Uncertainty quantification of chiral effective field theory

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UNIVERSITY OF TECHNOLOGY

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MARIE CURIE ACTIONS

Vetenskapsrådet

Acknowledgements

Bijaya Acharya, Mainz
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Kai Hebeler, Darmstadt
Gustav Jansen, ORNL

Contents of this talk

Truncation errors

deltafull vs deltaless

Optimization

Bayesian optimization

Combining errors

muonic deuterium

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What can they tell us?

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How to do this?

Overview

Nuclear physics spans a broad scientific scope. We would like to understand the origin, stability, and evolution of subatomic matter; how it organizes itself and what phenomena emerge…

Question: How does the nuclear chart emerge from QCD?

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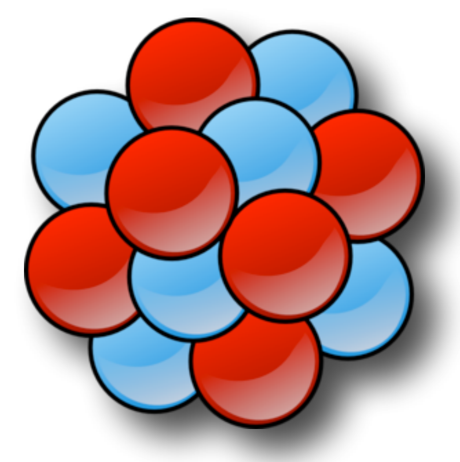
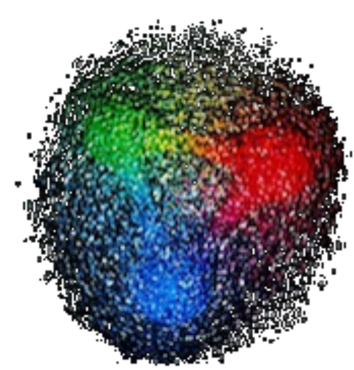
Question: How does the nuclear chart emerge from QCD?

$$\sum_{i=1}^{A} \frac{p_i^2}{2m_i} + \underbrace{\sum_{i<j=1}^{A} V_{ij} + \sum_{i<j<k=1}^{A} W_{ijk}}_{\text{chiral effective field theory}} |\Psi_A\rangle = E|\Psi_A\rangle$$



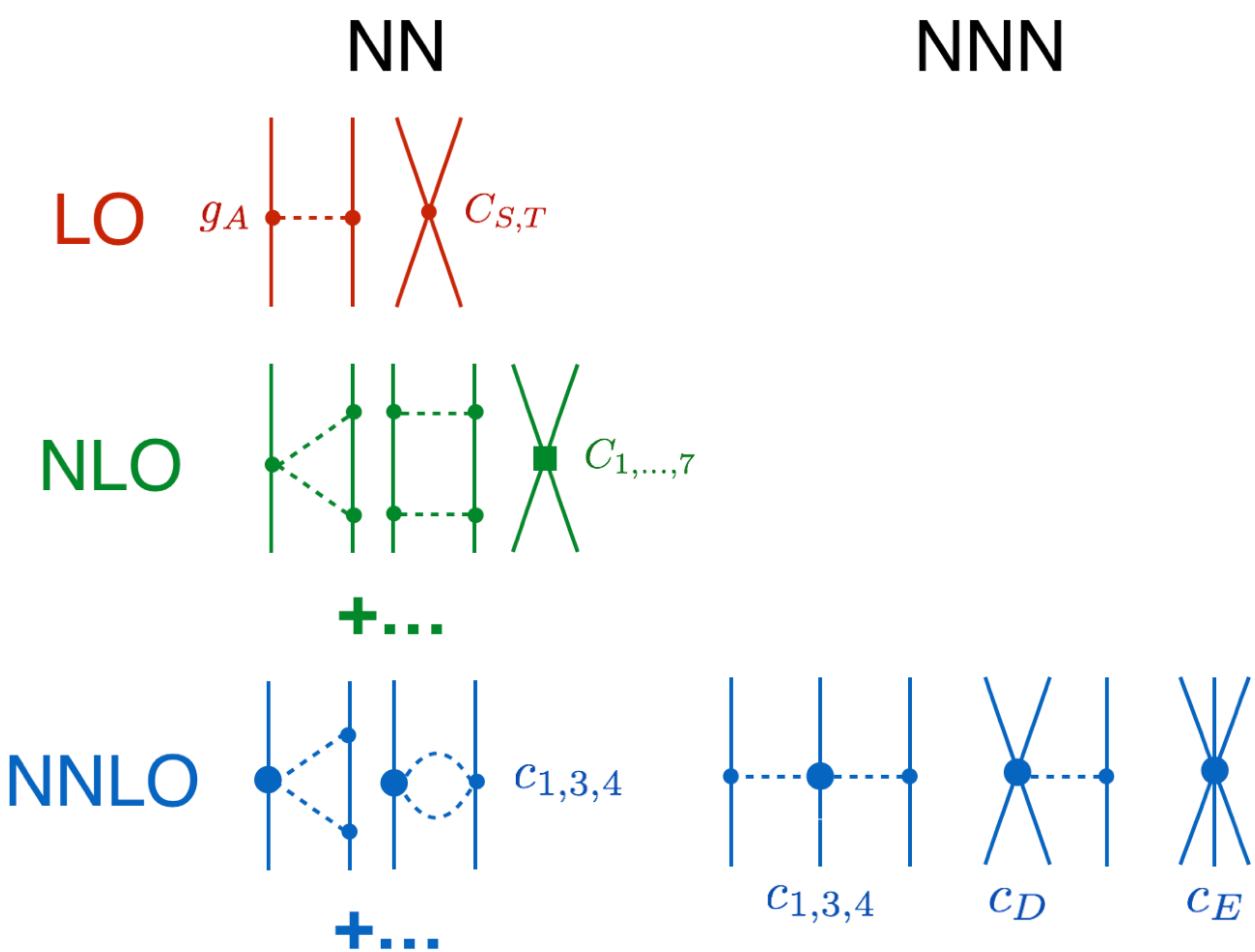


Truncation errors

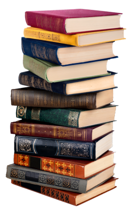
deltafull vs deltaless

Chiral effective field theory

*Nucleons interact via a potential built from perturbative pion contributions, and **indirectly** everything else.*



- Chiral symmetry dictates long-ranged physics (pion-exchange).
- 2N,3N,4N,… - forces
- Coupling constants fit from data ***once***
- On-going work: power counting, optimization strategies, uncertainty quantification.



Weinberg, van Kolck, Meissner, Epelbaum, Kaiser, Machleidt, Kaplan, Savage, Bernard, …

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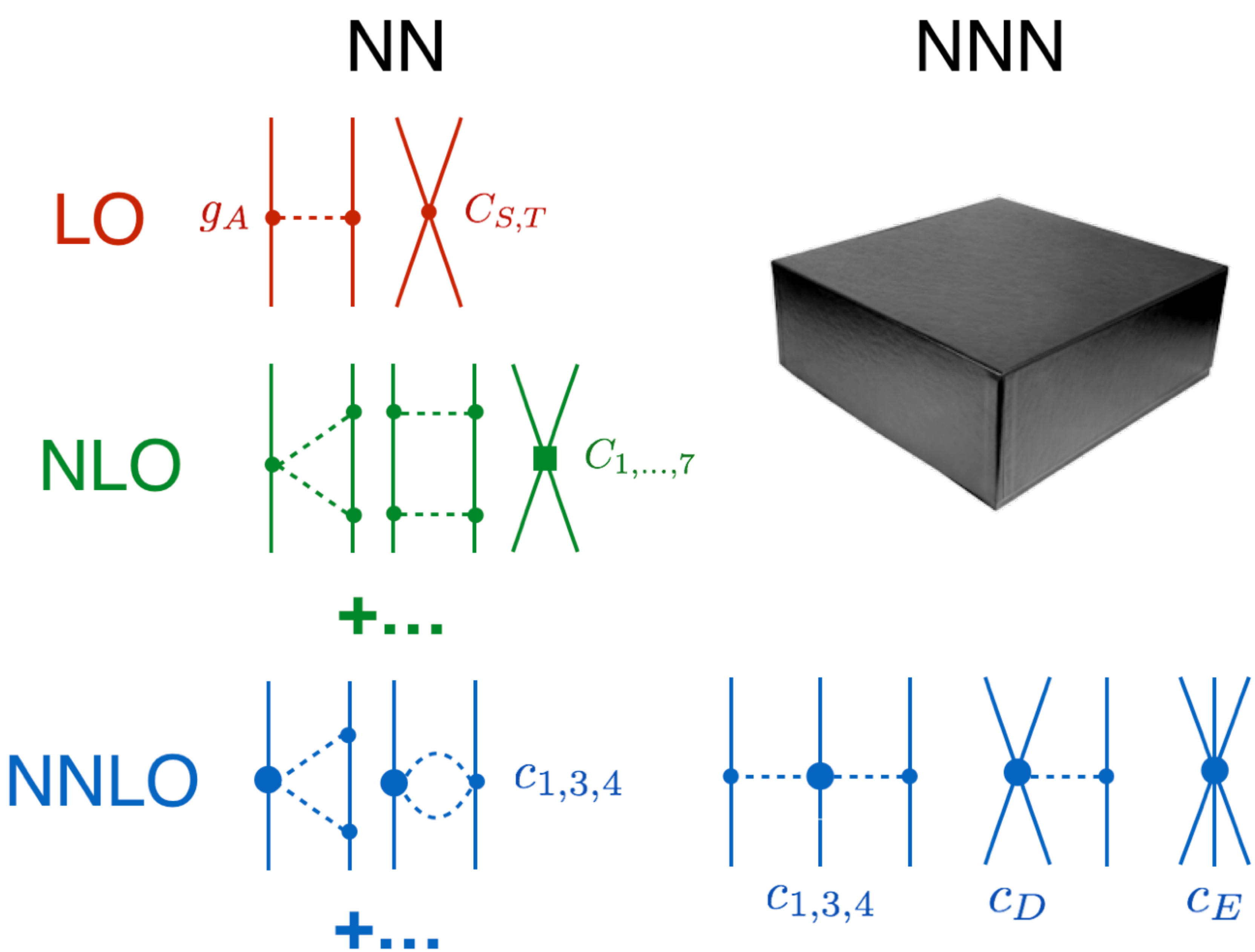

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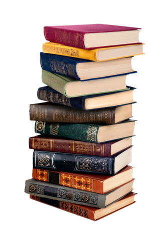

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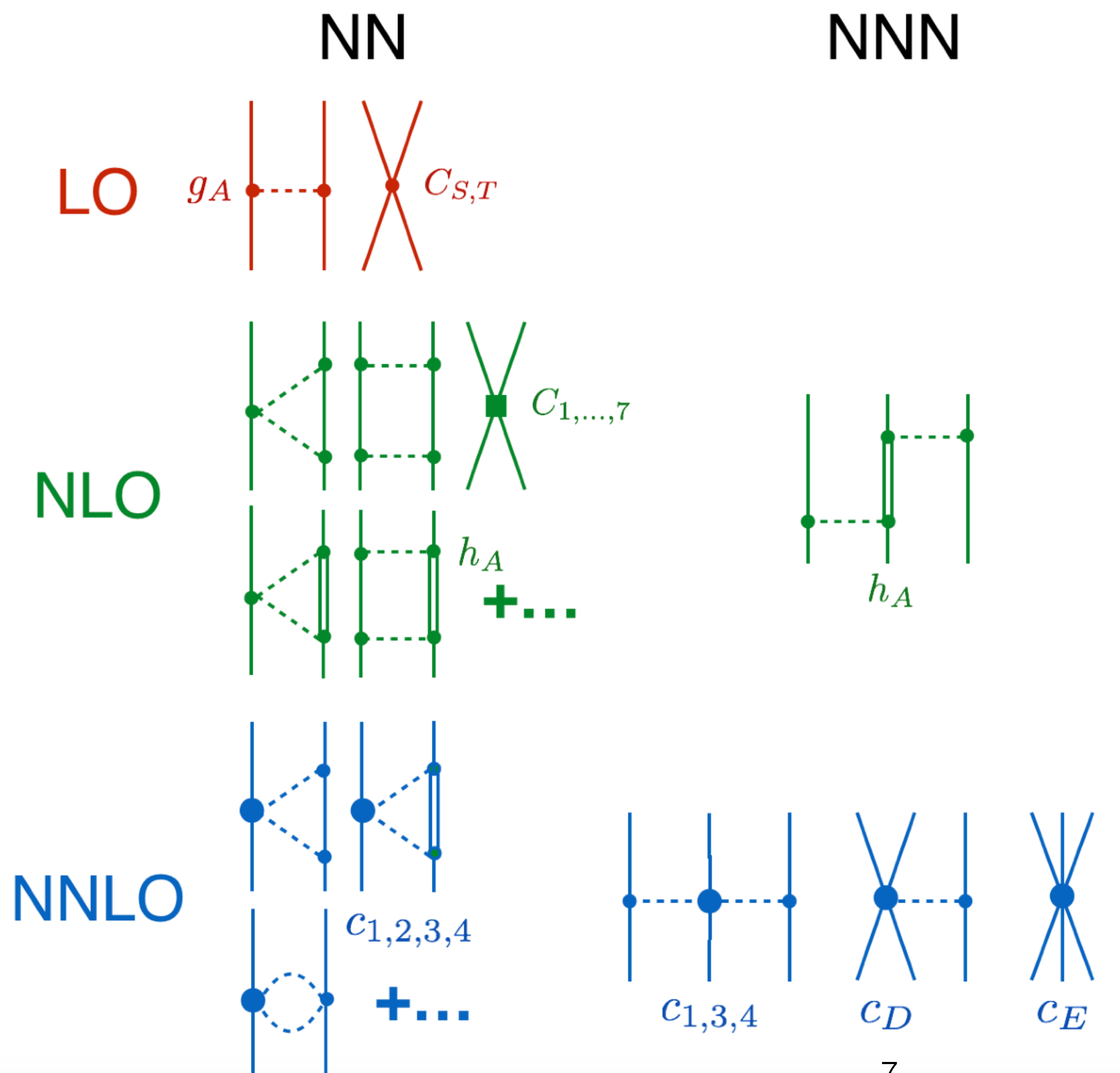
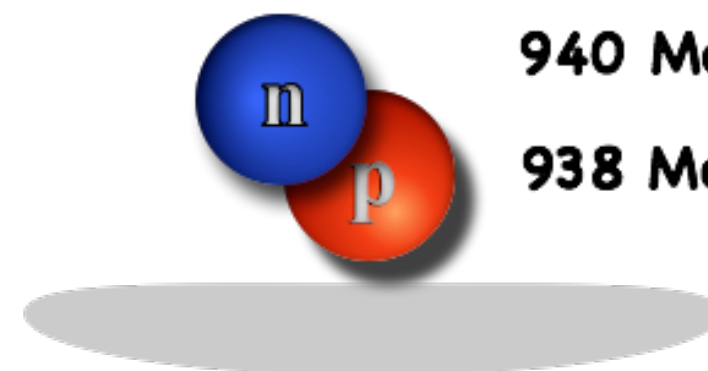
Δ-full Chiral EFT



1232 MeV

Proximity of the delta resonance motivates to explicitly including it in the effective Lagrangian.



940 MeV

938 MeV

$$\Delta \equiv m_\Delta - m_N = 293 MeV \approx 2.1 m_\pi$$

More *natural* values for the LECs!

But also more LECs and digrams (extensive N3LO)

Ordoñez, Ray, van Kolck 1994
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Δ-full Chiral EFT

1232 MeV

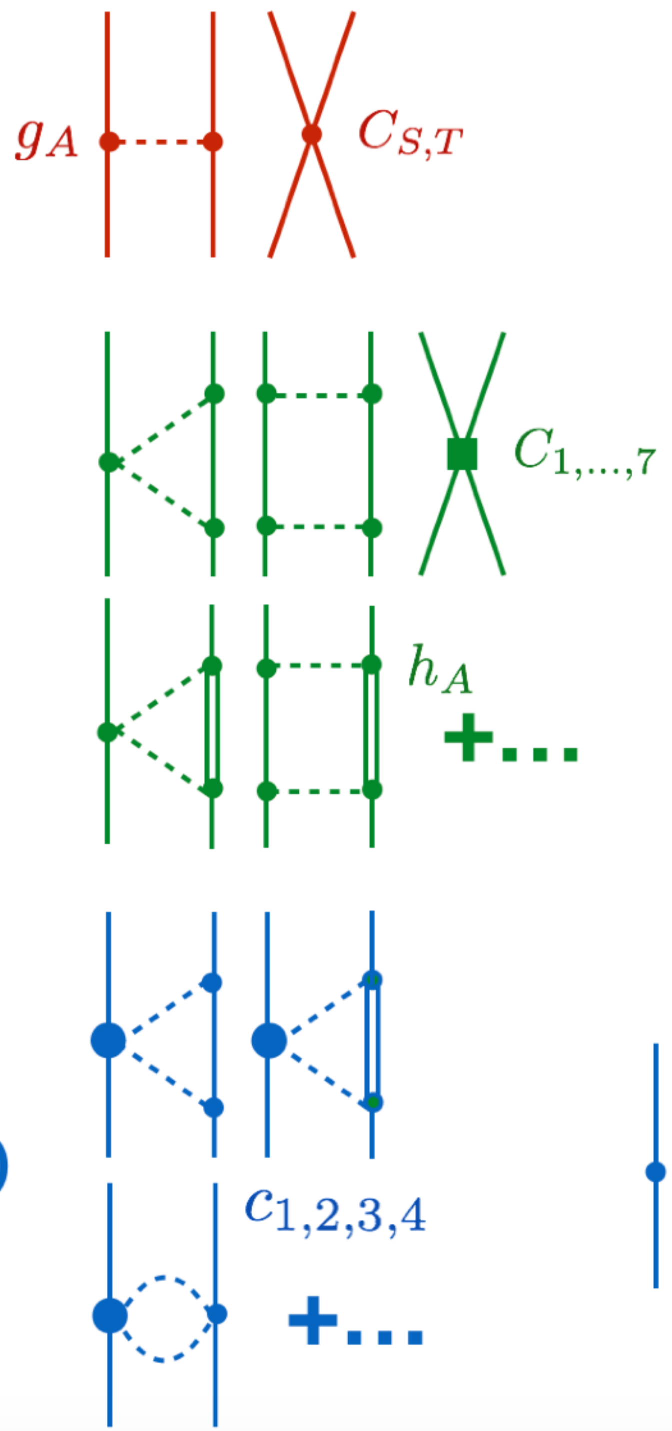
NN

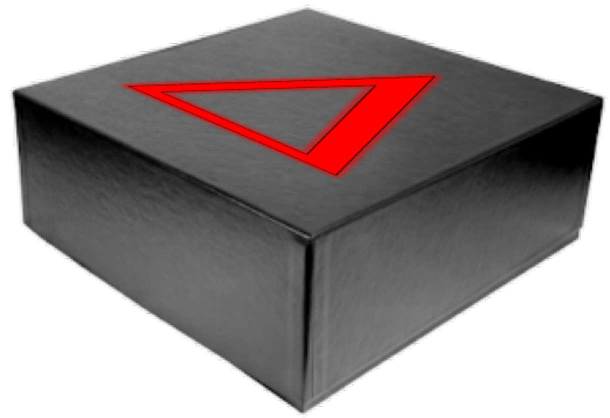
NNN

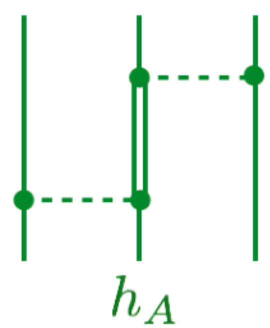
LO

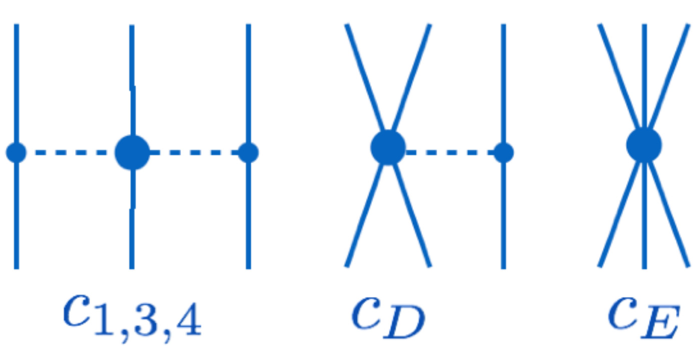
NLO

NNLO









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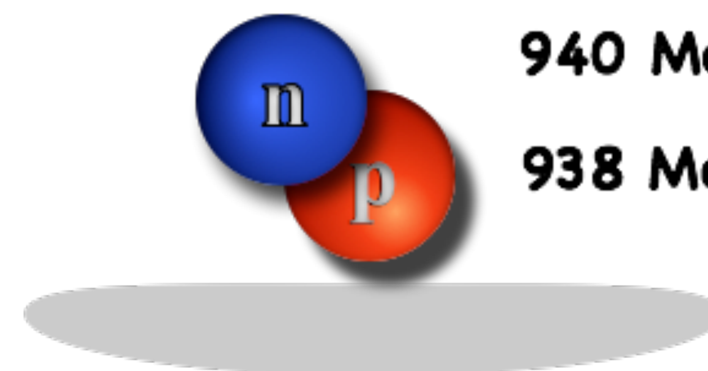

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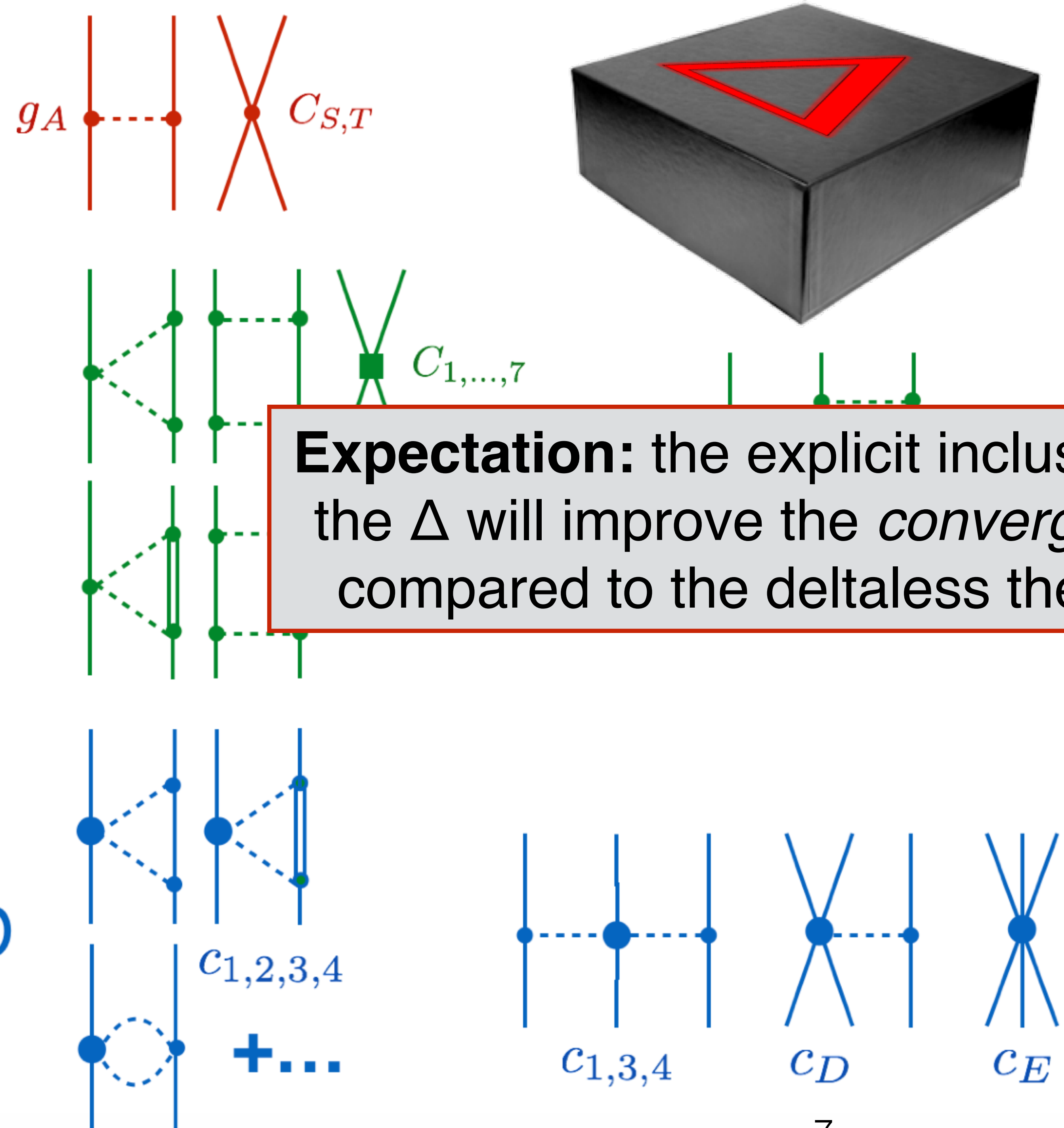
NN NNN

LO

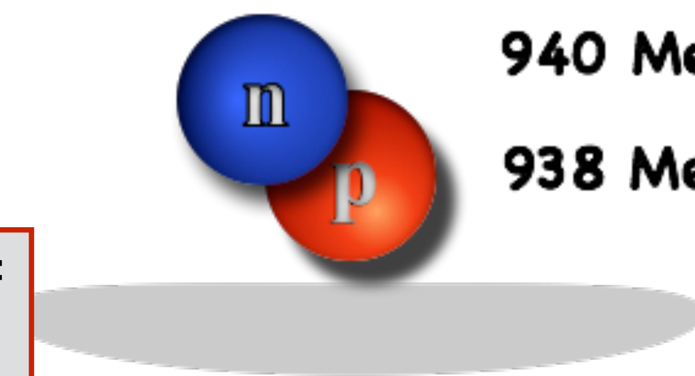
NLO

NNLO



Expectation: the explicit inclusion of the Δ will improve the *convergence* compared to the deltaless theory.

Proximity of the delta resonance motivates to explicitly including it in the effective Lagrangian.



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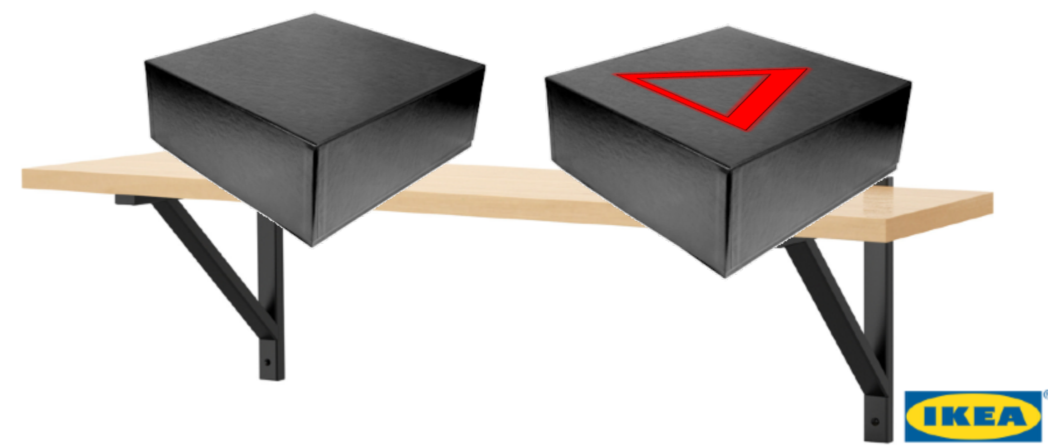
Δ-full/less interactions from the same fit strategy



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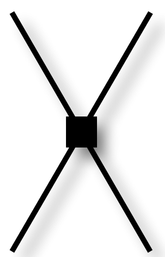
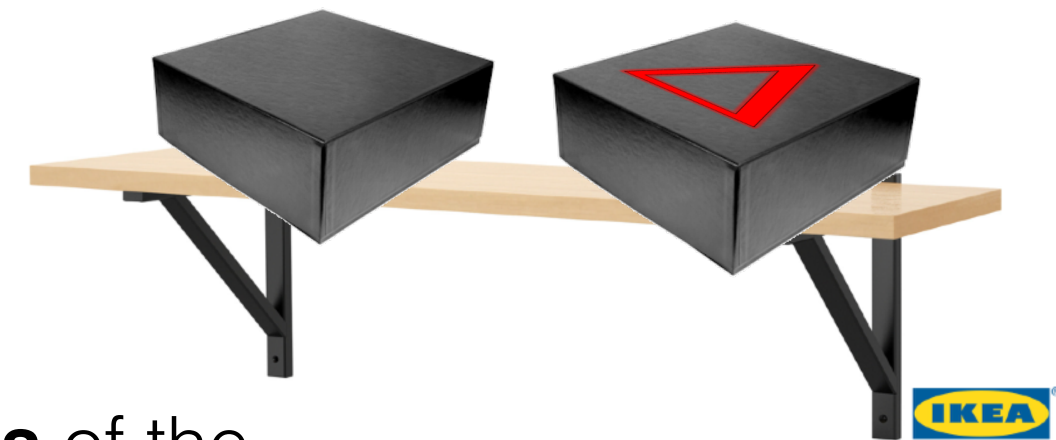


$$x_\star = \underset{x}{\operatorname{argmin}} \ \chi^2(x)$$

B. D. Carlsson et al. Phys. Rev. X **6**, 011019 (2016)
A. Eksröm et al. Phys. Rev. Lett. **110**, 192502 (2013)



partial-wave NN scattering **phase shifts** of the Granada group up to 200 MeV scattering energy in the laboratory system. R. Navarro-Perez et al, Phys. Rev. C **88**, 064002 (2013).

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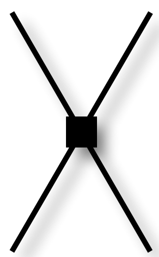

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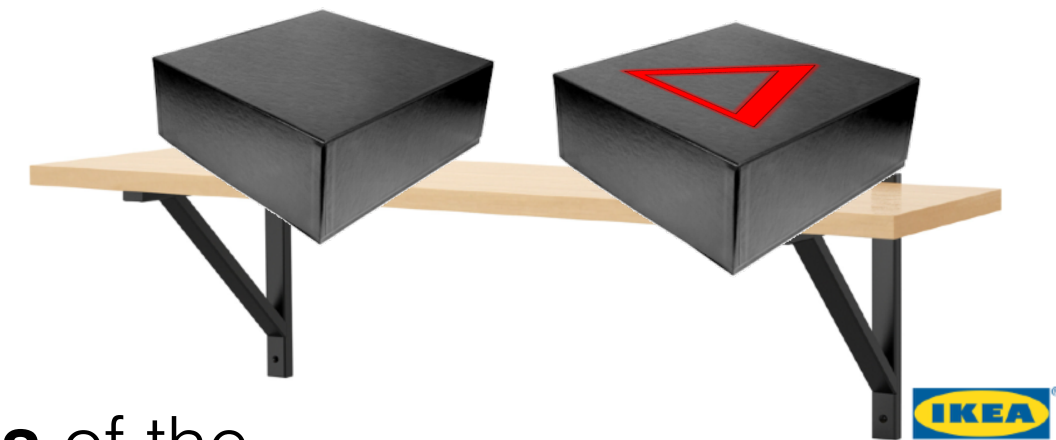

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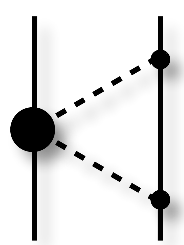

Sub-leading pi-N LECs precisely determined in recent **Roy-Steiner analysis.**

D. Siemens et al. Physics Letters B **770** (2017) 27–34

Δ−full

$$c_1 = -0.74(2)$$
$$c_2 = -0.49(17)$$
$$c_3 = -0.65(22)$$
$$c_4 = +0.96(11)$$
$$h_A = 1.40 \pm 0.05$$

....

Δ−less

$$c_1 = -0.74(2)$$
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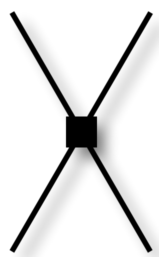

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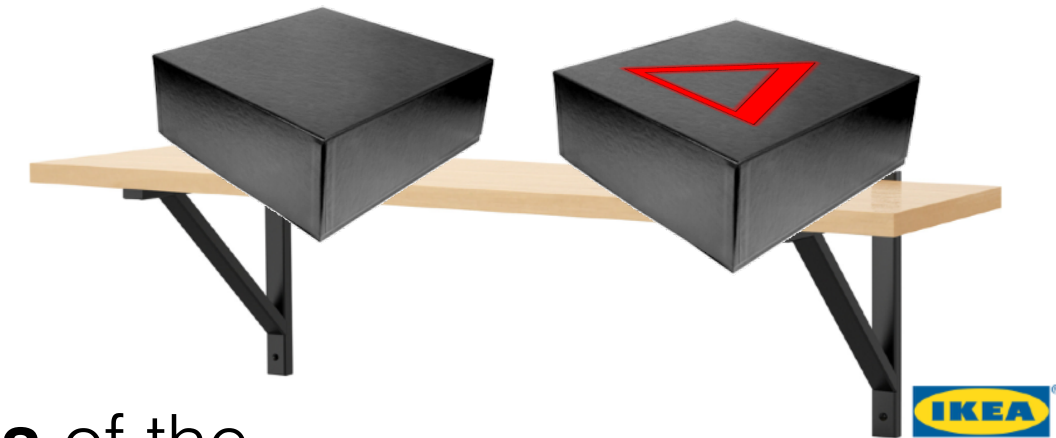

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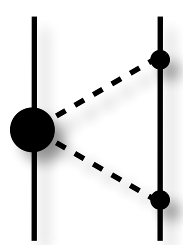

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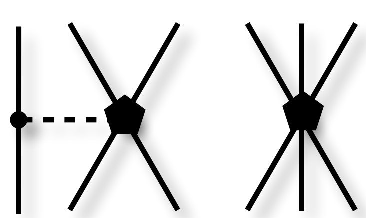

Determined from **NCSM** $E_{gs}(^4\text{He})$ && $R_{pt\text{-}p}(^4\text{He})$
n.b. only relevant at NNLO

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Estimating truncation errors

We truncate the chiral expansion at some finite order k

$$X = X_0 \sum_{n=0}^{\infty} c_n Q^n$$

Typically, $\{c_n\} \sim \mathcal{O}(1)$

Question: how to estimate the error in X due to truncation (k) in the EFT expansion, given explicit values for the (natural) coefficients $c_1, \ldots, c_k$?

$$X = X_0(c_0 Q^0 + \ldots c_k Q^k) + X_0(\underbrace{c_{k+1} Q^{k+1} + \ldots}_{\Delta_k})$$

That is, we seek $P(\Delta_k | c_0, \ldots, c_k)$

E. Epelbaum et al Phys. Rev. Lett. **115**, 122301 (2015)
R. J. Furnstahl et al, Phys. Rev. C **92**, 024005 (2015)

Up to factors of order unity, we can estimate the truncation error (degree of belief, evidential probability, …)

$$P(\Delta_k^{(1)}|c_0,\ldots,c_k) \qquad \sigma_X(\mathrm{N}j\mathrm{LO}) = X_0 Q^{j+2}\max(|c_0|,|c_1|,\ldots,|c_{j+1}|)$$

$$Q = \left(\frac{p}{\Lambda_b}\right) \quad p = \begin{cases} M_\pi \\ k_F \end{cases} \quad \Lambda_b = 500\,\mathrm{MeV}$$

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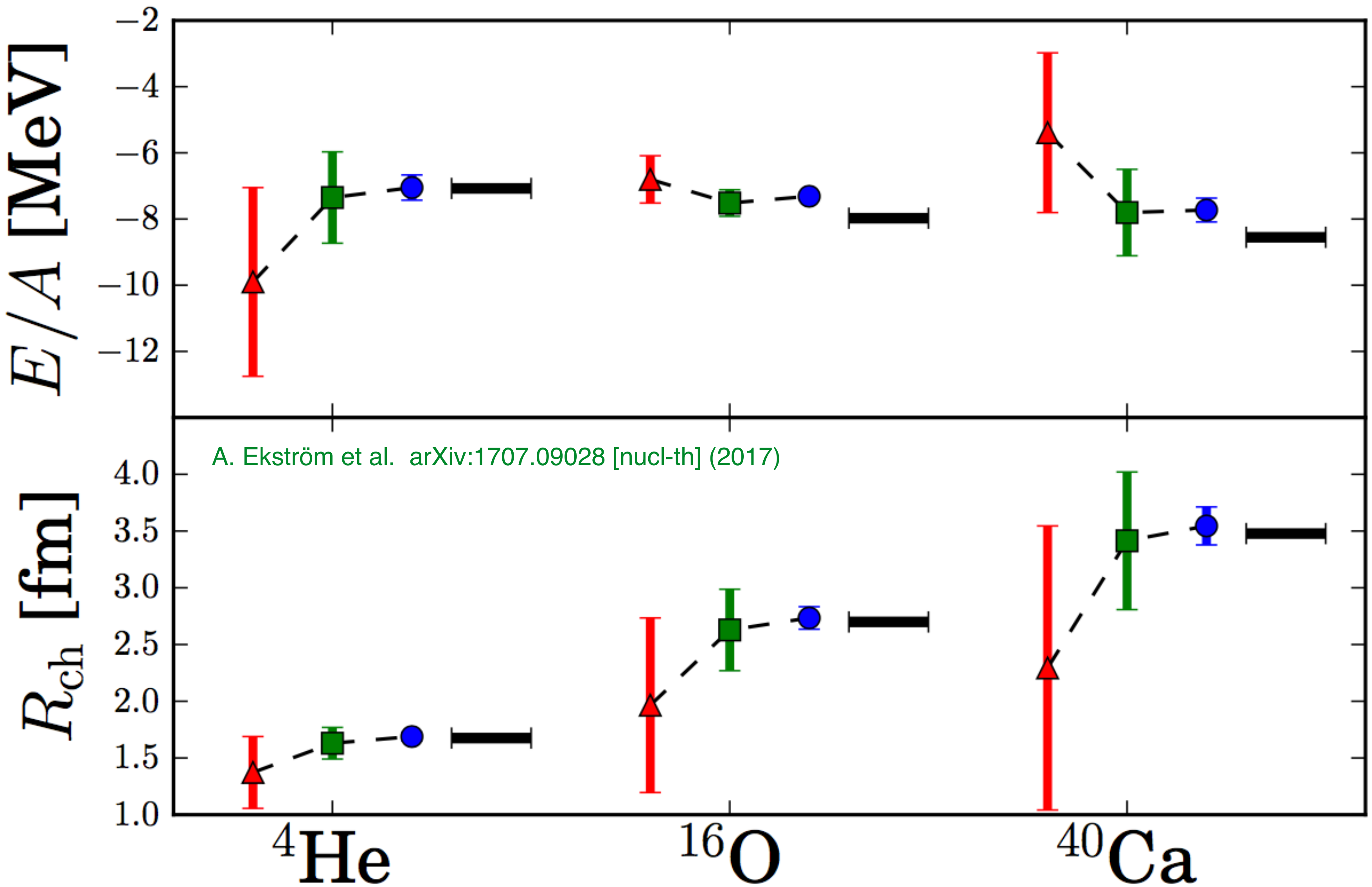

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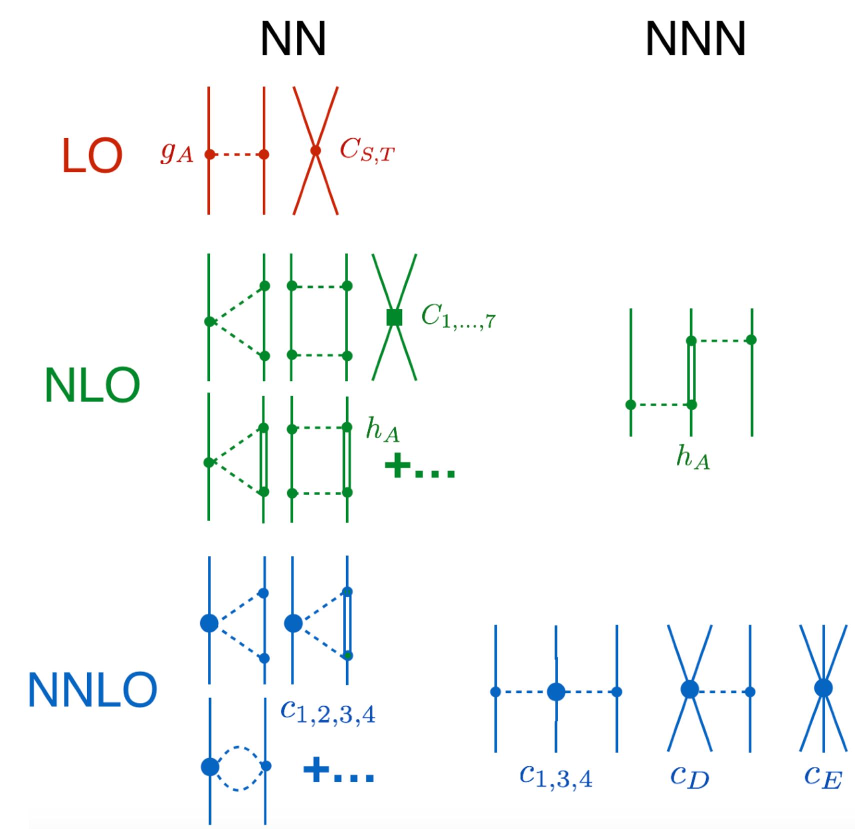

