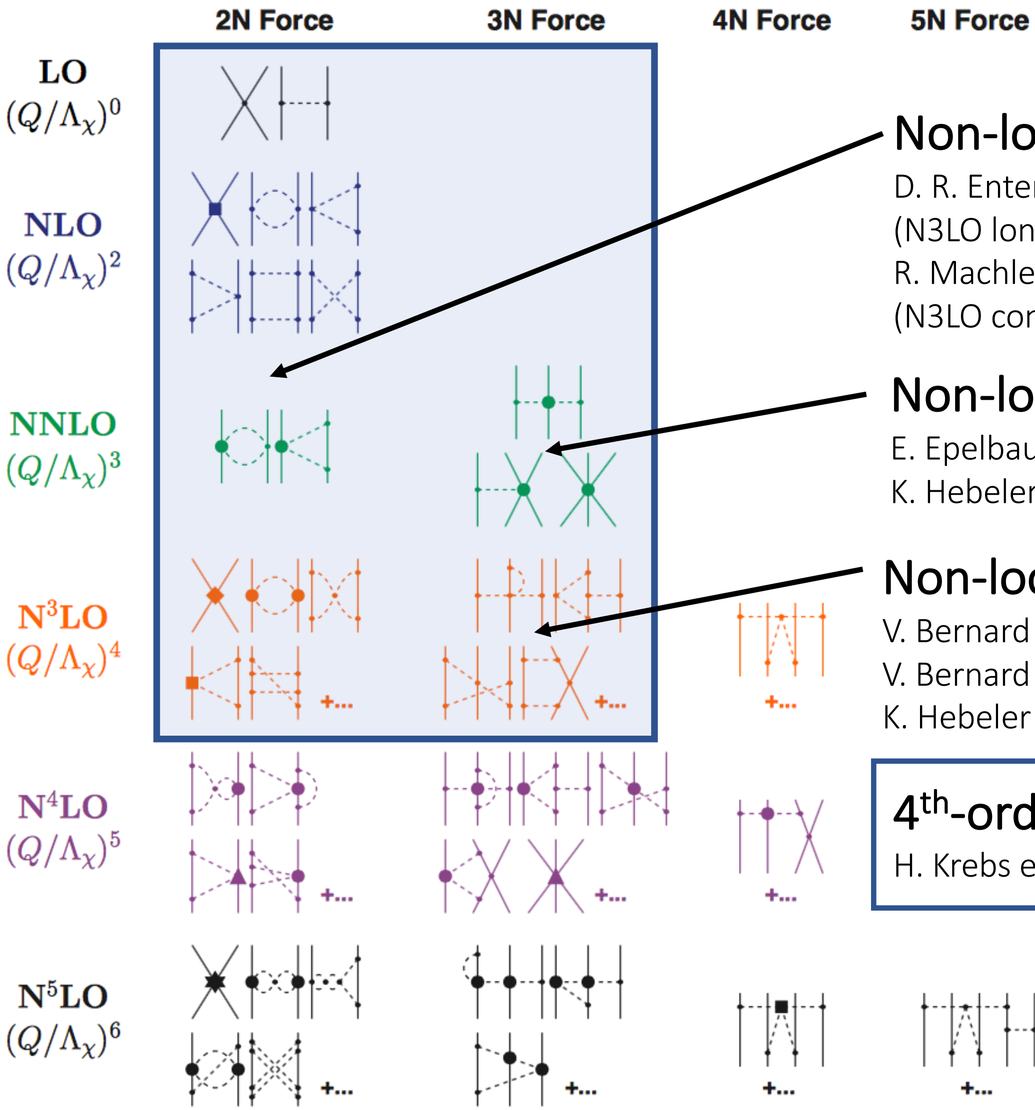
$$\sigma^{(\text{amp})}_{\text{model}} = C \left(\frac{Q}{\Lambda} \right)^{\nu+1}$$



B. D. Carlsson et al. PRX 6 011019 (2016)
A. Ekström et al. PRC 91 051301(R) (2015)

Objective function

$$\chi^2(\mathbf{p}) = \sum_i \left(\frac{\mathcal{O}_{i,\mathrm{theo}}(\mathbf{p}) - \mathcal{O}_{i,\mathrm{exp}}}{\sigma_{i,\mathrm{tot}}} \right)^2$$



Non-local, 2NF up to N3LO

D. R. Entem et al. PRC 91, 014002 (2015)
(N3LO long-ranged part)
R. Machleidt et al. Phys. Rep. 503 (2011)
(N3LO contact potential)

26 contacts
4 c_i's + 4 d_i's

Non-local, leading 3NF

E. Epelbaum et al. PRC 66, 064001 (2002)
K. Hebeler et al. PRC 91, 044001 (2015)

c_D c_E
3 c_i's

Non-local, sub-leading 3NF

V. Bernard et al. PRC 77, 064004 (2008)
V. Bernard et al. PRC 84, 054001 (2011)
K. Hebeler et al. PRC 91, 044001 (2015)

c_S c_T

4^{th}-order πN scattering

H. Krebs et al. PRC 85, 054006 (2015)

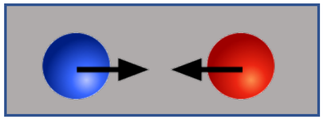
5 e_i's

Total 41 unique LECs of interest

Figure from: R. Machleidt and F. Sammarruca, Phys. Scr. **91** (2016) 083007

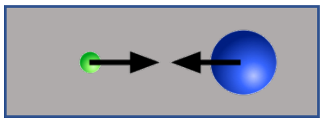
Experimental data

$$\chi^2(\mathbf{p}) = \sum_i \left(\frac{\mathcal{O}_{i,\mathrm{theo}}(\mathbf{p}) - \mathcal{O}_{i,\mathrm{exp}}}{\sigma_{i,\mathrm{tot}}} \right)^2$$



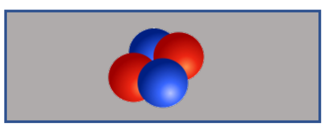
Granada NN database (0-290 MeV)

R. Navarro Pérez et al. PRC 88, 064002 (2013)



Washington Institute WI08 πN database (0-70 MeV)

R. Workman et al. PRC 86, 035202 (2012)



	Experimental value	$\sigma_{\mathrm{exp+method}}$
$E(^2\mathrm{H})$	$-2.22456627(46)$	0.22×10^{-3}
$E(^3\mathrm{H})$	$-8.4817987(25)$	0.028
$E(^3\mathrm{He})$	$-7.7179898(24)$	0.019
$E(^4\mathrm{He})$	$-28.2956099(11)$	0.11
$r_{\mathrm{pt\text{-}p}}(^2\mathrm{H})$	1.97559(78)[a]	0.79×10^{-3}
$r_{\mathrm{pt\text{-}p}}(^3\mathrm{H})$	1.587(41)	0.041
$r_{\mathrm{pt\text{-}p}}(^3\mathrm{He})$	1.7659(54)	0.013
$r_{\mathrm{pt\text{-}p}}(^4\mathrm{He})$	1.4552(62)	0.0071
$Q(^2\mathrm{H})$	0.27(1)[b]	0.01
$E^1_A(^3\mathrm{H})$	0.6848(11)	0.0011

Multiple minima

41-dim LEC space!

Boris Carlsson

Fit πN-sector to πN data → Fit NN contacts to NN phase *phase shifts* → Fit NN contacts to NN data → Fit cD/cE to A=3 data → Simultaneous optimization

Number of optima at each stage in the optimization

2^5x5=160	**2^5x4=128**	**160**	**104**

c_1	$-0.69(50)$
c_2	$+3.0(14)$
c_3	$-4.12(32)$
c_4	$+5.35(81)$
d_1+d_2	$+6.22(44)$
d_3	$-5.31(30)$
d_5	$-0.46(18)$
$d_{14}-d_{15}$	$-11.00(42)$
e_{14}	$-0.63(95)$
e_{15}	$-7.7(26)$
e_{16}	$+5.9(49)$
e_{17}	$+2.1(18)$
e_{18}	$-8.1(42)$

Fit NN contacts to NN phase shifts		Fit NN contacts to NN data	
$^1S_0$:	2	$^1S_0$:	2
$^3S_1$, $^3D_1$, $^3S_1$-$^3D_1$	5	$^3S_1$, $^3D_1$, $^3S_1$-$^3D_1$	4
$^1P_1$, $^3P_0$, $^3P_1$, $^3P_2$-$^3F_2$	2/chn	$^1P_1$, $^3P_0$, $^3P_1$, $^3P_2$-$^3F_2$	2/chn

Some cases with two cD/cE - optima

(Λ=500 MeV)