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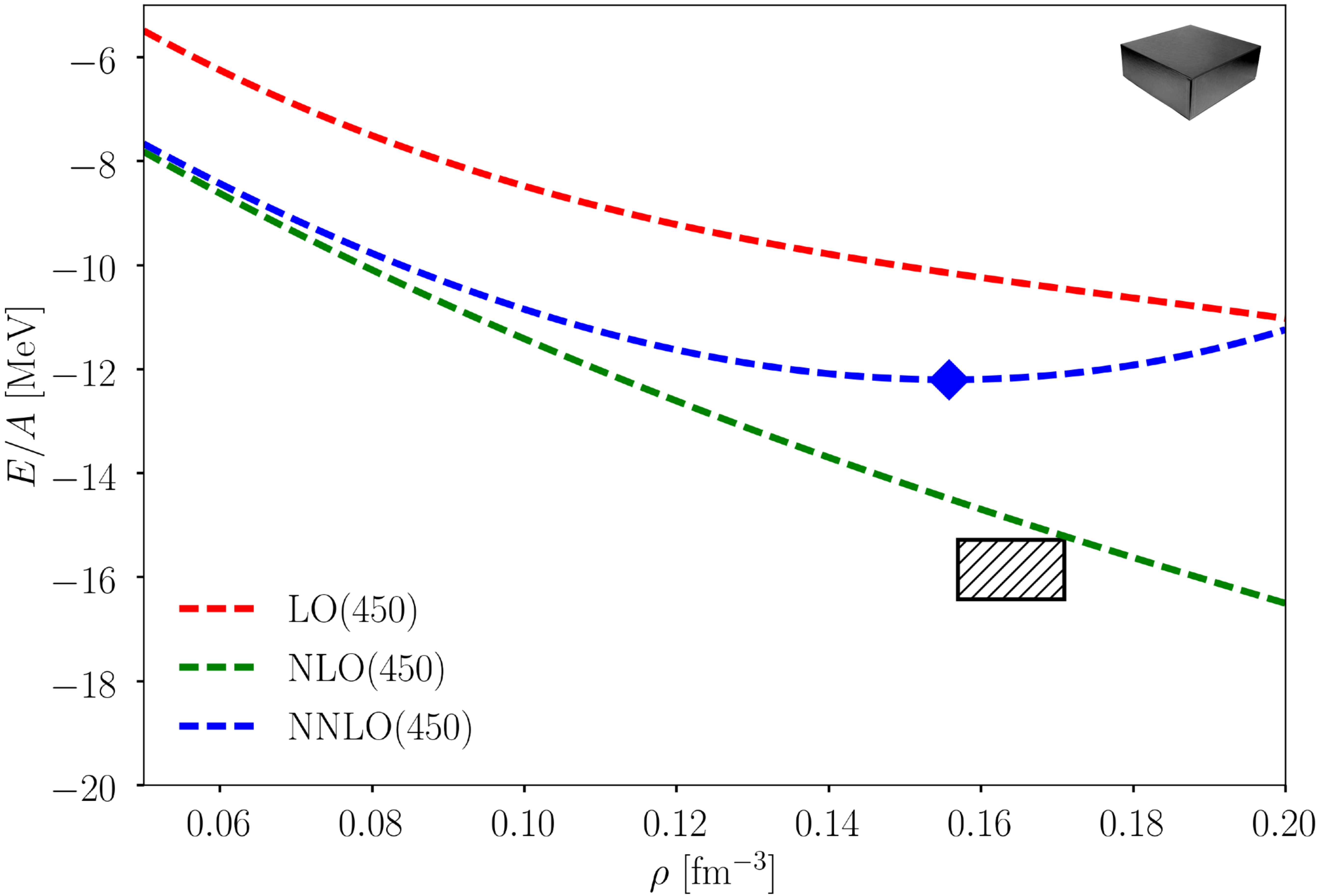
LO(450)
NLO(450)
NNLO(450)
E/A [MeV]
ρ [fm^{-3}]
−6
−8
−10
−12
−14
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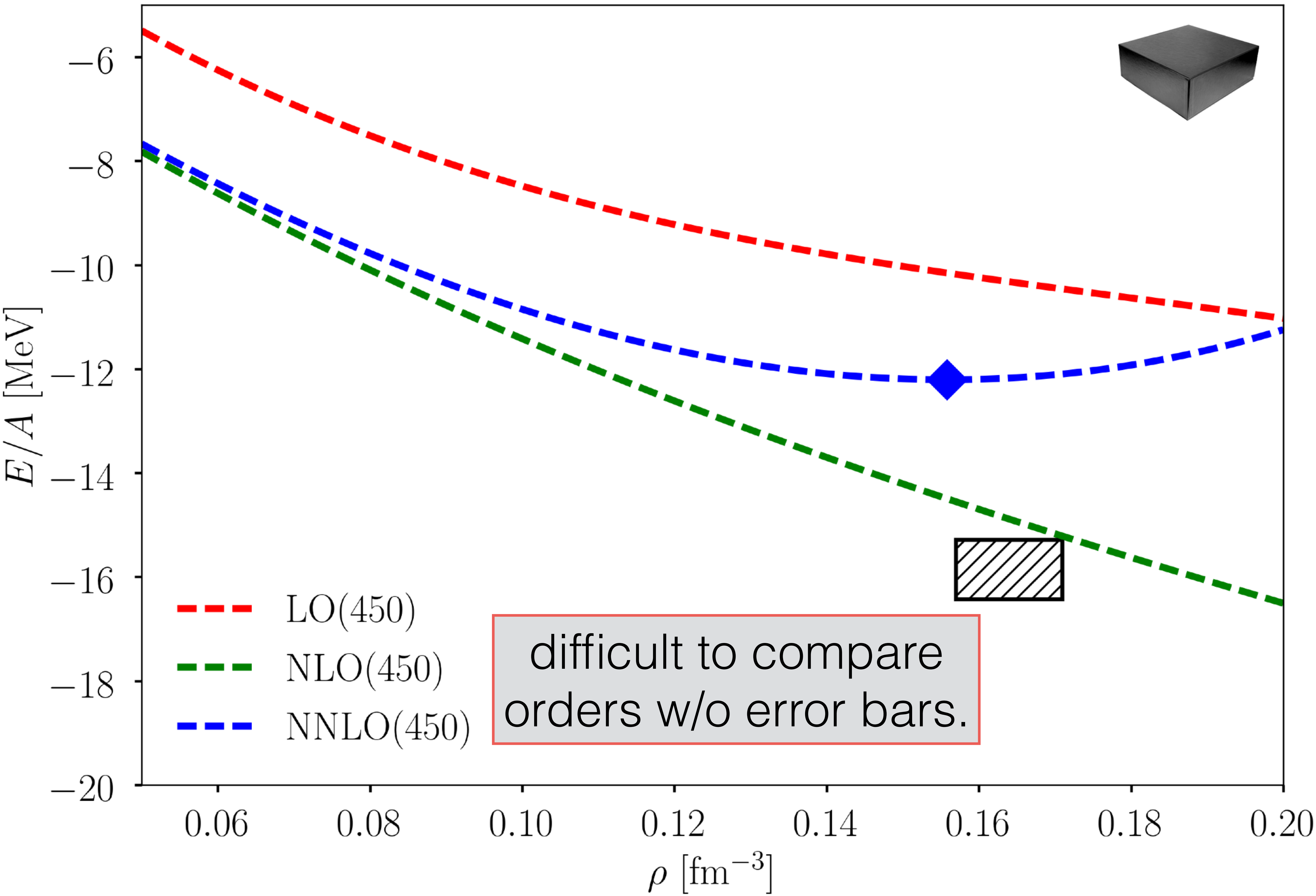
−18
−20
0.06
0.08
0.10
0.12
0.14
0.16
0.18
0.20



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0.10
0.12
0.14
0.16
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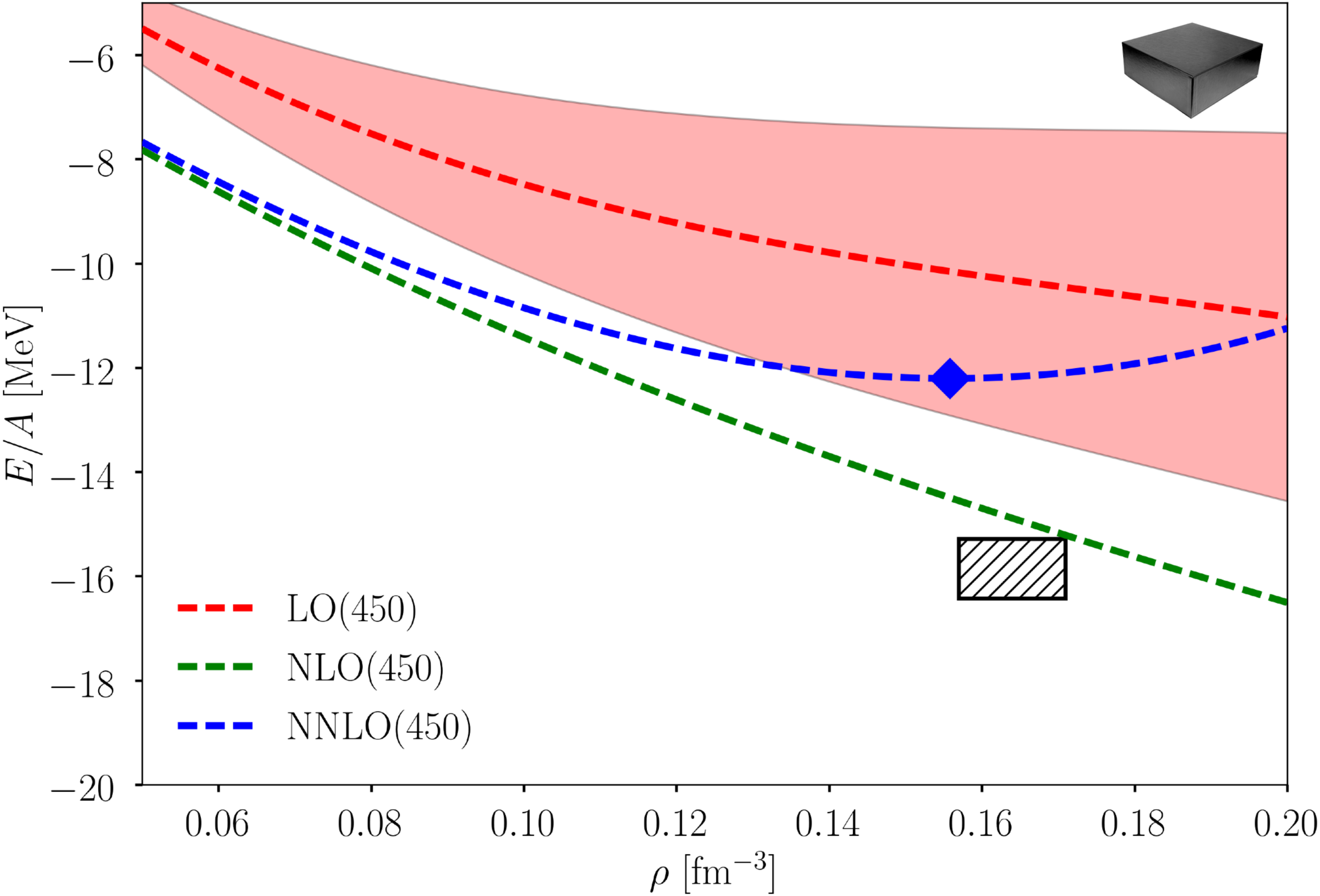
0.20
ρ [fm^{-3}]
LO(450)
NLO(450)
NNLO(450)
difficult to compare
orders w/o error bars.



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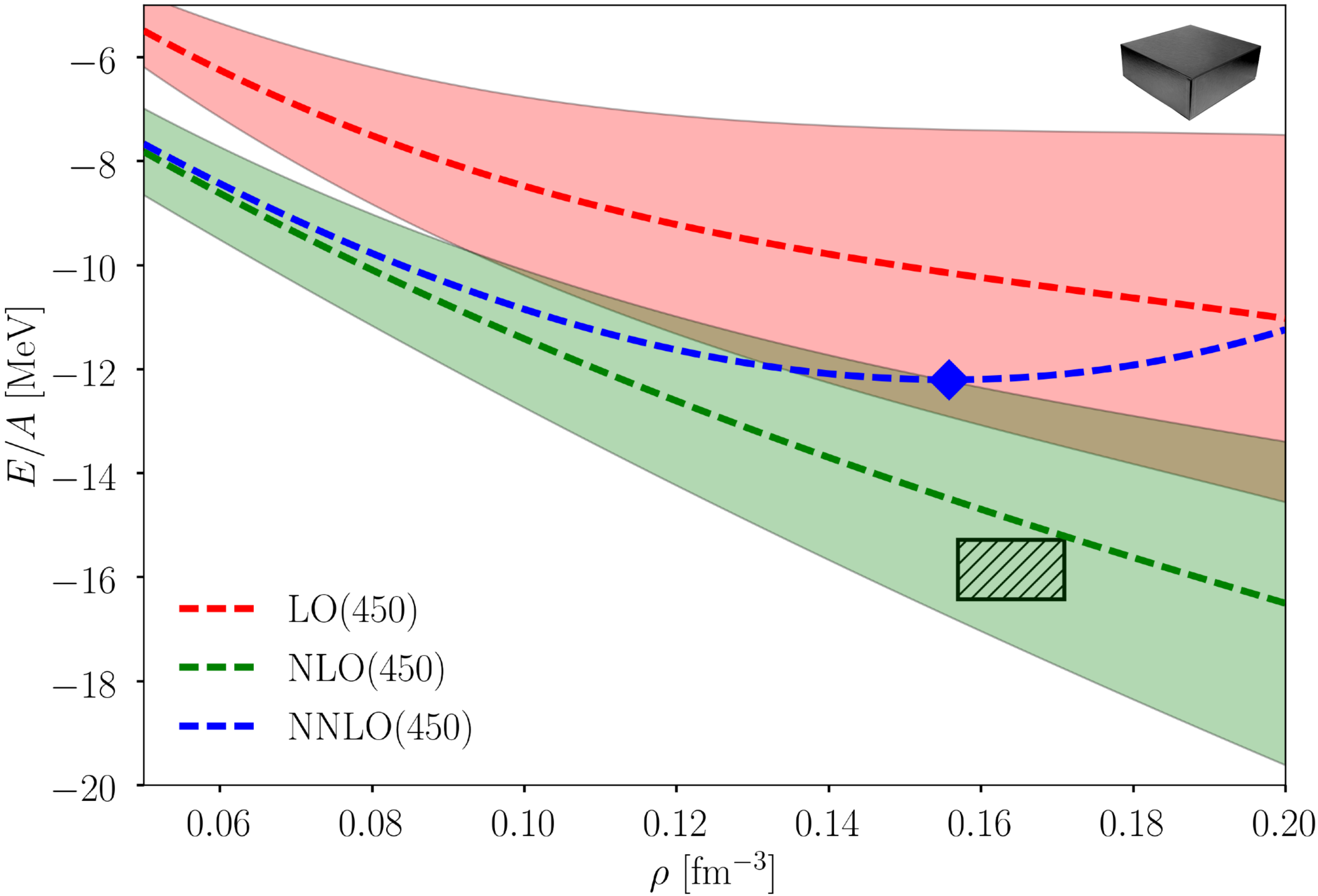

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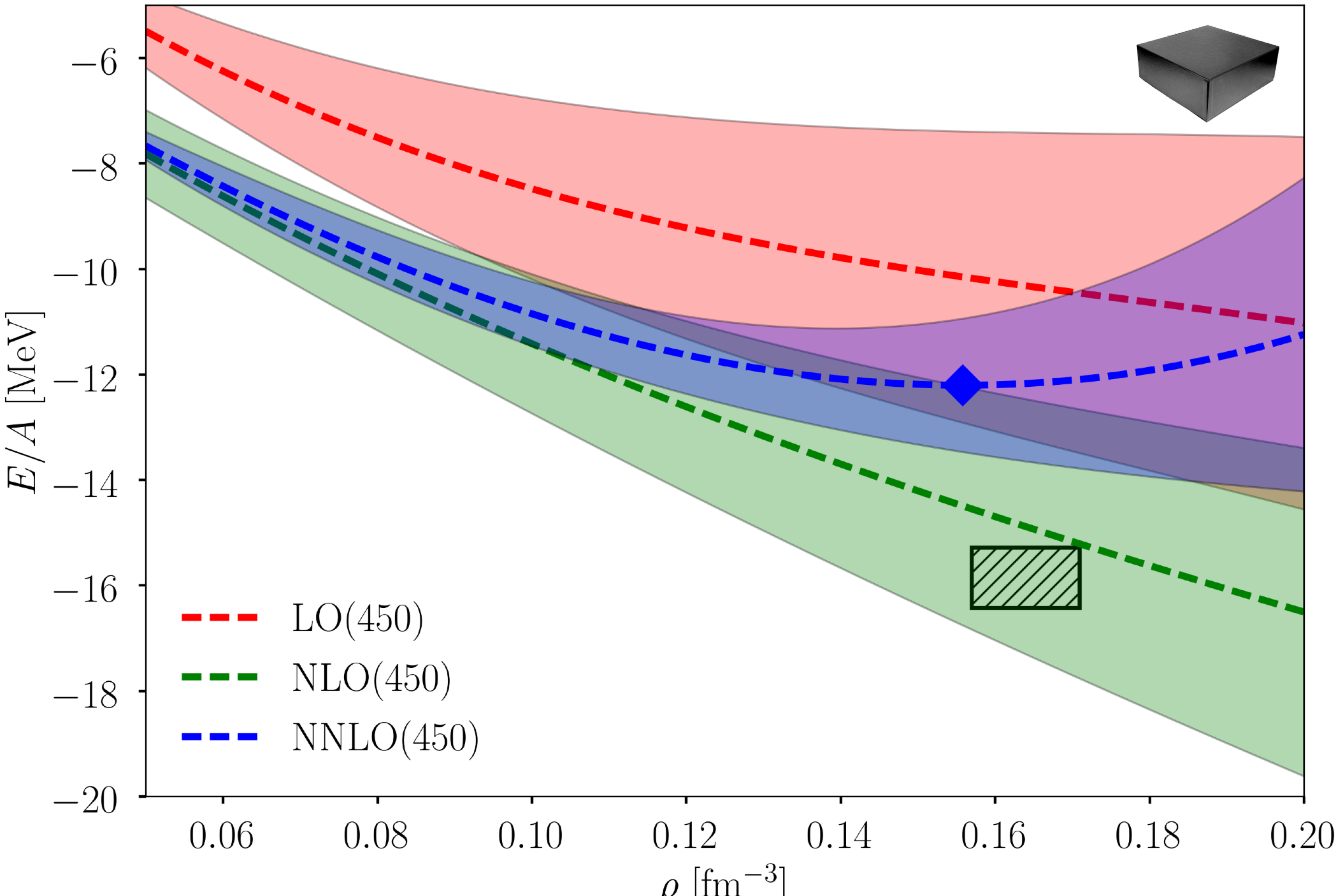

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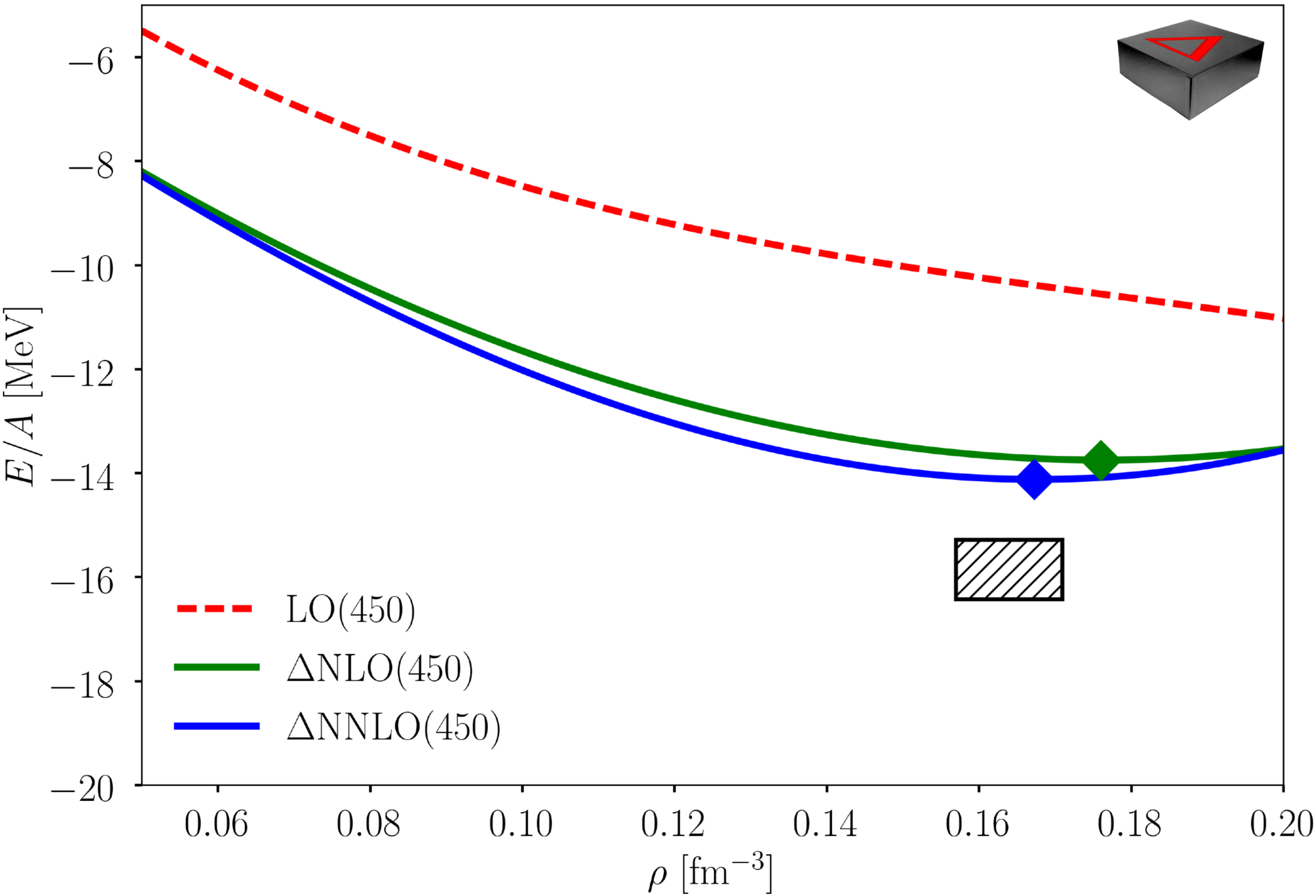

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−20
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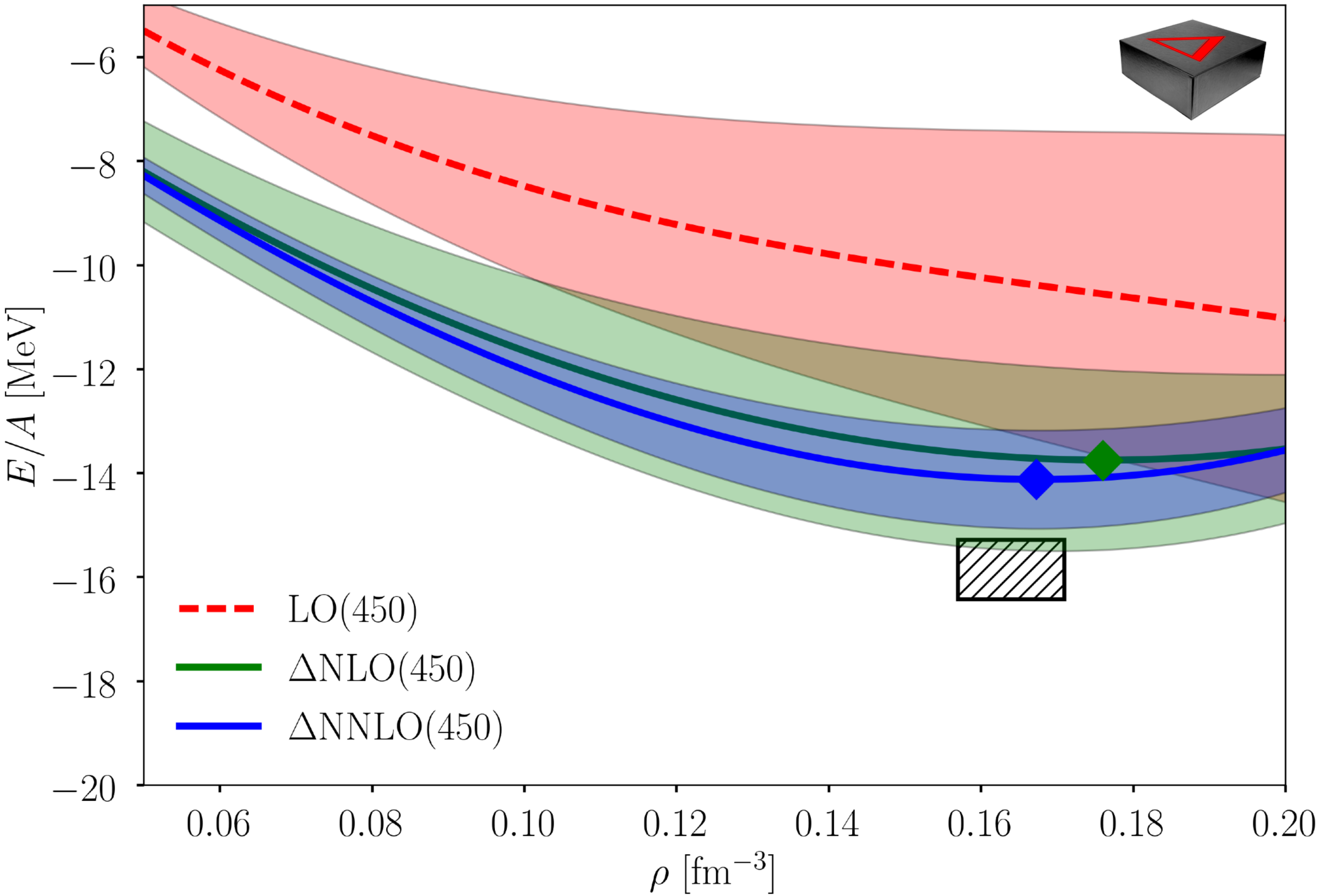
0.10
0.12
0.14
0.16
0.18
0.20
ρ [fm⁻³]
LO(450)
ΔNLO(450)
ΔNNLO(450)



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E/A [MeV]
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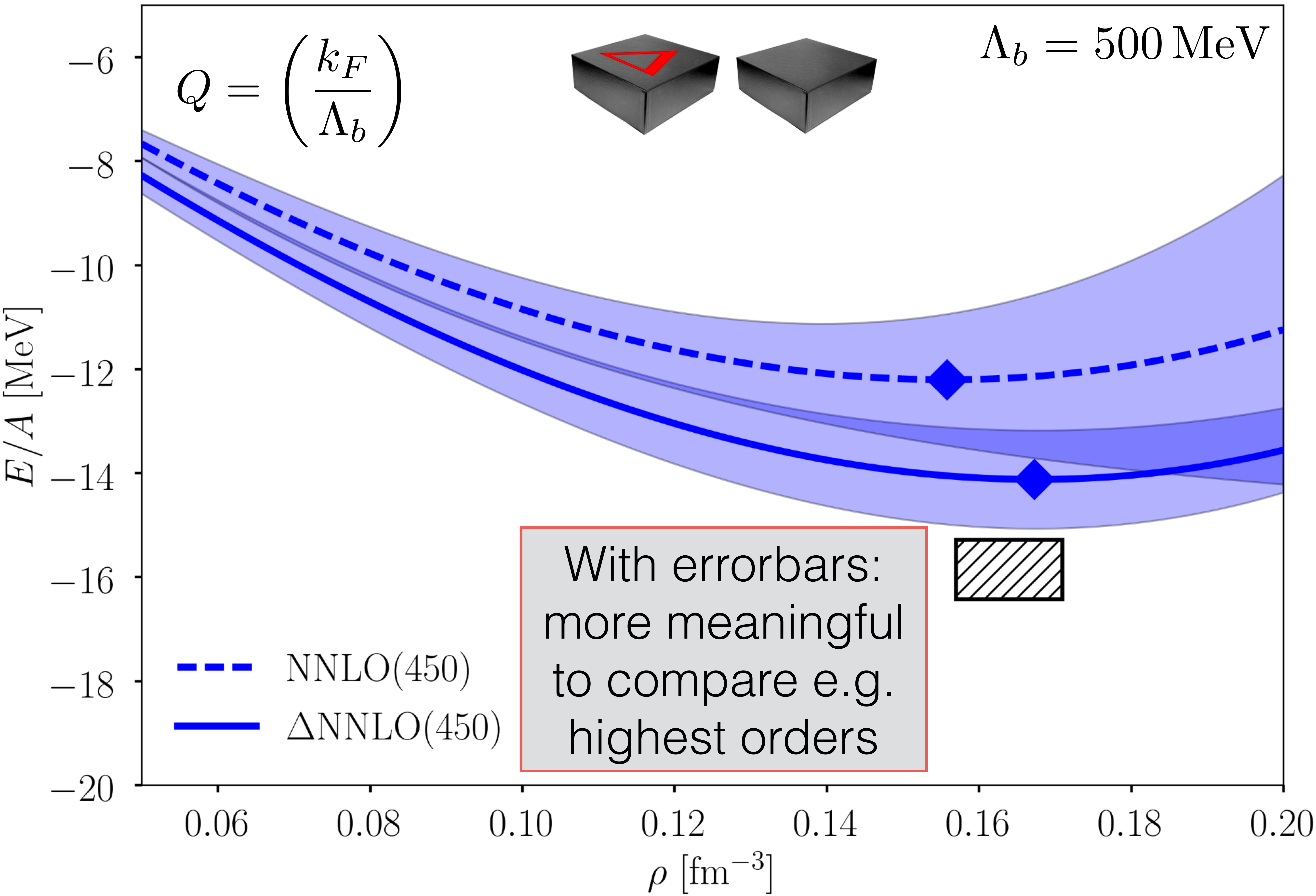
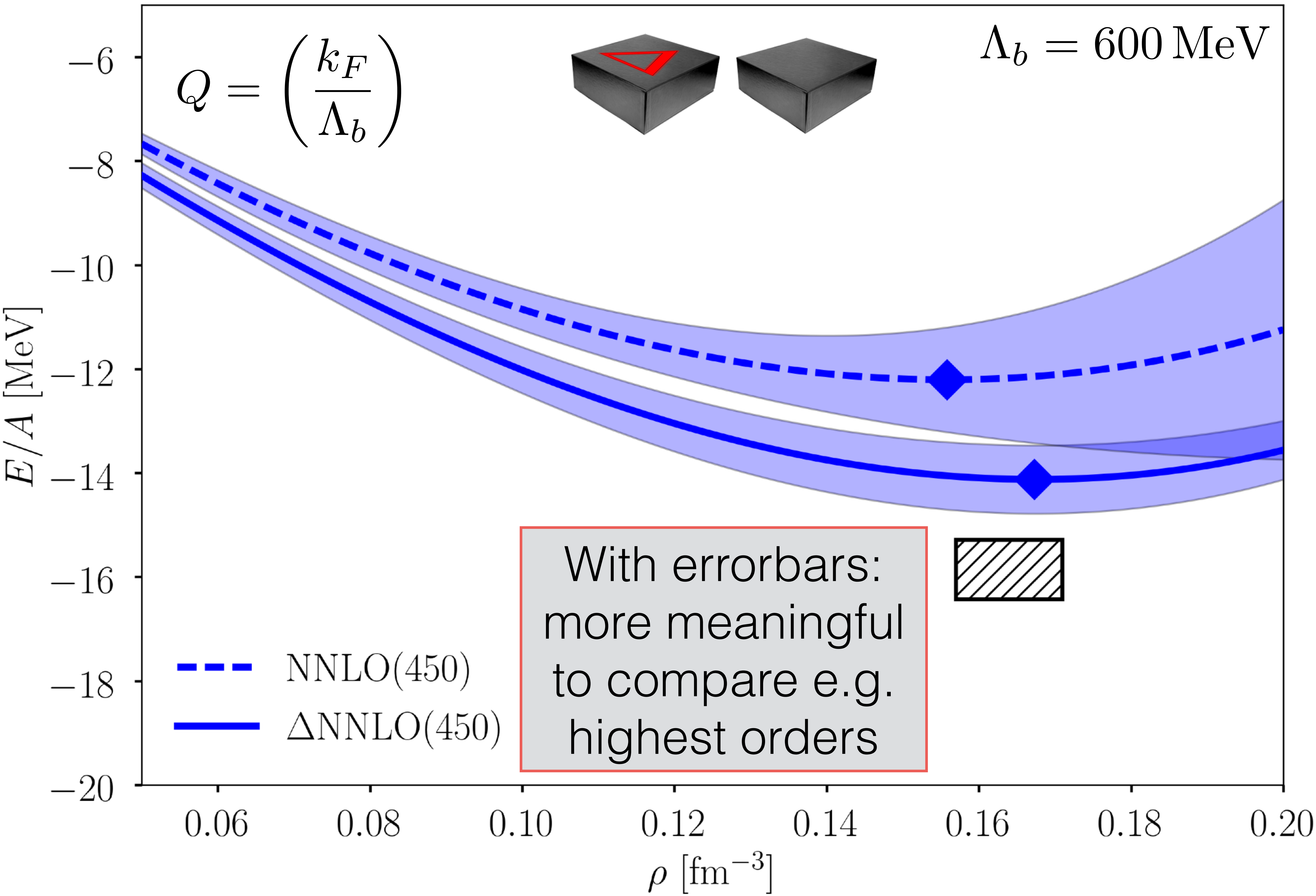
0.20
ρ [fm^{-3}]
LO(450)
ΔNLO(450)
ΔNNLO(450)


$Q = \left(\frac{k_F}{\Lambda_b}\right)$
$\Lambda_b = 500\,\mathrm{MeV}$
E/A [MeV]
ρ [fm^{-3}]
NNLO(450)
ΔNNLO(450)
With errorbars: more meaningful to compare e.g. highest orders



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ρ [fm^{-3}]
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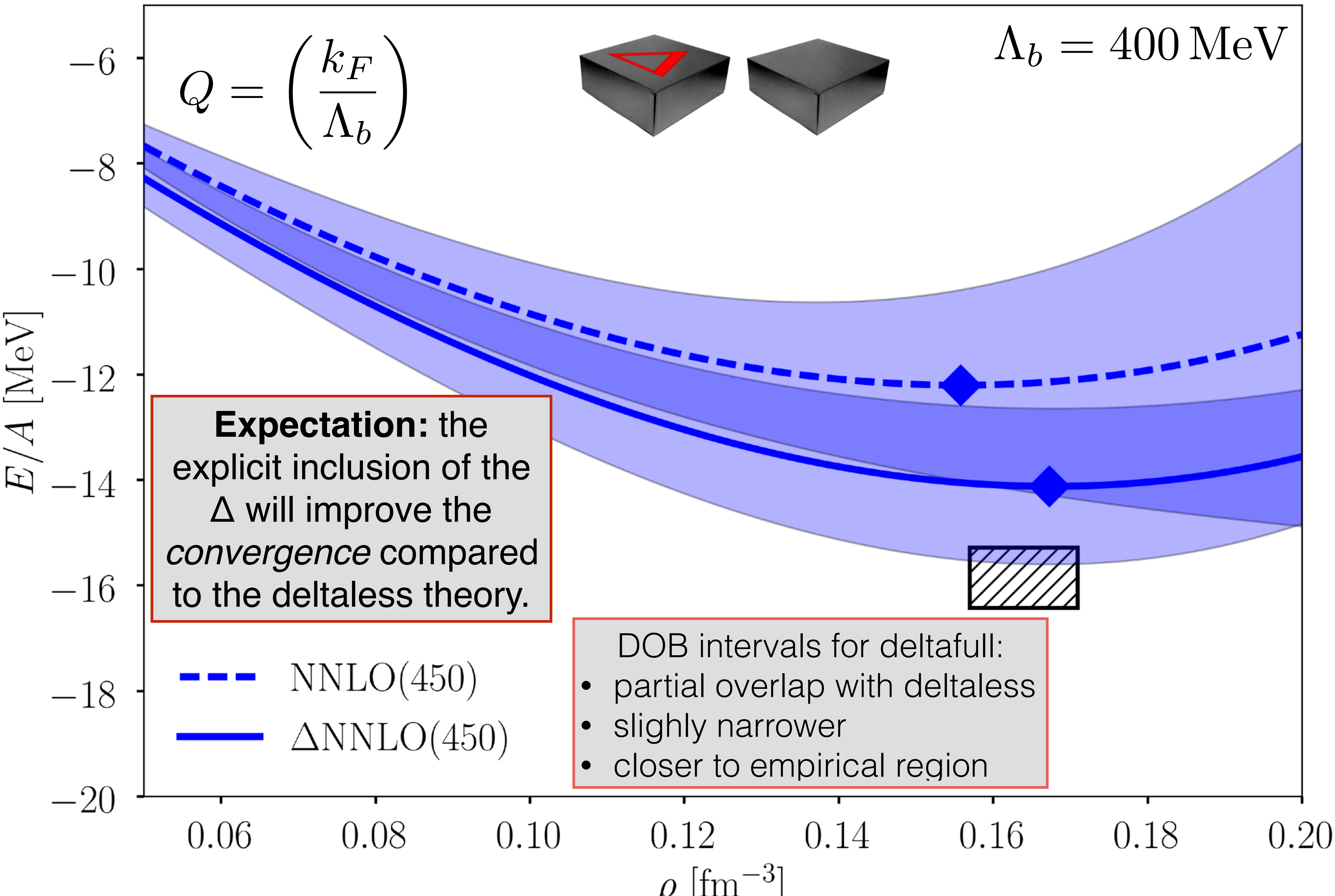
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0.12
0.14
0.16
0.18
0.20
Expectation: the explicit inclusion of the Δ will improve the *convergence* compared to the deltaless theory.
NNLO(450)
ΔNNLO(450)
DOB intervals for deltafull:
• partial overlap with deltaless
• slighly narrower
• closer to empirical region

Optimization

Bayesian optimization

Bayesian Optimization

Scenario: the function f that we wish to minimize is **expensive to evaluate**, and its exact functional form is unavailable for whatever reason.

No more information is available to us.