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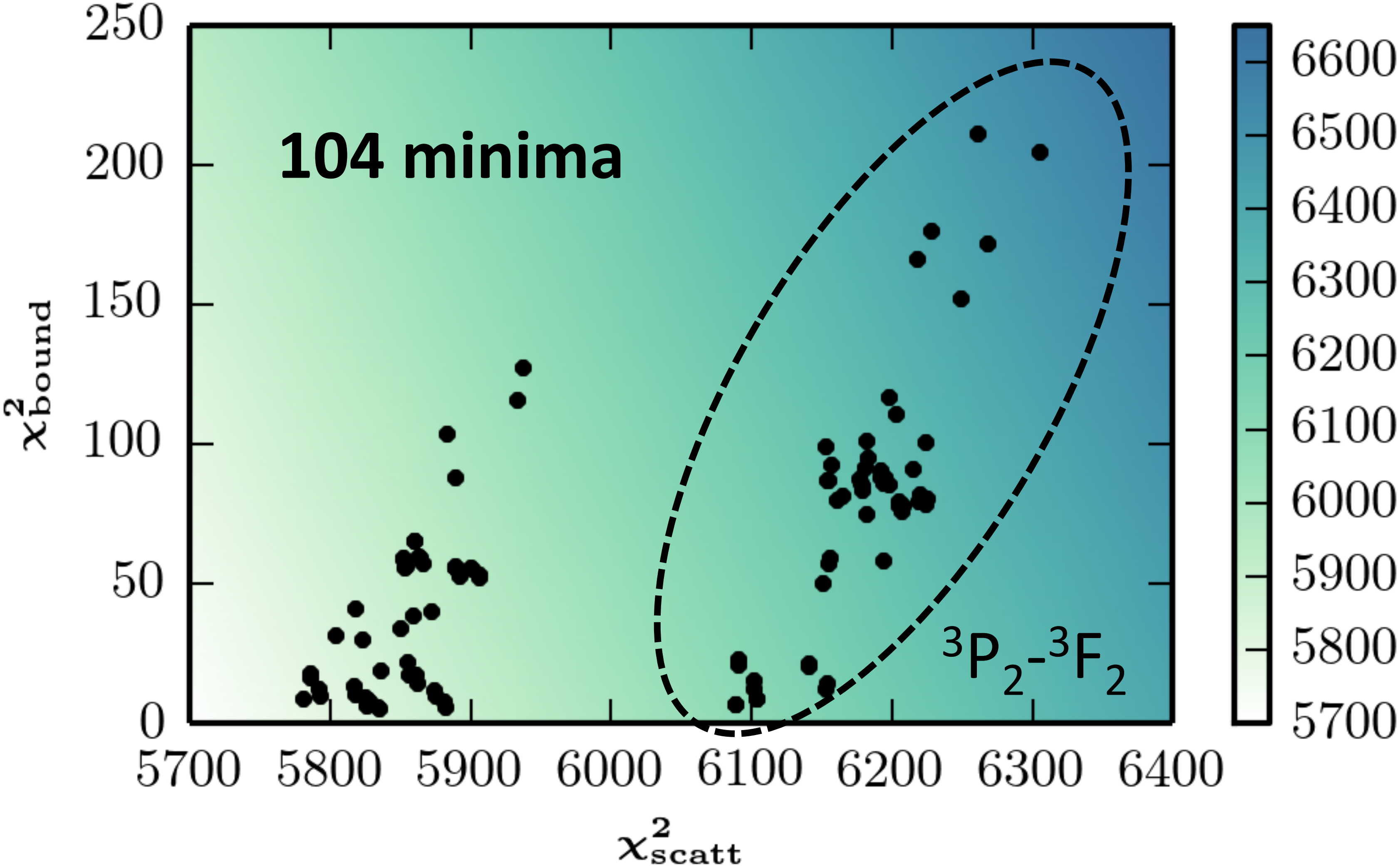
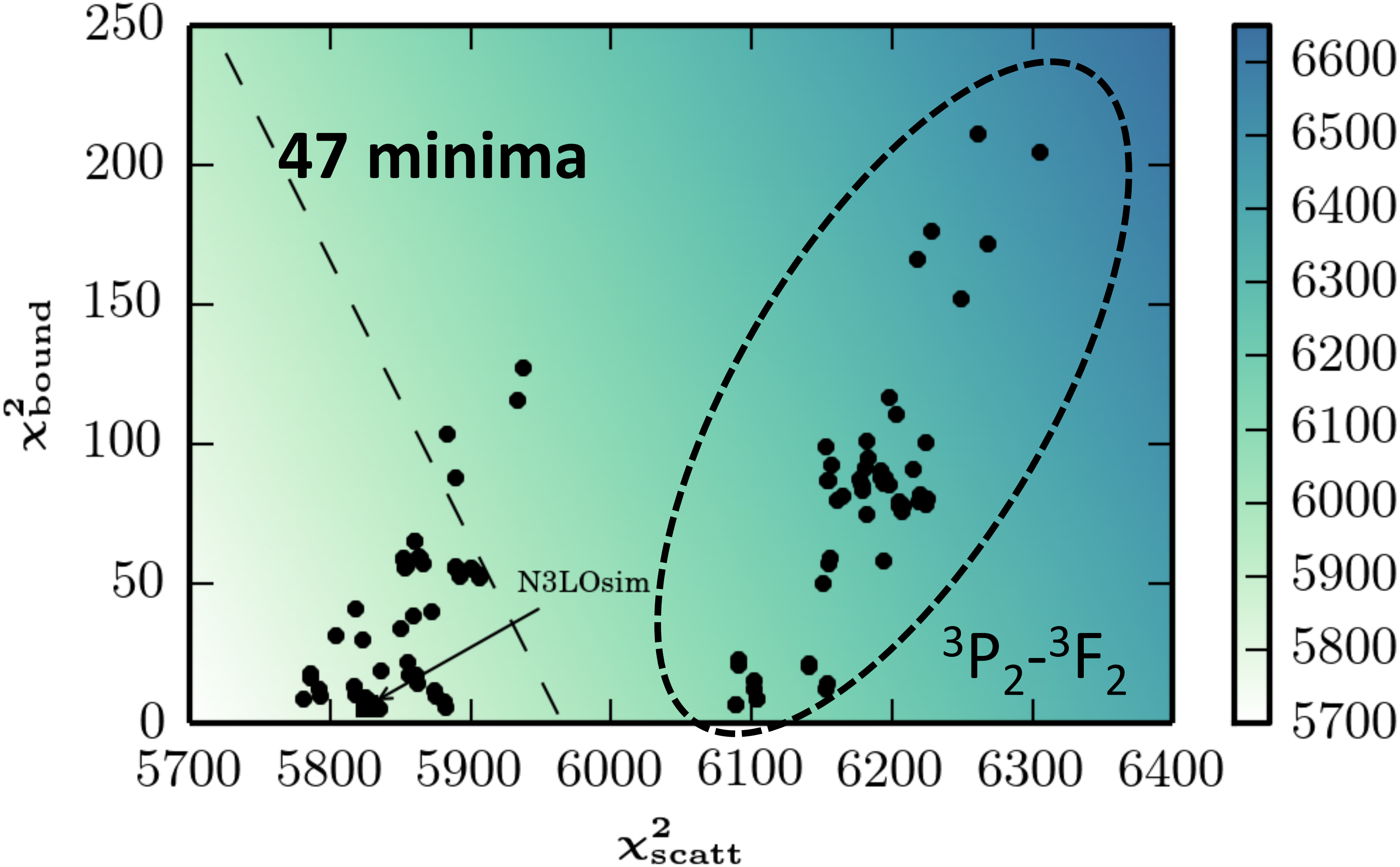
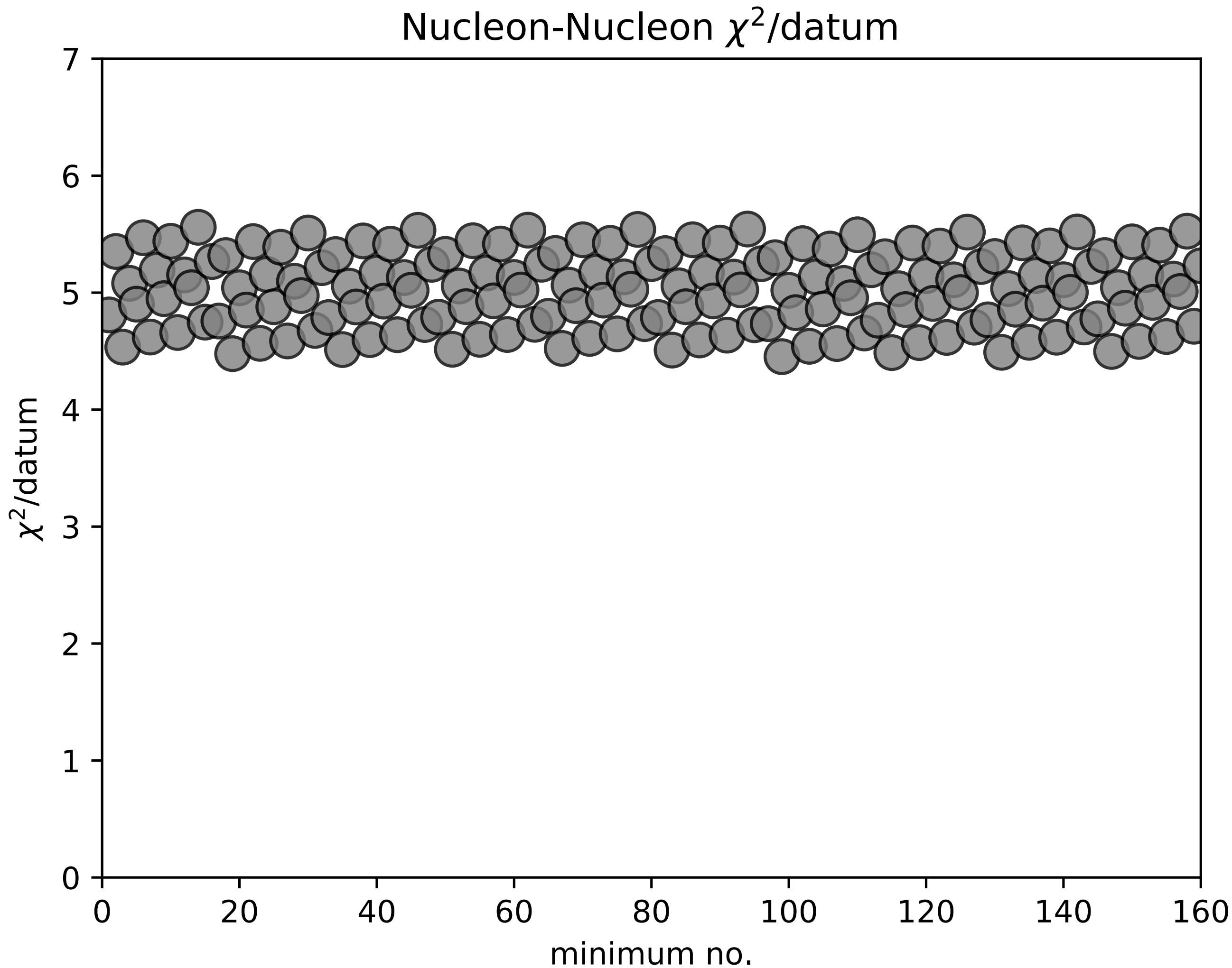
Multiple minima at N3LO: overview



Multiple minima at N3LO: overview



Fit πN-sector to πN data → Fit NN contacts to NN phase *phase shifts* → Fit NN contacts to NN data → Fit cD/cE to A=3 data → Simultaneous optimization



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Progress in Ab Initio Techniques in Nuclear Physics, TRIUMF, Feb 28 - March 3, 2017.

- Fit πN-sector to πN data
- Fit NN contacts to NN phase *phase shifts*
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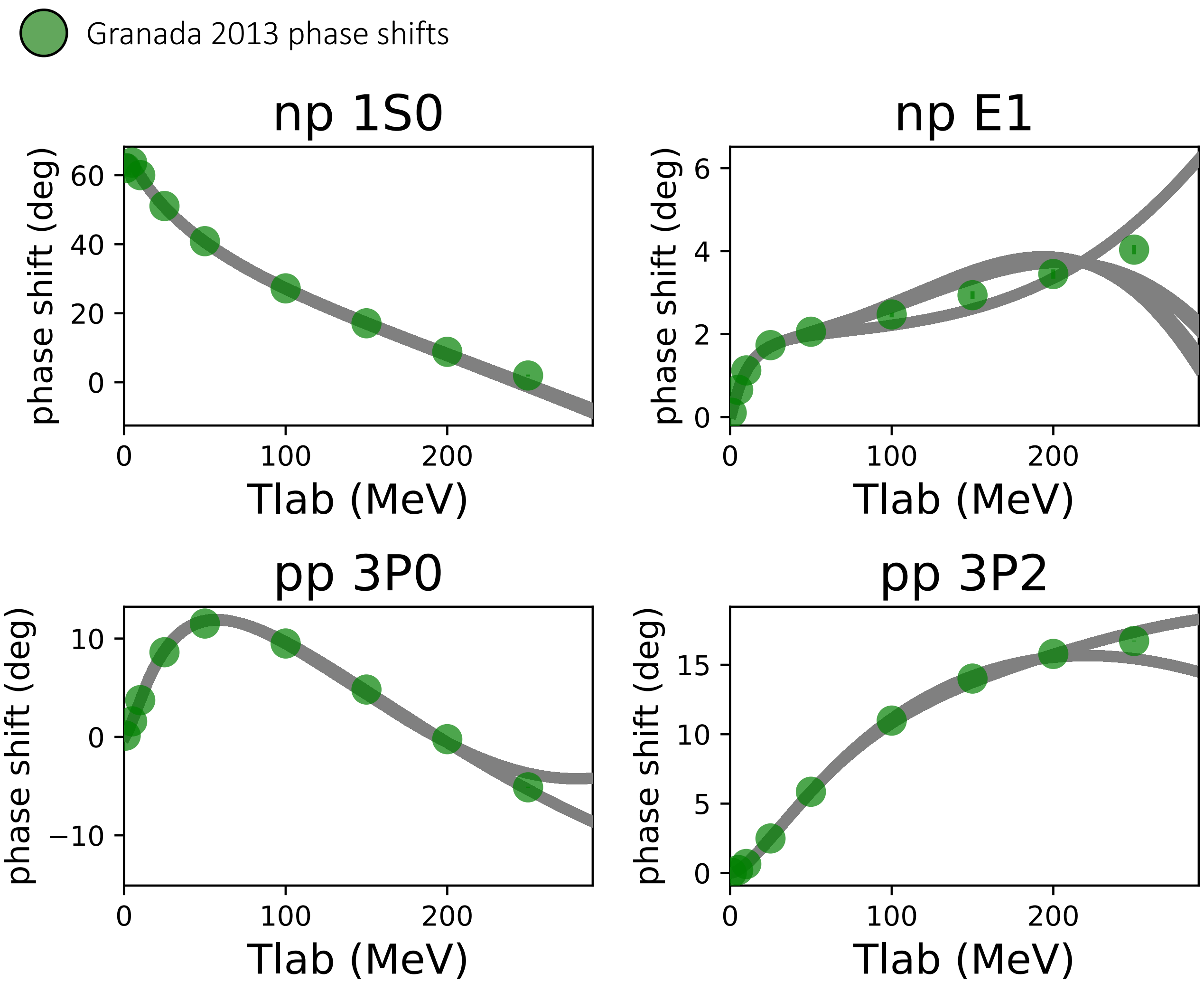
- Fit cD/cE to A=3 data
- Simultaneous optimization