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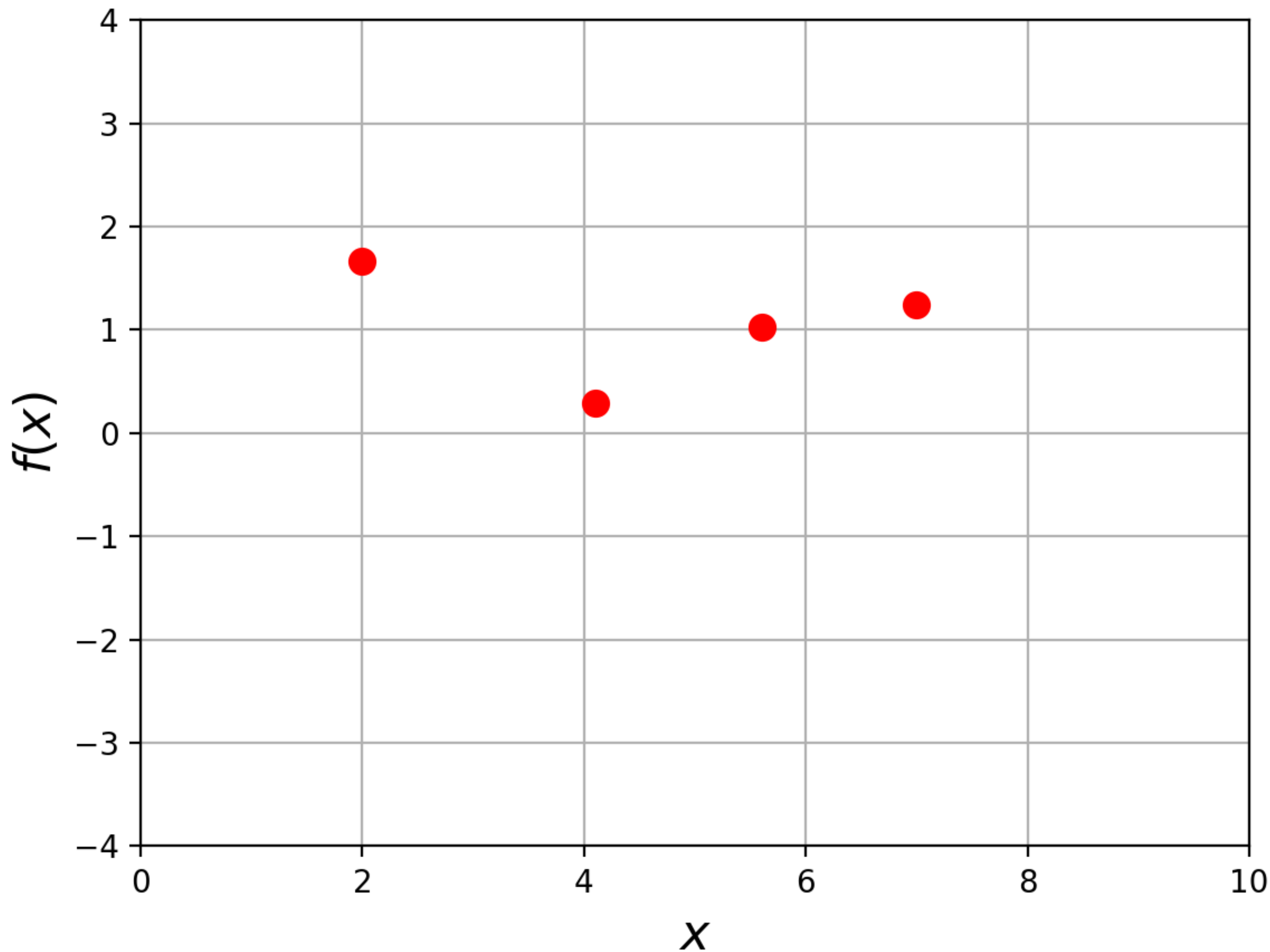
usually we know (guess) parameter domain



4
3
2
1
0
−1
−2
−3
−4
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Scenario: the function f that we wish to minimize is expensive to evaluate, and its exact functional form is unavailable for whatever reason.

No more information is available to us.

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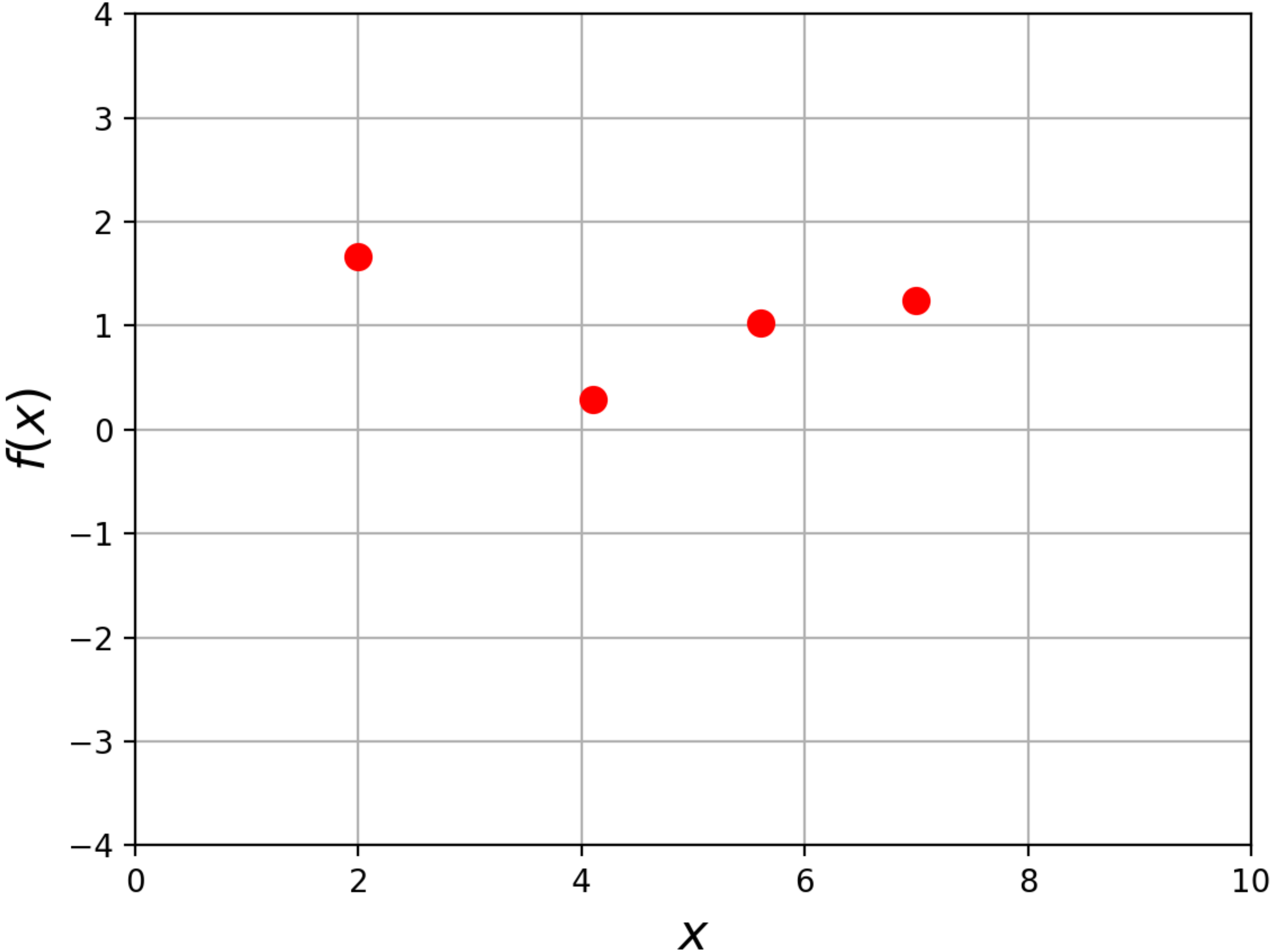

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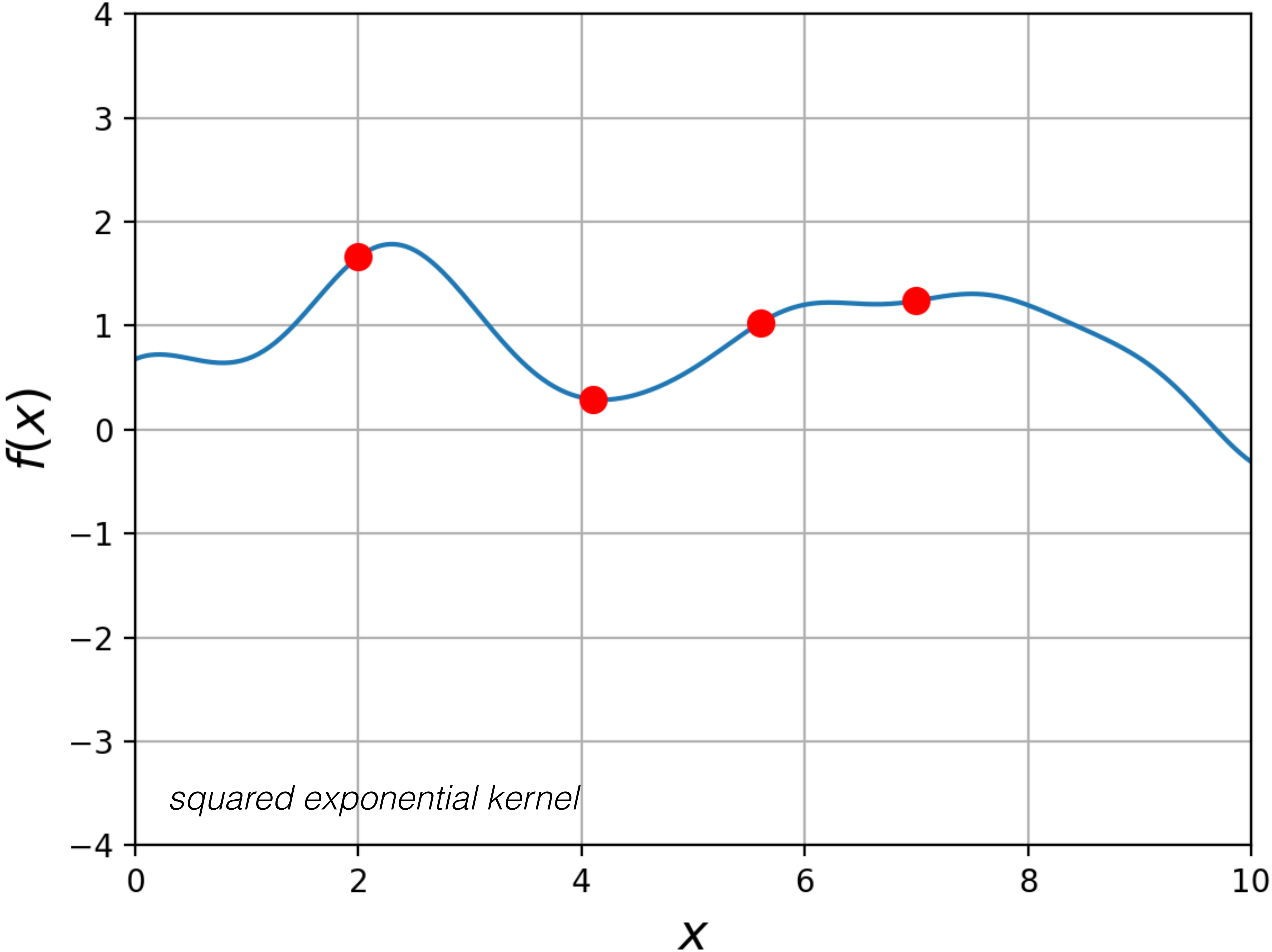
$f(x)$


4
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f(x)
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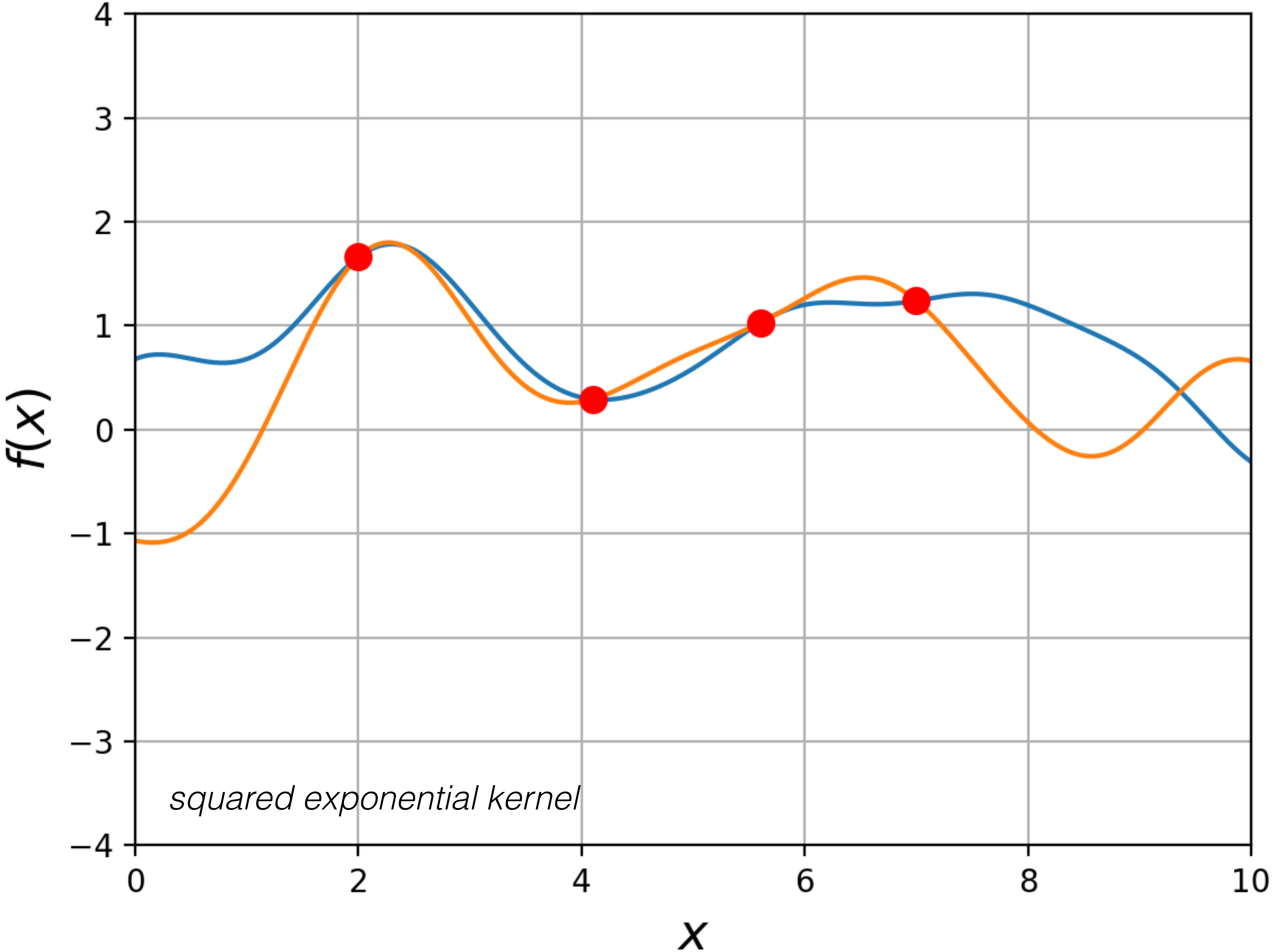
x
squared exponential kernel



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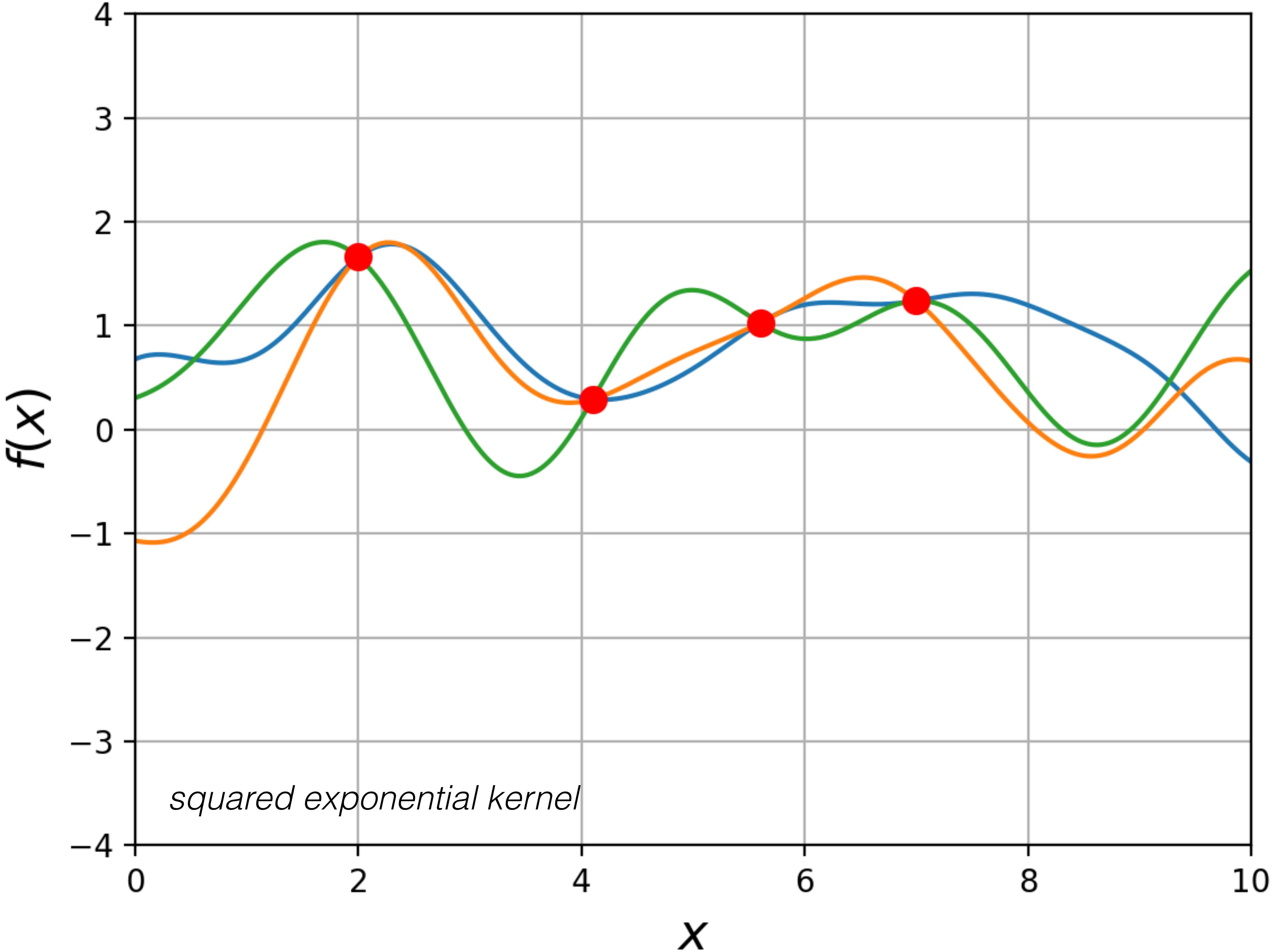

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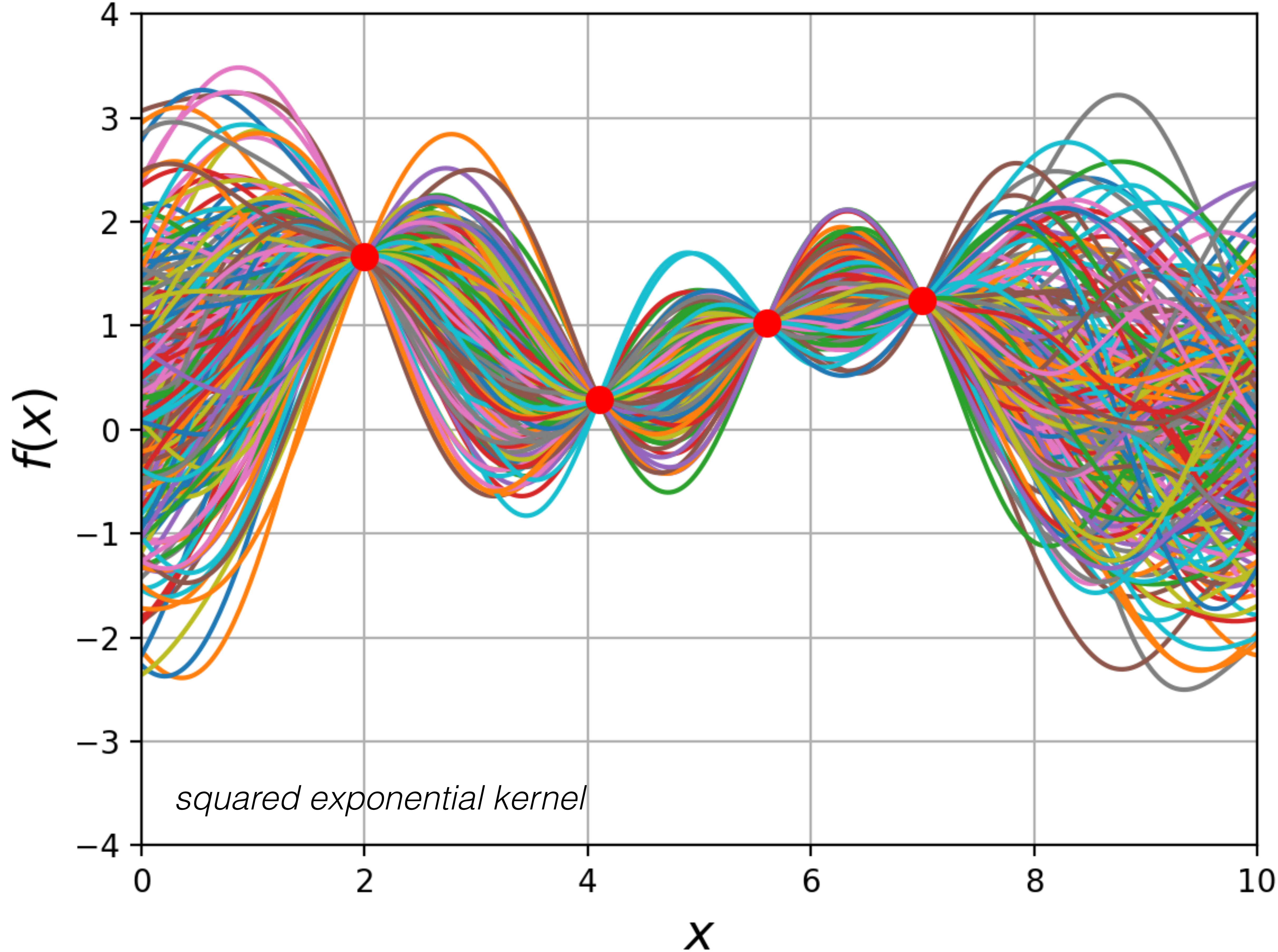

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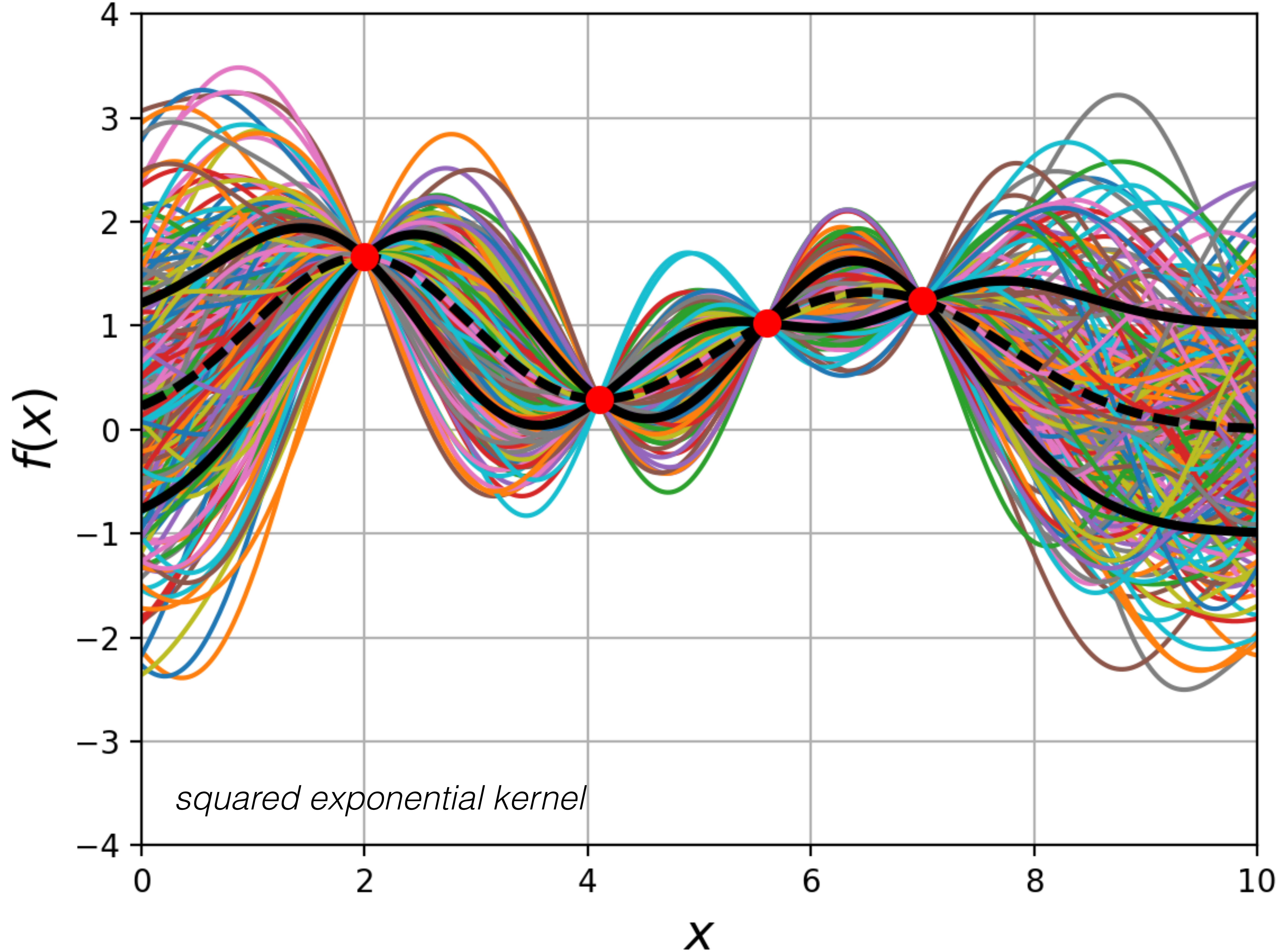

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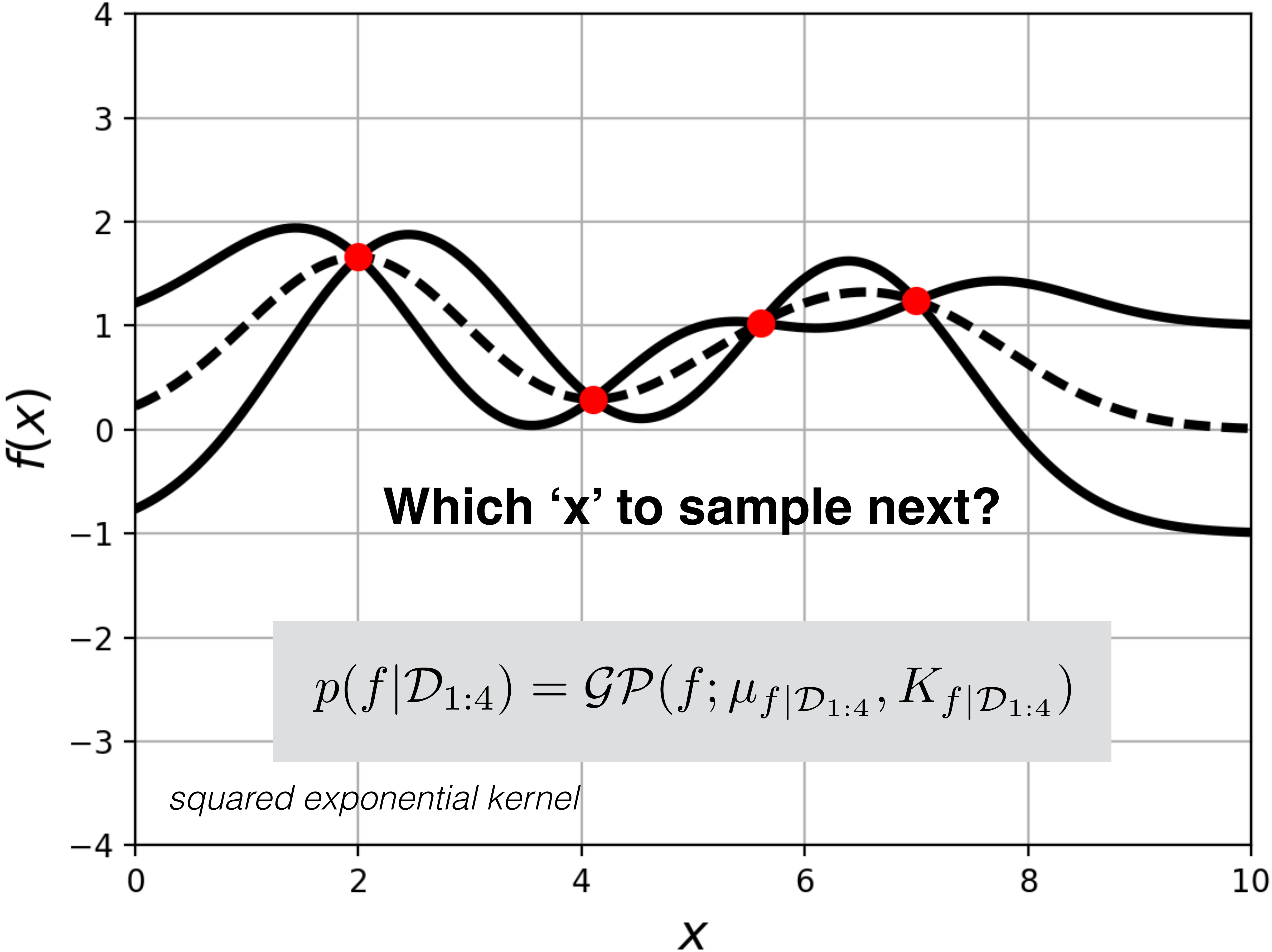
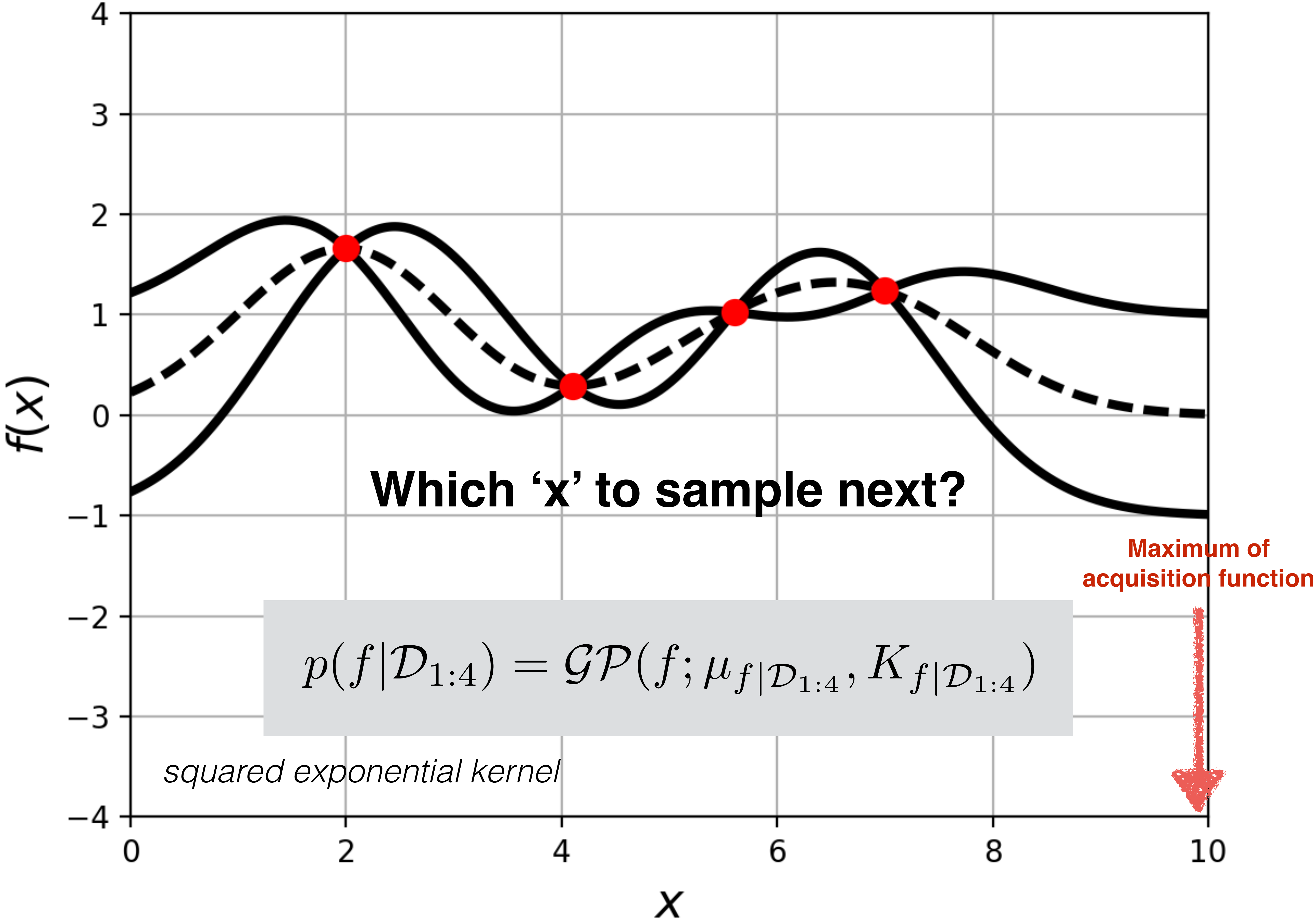


$$p(f|\mathcal{D}_{1:4}) = \mathcal{GP}(f; \mu_{f|\mathcal{D}_{1:4}}, K_{f|\mathcal{D}_{1:4}})$$



4
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f(x)
x
Which 'x' to sample next?
Maximum of
acquisition function
$p(f|\mathcal{D}_{1:4}) = \mathcal{GP}(f; \mu_{f|\mathcal{D}_{1:4}}, K_{f|\mathcal{D}_{1:4}})$
squared exponential kernel

Expected Improvement (EI) acquisition function

utility function: $u(x) = \max(0, f_{\min} - f(x))$

We need to find the argmax of the acquisition function

$$x_{n+1} = \operatorname{argmax} \mathcal{A}(x)$$

$$\mathcal{A}(x) = \langle u(x) \rangle = \int_{f(x)} \max(0, f_{\min} - f(x)) p(f(x)|\mathcal{D}_{1:n})\, df$$

$$= (f_{\min} - \mu(x)_{\mathcal{D}})\Phi\left(\frac{f_{\min} - \mu(x)_{\mathcal{D}}}{\sigma(x)_{\mathcal{D}}}\right) + \sigma(x)_{\mathcal{D}}\mathcal{N}\left(\frac{f_{\min} - \mu(x)_{\mathcal{D}}}{\sigma(x)_{\mathcal{D}}}; 0, 1\right)$$

Exploitation

sampling areas of likely improvement

Exploration

sampling areas of high uncertainty

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Too much => local minimization

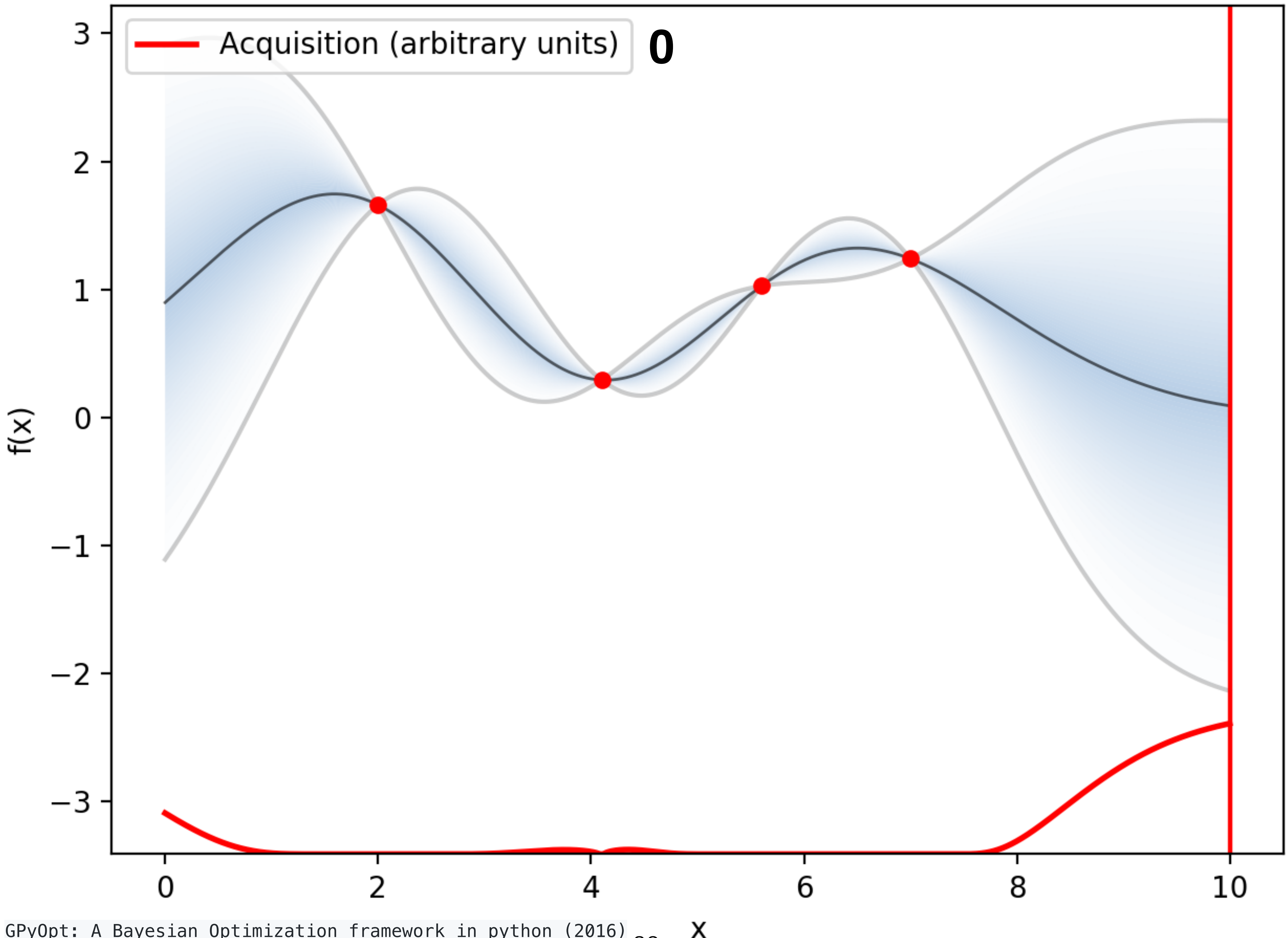
Exploitation

sampling areas of likely improvement

Exploration

sampling areas of high uncertainty

Too much => wasted iterations



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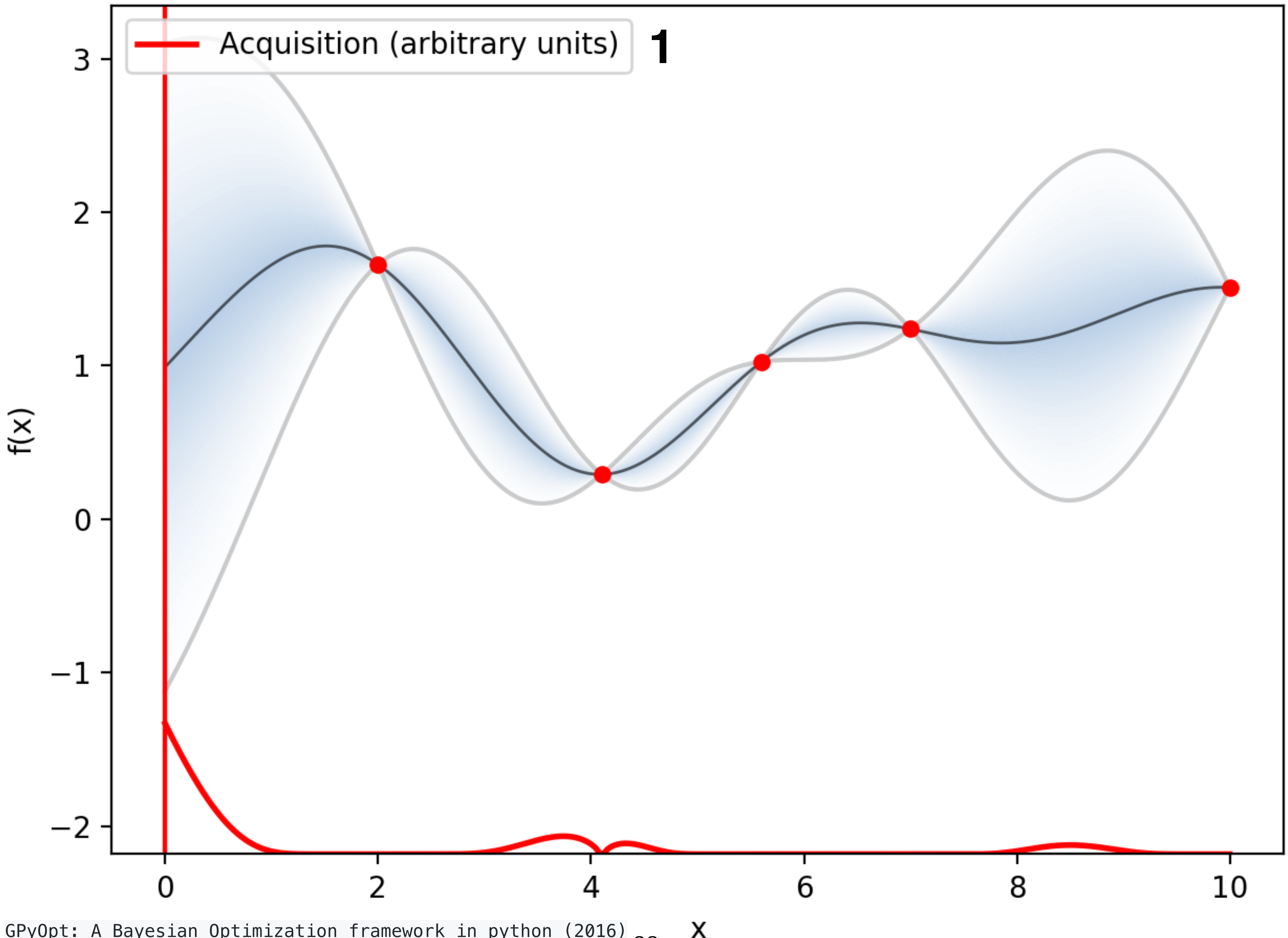

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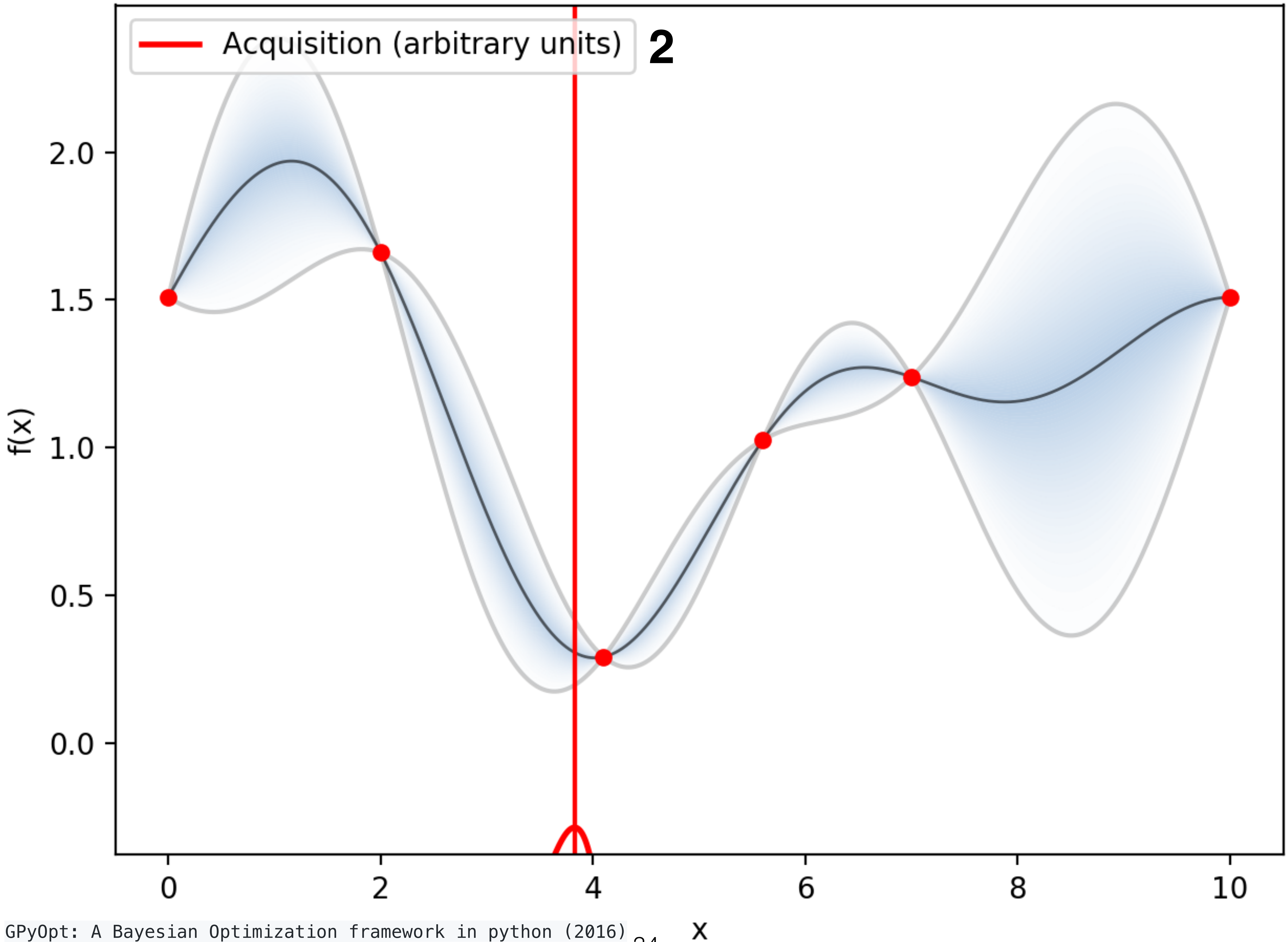

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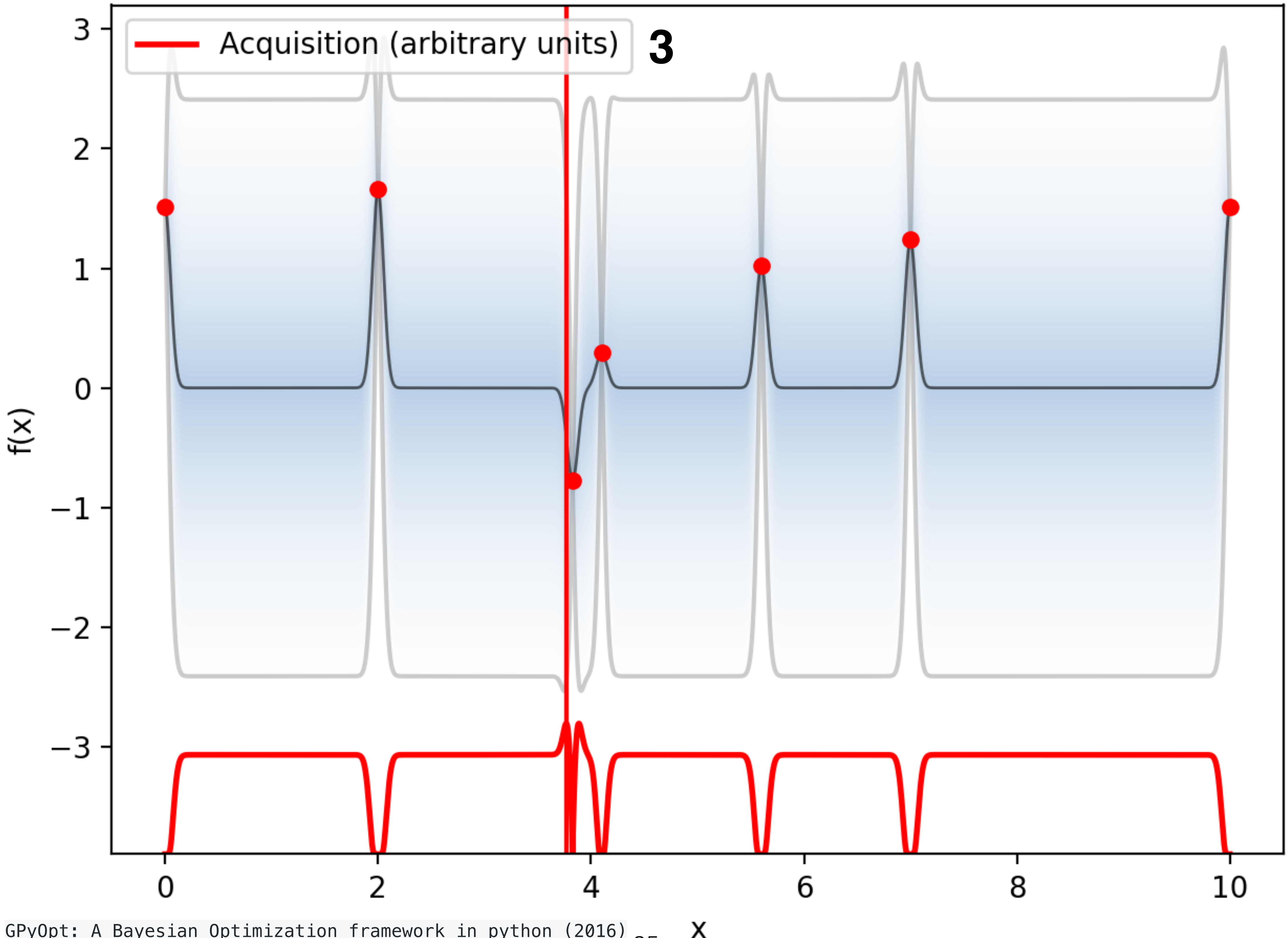

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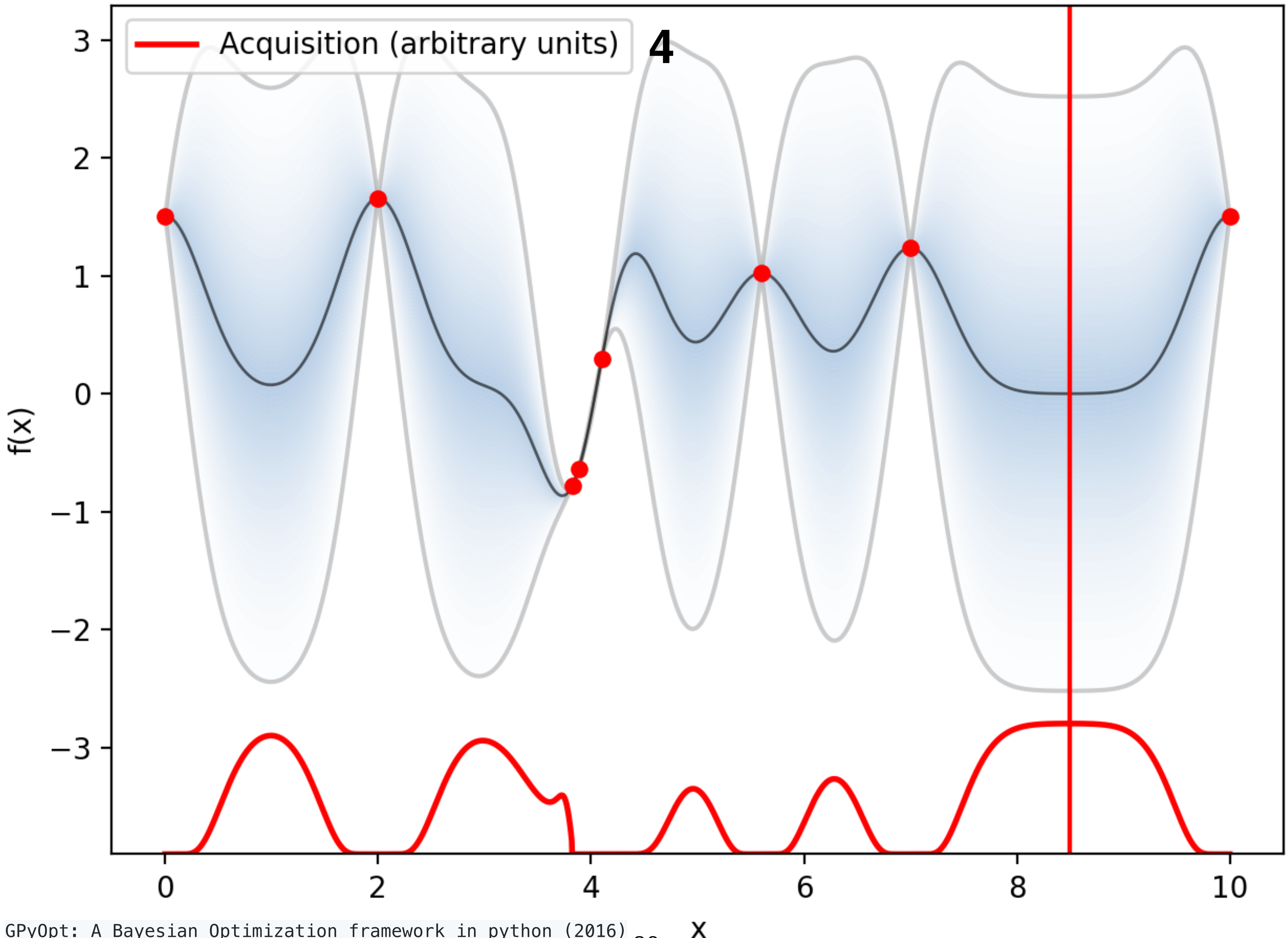

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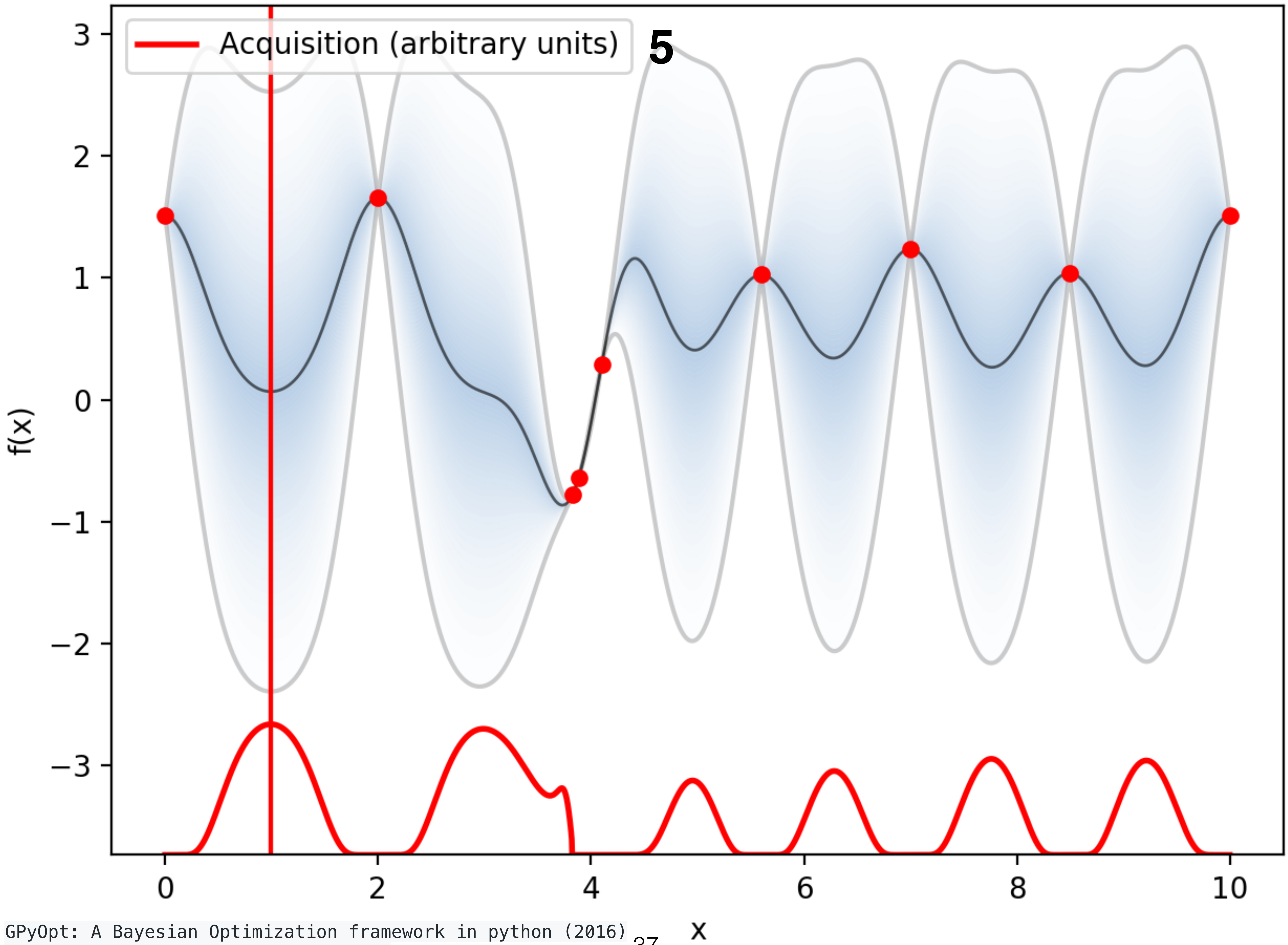

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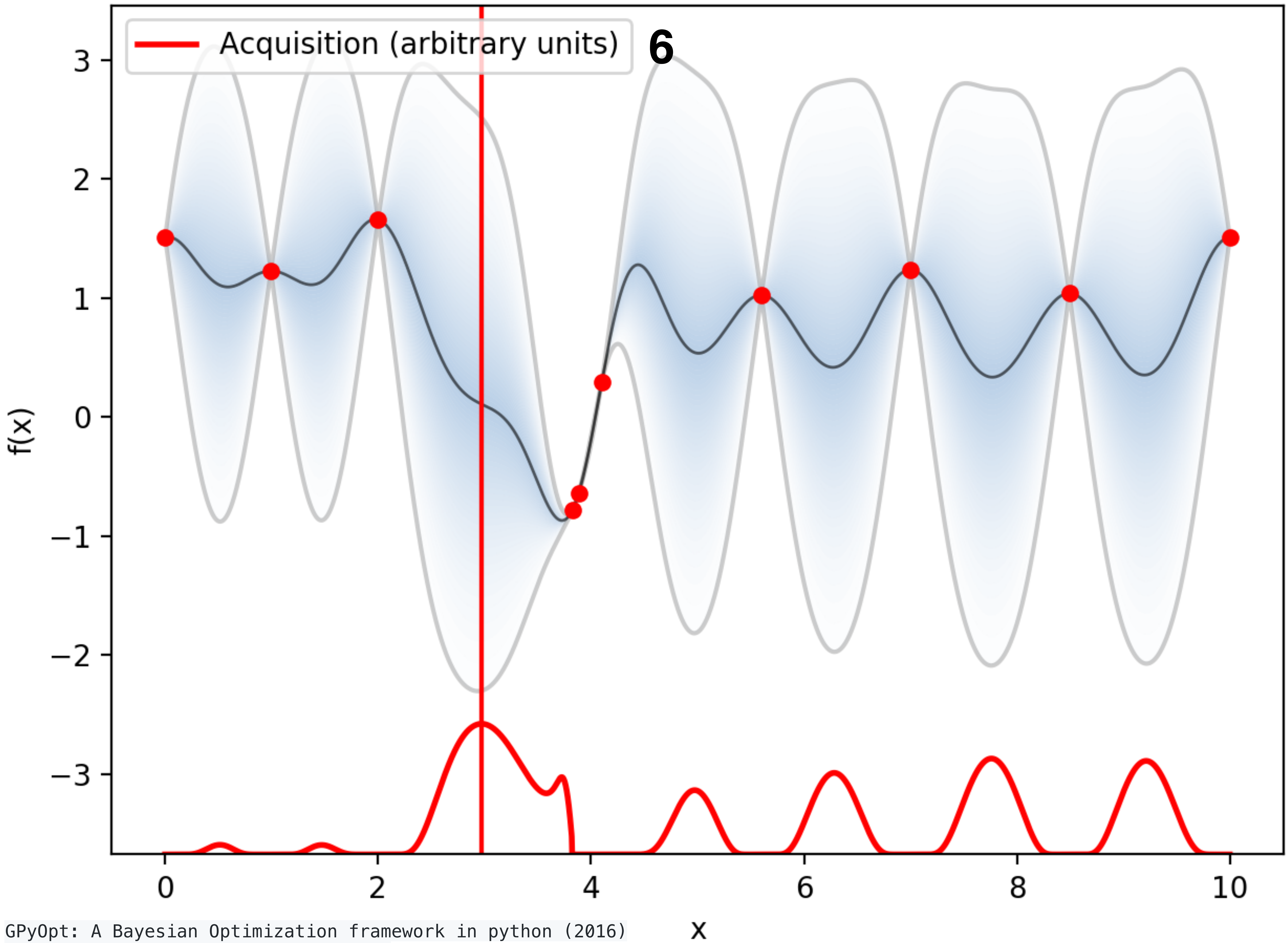

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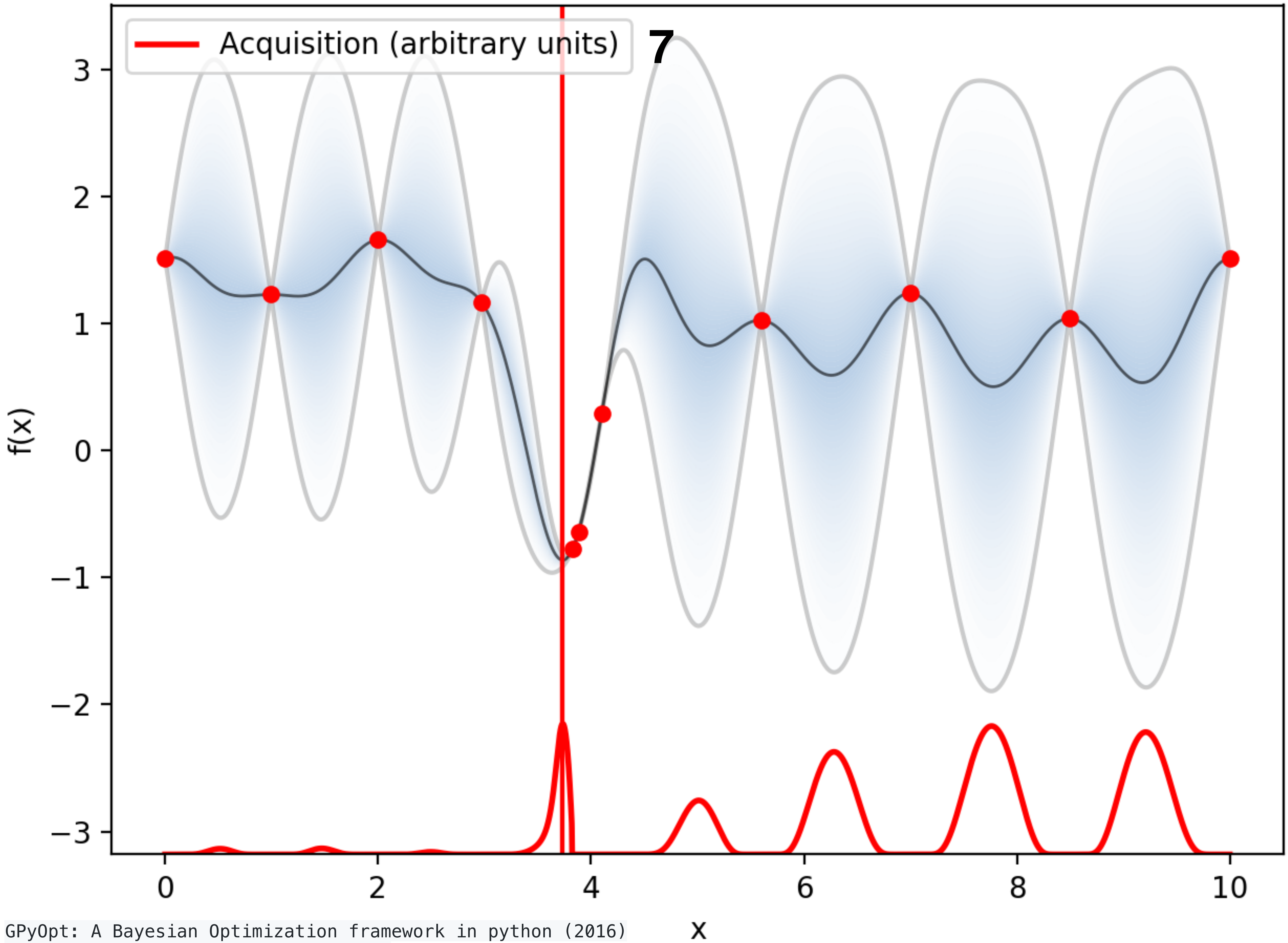

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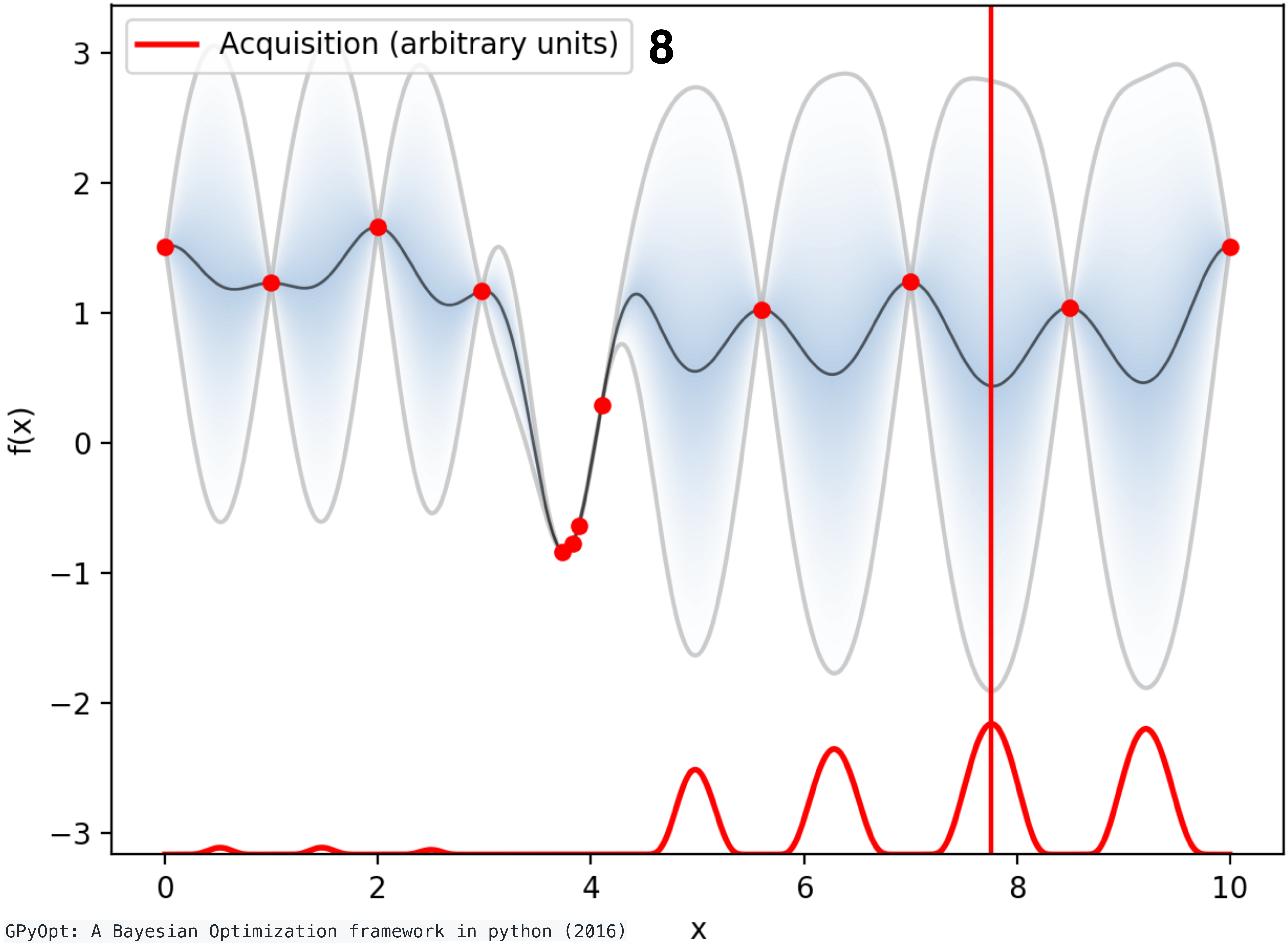

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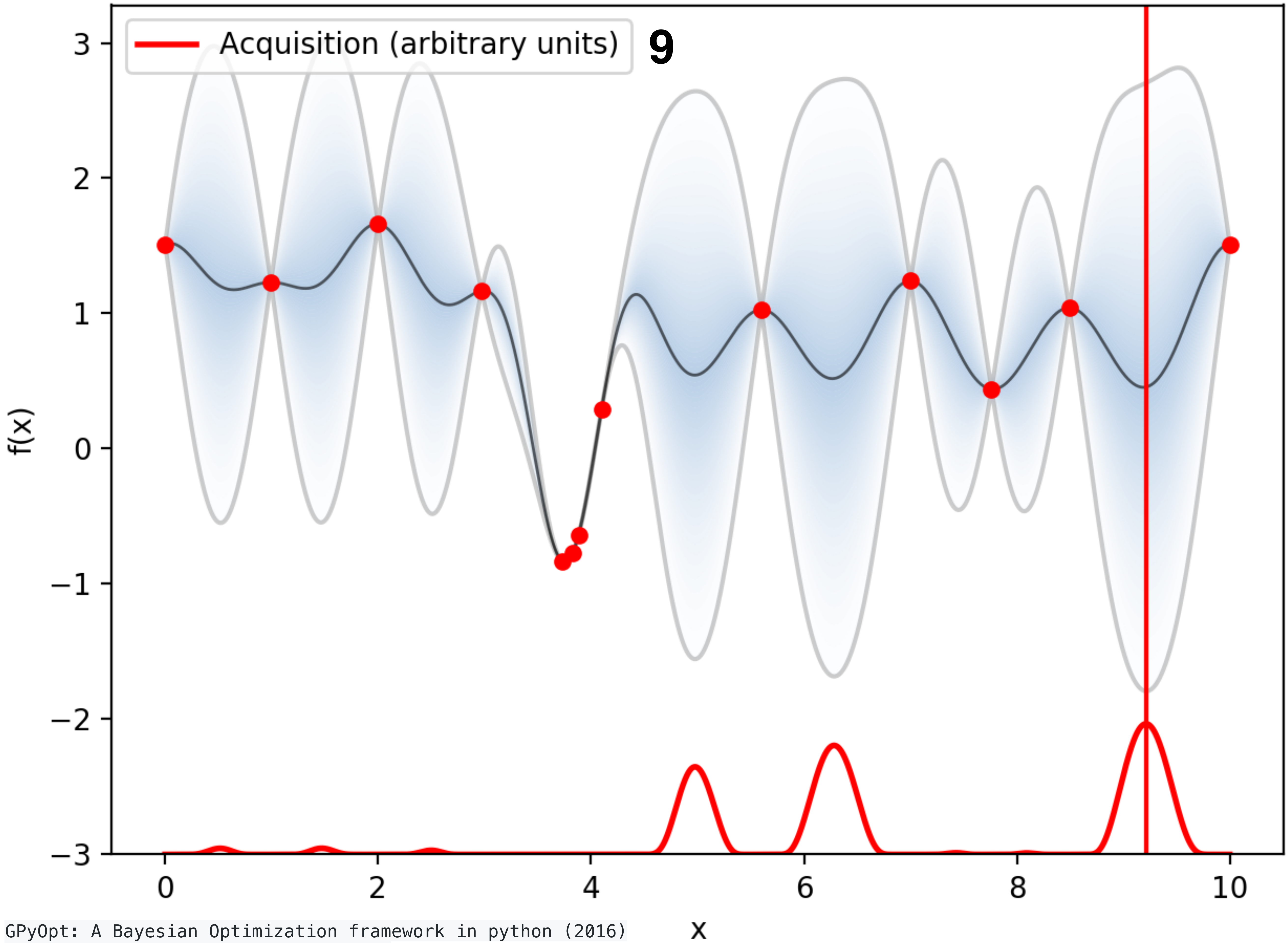

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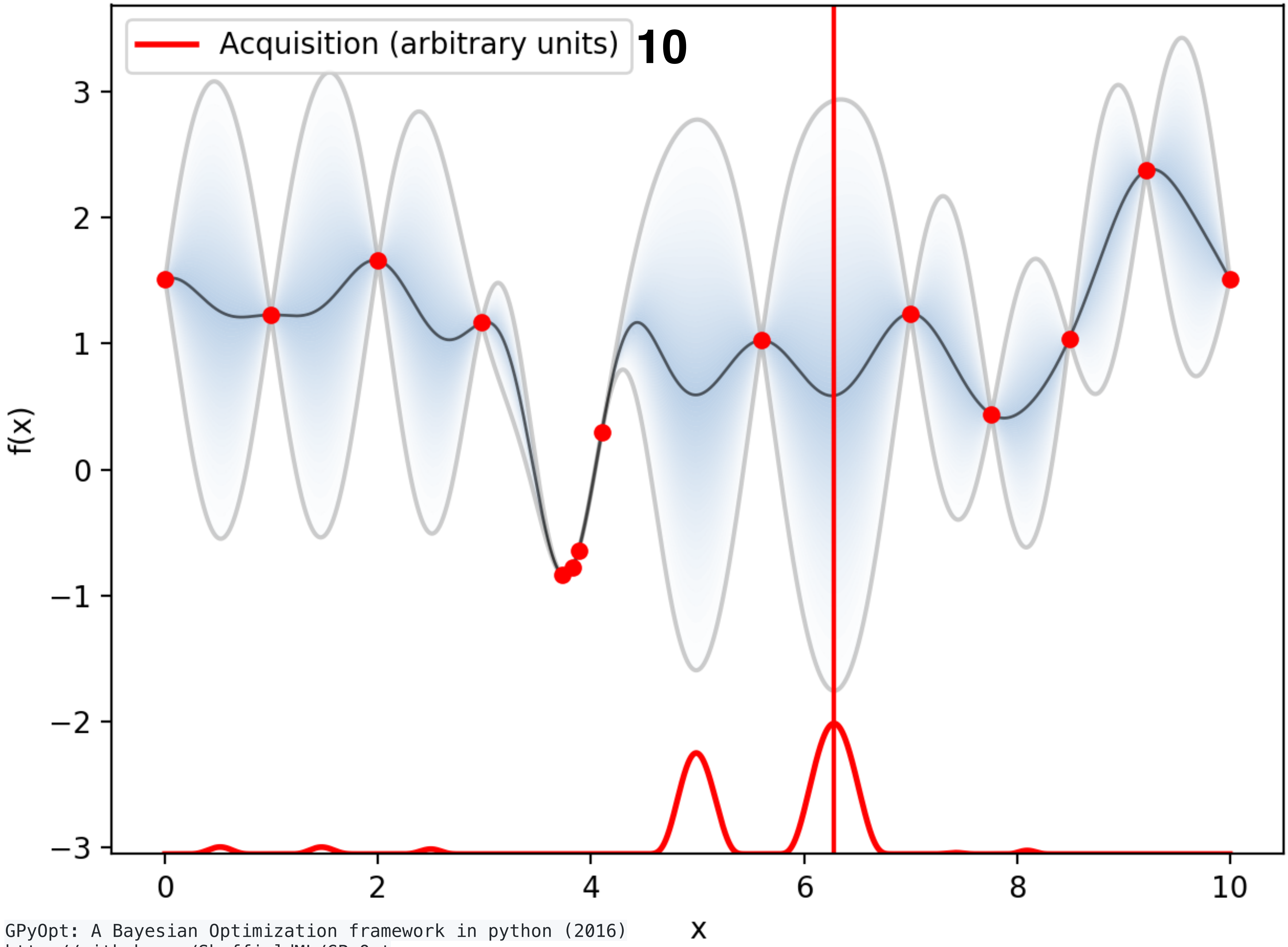

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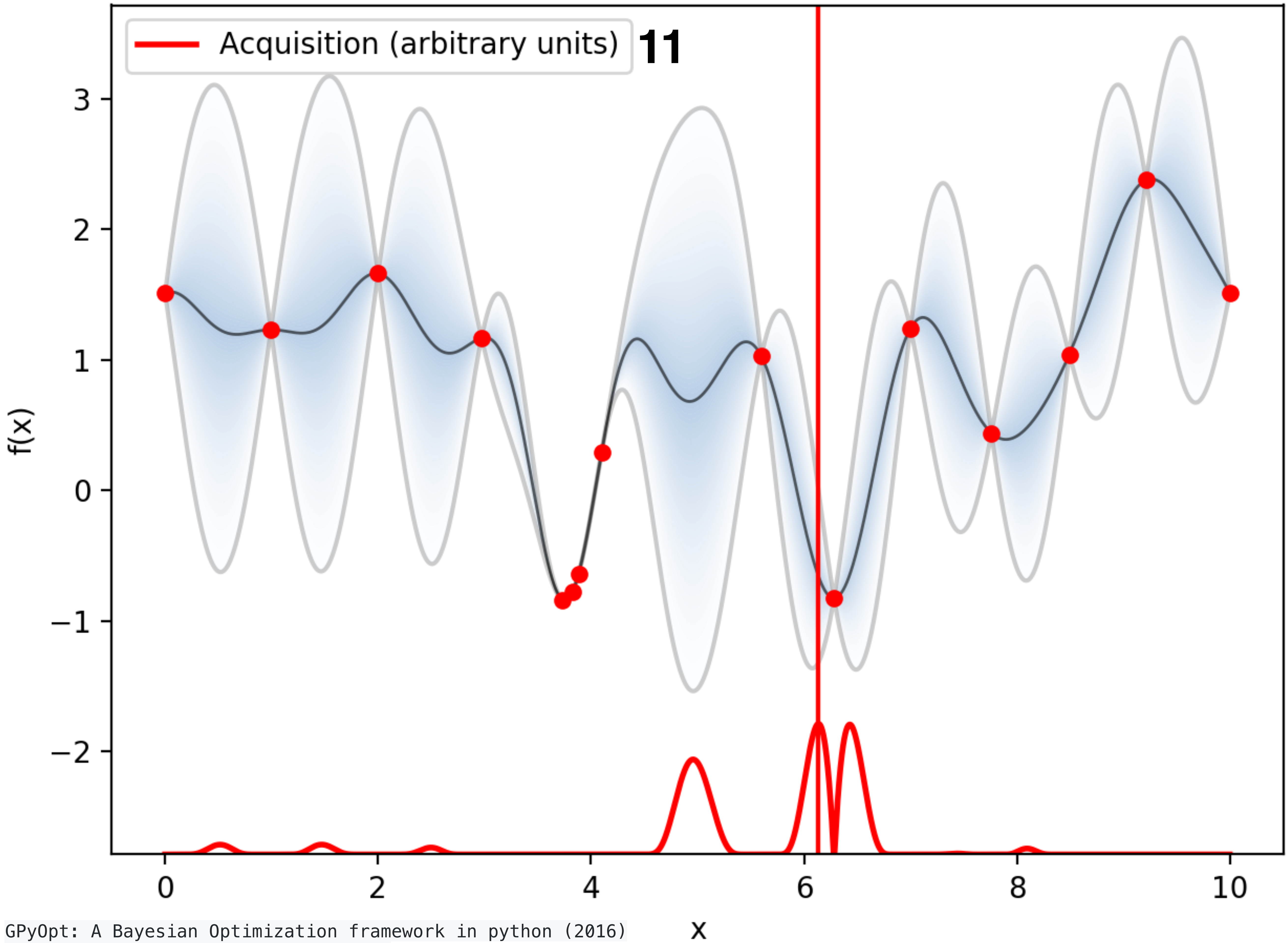