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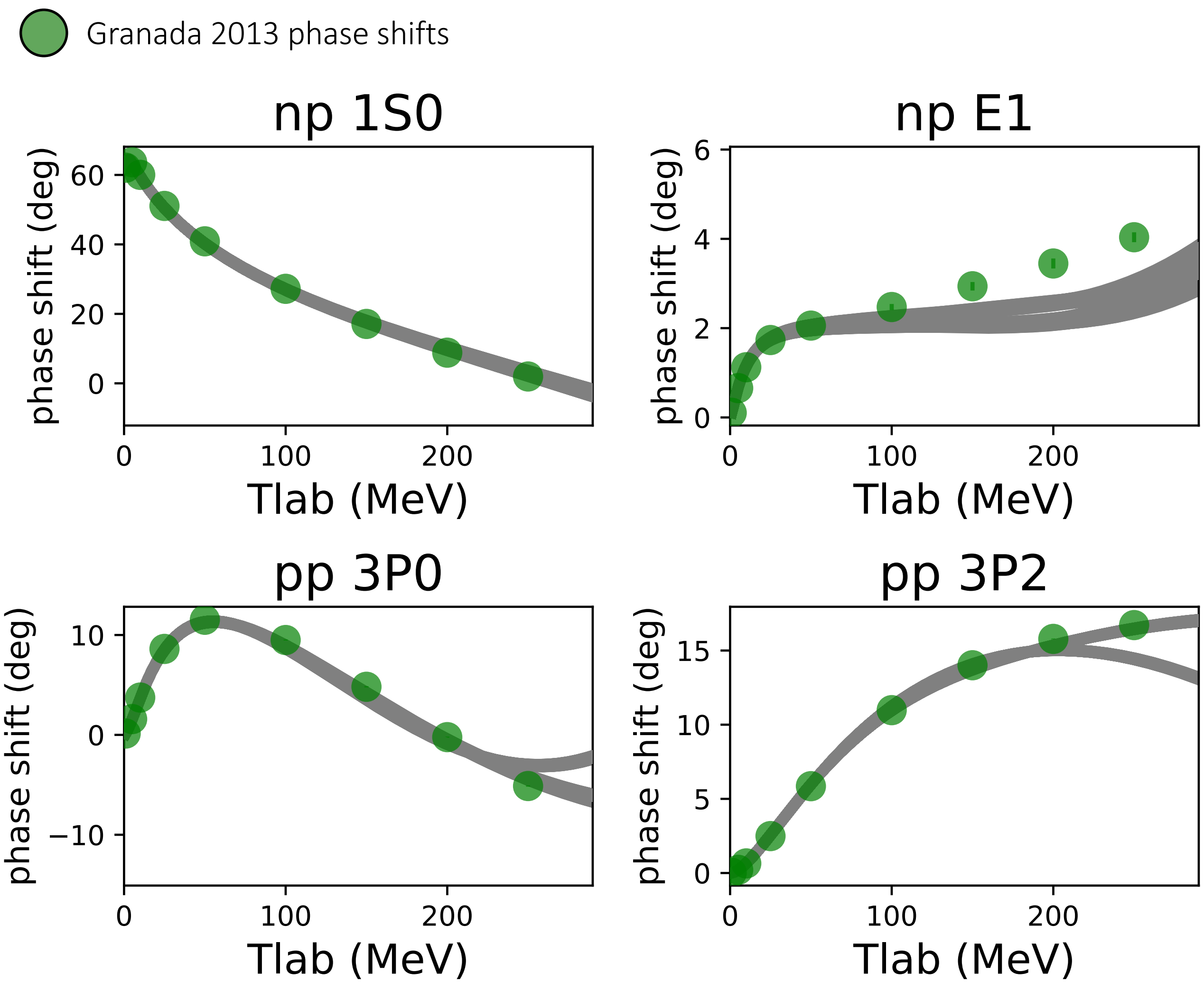

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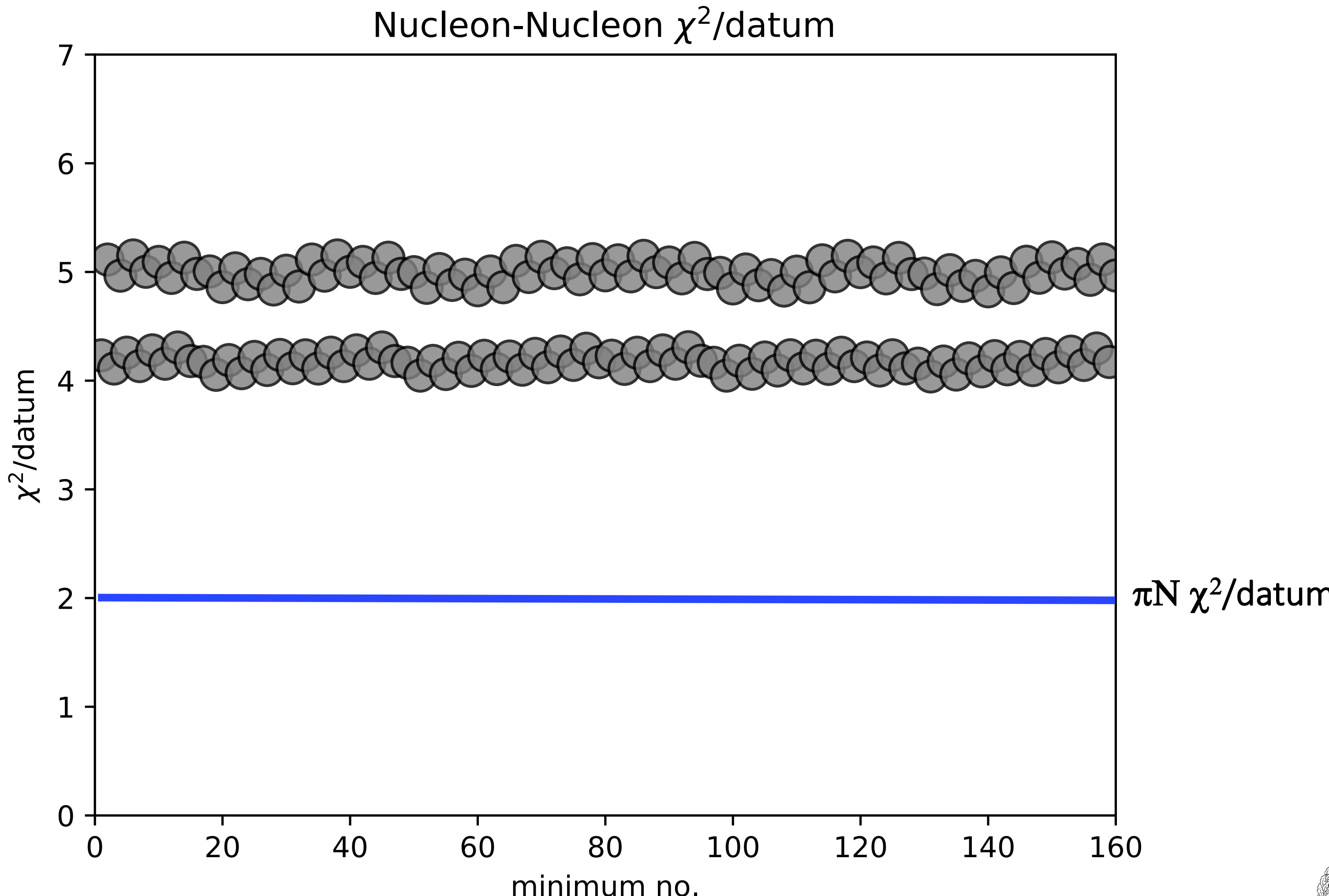
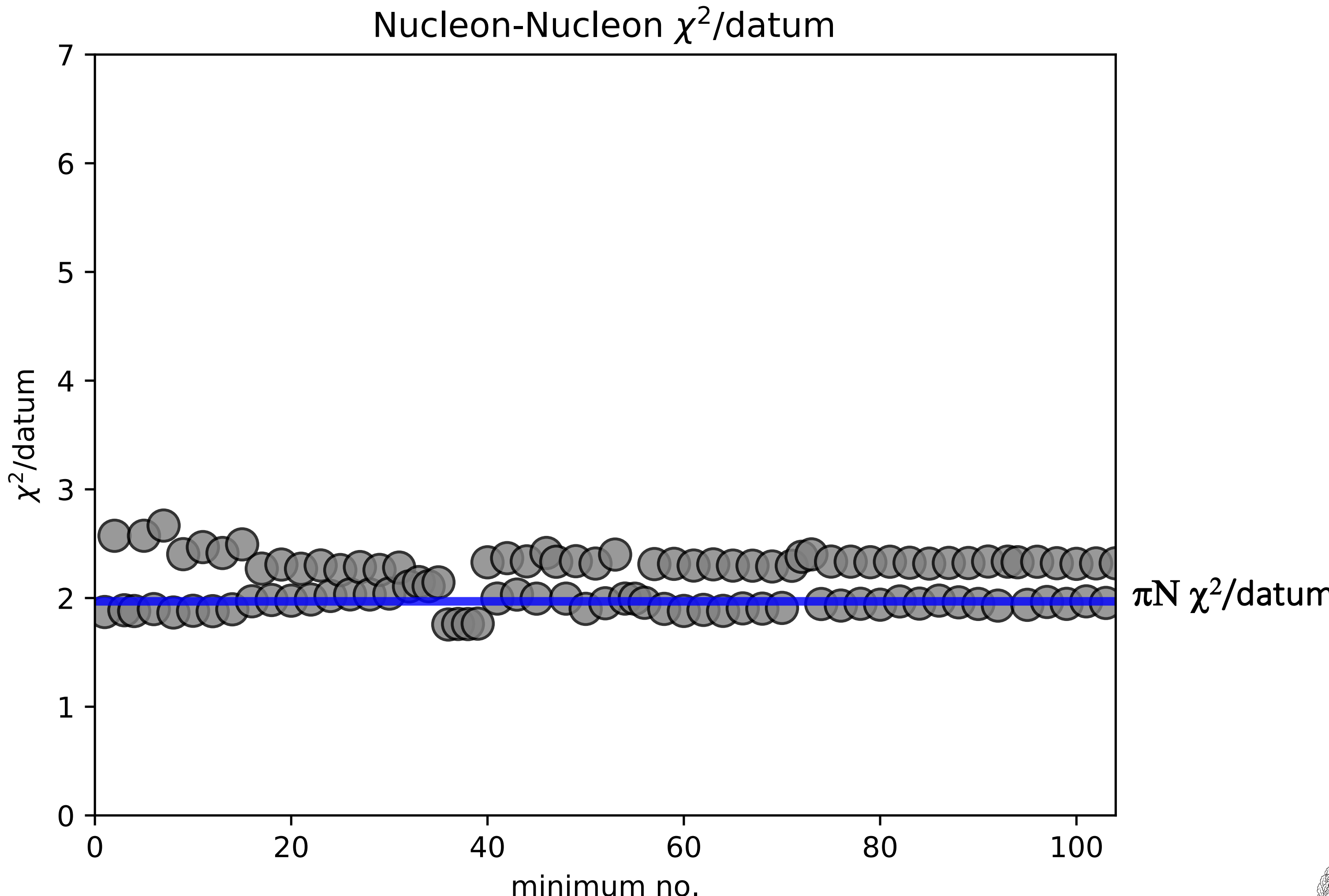