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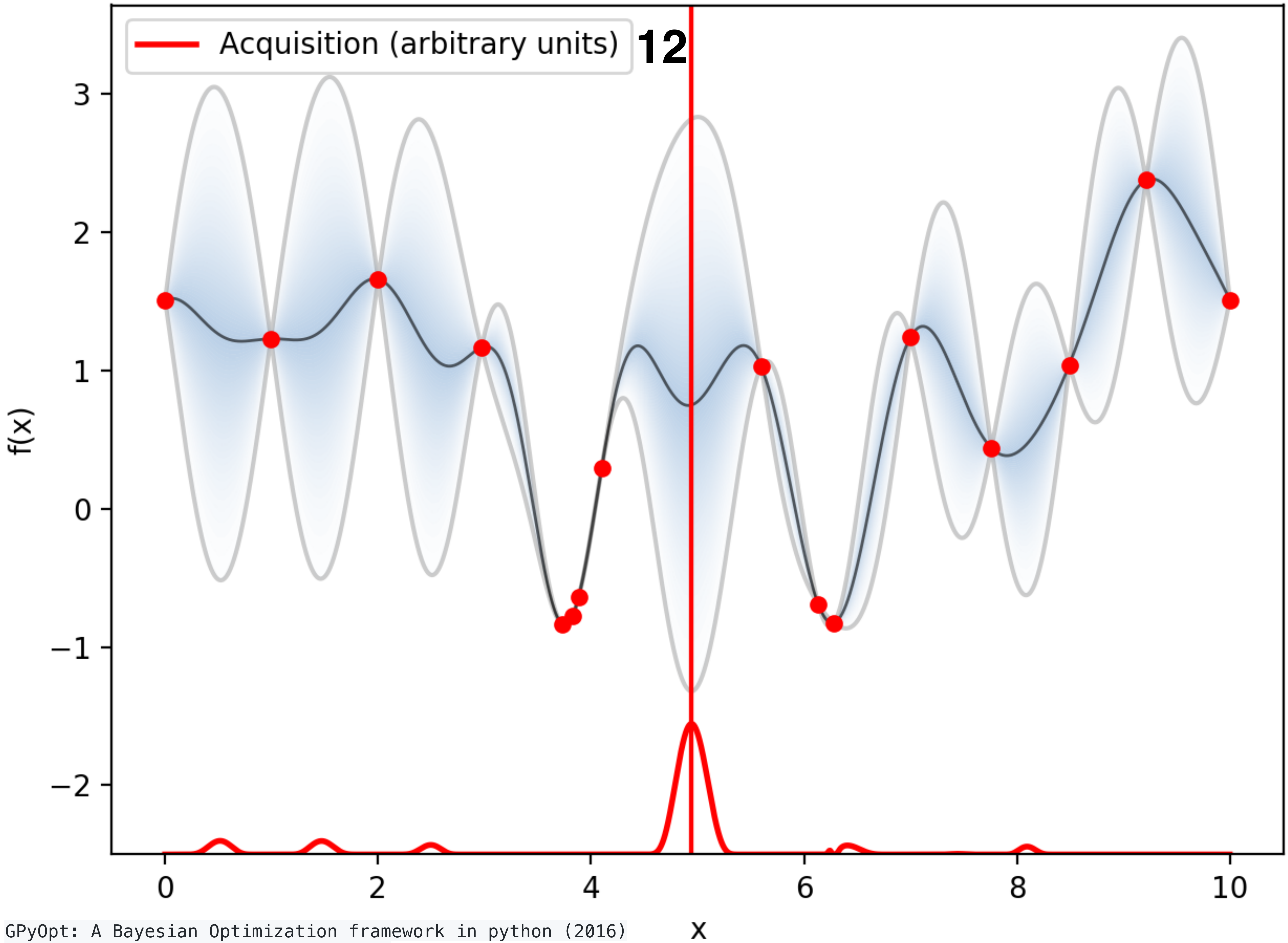

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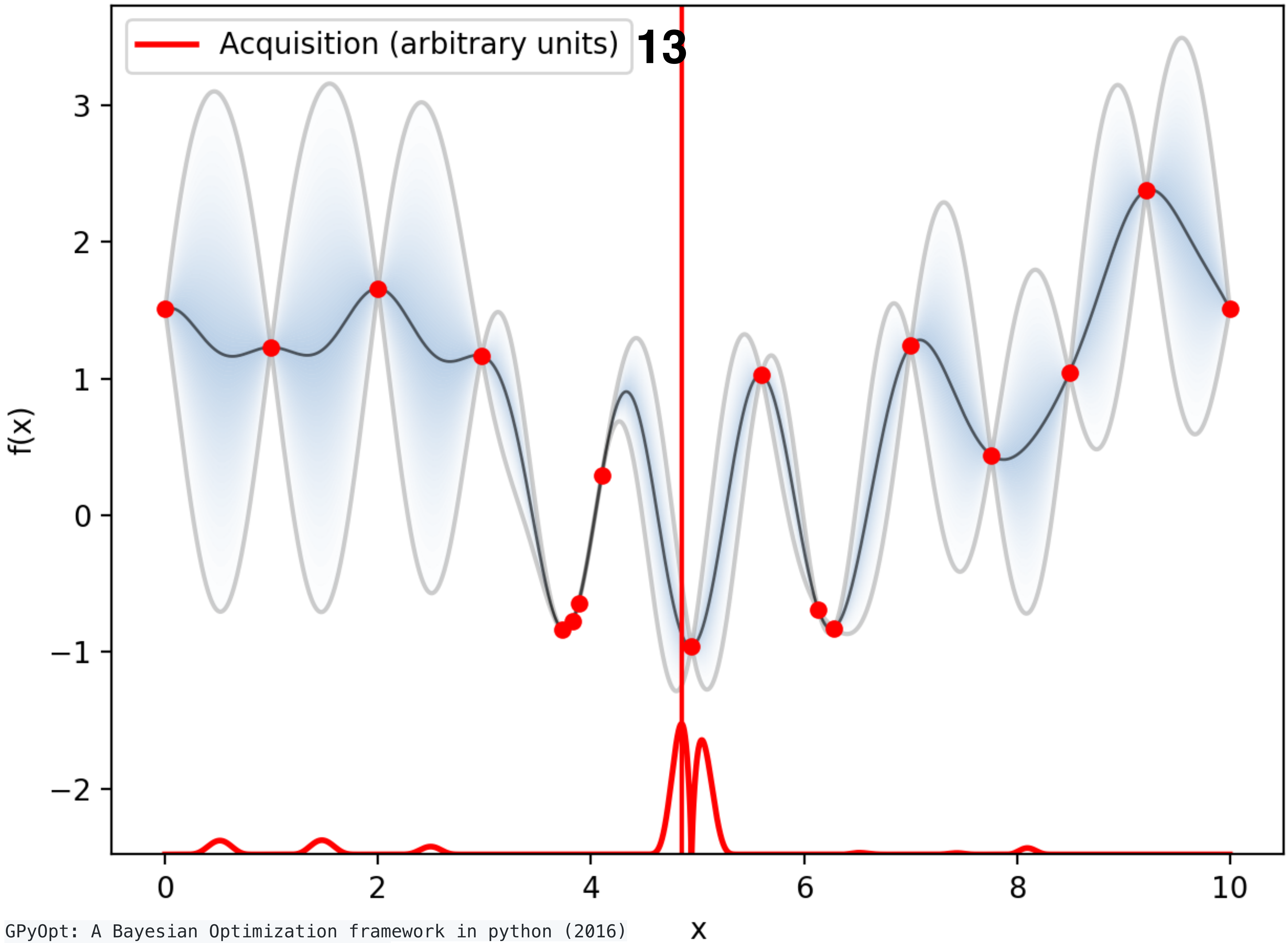

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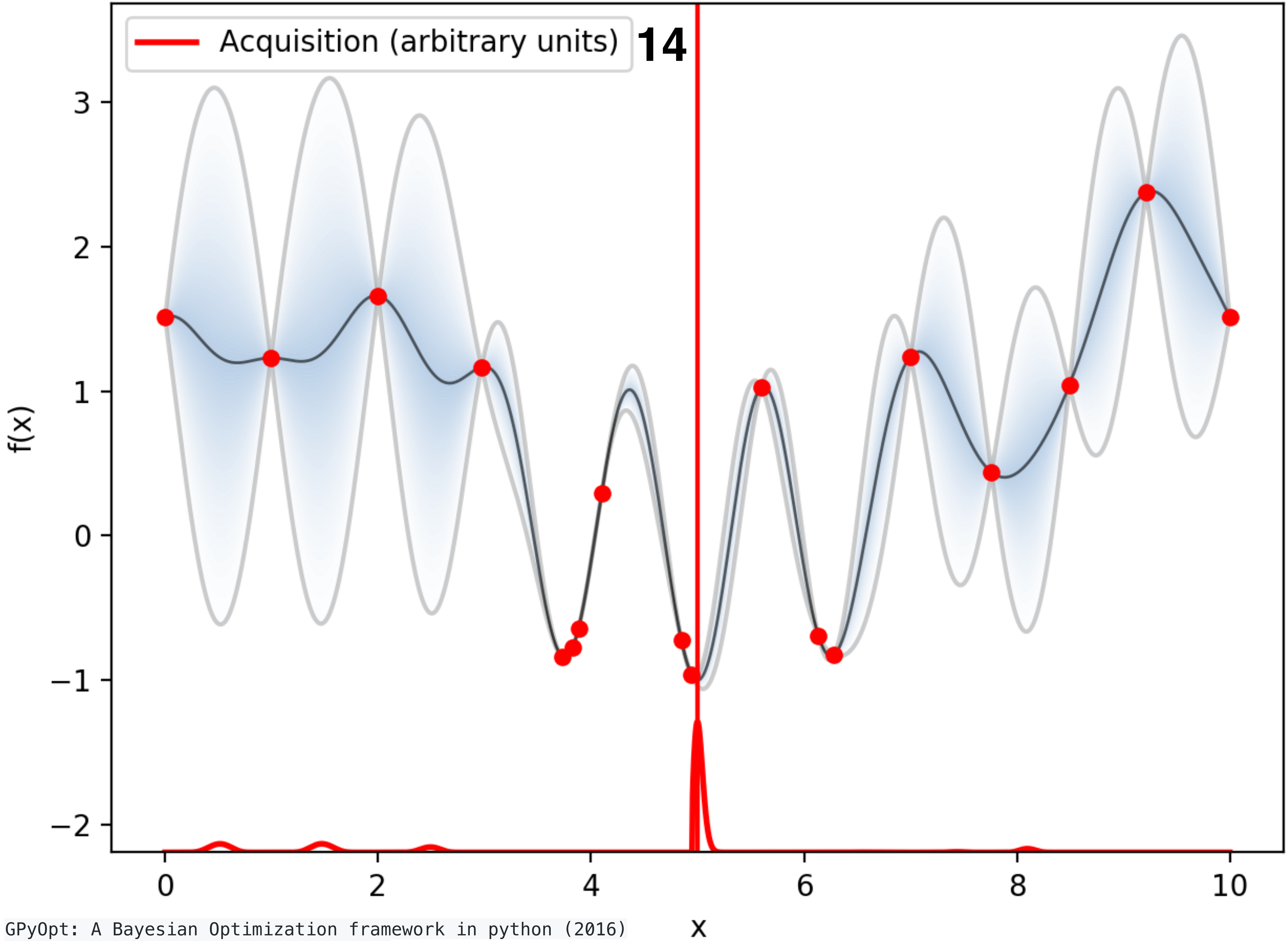

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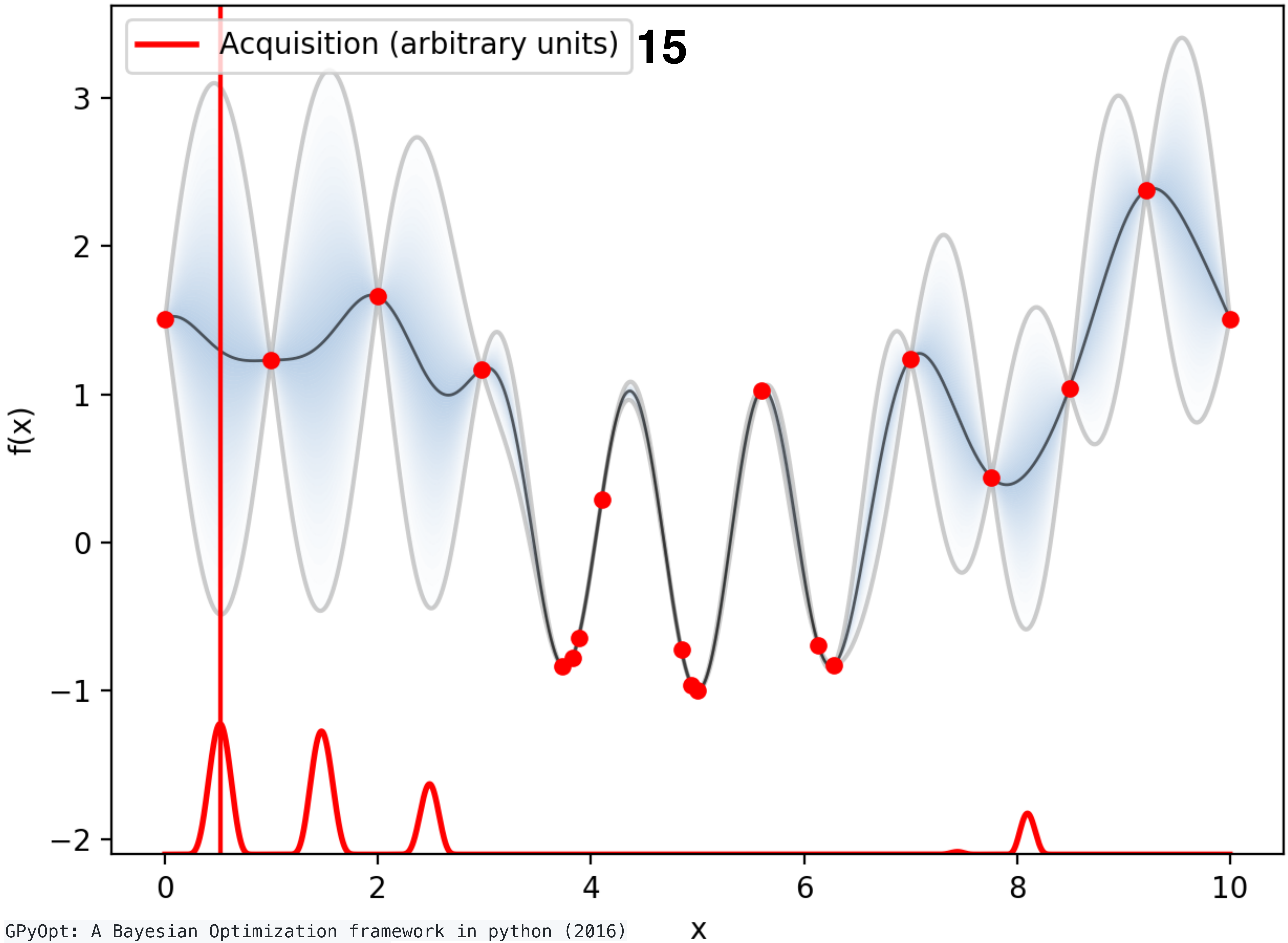

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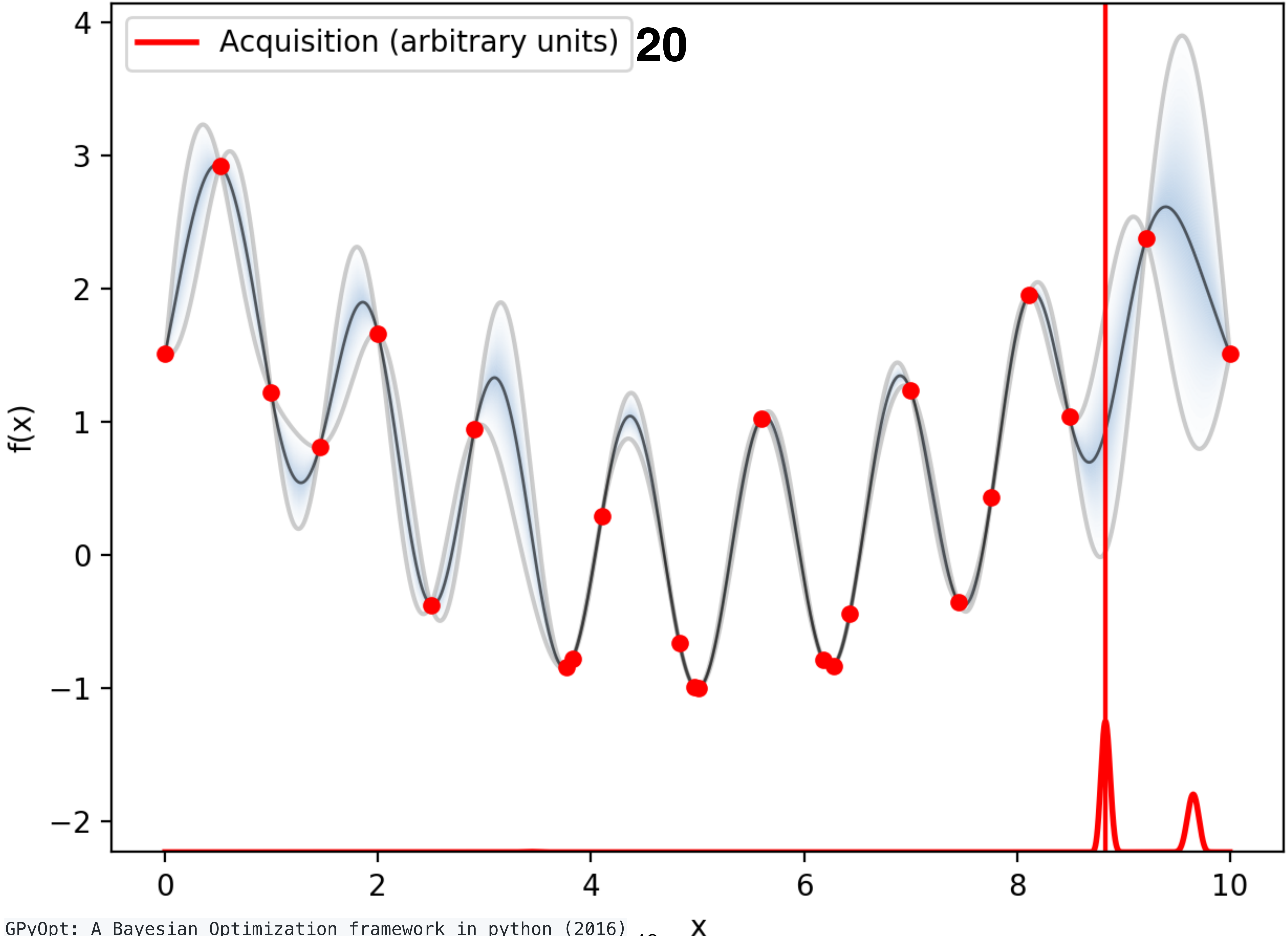

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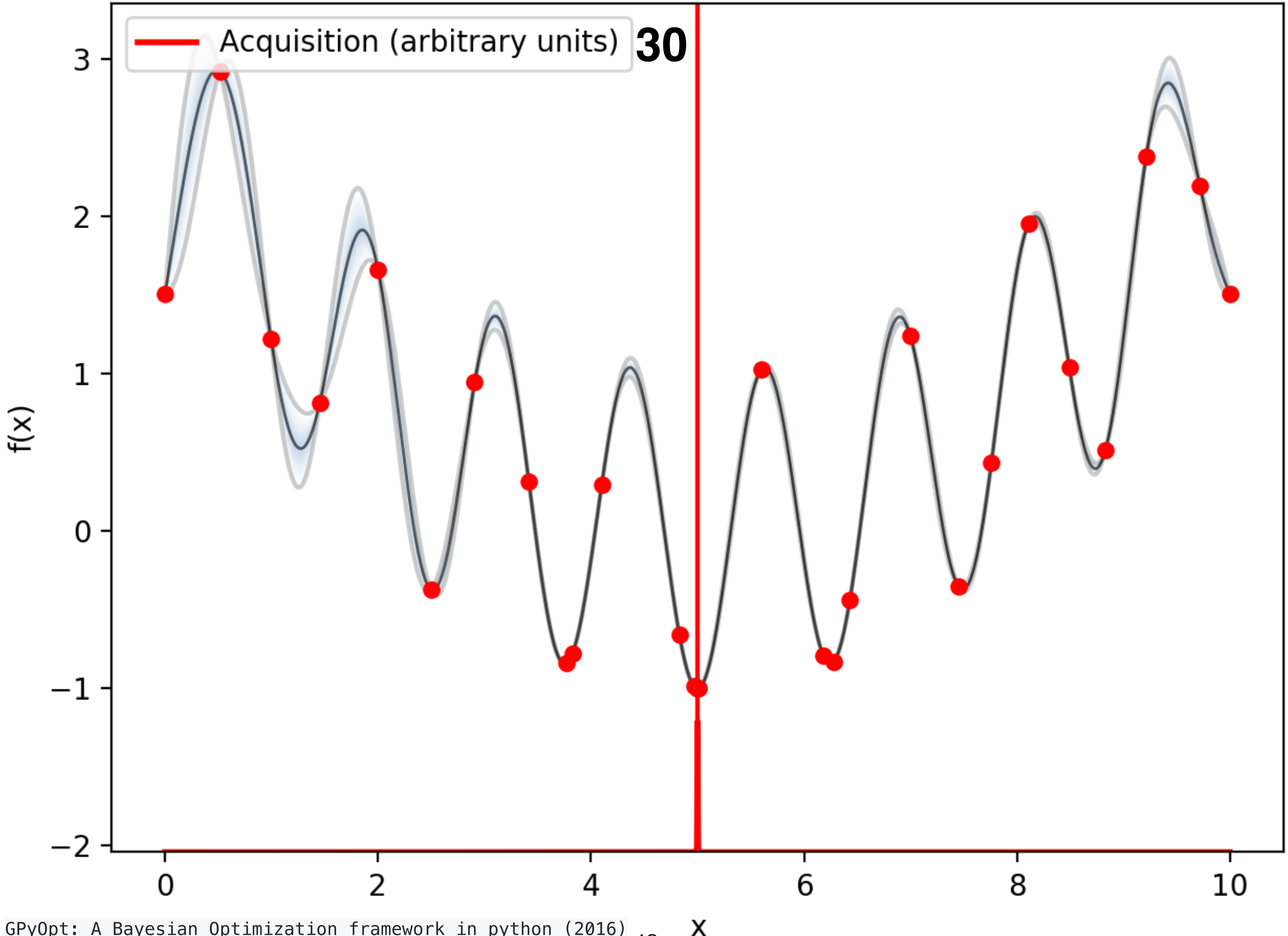

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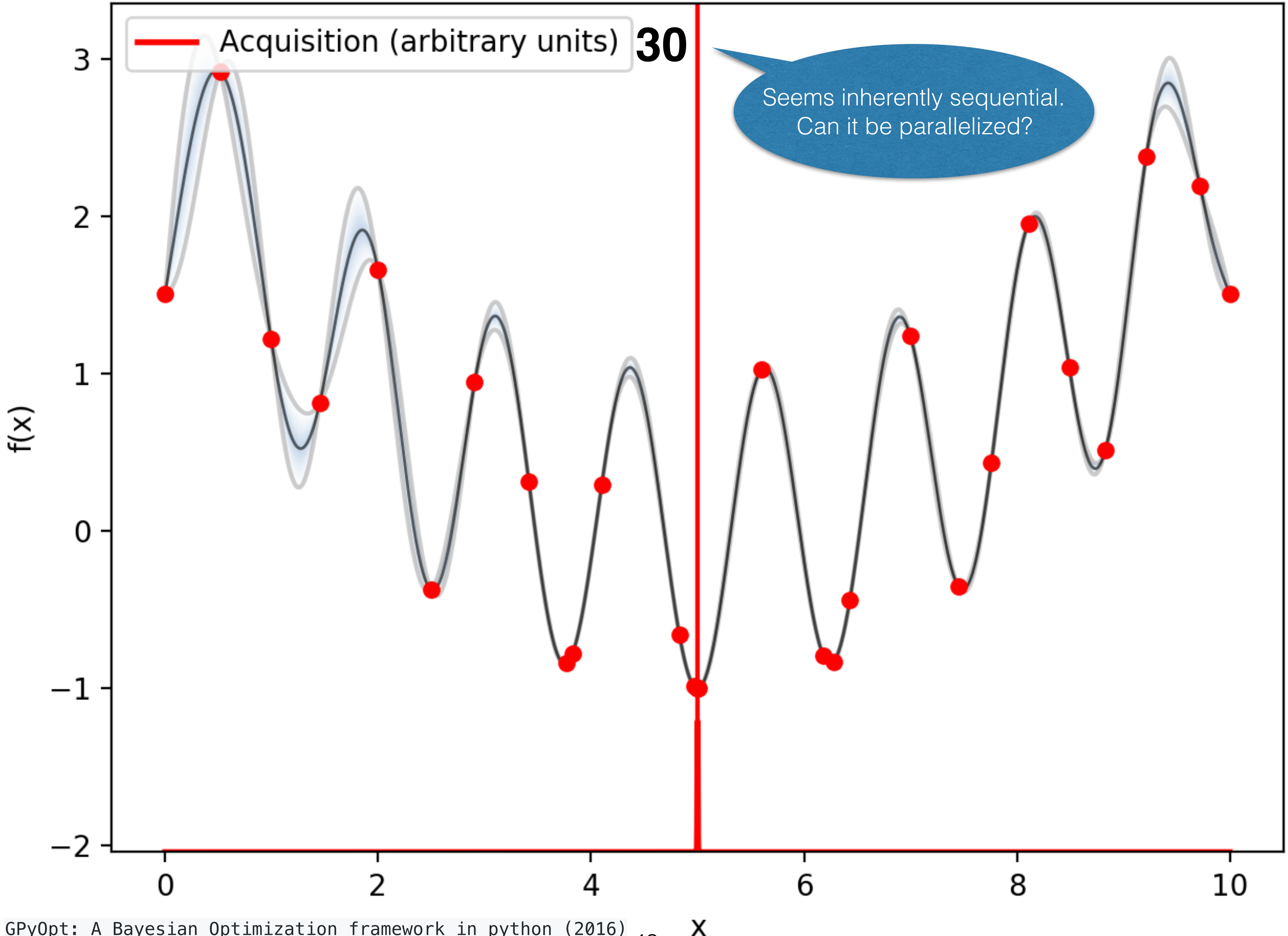

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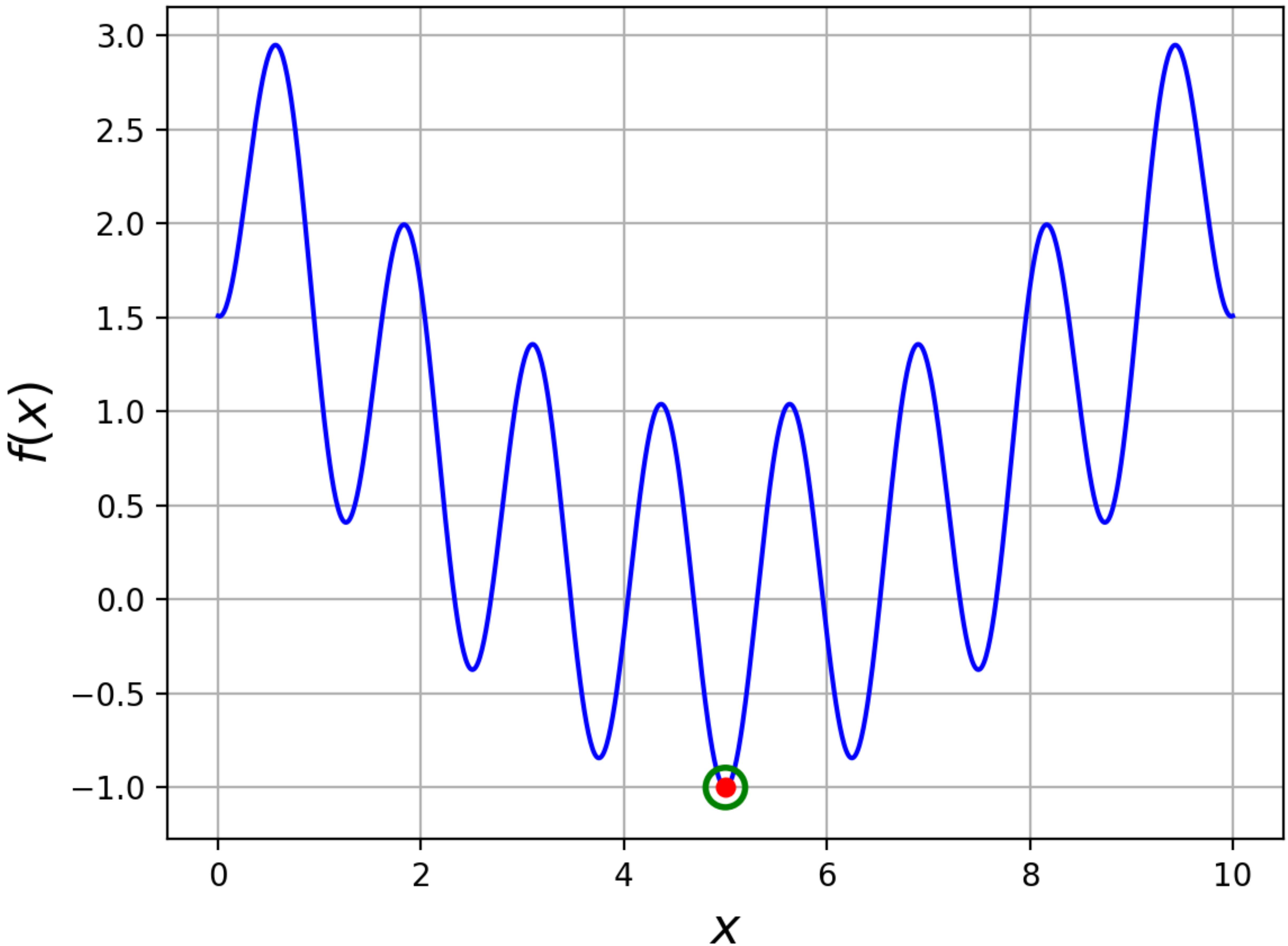
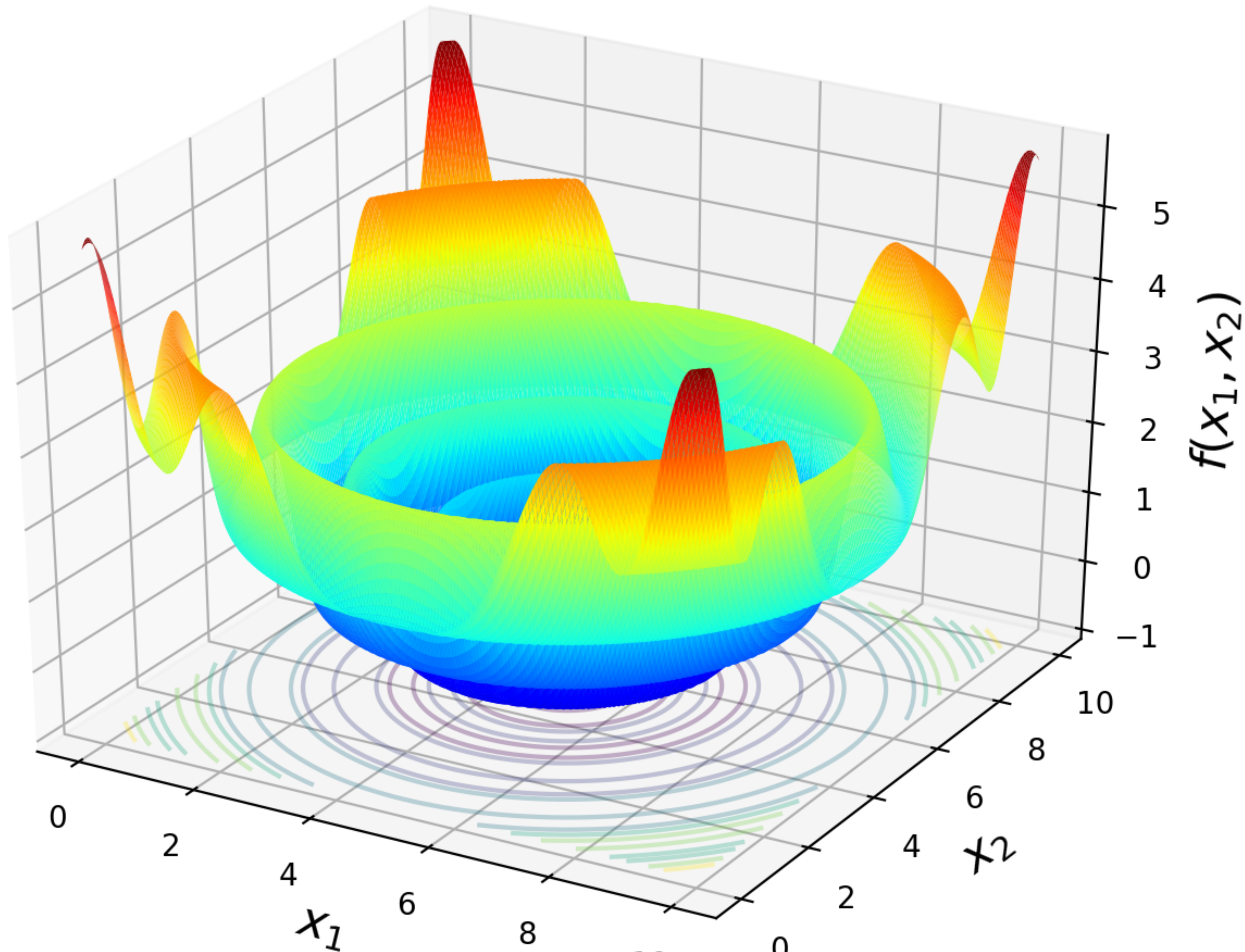
DeflectedCorrugatedSpring

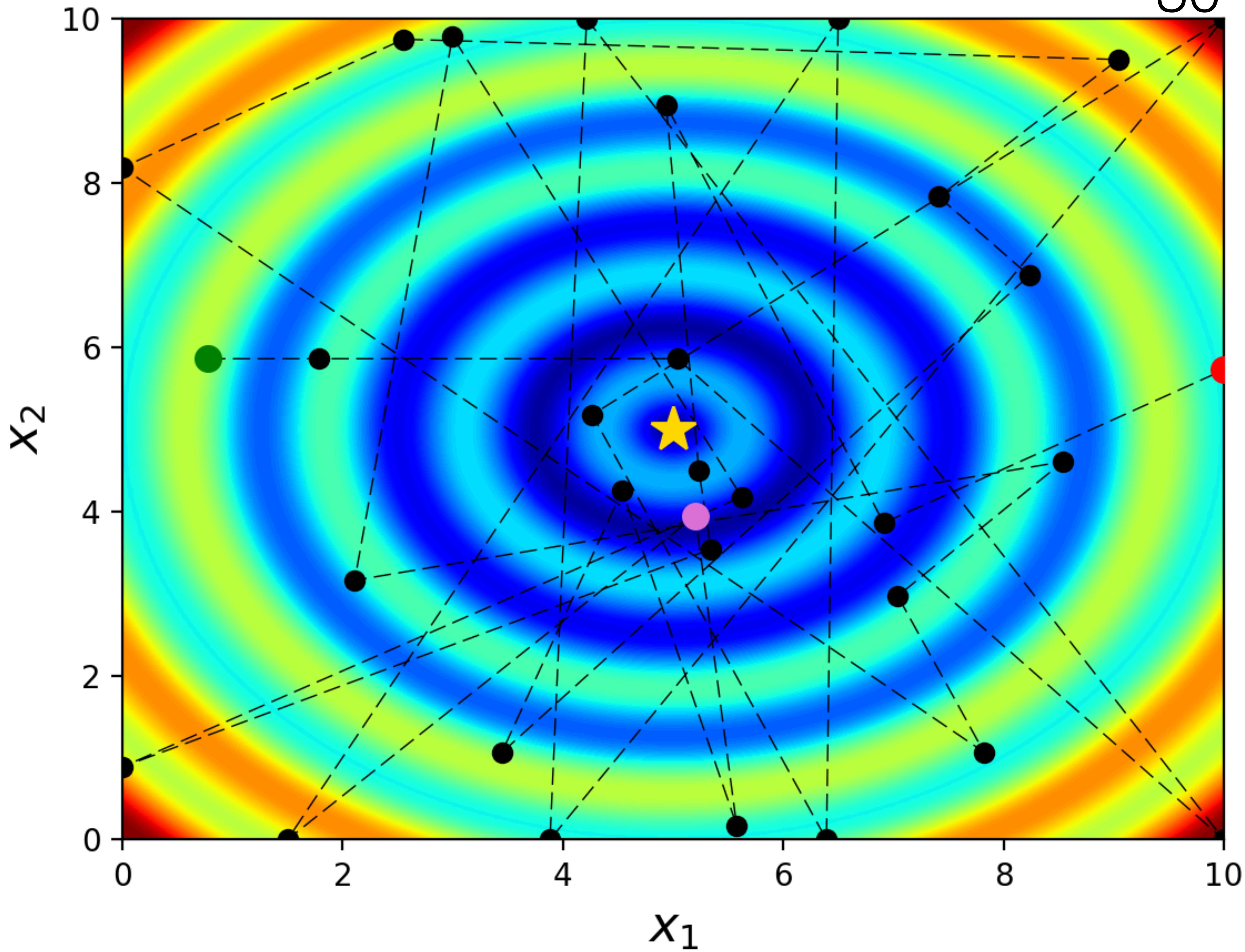


N-dim more challenging



N-dim more challenging

30



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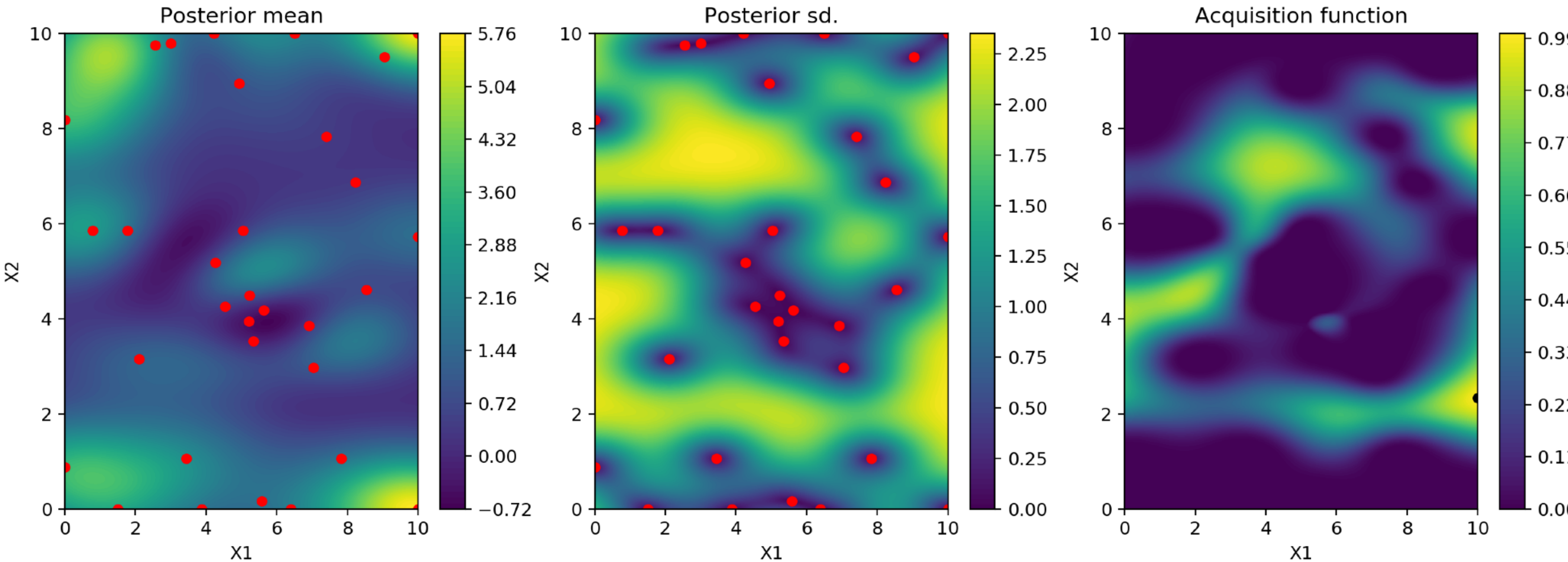

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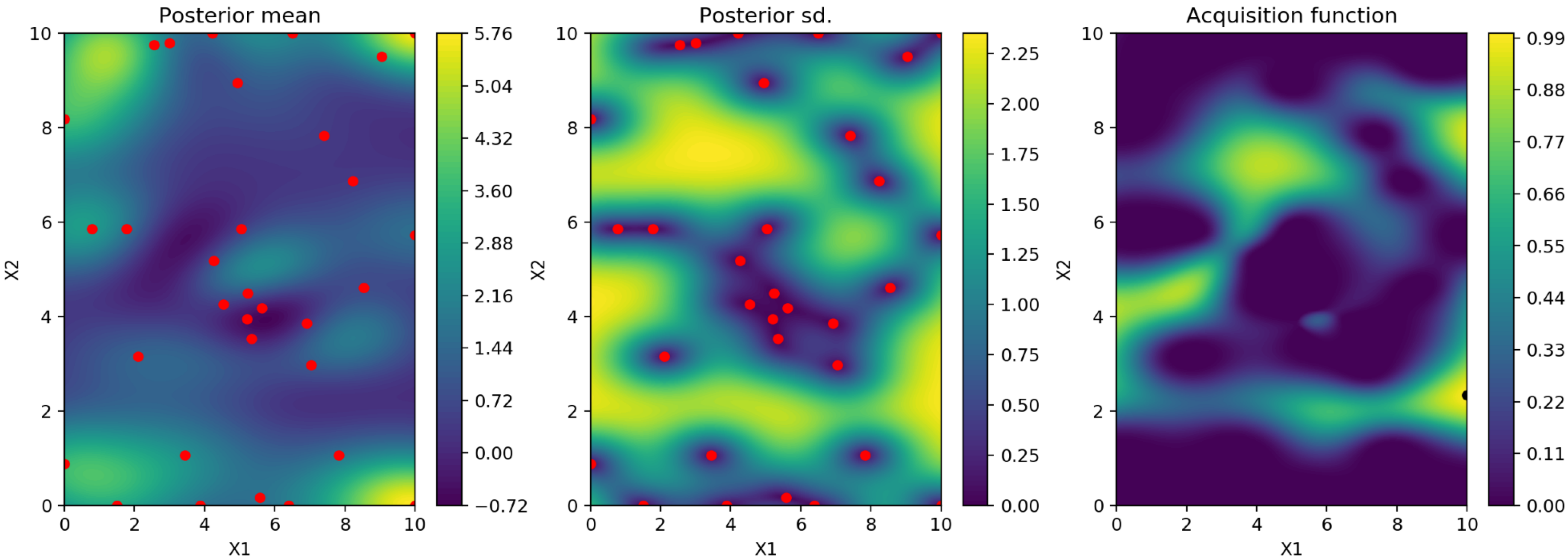

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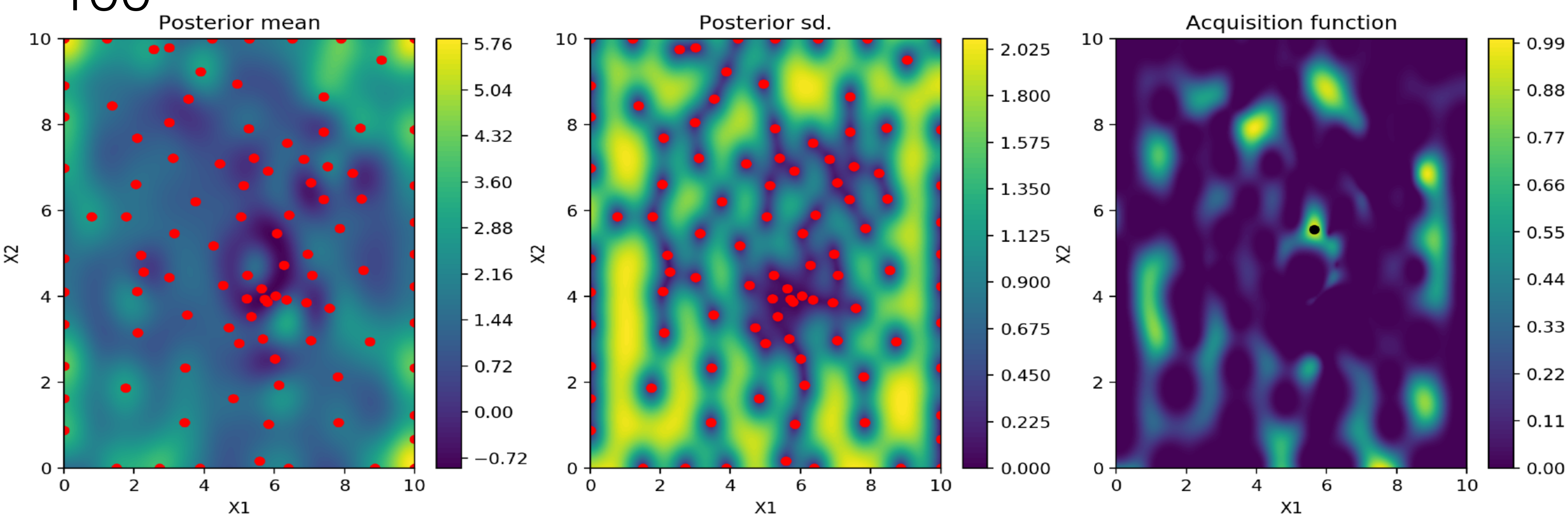

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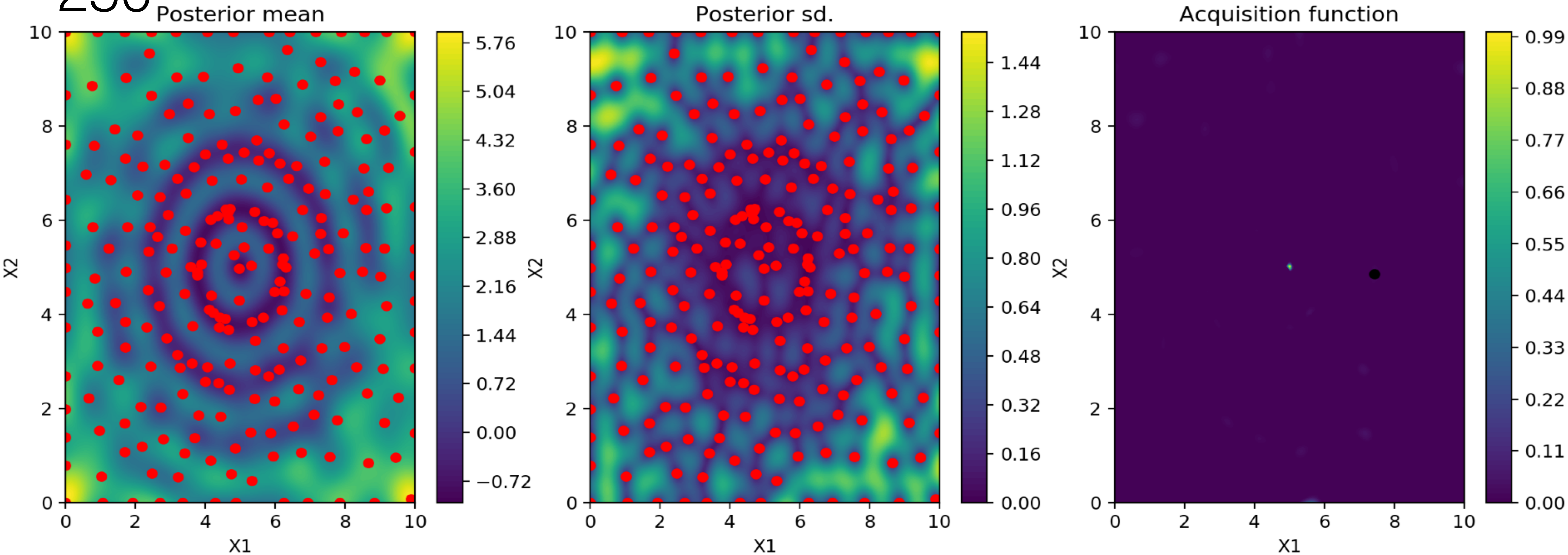
250



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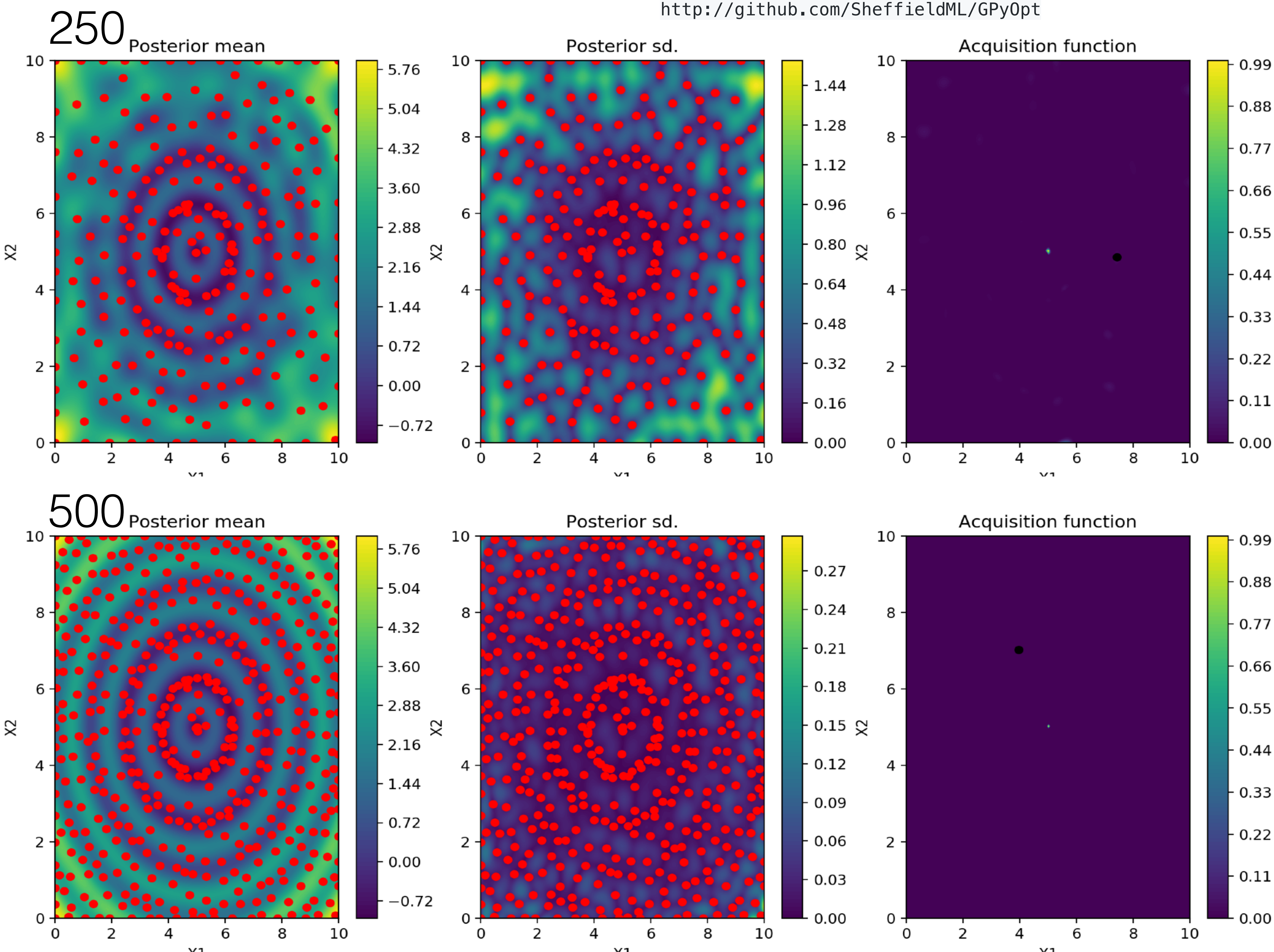
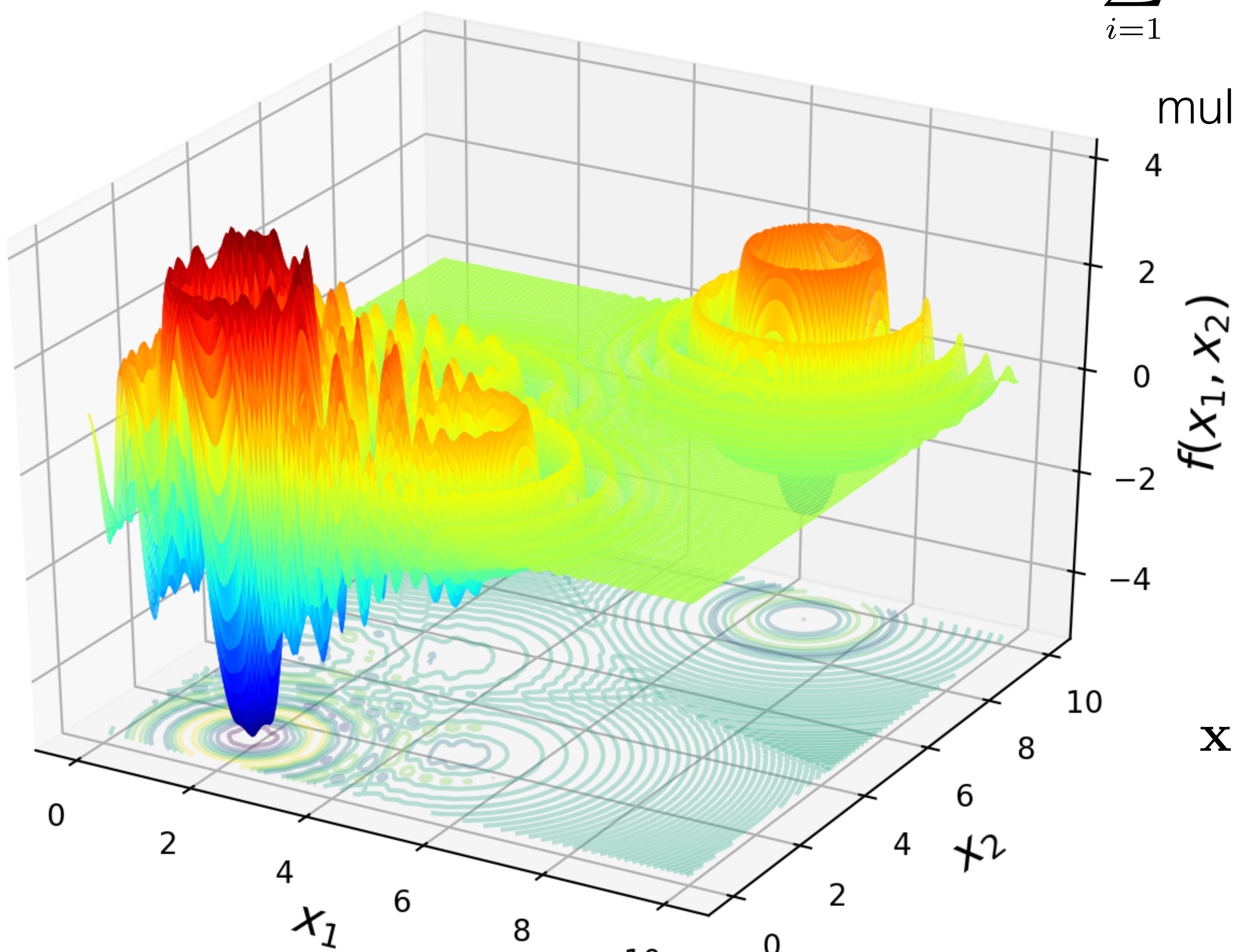


Langermann function

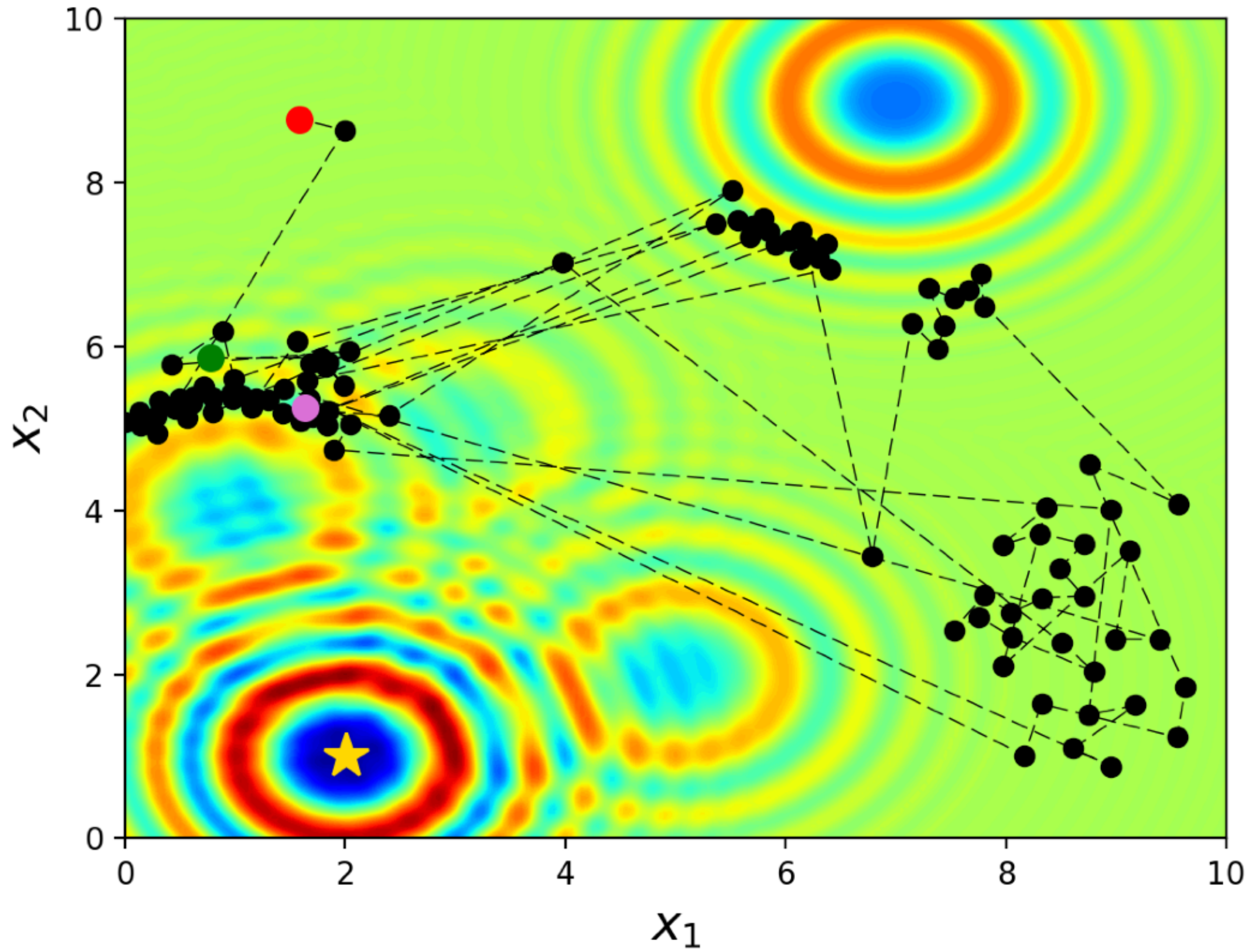
$$f_{\text{Langermann}}(\mathbf{x}) = -\sum_{i=1}^{5} \frac{c_i \cos\left\{\pi\left[(x_1-a_i)^2+(x_2-b_i)^2\right]\right\}}{e^{\frac{(x_1-a_i)^2+(x_2-b_i)^2}{\pi}}}$$

multimodal optimization problem



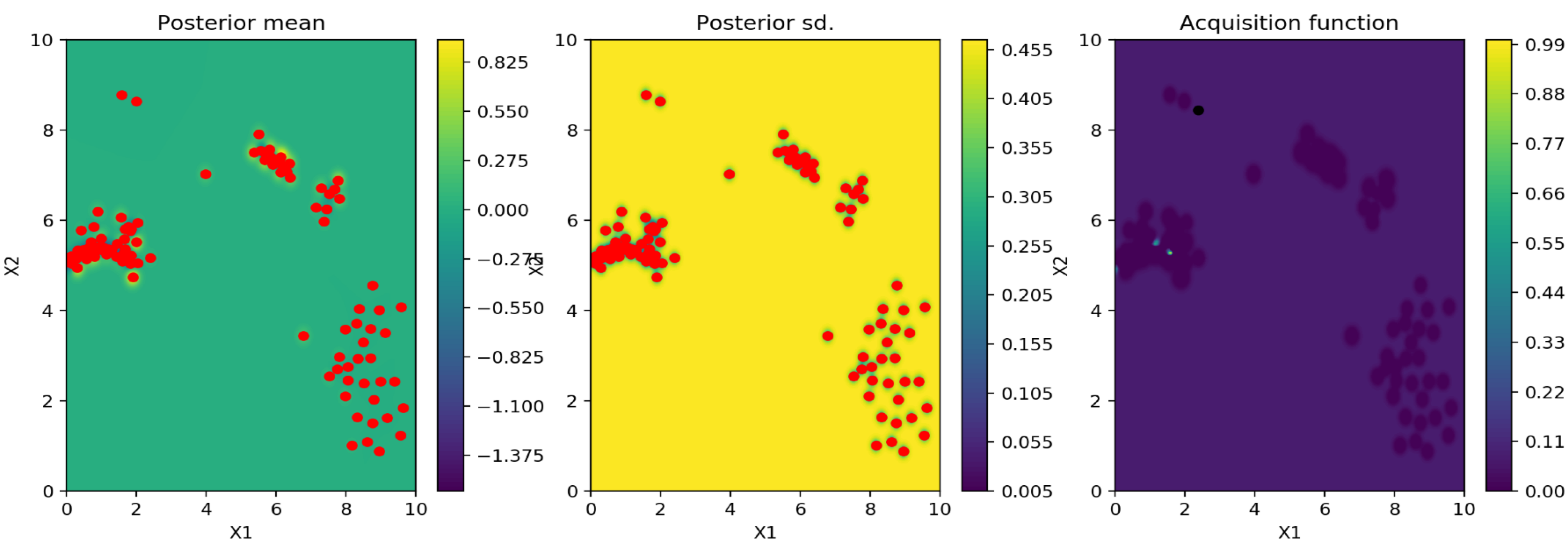
Choice of GP-kernel will affect the posterior distribution of functions.

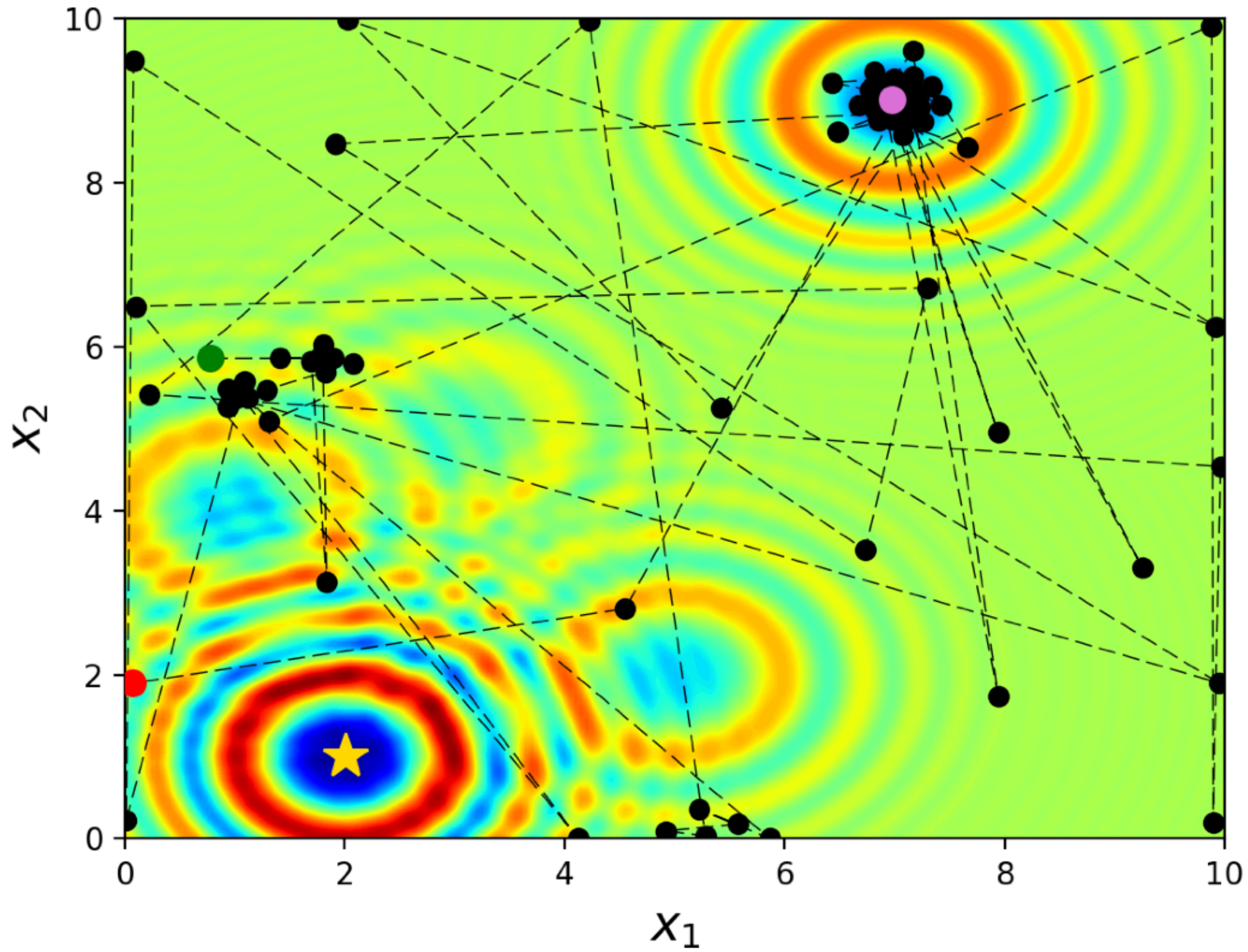
$$f(\mathbf{x}) = -5.1621259 \text{ for}$$
$$\mathbf{x} = [2.00299219, 1.006096]$$



100 iterations
Acq.: Expected Improvement
GP-kernel: **Squared exponential**

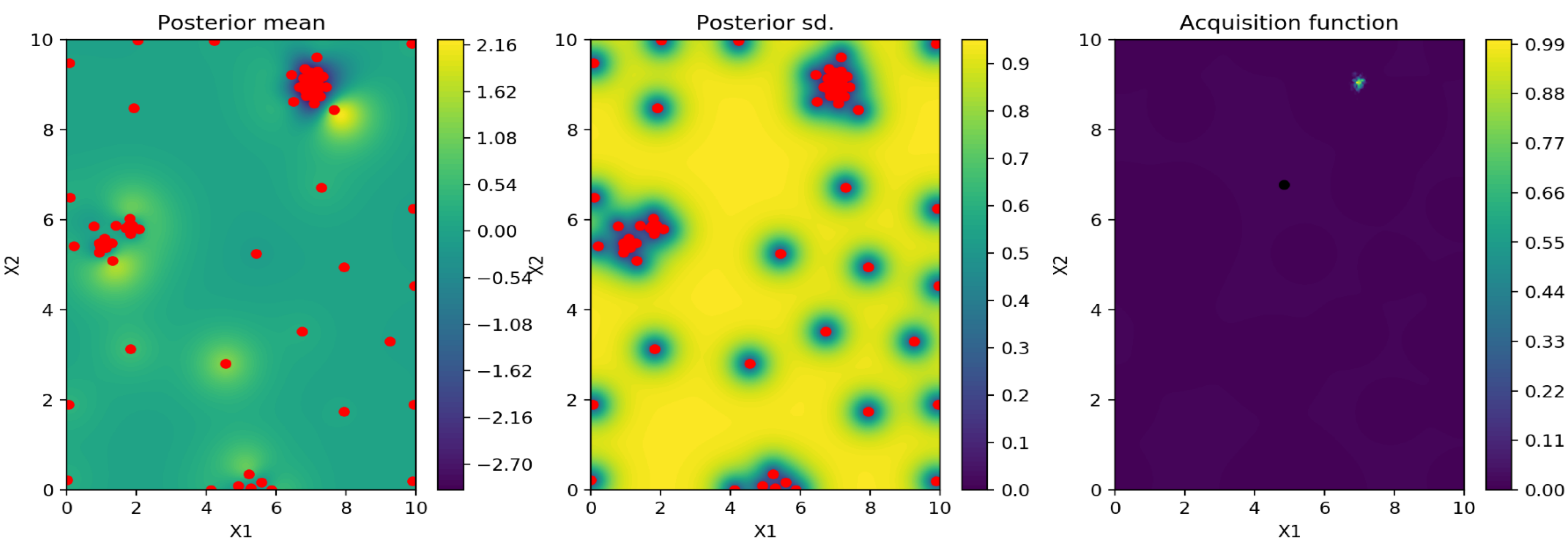
Doesn’t pick up on the structured details of the Langermann function



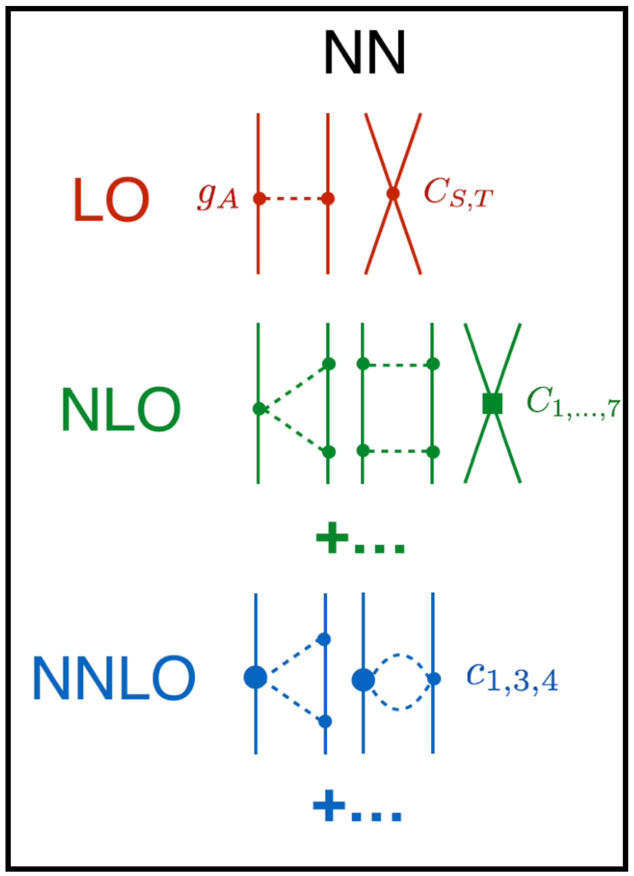


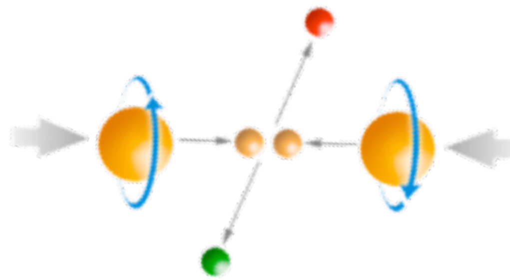
100 iterations
Acq.: Expected Improvement
GP-kernel: Matern 3/2
(exponential * linear)

A Matern 3/2 kernel does at better job, although in this run it does not find the global minimum.



NN scattering at NNLO(500)





Proton-Neutron scattering data < 75 MeV

R. Navarro-Perez et al, Phys. Rev. C **88**, 064002 (2013).

Model has 12 LECs/parameters that we vary

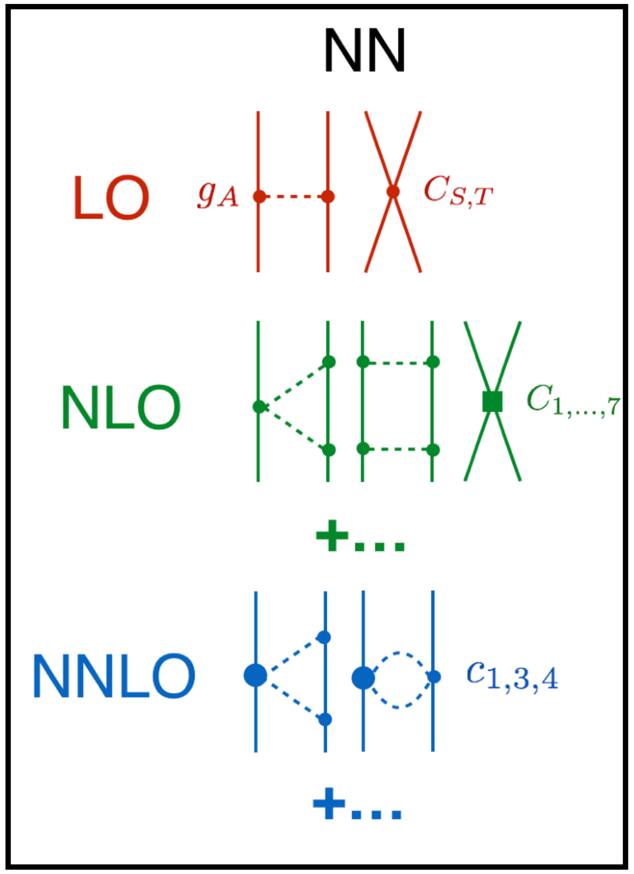
$$x = [\tilde{C}_{1S0}^{(np)}, \tilde{C}_{3S1}, C_{1S0}, C_{3S1}, C_{E1}, C_{1P1}, C_{3P0}, C_{3P1}, C_{3P2}]$$

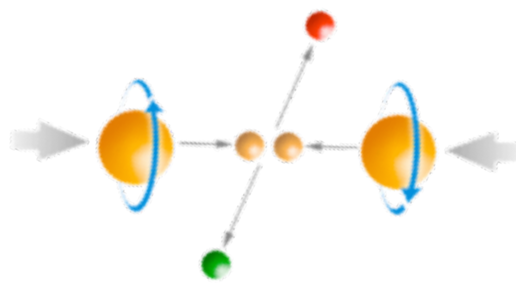
$$x_\star = \underset{x}{\operatorname{argmin}}\ \chi^2(x)$$

$$x \in X$$

parameter domain will matter!

NN scattering at NNLO(500)





Proton-Neutron scattering data < 75 MeV

R. Navarro-Perez et al, Phys. Rev. C **88**, 064002 (2013).

Model has 12 LECs/parameters that we vary

$$x = [\tilde{C}^{(np)}_{1S0}, \tilde{C}_{3S1}, C_{1S0}, C_{3S1}, C_{E1}, C_{1P1}, C_{3P0}, C_{3P1}, C_{3P2}]$$

$$x_\star = \underset{x}{\operatorname{argmin}} \; \chi^2(x)$$

$x \in X$

parameter domain will matter!

Let's try three different ones.

X1: "informed"
X2: "ignorant"
X3: "crazy"

5 random draws in each domain

MORE STATS NEEDED

X	$\tilde{C}^{(np)}_{1S0}$	$\tilde{C}_{3S1}$	C_{1S0}	$C_{3S1}-C_{3P2}$	c_1	c_3	c_4
X_1	$(-0.2,-0.1)$	$(+2,+3)$	$(-0.2,-0.1)$	$(-1,+1)$	$(-0.76,-0.72)$	$(-3.66,-3.56)$	$(+2.41,+2.47)$
X_2	$(-5.0,+5.0)$	$(-5,+5)$	$(-5.0,+5.0)$	$(-5,+5)$	$(-0.76,-0.72)$	$(-3.66,-3.56)$	$(+2.41,+2.47)$
X_3	$(-5.0,+5.0)$	$(-5,+5)$	$(-5.0,+5.0)$	$(-5,+5)$	$(-5.00,+5.00)$	$(-5.00,+5.00)$	$(-5.00,+5.00)$

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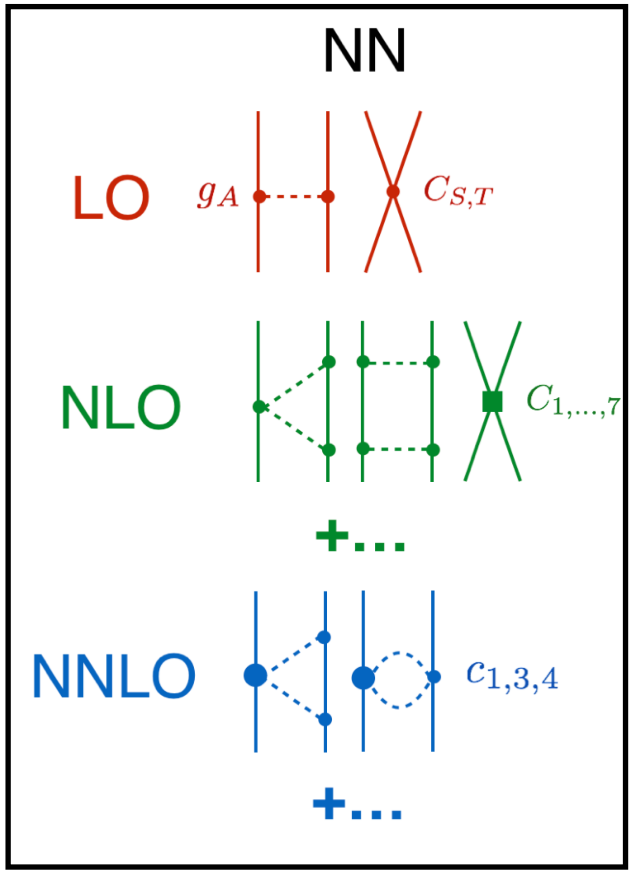

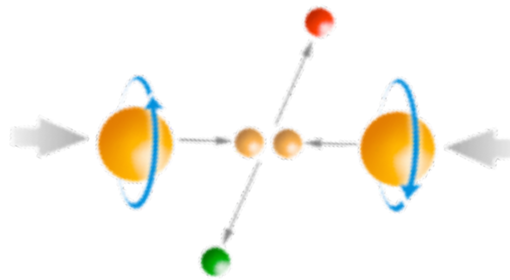

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$$x_\star = \underset{x}{\operatorname{argmin}} \; \chi^2(x)$$

How many random starting points typically 'needed' in N-dim space? (2N, Nlog(N), … ?)

Let's try three different ones.