1. Fit πN-sector to πN data
2. Fit NN contacts to NN phase *phase shifts*
3. Fit NN contacts to NN data
4. Fit cD/cE to A=3 data
5. Simultaneous optimization



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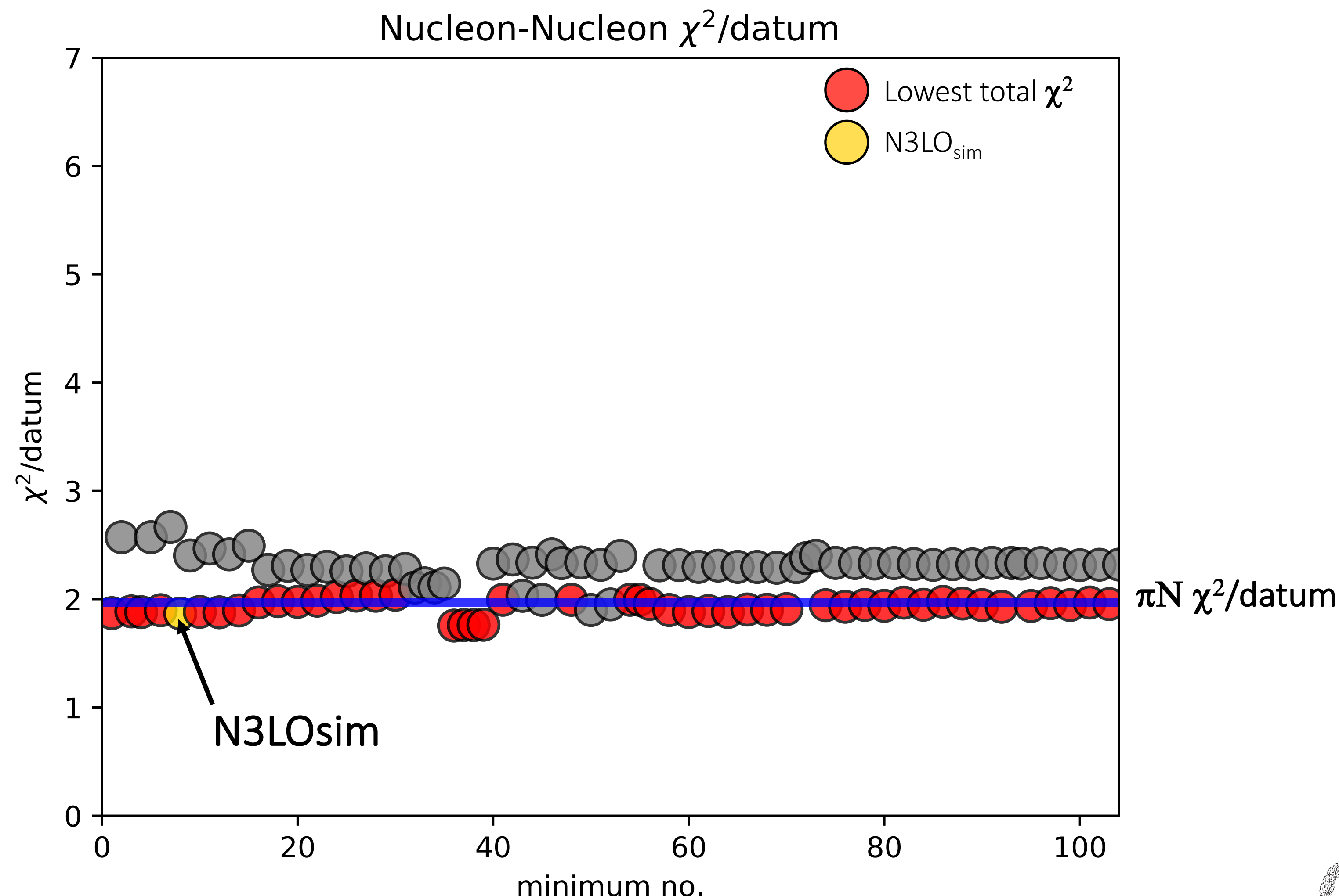

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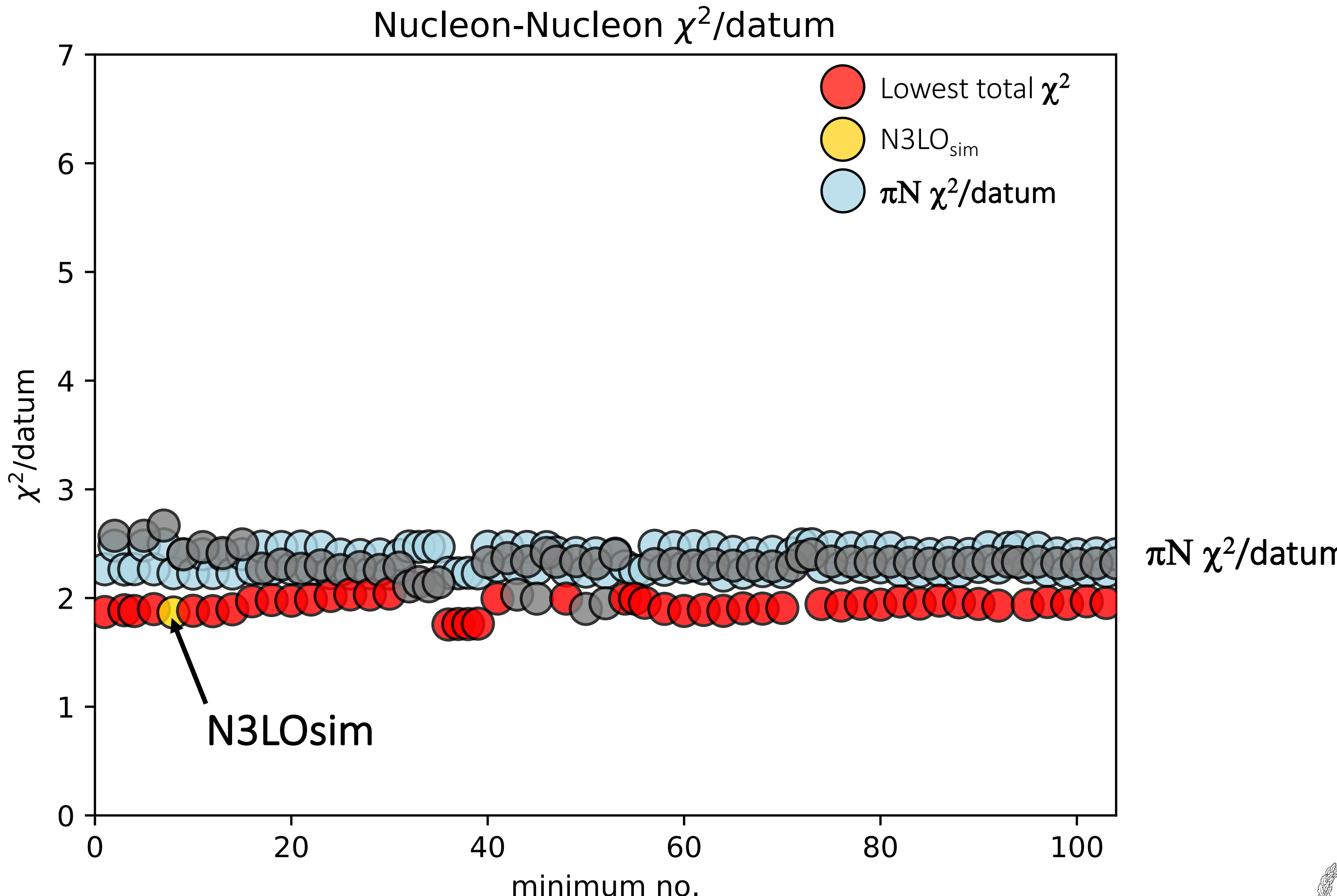

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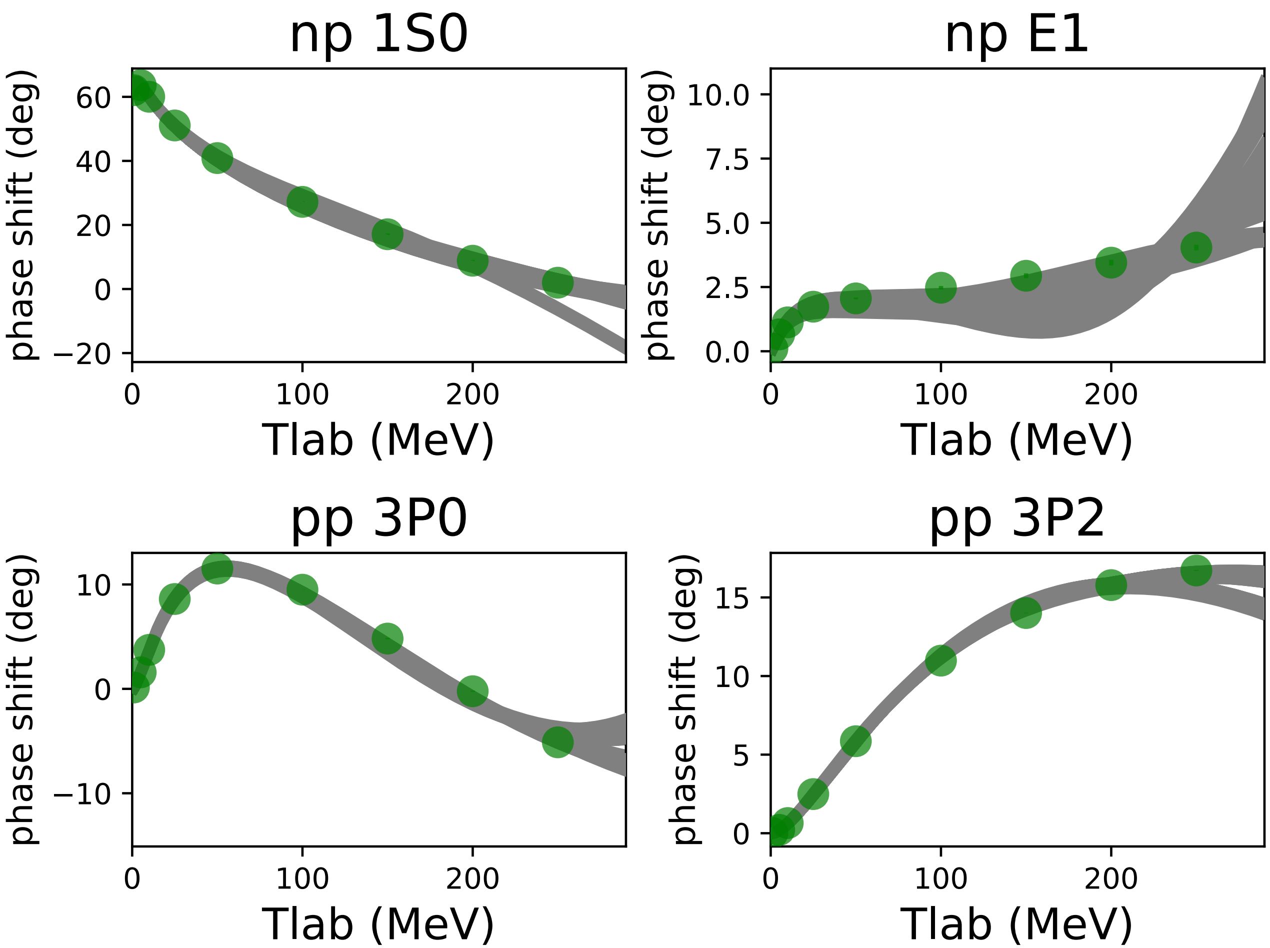

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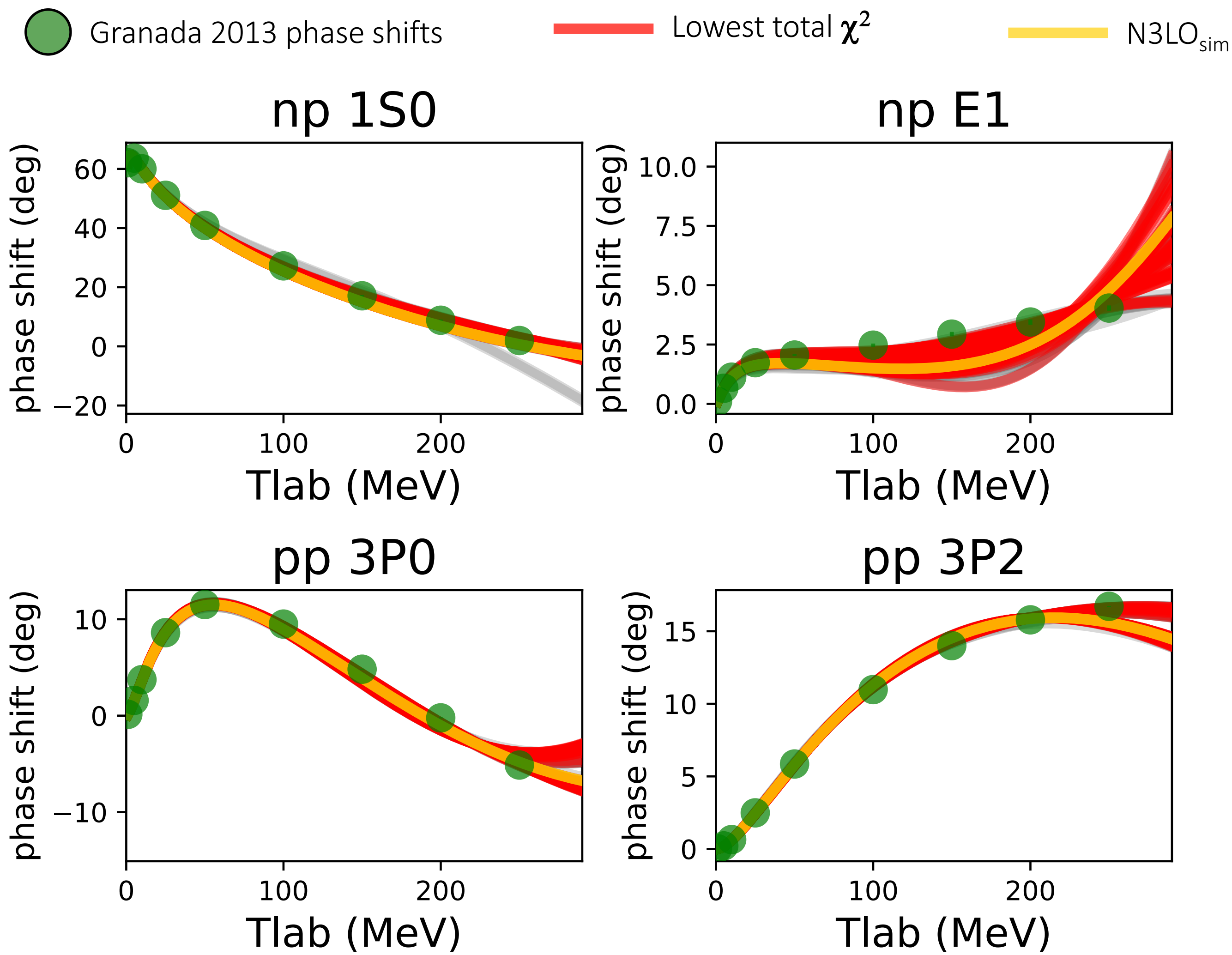

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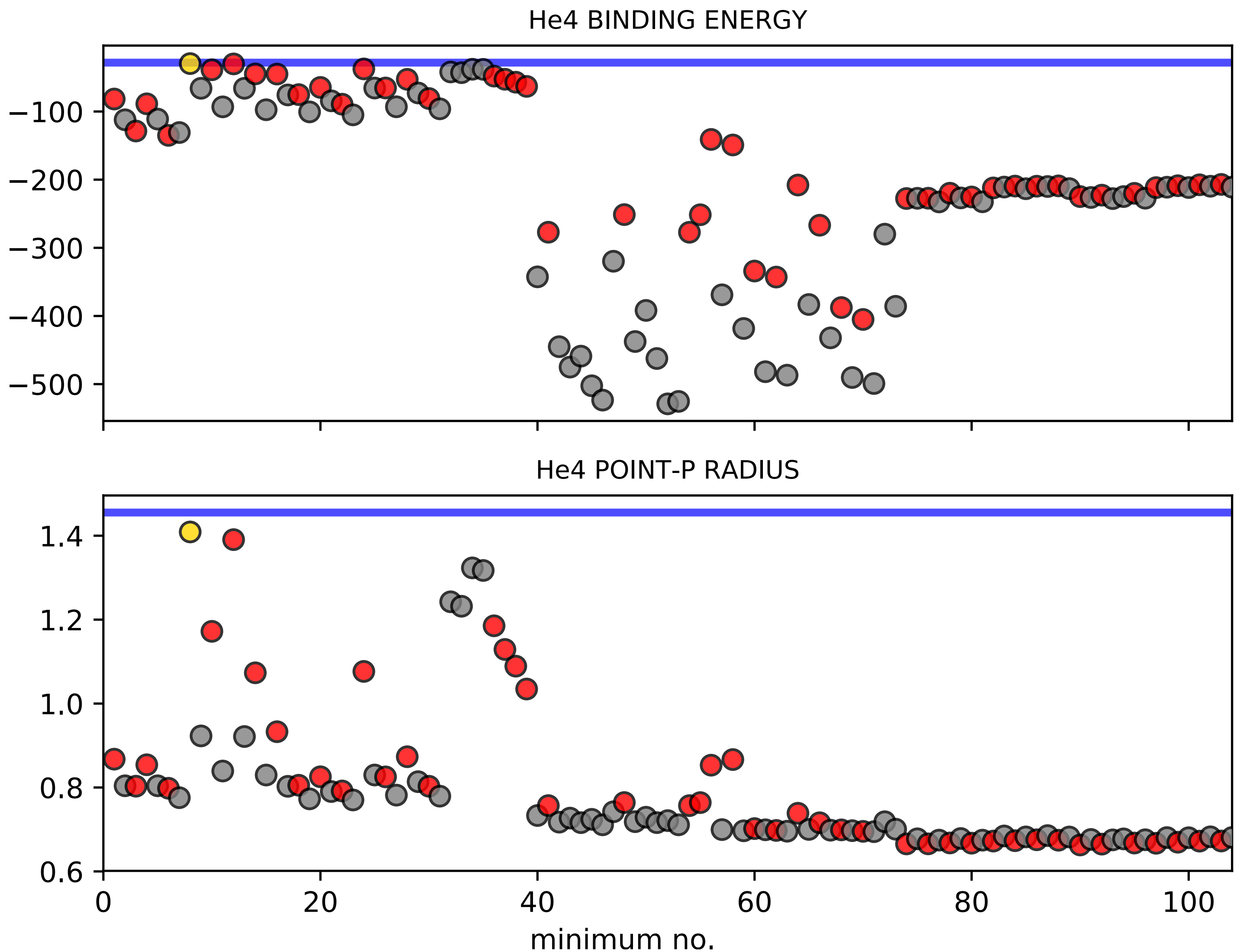
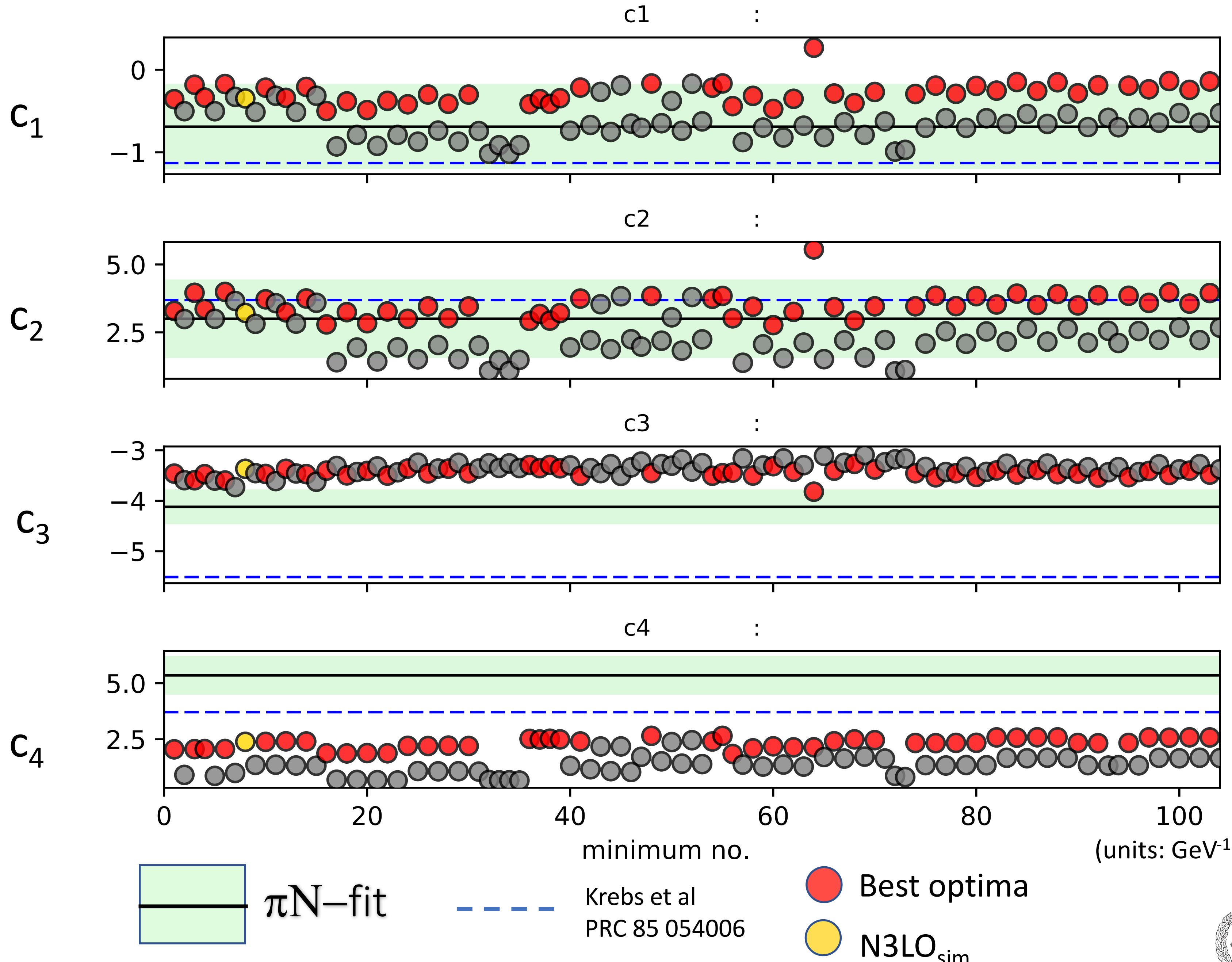



c1 :
c2 :
c3 :
c4 :
c_1
c_2
c_3
c_4
minimum no.
(units: GeV-1)
πN–fit
Krebs et al
PRC 85 054006
Best optima
N3LOsim