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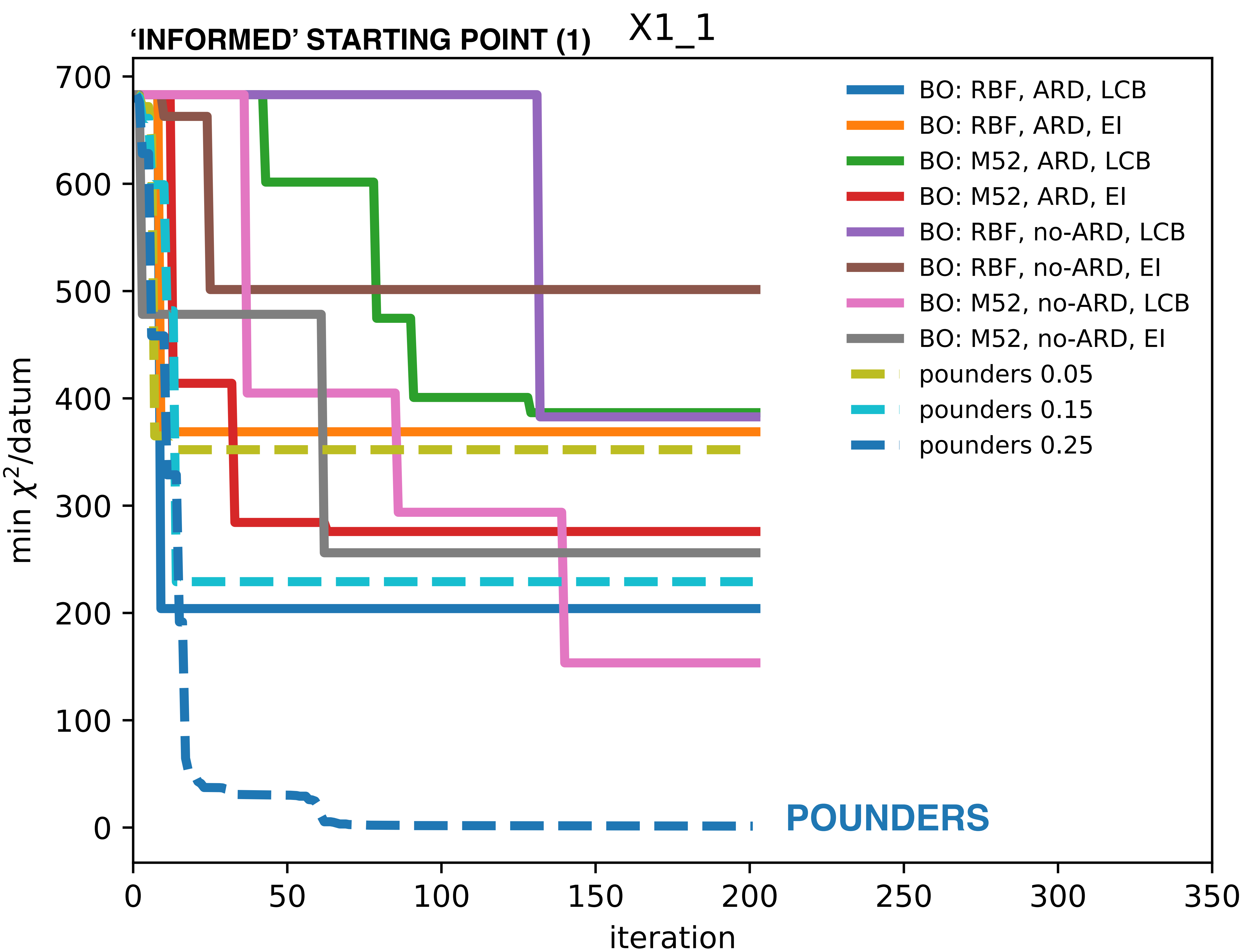
5 random starting points in each parameter domain



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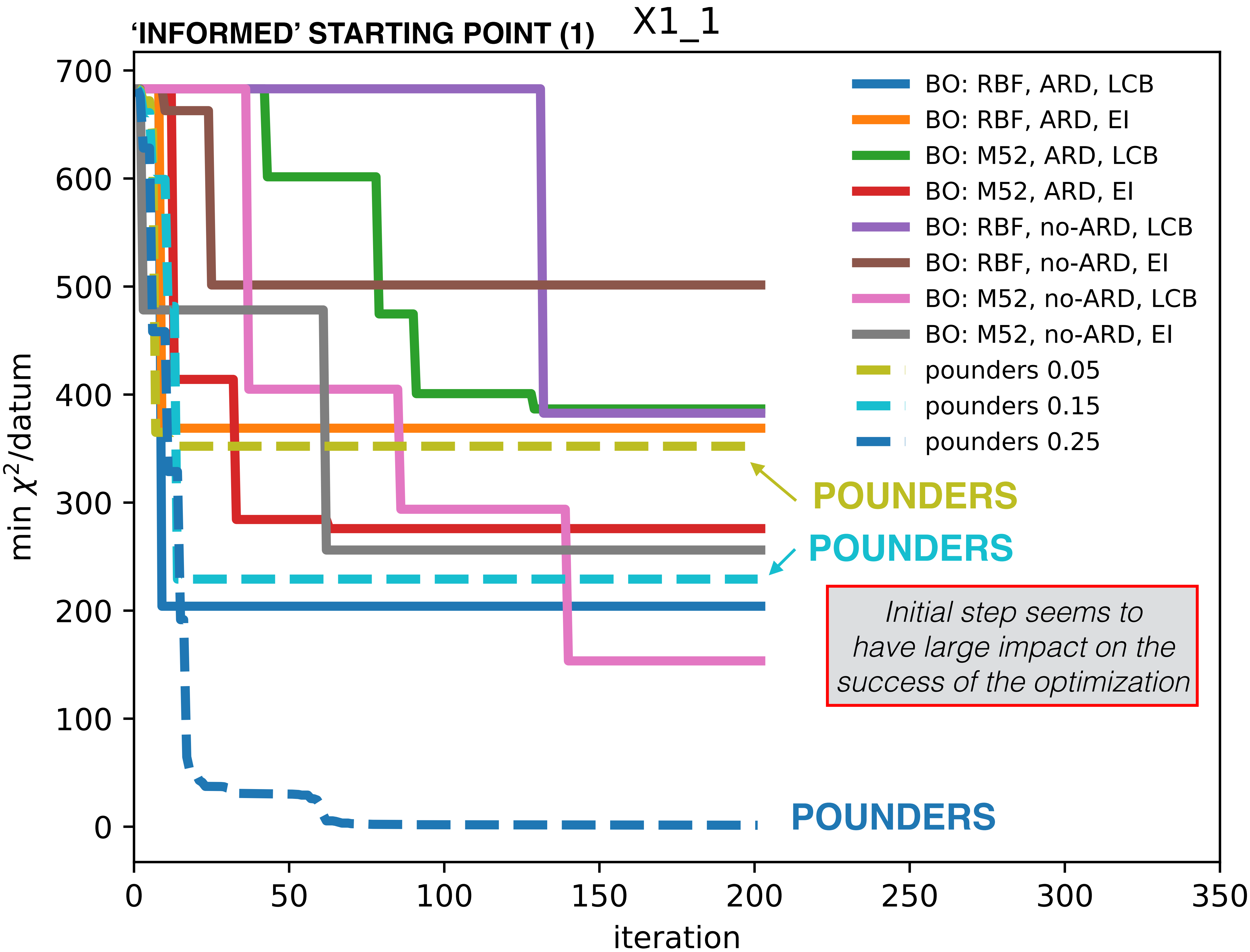

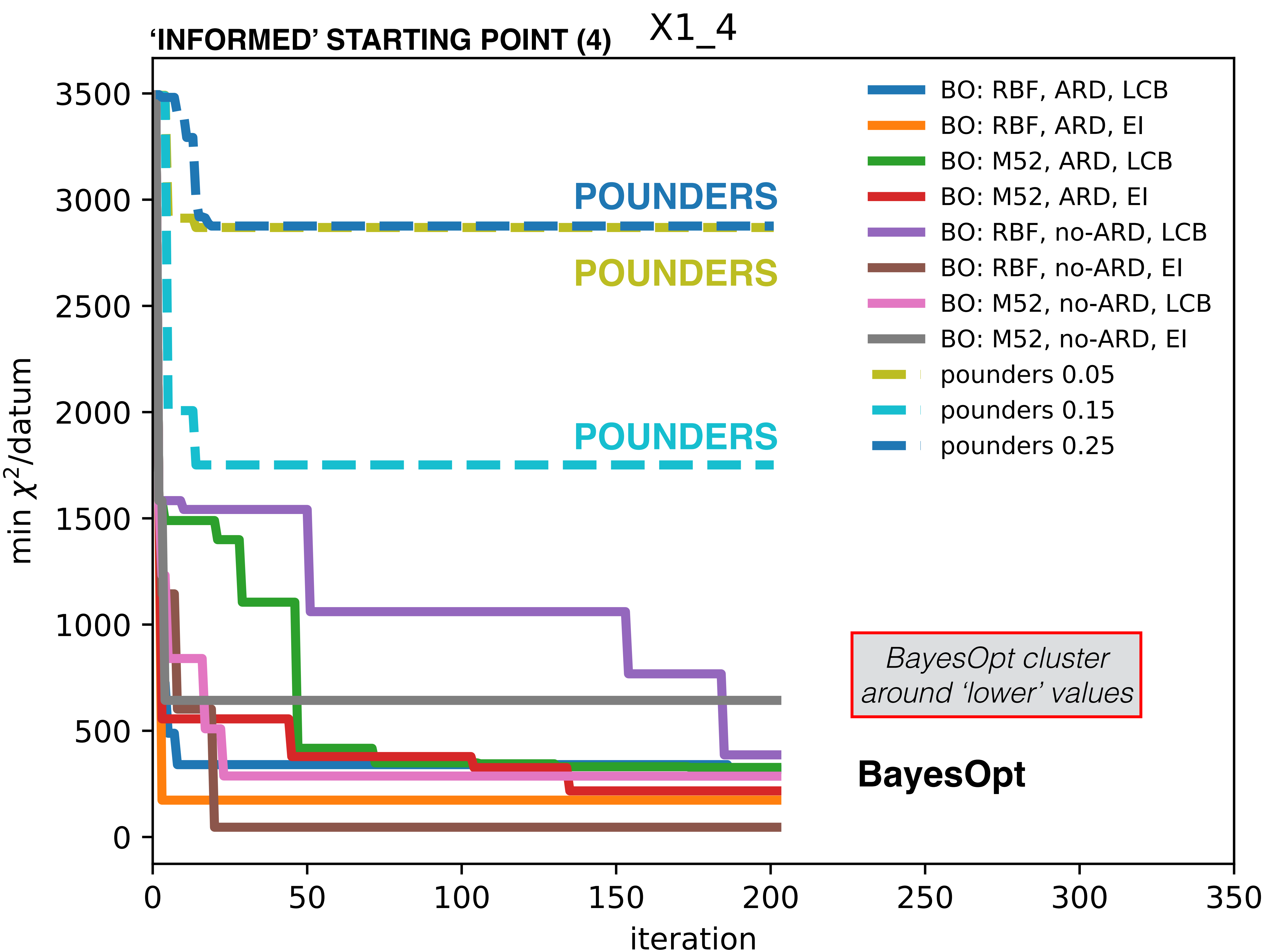

‘INFORMED’ STARTING POINT (4)
X1_4
POUNDERS
POUNDERS
POUNDERS
BO: RBF, ARD, LCB
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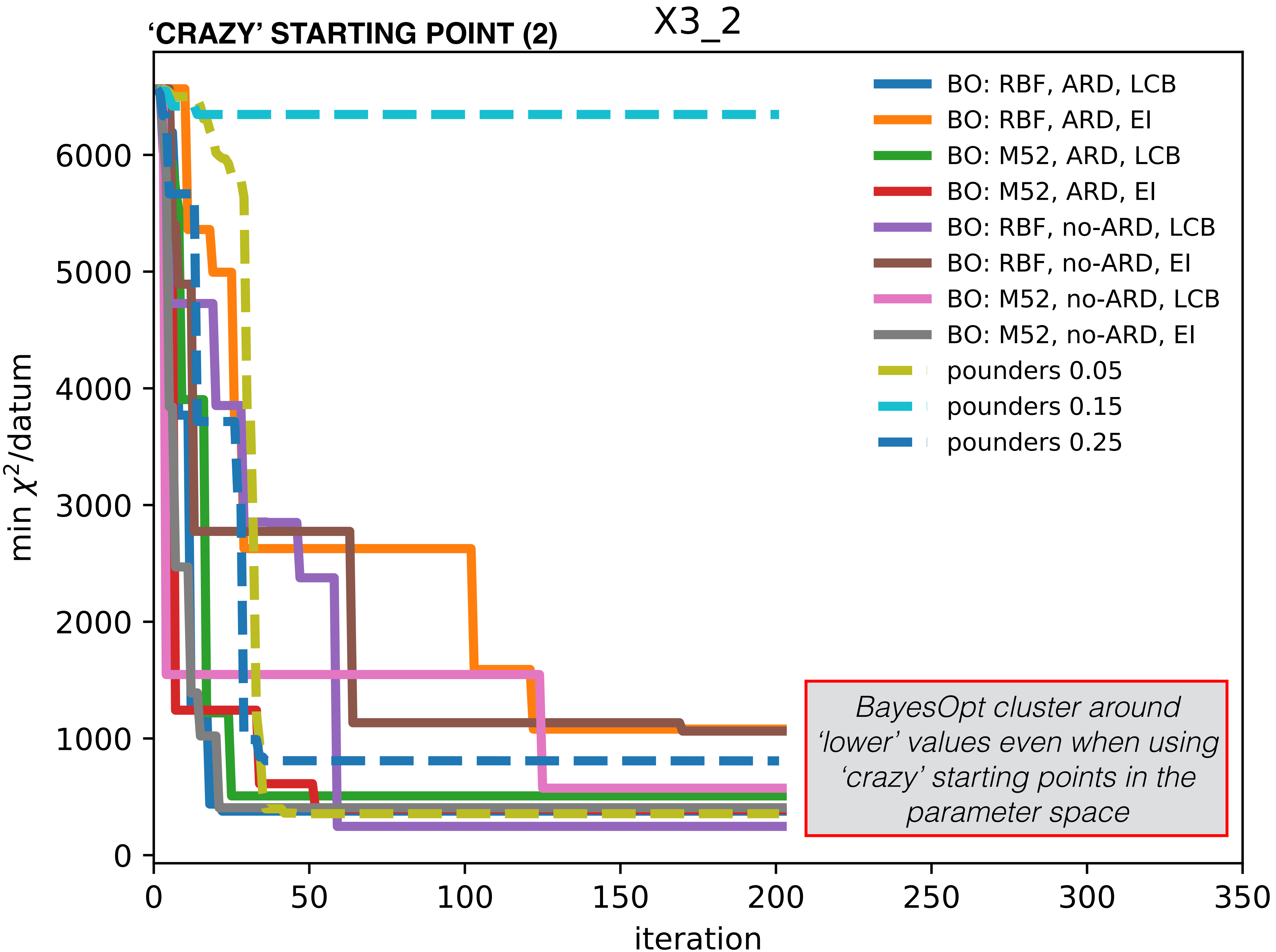
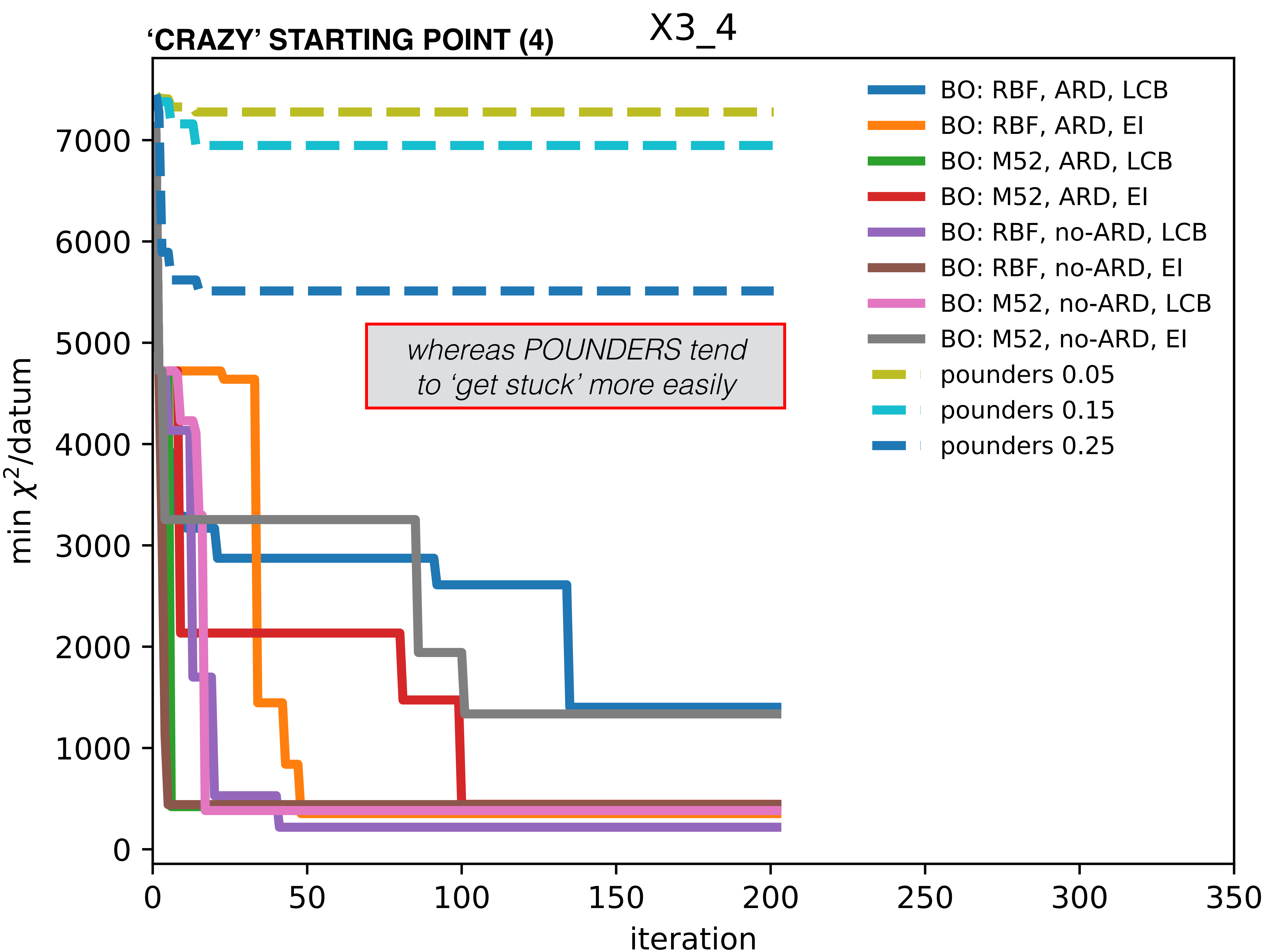
pounders 0.05
pounders 0.15
pounders 0.25
BayesOpt cluster around ‘lower’ values
BayesOpt
min χ^2/datum
iteration
0
500
1000
1500
2000
2500
3000
3500
0
50
100
150
200
250
300
350

‘CRAZY’ STARTING POINT (2)




'CRAZY' STARTING POINT (4)
X3_4
whereas POUNDERS tend
to 'get stuck' more easily
BO: RBF, ARD, LCB
BO: RBF, ARD, EI
BO: M52, ARD, LCB
BO: M52, ARD, EI
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Fingerspitzengefühl

POUNDERS:

- **Rather little tuning necessary (mainly initial step length).**
- **Scales rather well with dimensionality (at least computationally)**
- **Not much exploration.**
- **Sensitive to starting point.**

BayesOpt:

- **Exploration - Exploitation benefits.**
- **Seems to be less sensitive to starting point.**
- **Much tuning (Acuisition func, kernel, …). Determines success.**
- **Poor scaling with dimensionality (subspace projection?)**

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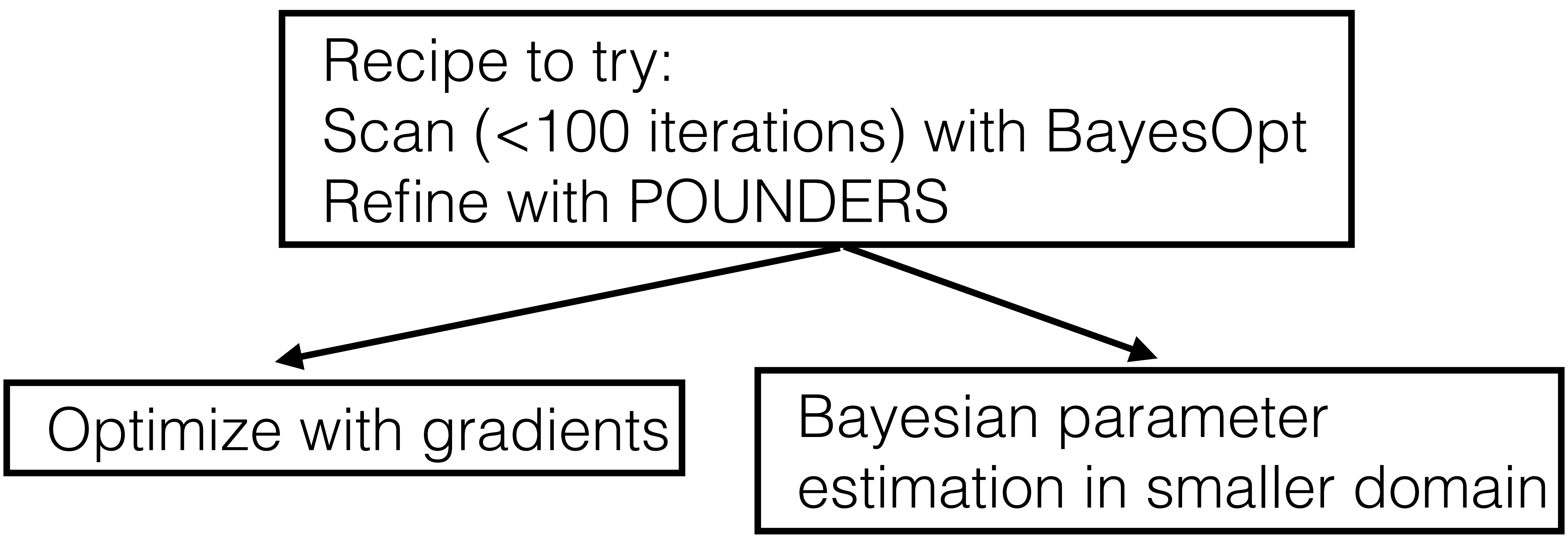

Combining errors

muonic deuterium

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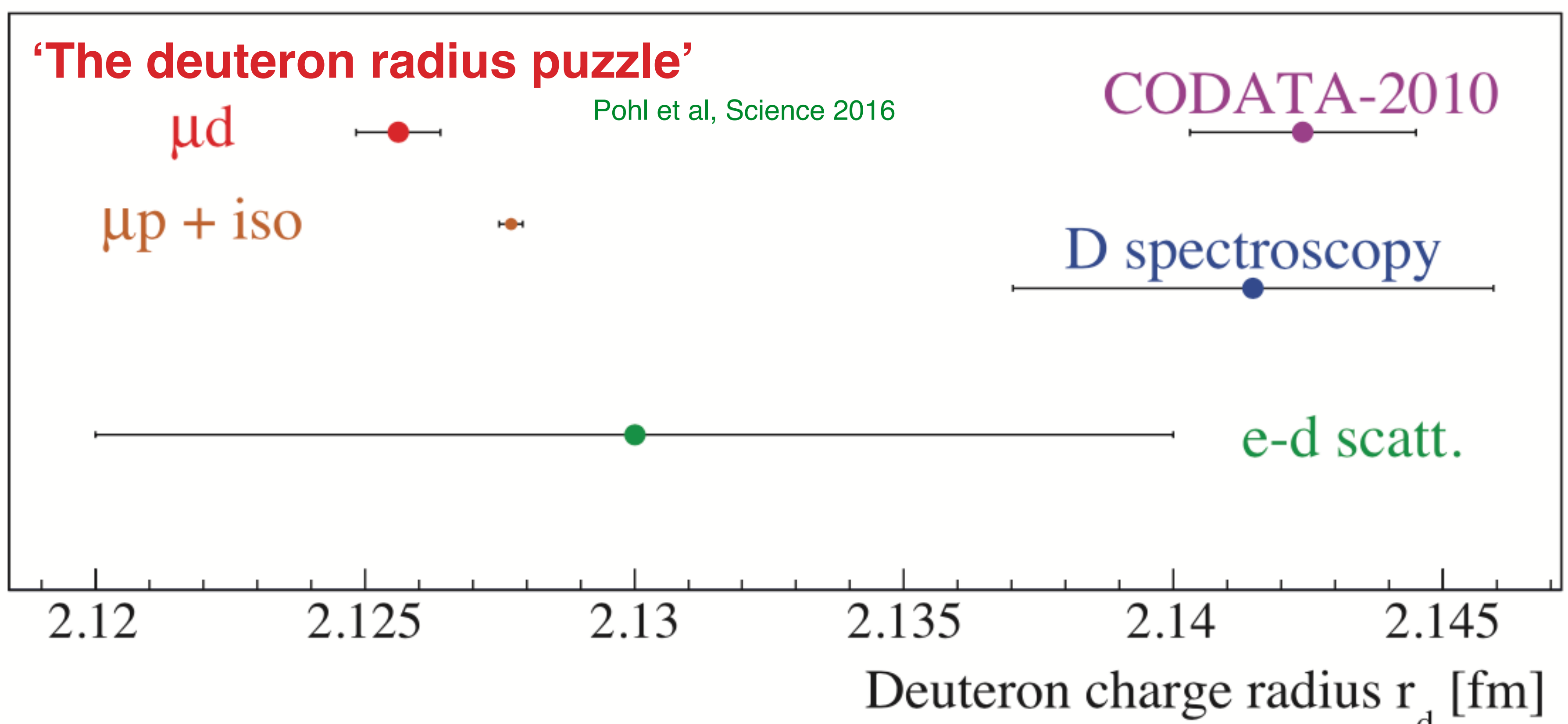
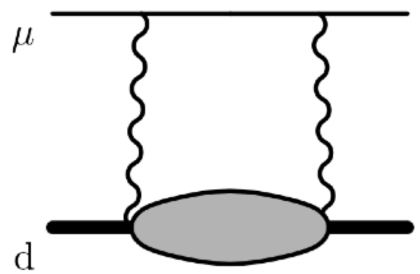
'proton radius puzzle'

Pohl et al, Nature 2010
Antognini et al, Science 2013
Beyer et al, Science 2017



The energy levels of muonic atoms are very sensitive to effects of quantum electrodynamics (QED), **nuclear structure**, and recoil, since the muon is about 206 times heavier than the electron

‘Two-Photon Exchange’



The inelastic contributions (‘nuclear polariztion’ / Two-Photon Exchange [TPE]) comes from nuclear theory. It is currently the limiting uncertainty in the extraction of the charge radius from laser spectroscopy of the Lamb shift.

$$\delta^{\mathrm{LS}}_{\mathrm{exp}} = \delta^{\mathrm{LS}}_{\mathrm{QED}} + \delta^{\mathrm{LS}}_{\mathrm{TPE}} - \delta^{\mathrm{LS}}_{\mathrm{rad.-dep.}} \cdot r_d^2$$

Pohl et al, Science 2016

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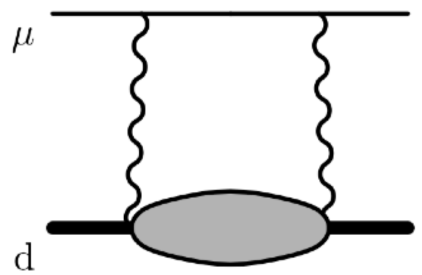

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$228.7766(10)\,\mathrm{meV}$

$202.8785(34)\,\mathrm{meV}$ $1.7096(200)\,\mathrm{meV}$ $-6.1103(3)\,\mathrm{meV/fm^2}$

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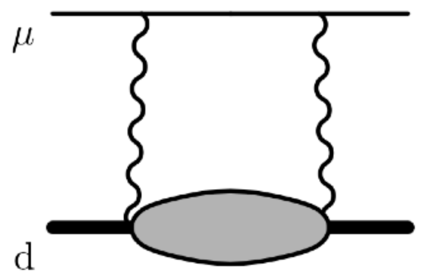

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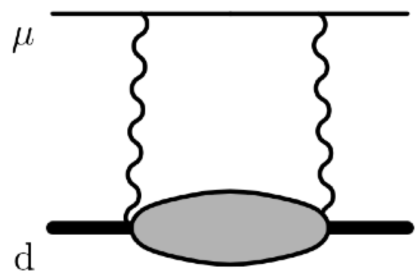

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depends on NN-pot

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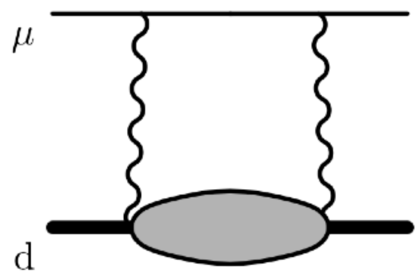

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$$r_d(\mu - d) = 2.12562(13)_{\rm exp}(77)_{\rm theo}\,\text{fm} = 2.12562(78)\,\text{fm}$$

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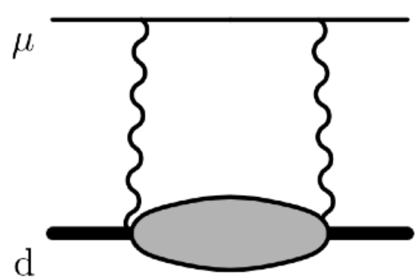

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added in quadrature

‘exp error’ ‘QED error’ ‘TPE error’ ‘mass error’

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‘exp error’

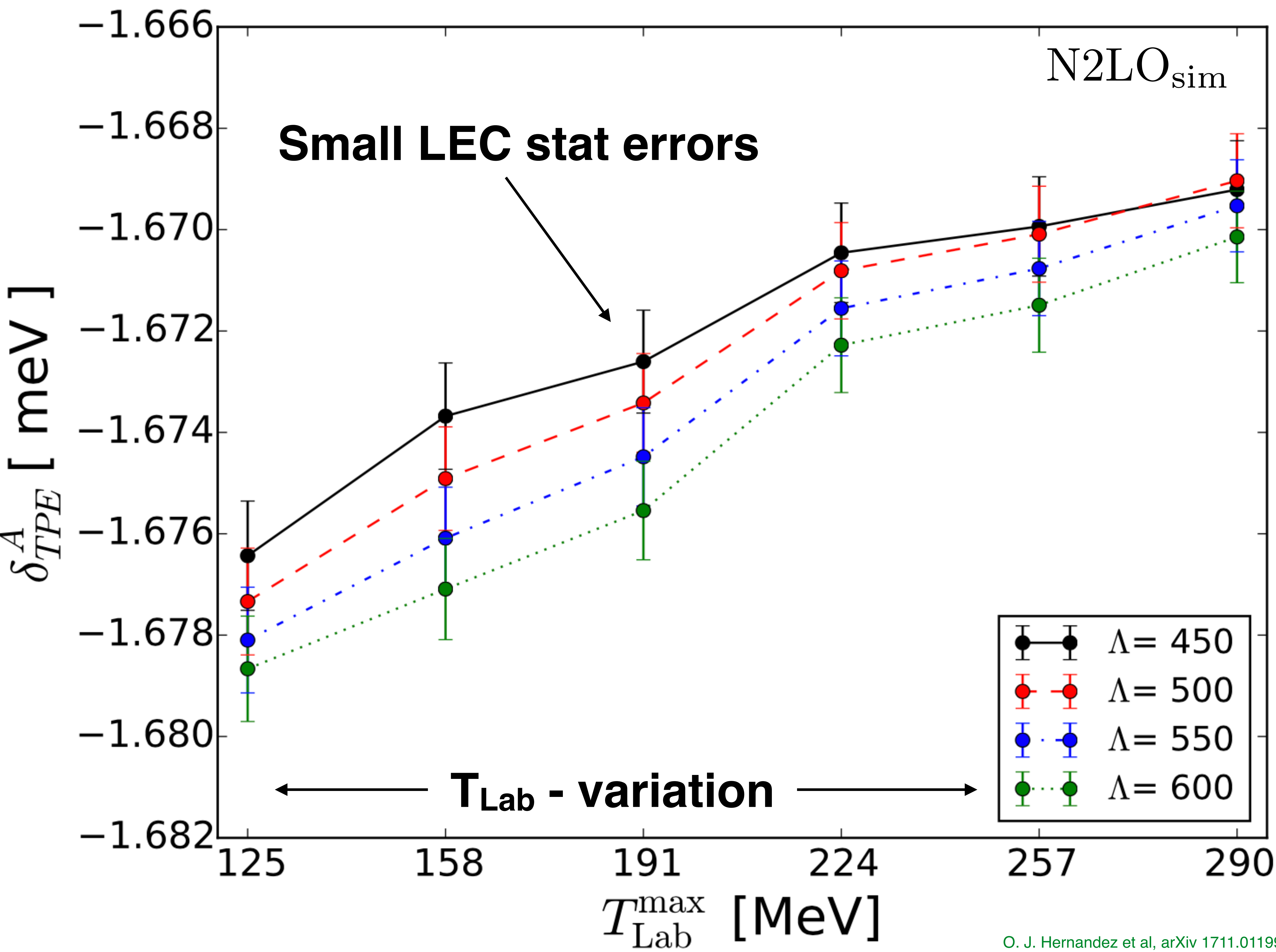
$$\delta^A_{\rm TPE} = \delta^{(0)} + \delta^{(1)} + \delta^{(2)} + \delta^{(1)}_{\rm NS} + \delta^{(2)}_{\rm NS} + \delta^A_{\rm Zem}$$

‘theory error’

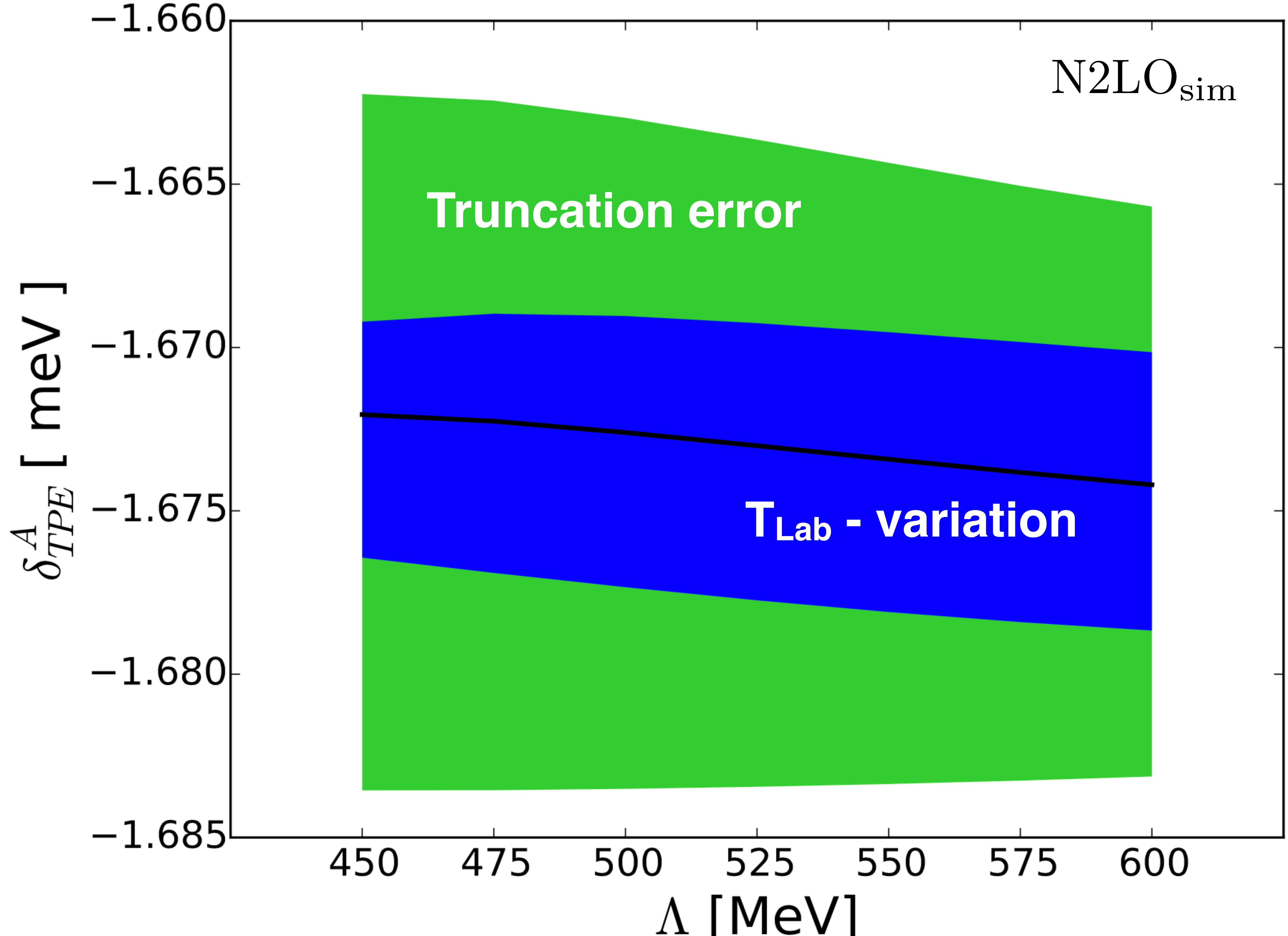
$$r_d(\mu - d) = 2.12562(13)_{\rm exp}(77)_{\rm theo}\ \text{fm} = 2.12562(78)\ \text{fm}$$

$\sigma_{\rm theo}$ is 98% TPE

Pohl et al, Science 2016



O. J. Hernandez et al, arXiv 1711.01199 (2017)



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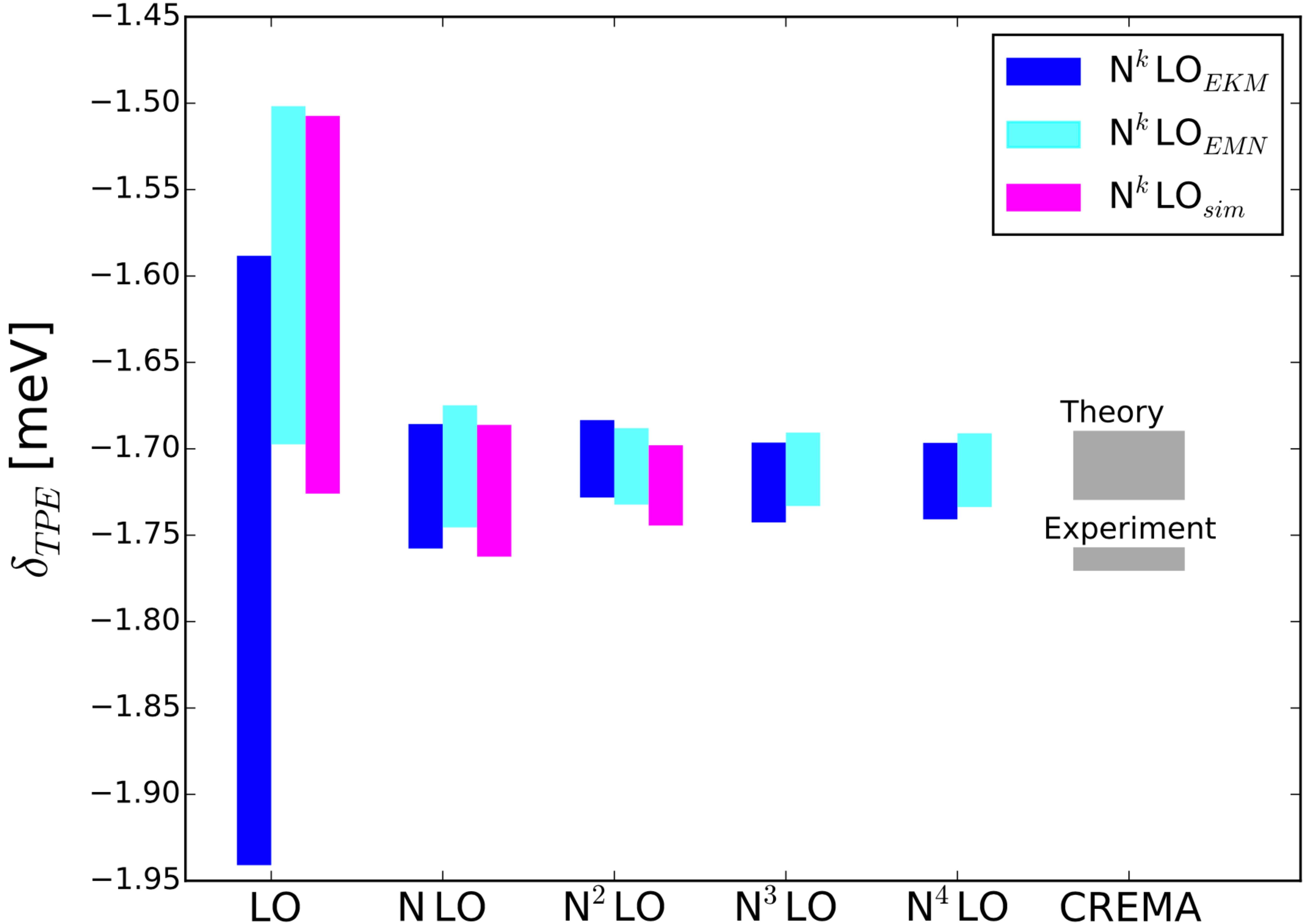

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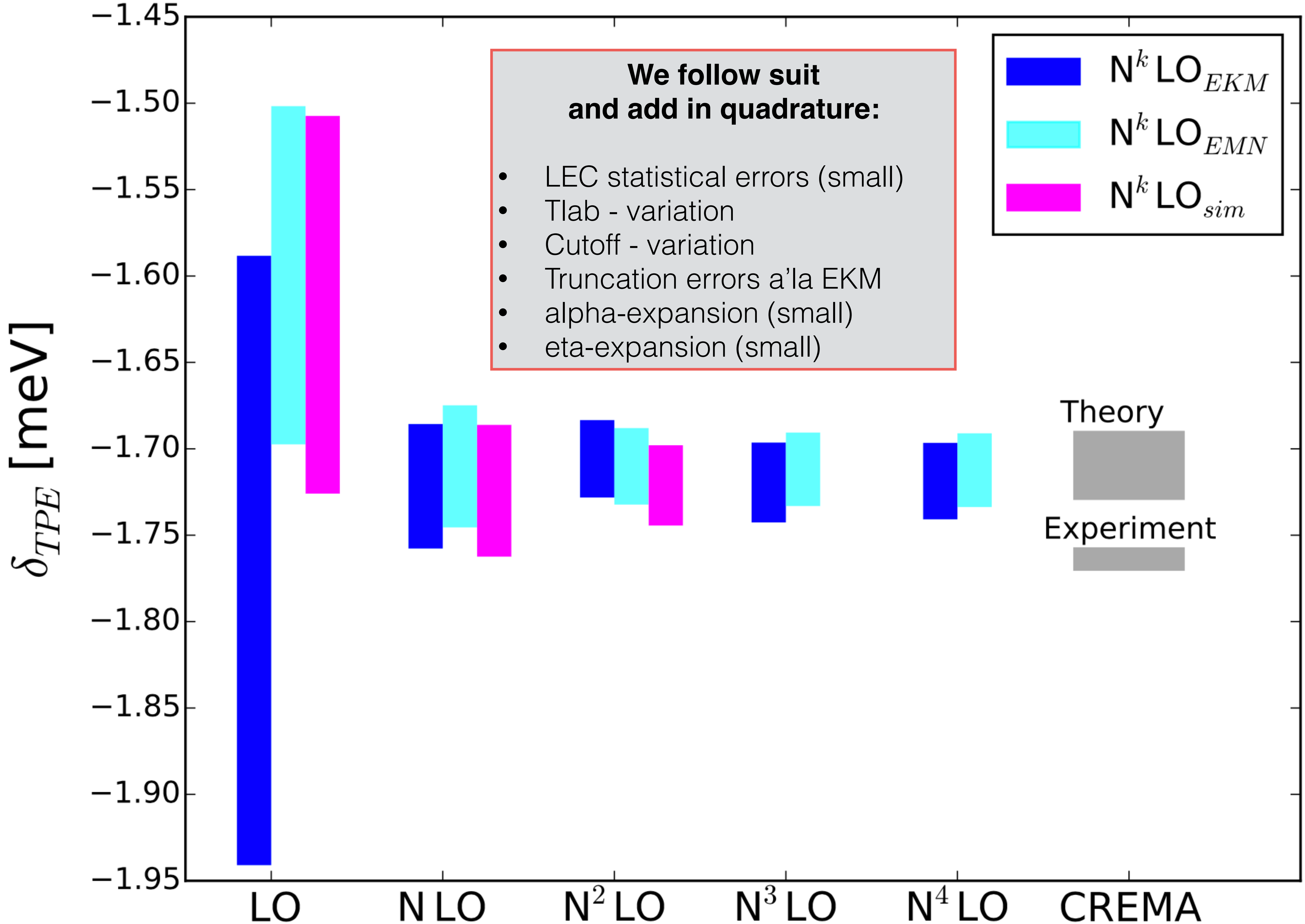