Using “Roy-Steiner" πN-LECs

Constraining the objective function to keep πN LECs close to values from Roy-Steiner analysis in *M. Hoferichter et al. PRL 115, 192301 (2015)*

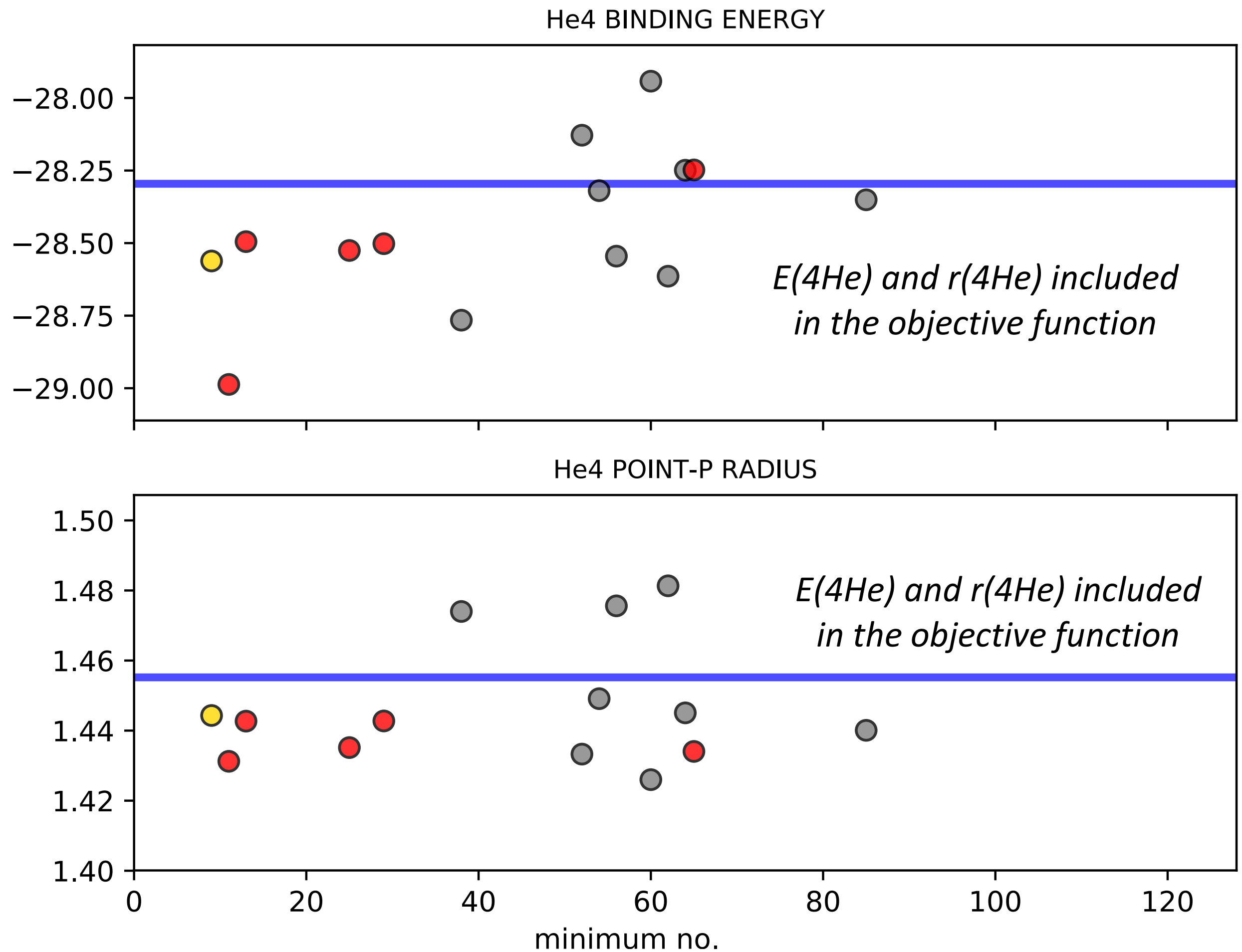
A simultaneous optimization of this objective function also leads to a good description on all NN and NNN data. For instance NN χ^2/datum = 2.5. Most LECs remain in the Roy-Steiner region (to ~1 sigma), only c_1 and c_3 depart, 6 and 31 sigma, to -0.96 GeV^{-1} and -3.76 GeV^{-1}, respectively.

However, predictions with N3LO non-local NN+3NF for ^{4}He disagree with experiment

E(4He) = -38 MeV
R(4He) = 1.05 fm

Keeping only the minima with energies and radii within +- 1 MeV and +- 0.03 fm

Still several minima



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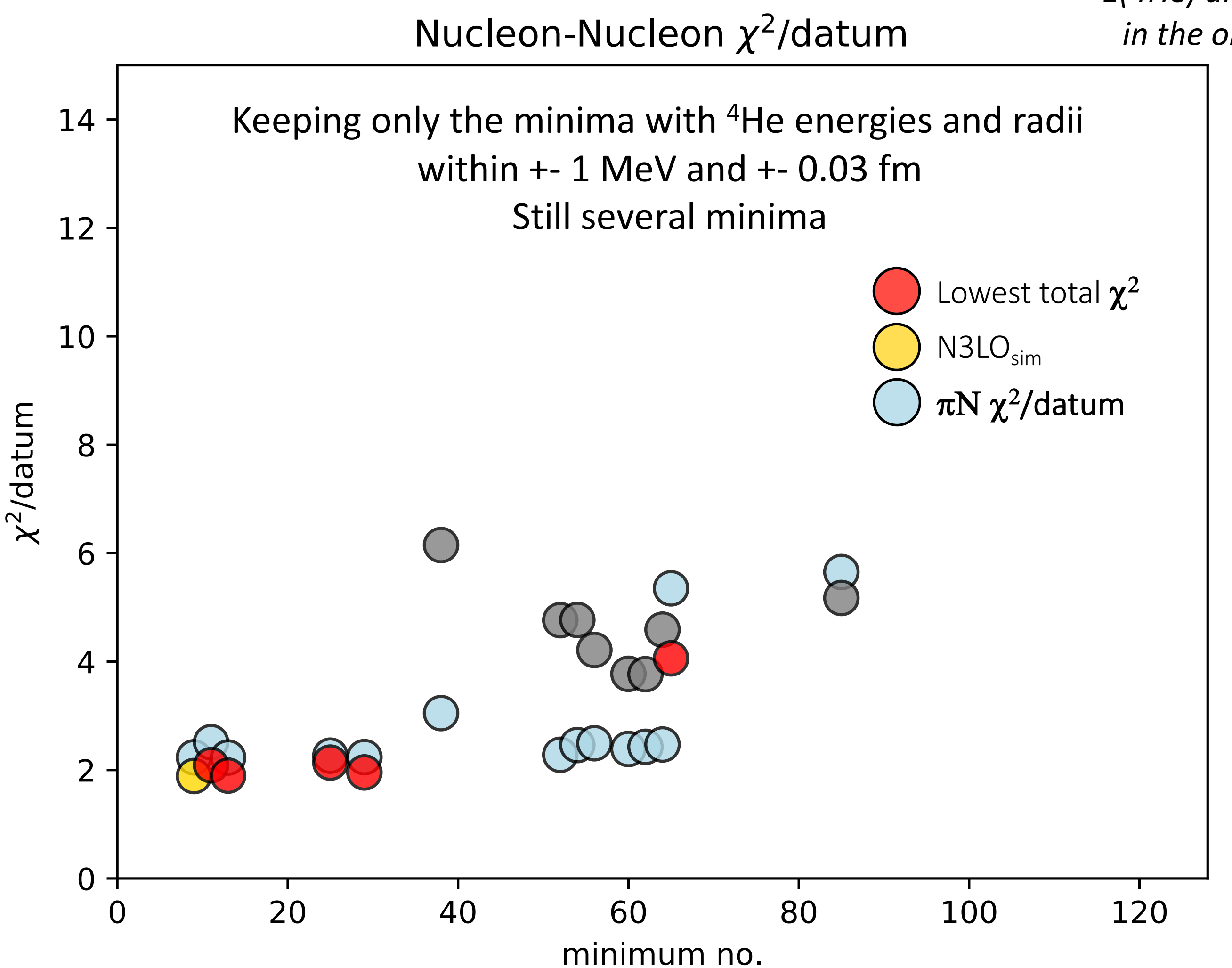
E(4He) and r(4He) included in the objective function



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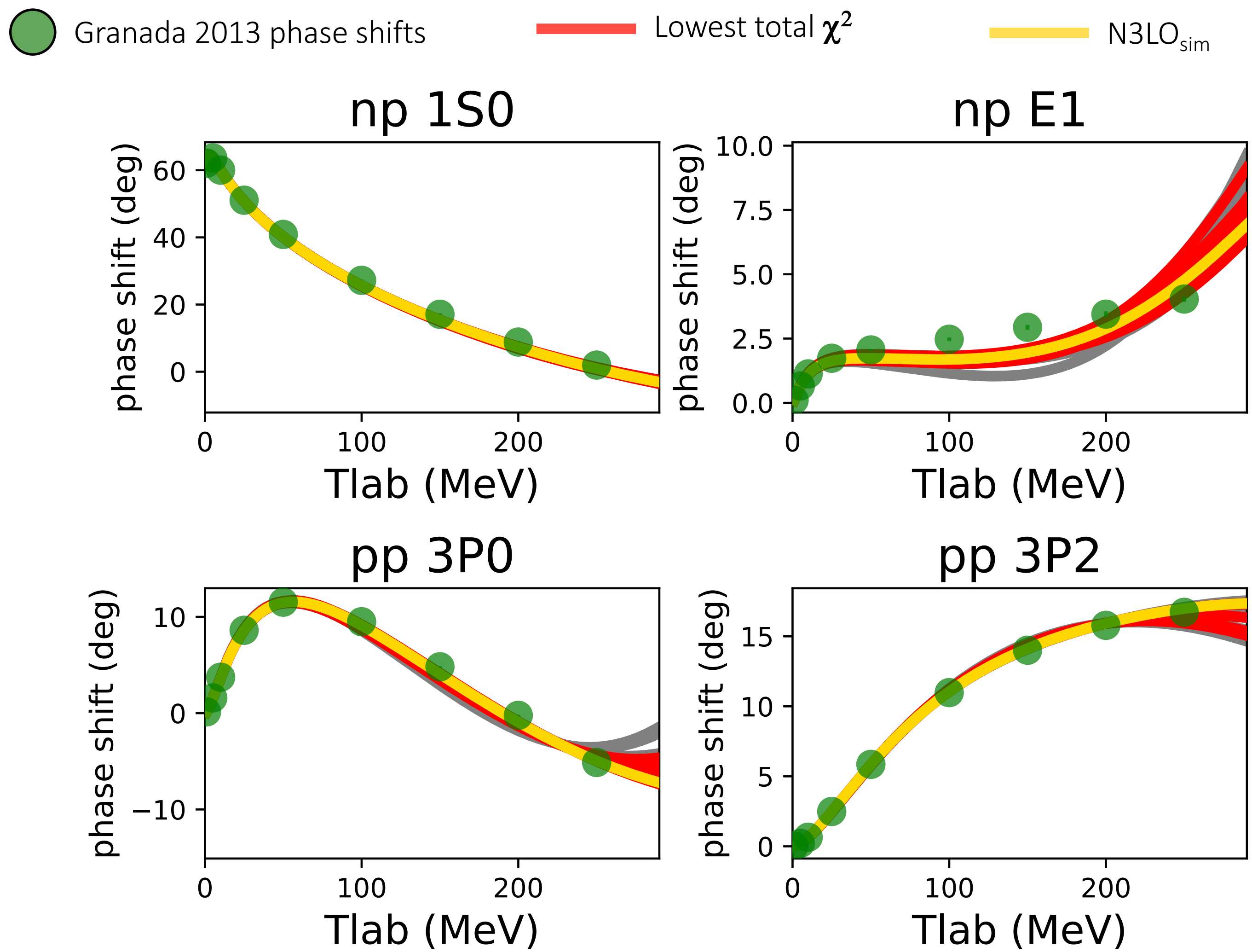
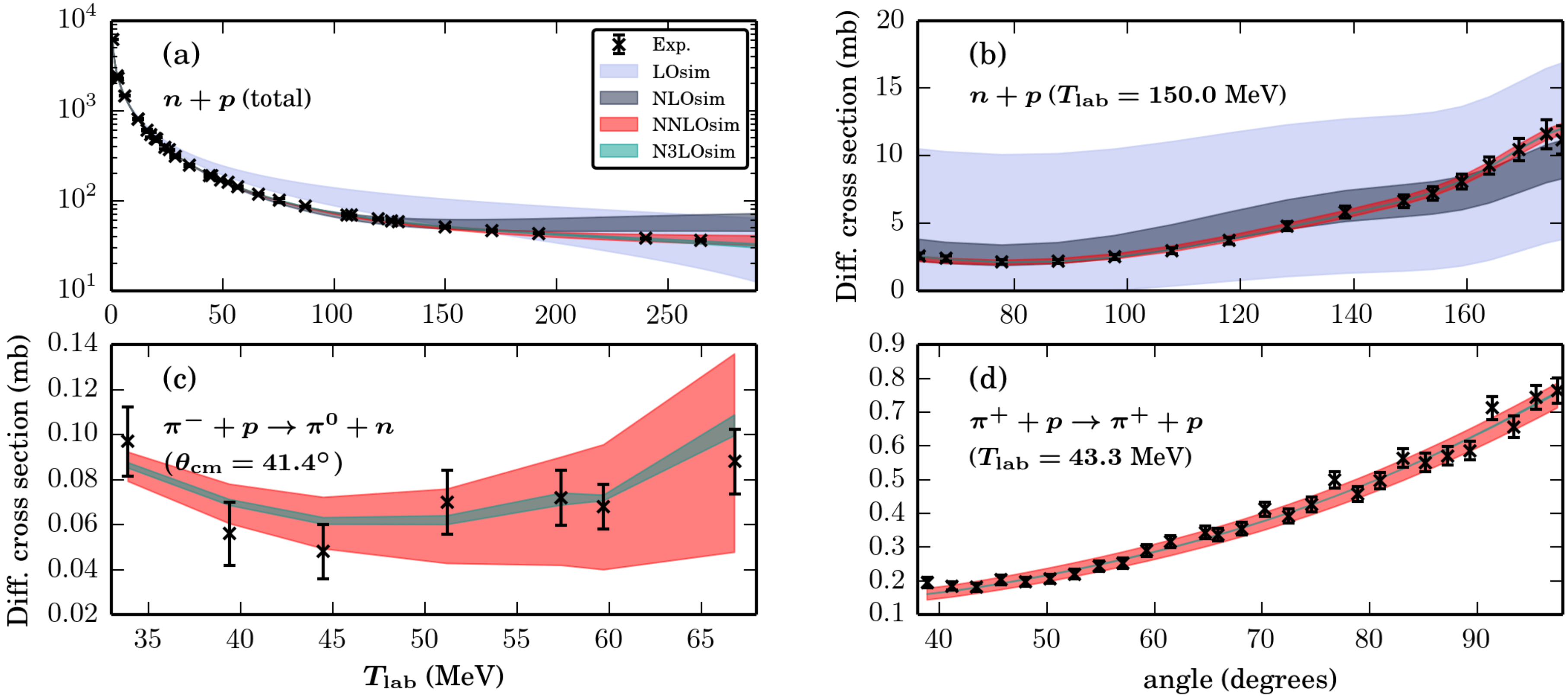
Fit πN-sector to πN data → Fit NN contacts to NN phase *phase shifts* → Fit NN contacts to NN data → Fit cD/cE to A=3 data → **Simultaneous optimization**

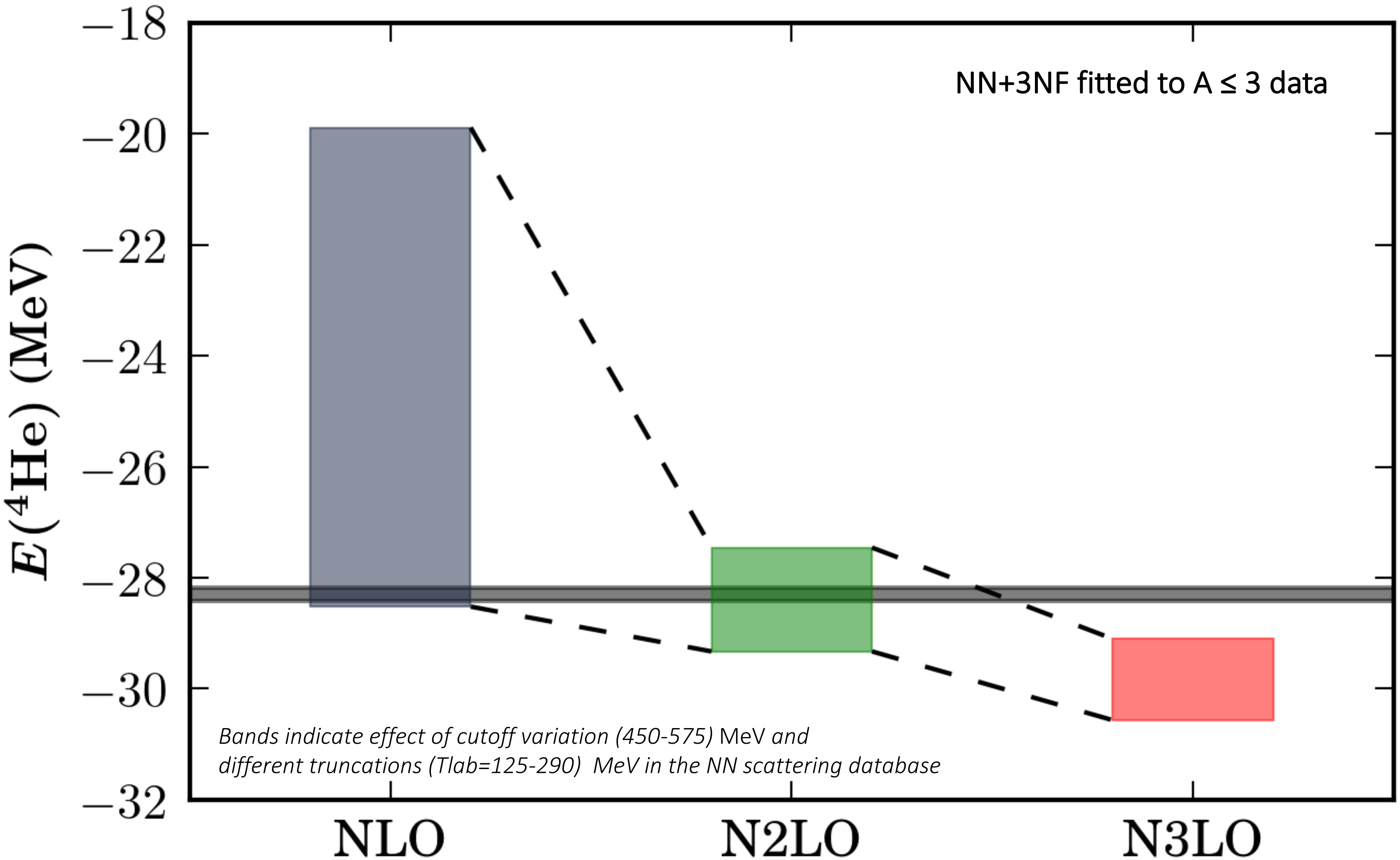
Keeping only the minima with ^{4}He energies and radii within +- 1 MeV and +- 0.03 fm



Scattering observables



Non-local chiral interactions (sim)



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Hessian method for UQ

Approximate the objective function with a quadratic form in the vicinity of the optimum

$$\chi^2(\mathbf{p_0} + \Delta\mathbf{p}) - \chi^2(\mathbf{p_0}) \approx \frac{1}{2}(\Delta\mathbf{p})^T \left[\mathbf{H}|_{\mathbf{p_0}}\right](\Delta\mathbf{p})$$

The covariance matrix can be computed from the inverse of the Hessian. This follows from a quadratic approximation to the log-likelihood function.

$$\mathrm{Cov}(\mathbf{p_0}) \sim \left[\mathbf{H}|_{\mathbf{p_0}}\right]^{-1}$$

Expand observables similarly, to second order

$$\mathcal{O}(\mathbf{p_0} + \Delta\mathbf{p}) - \mathcal{O}(\mathbf{p_0}) \approx \left(\Delta\mathbf{p}^T\right)\mathbf{J}_{\mathcal{O}} + \frac{1}{2}\left(\Delta\mathbf{p}^T\right)\mathbf{H}_{\mathcal{O}}\left(\Delta\mathbf{p}\right)$$

The covariance between two observables is then given by

$$\mathrm{Cov}(\mathcal{O}_A, \mathcal{O}_B) \approx \mathbf{J}^T_{\mathcal{O}_A}\mathrm{Cov}(\mathbf{p_0})\mathbf{J}_{\mathcal{O}_B} + \text{second order}$$

Hessian method for UQ

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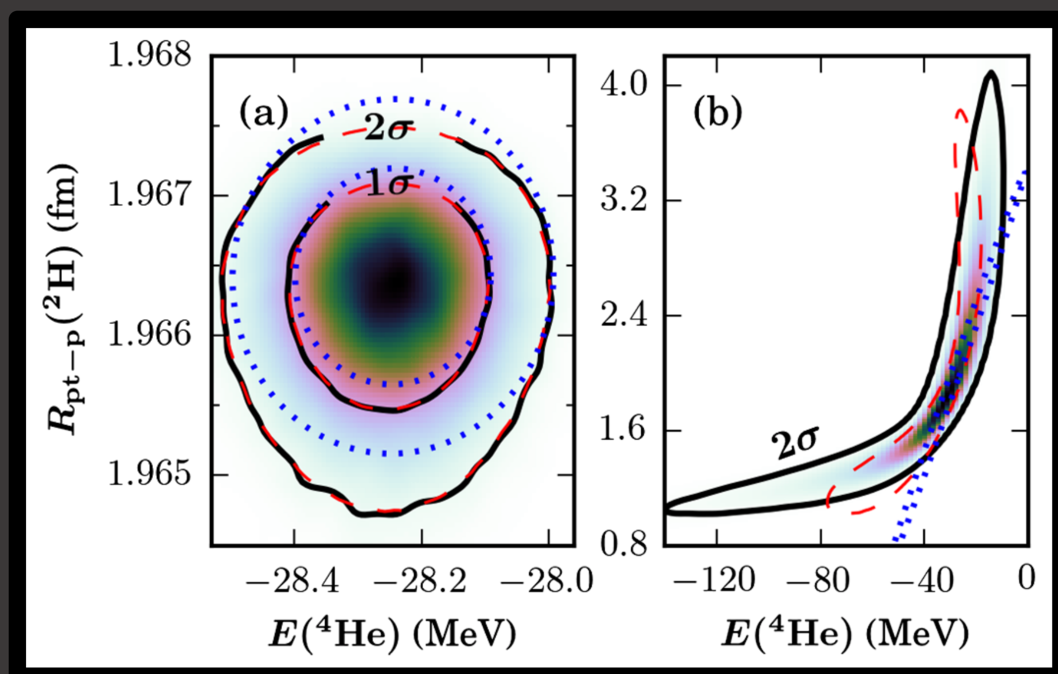
- 🙂 Very ”portable” once you have the covariance matrix
- 🙂 Facilitates correlation studies in several observables

- 😡 Gradients can be costly to compute
- 😡 Relies on second order approximation to the objective function



B. D. Carlsson et al. PRX 6 011019 (2016)

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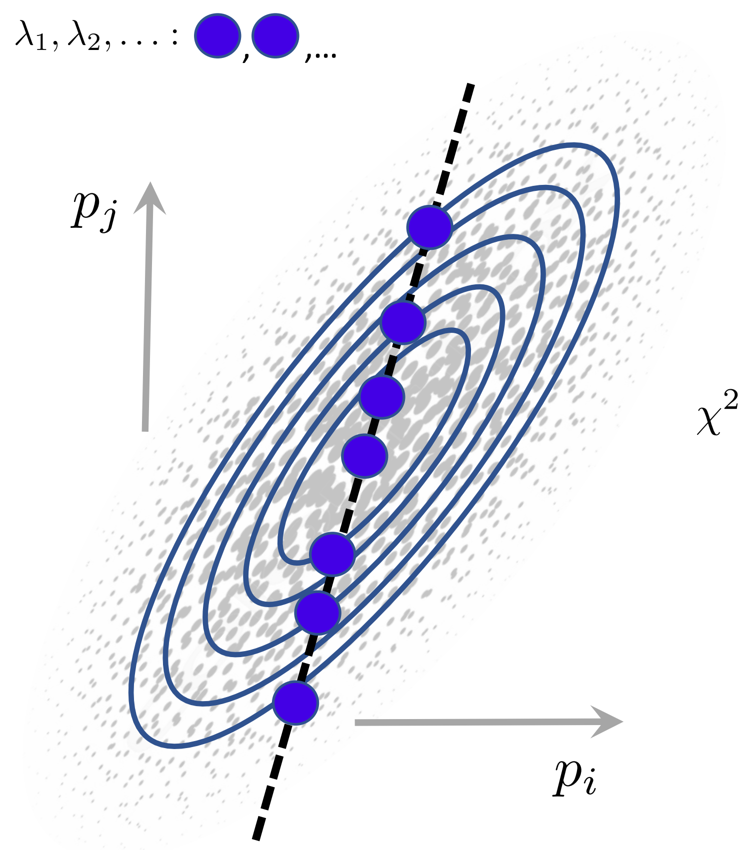
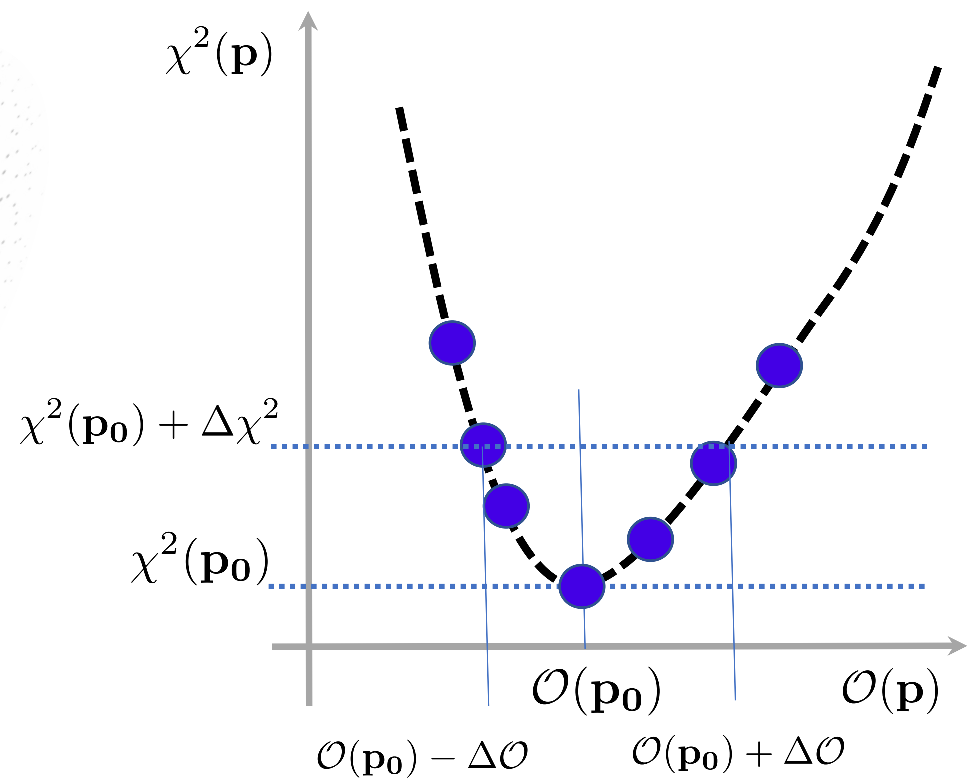
Lagrange multiplier optimization

$$F(\mathbf{p}, \lambda) = \chi^2(\mathbf{p}) + \lambda \cdot \mathcal{O}(\mathbf{p})$$

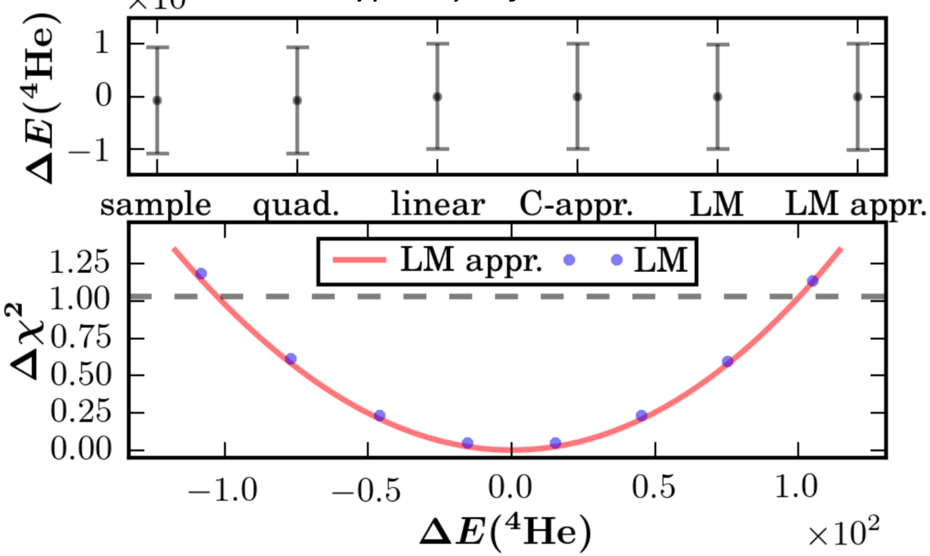




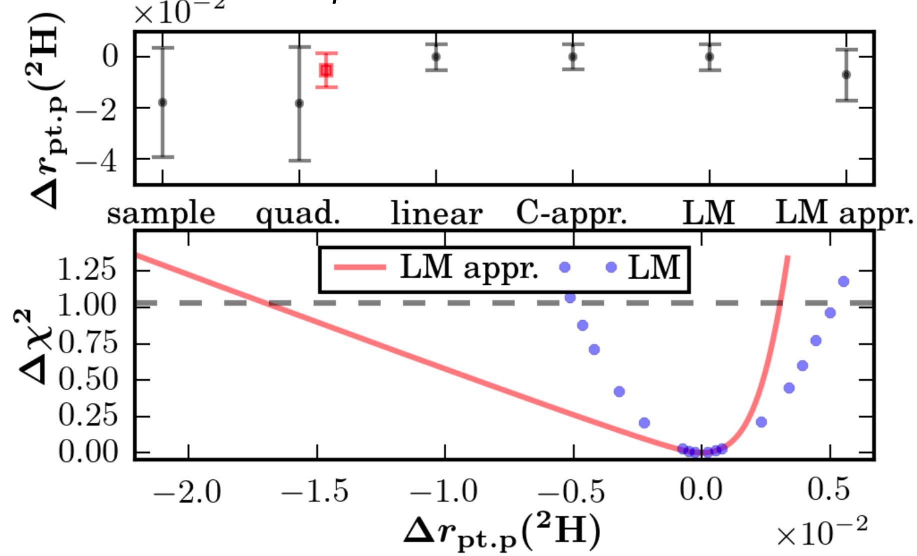
Quick Comparison

B. D. Carlsson *accepted Phys. Rev. C* (arXiv:1611.03691)

When LECs are well-constrained by data,
It is typically safe to use Hessian UQ.



If the LEC errors are large, the Lagrange
Multiplier method will be more accurate.



Sample = 10^5 MC samples of observable response using LECs drawn from the covariance matrix
Quad. = Hessian UQ with observables expanded in the LECs to second order.
Linear = Same as "quad", but linear approximation
C-appr = Same as "linear", but also linear approximation of Hessian matrix.
LM = Lagrange-Multiplier method
LM appr. = Quadratic approximation to LM method.

Simulated larger error bars enhances the non-quadratic shape of the chi-squared surface.

Red error bar: accounting for higher-order terms improves the picture.

MC sample overestimates dramatically.

Summary

- ”Standard” pool of fit data insufficient to identify a single set of LECs at N3LO.
- Need more data to filter minima and better inform the N3LO interaction. *Many good suggestions during the workshop.* (scattering observables, heavier nuclei, matter, LQCD).
- Non-local N3LO 3NF is not a small correction to ^{4}He.
- Lagrangian multiplier optimization is a convenient and derivative free method for UQ.

Thank You