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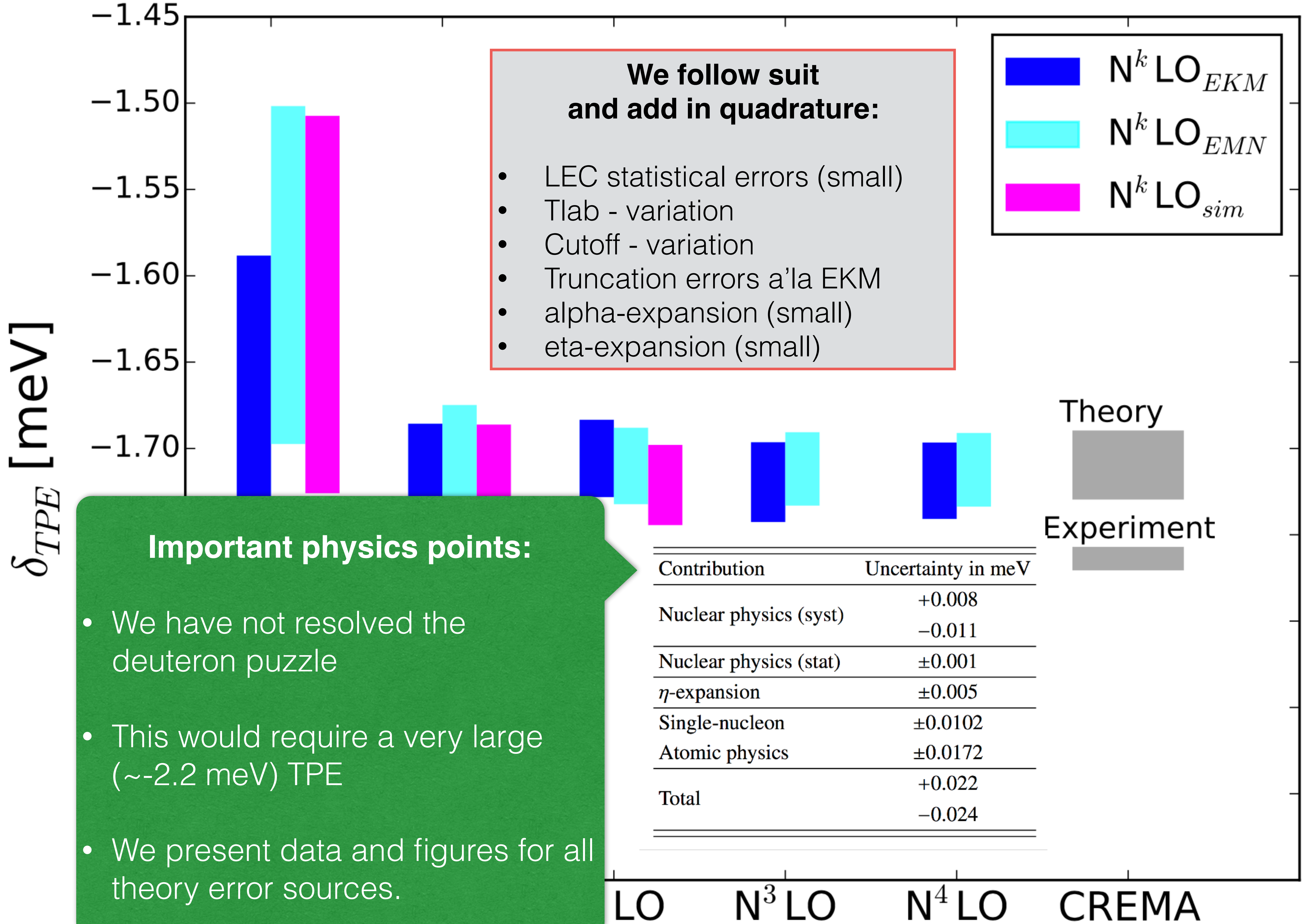


We follow suit and add in quadrature:

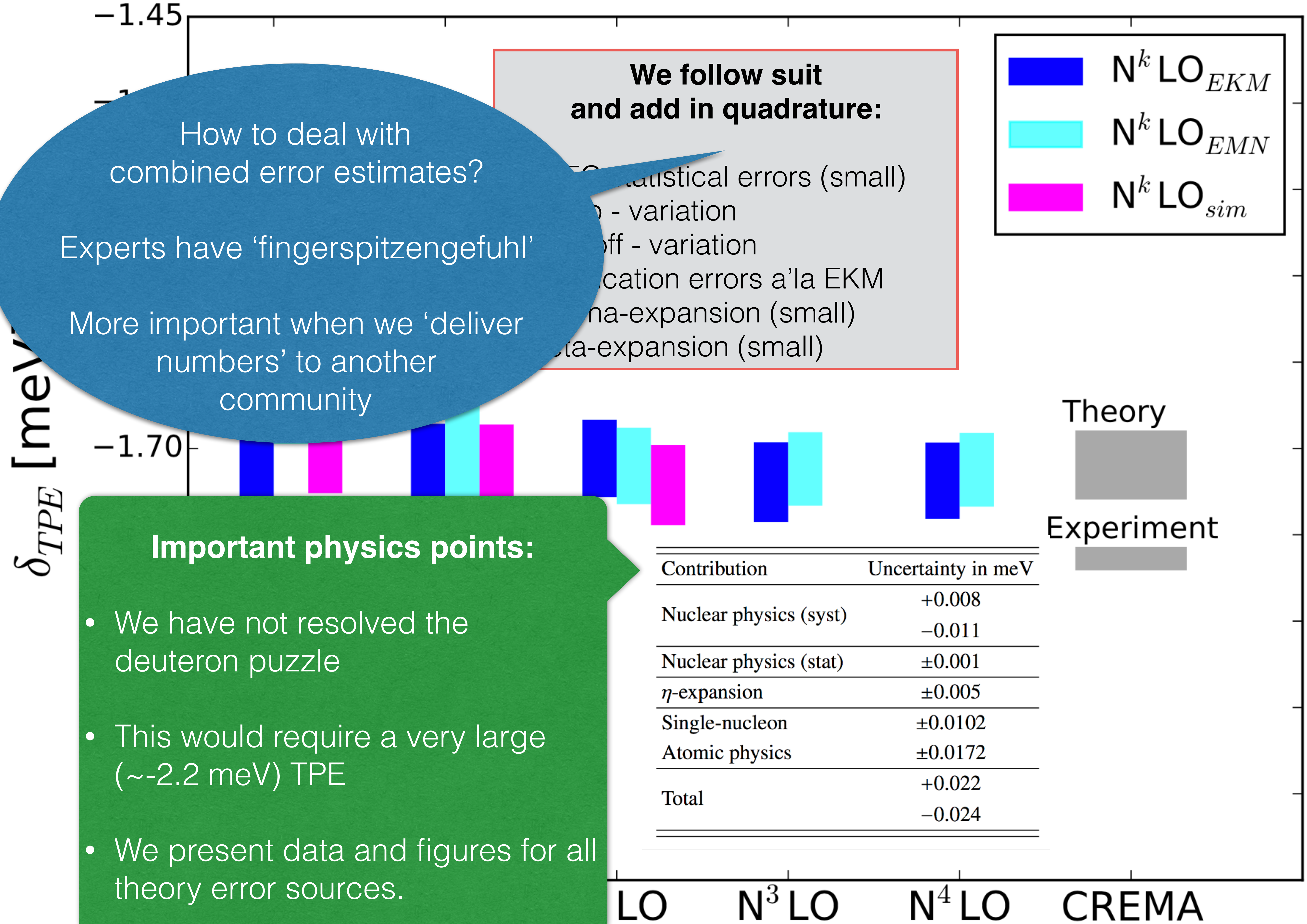
- LEC statistical errors (small)
- Tlab - variation
- Cutoff - variation
- Truncation errors a'la EKM
- alpha-expansion (small)
- eta-expansion (small)

Important physics points:

- We have not resolved the deuteron puzzle
- This would require a very large (~-2.2 meV) TPE
- We present data and figures for all theory error sources.

Contribution	Uncertainty in meV
Nuclear physics (syst)	+0.008 / −0.011
Nuclear physics (stat)	±0.001
η-expansion	±0.005
Single-nucleon	±0.0102
Atomic physics	±0.0172
Total	+0.022 / −0.024

O. J. Hernandez et al, arXiv 1711.01199 (2017)



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How to deal with combined error estimates?

Experts have 'fingerspitzengefuhl'

More important when we 'deliver numbers' to another community

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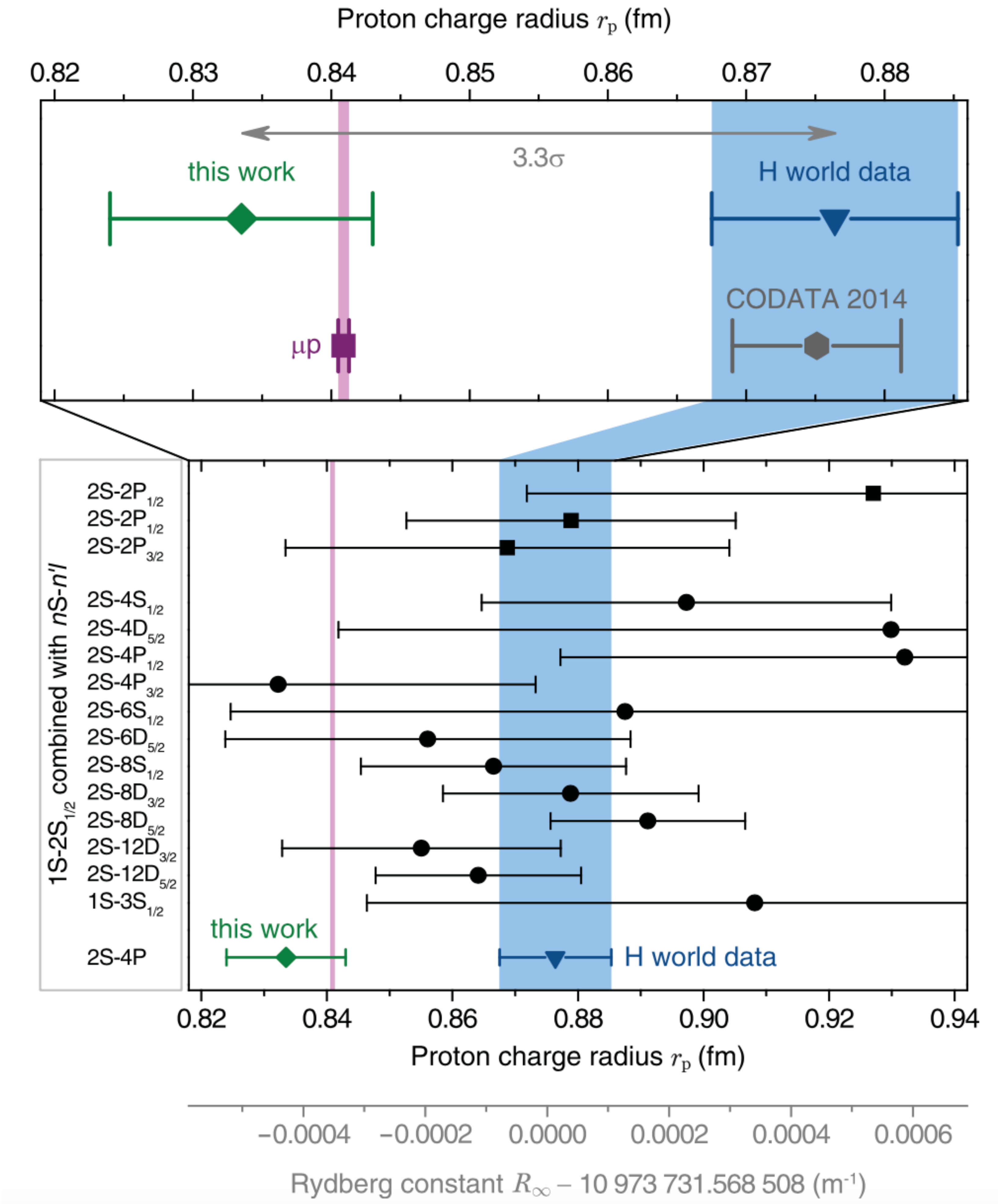
Summary

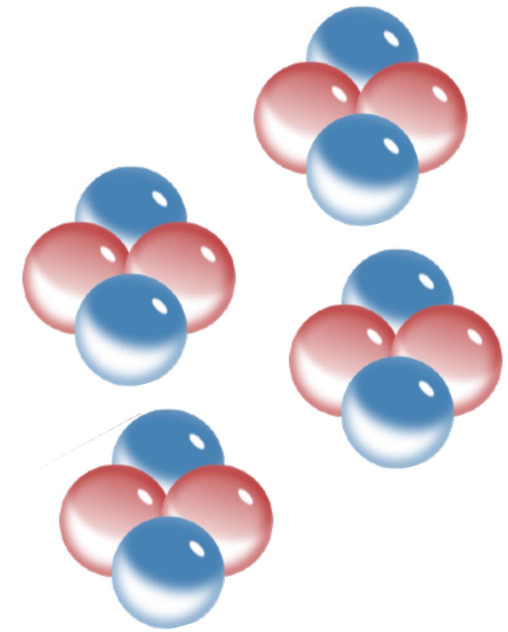
- Approximate DOB intervals support the *expected improved convergence for deltafull EFT.*
- Bayesian optimization could be useful for optimizing interactions from expensive ab initio calculations.
- Several sources of uncertainty very common. How can we ‘best’ combine/report a conglomerated value?

Thanks for your attention!



Beyer et al., Science 358, 79–85 (2017)

Stability with respect to alpha breakup



Several recent calculations observe that, contrary to well-established experiments, ^{16}O is not stable against decay into 4α particles

- Lattice EFT calculations (improved LO interaction "A") (observed for ^{8}Be, ^{12}C, ^{16}O, ^{20}Ne) S. Elhatisari et al. Phys. Rev. Lett. **117**, 132501 (2016)
- Pionless EFT calculations at LO L. Contessit et al. arXiv:1701.06516 [nucl-th] (2017)
- Chiral EFT calculations using optimized $NNLO_{sim}$ B. D. Carlsson et al. Phys. Rev. X **6**, 011019 (2016)
- Δ-less chiral EFT calculations LO, NLO, NNLO A. Ekström et al. arXiv:1707.09028 [nucl-th] (2017)

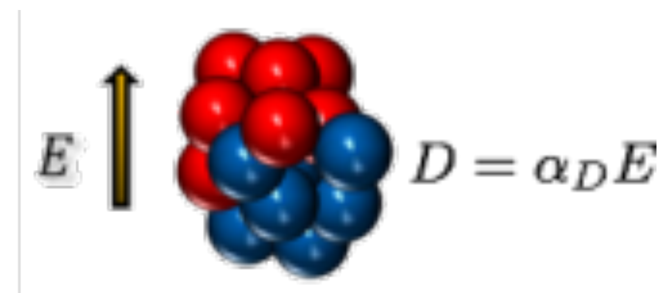
The Δ-full NLO, NNLO interactions yield ^{16}O (and ^{40}Ca) stable with respect to α breakup A. Ekström et al. arXiv:1707.09028 [nucl-th] (2017)

Coupled-cluster calculations in the Lambda-CCSD(T) formulation, hw=16, E3max=16hw, 3NF-NO2b HF

TABLE II. Binding energies (E) (in MeV), charge radii (in fm), proton point radii (in fm), neutron point radii (in fm), and neutron skin (in fm) for ^{8}He, ^{16,22,24}O, and ^{40,48}Ca at ΔNLO and ΔNNLO, and compared to experiment.

	E			R_{ch}			R_{p}		R_{n}		R_{skin}	
	ΔNLO	ΔNNLO	Exp. [65]	ΔNLO	ΔNNLO	Exp. [51]	ΔNLO	ΔNNLO	ΔNLO	ΔNNLO	ΔNLO	ΔNNLO
^{8}He	27.5	27.0	31.40	1.90	1.97	1.924(31)	1.77	1.85	2.63	2.70	0.85	0.85
^{16}O	120.3	117.0	127.62	2.63	2.73	2.699(5)	2.49	2.61	2.47	2.58	−0.02	−0.03
^{22}O	146.2	145.4	162.04	2.66	2.77		2.54	2.66	2.88	3.00	0.34	0.34
^{24}O	152.2	151.6	168.96	2.70	2.81		2.59	2.71	3.11	3.22	0.52	0.51
^{40}Ca	312.2	309.1	342.05	3.41	3.55	3.478(2)	3.31	3.45	3.26	3.40	−0.05	−0.05
^{48}Ca	373.4	373.8	416.00	3.45	3.56	3.477(2)	3.36	3.47	3.51	3.62	0.15	0.15

- 😀 ΔNNLO *predicts* E and R_{ch} rather well.
- 😀 Neutron skin in ^{48}Ca consistent with estimated ranges: 0.14–0.20 fm from E-dipole polarizability & ab intio predictions 0.12-0.15 fm
- 😀 Low-lying states in ^{17}O in good agreement with data.
- 🙁 ^{25}O is bound at ΔNNLO with respect to ^{24}O by about 0.5 MeV
- 🙁 2^{+} state in ^{24}O is too low compared to experiment.

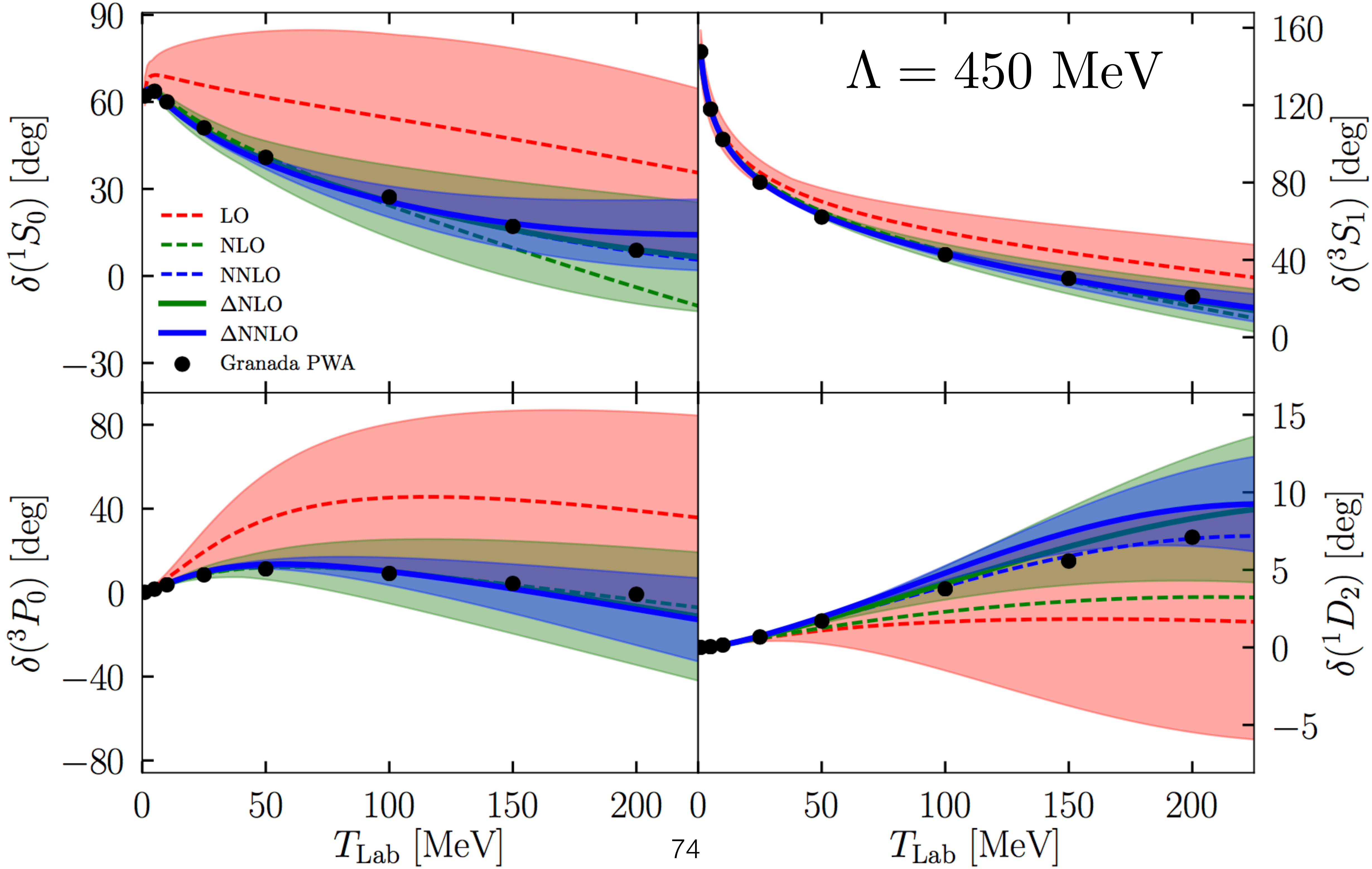


$$\alpha_D = 2\alpha \int \frac{R(w)}{\omega} d\omega$$

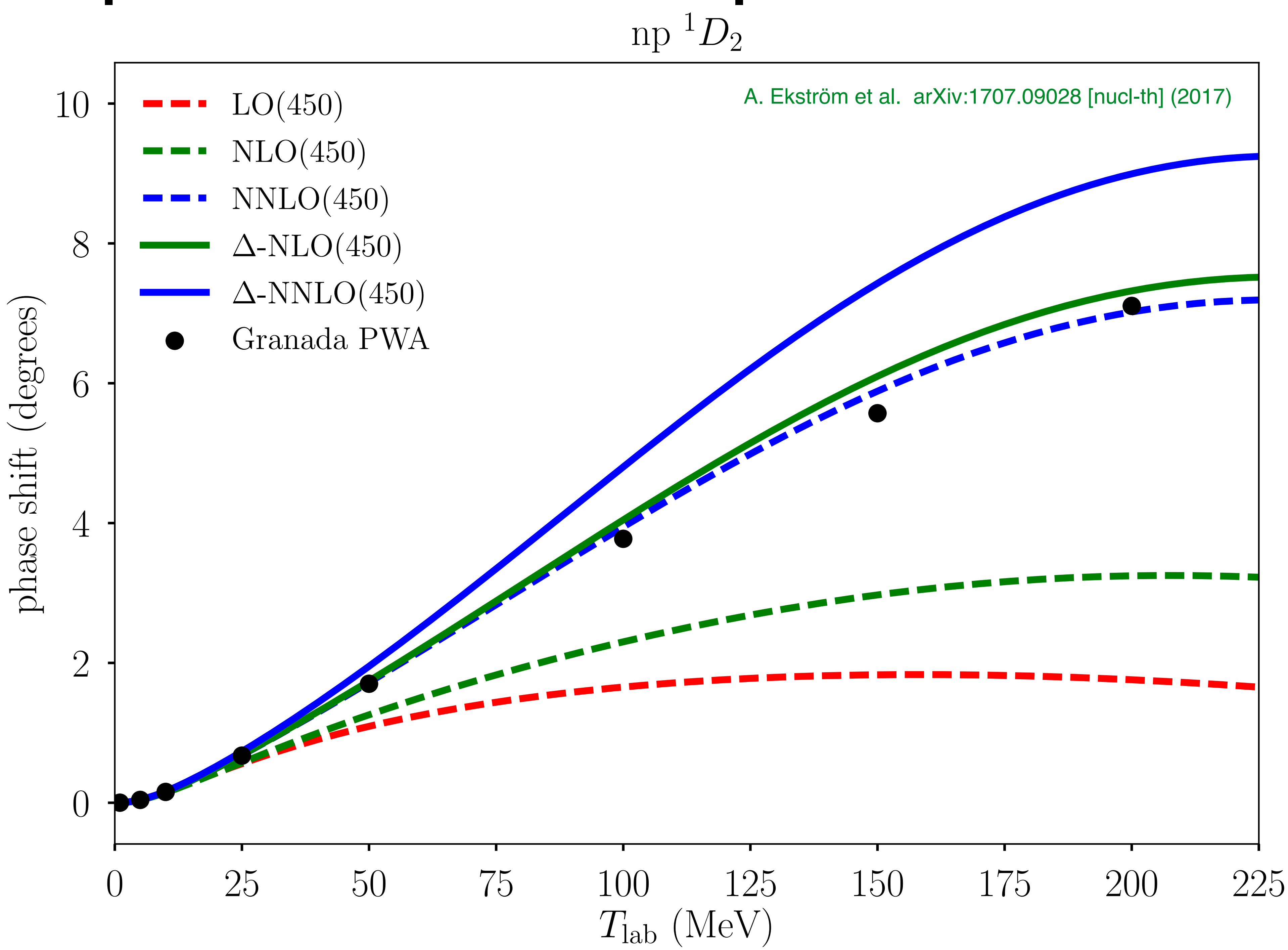
$$R_{\mathrm{skin}} = R_n - R_p$$

G. Hagen, et al. Nature Physics **12**, 186–190 (2016)
J. Birkhan, et al. PRL **118**, 252501 (2017)

Phase shifts, truncation errors

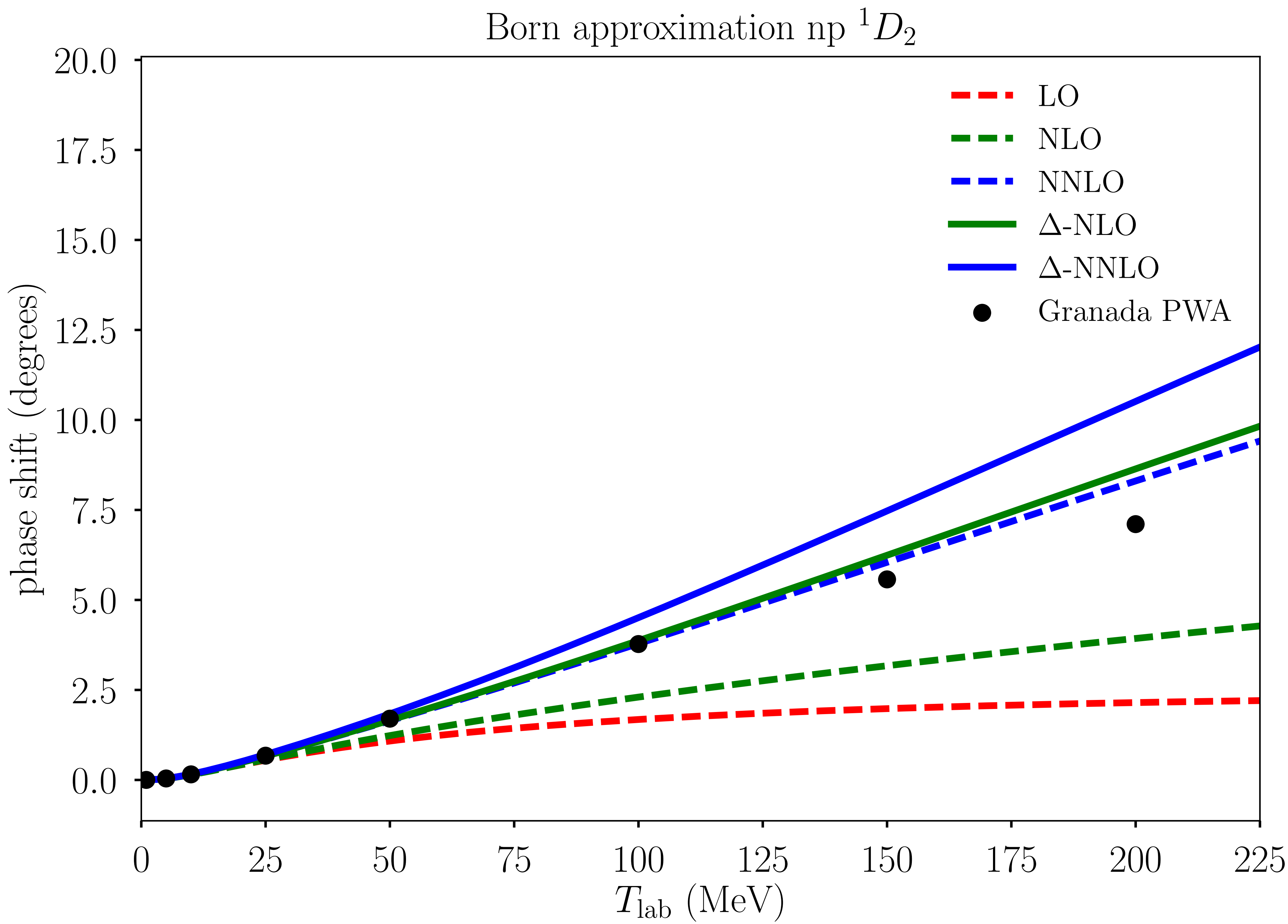


Peripheral NN-phase shifts

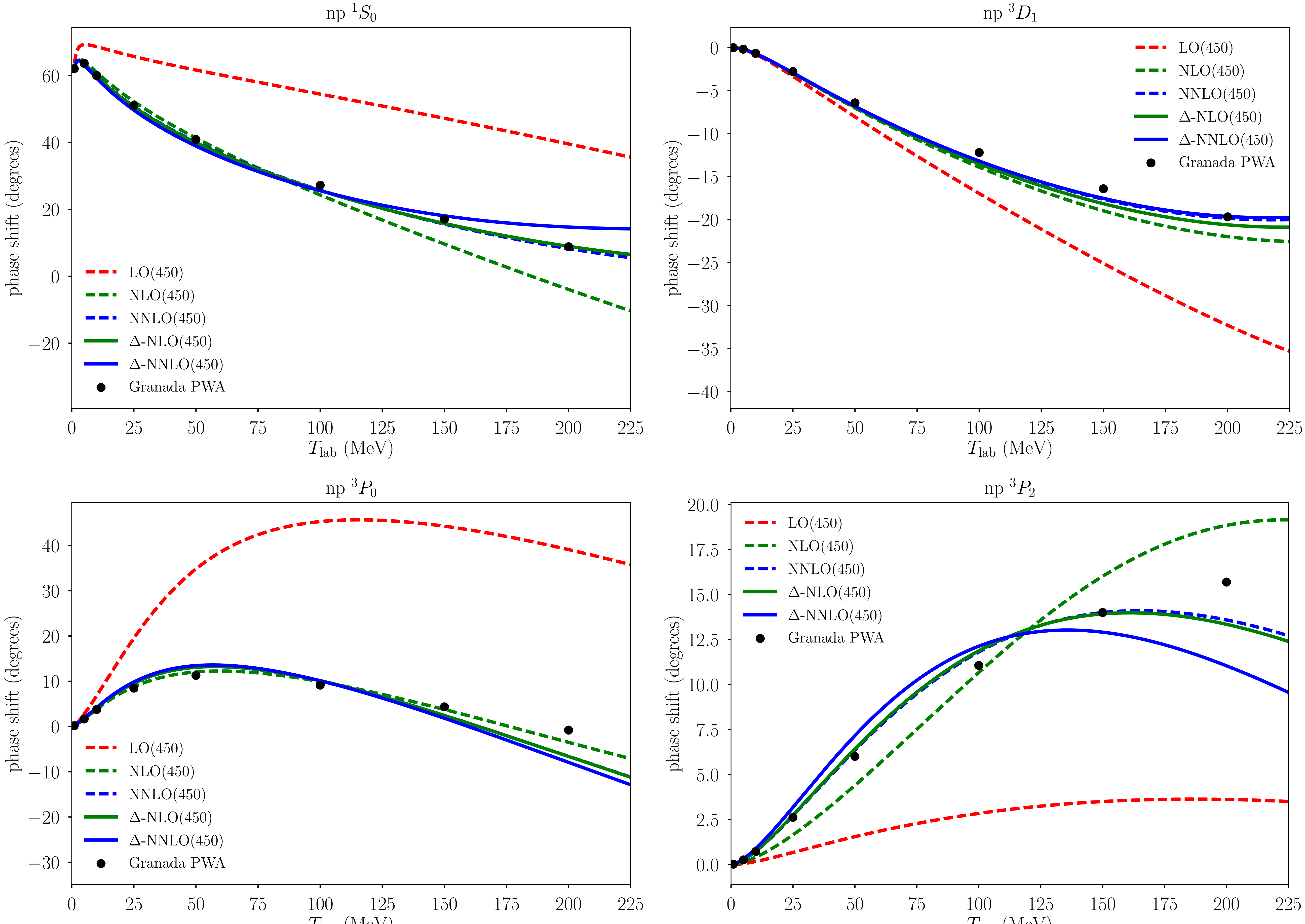


Δ-NLO $\approx$ NNLO

H. Krebs et al. Eur. Phys. J. A **32**, 127-137 (2007)



Born approximation np $^1D_2$
LO
NLO
NNLO
Δ-NLO
Δ-NNLO
Granada PWA
phase shift (degrees)
T_{lab} (MeV)
0.0
2.5
5.0
7.5
10.0
12.5
15.0
17.5
20.0
0
25
50
75
100
125
150
175
200
225

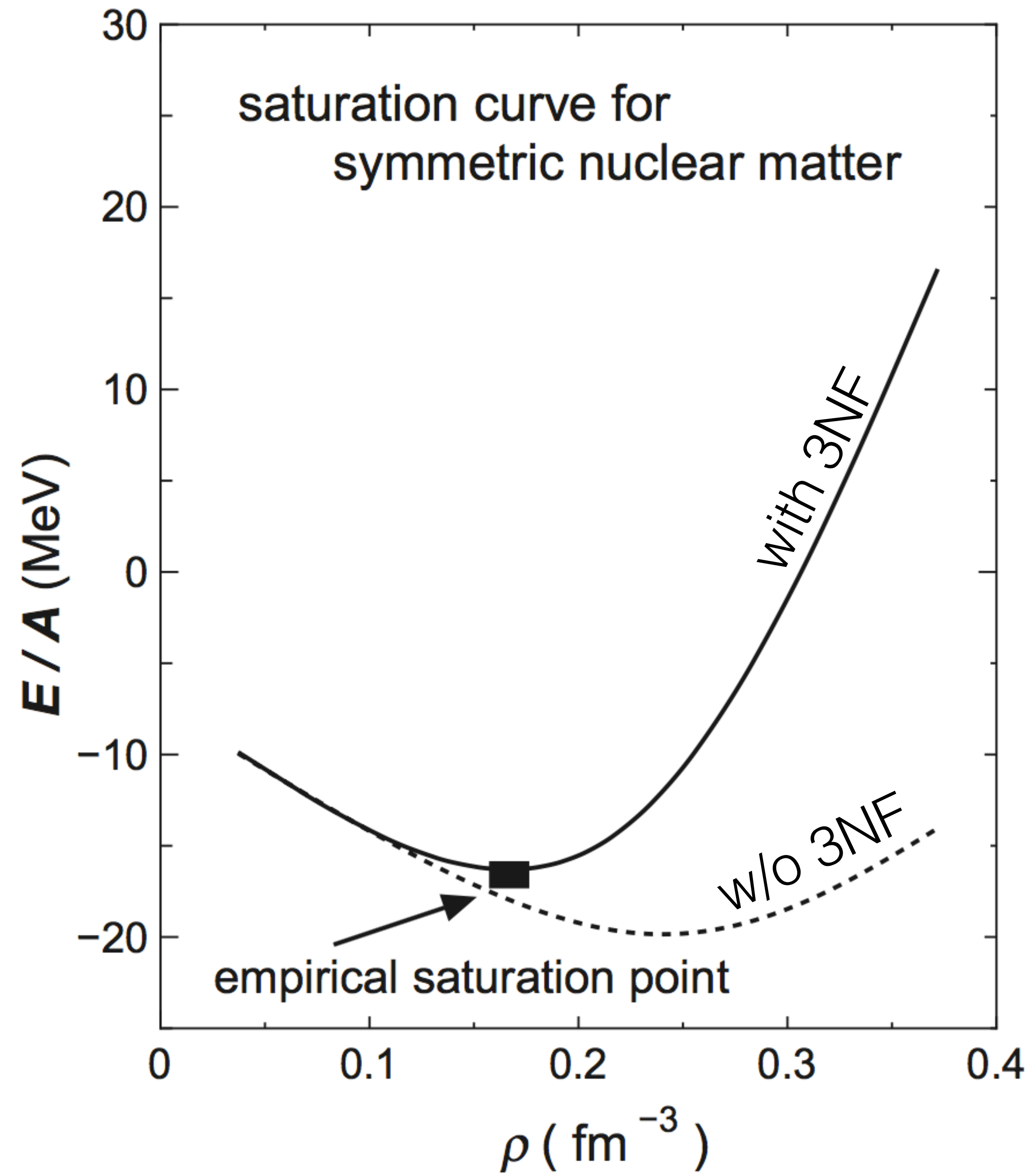


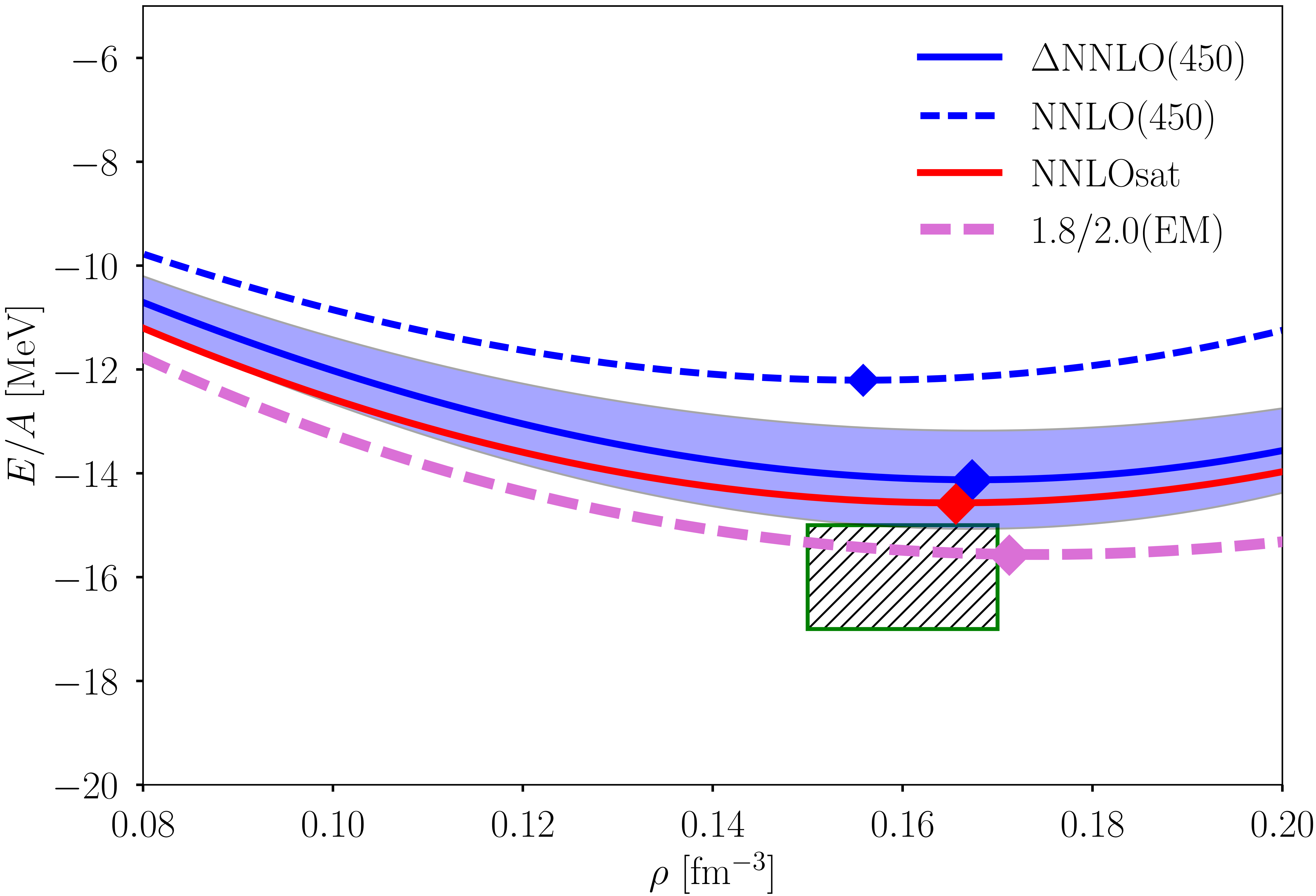
A. Ekström et al. arXiv:1707.09028 [nucl-th] (2017)

Saturation in nuclear matter

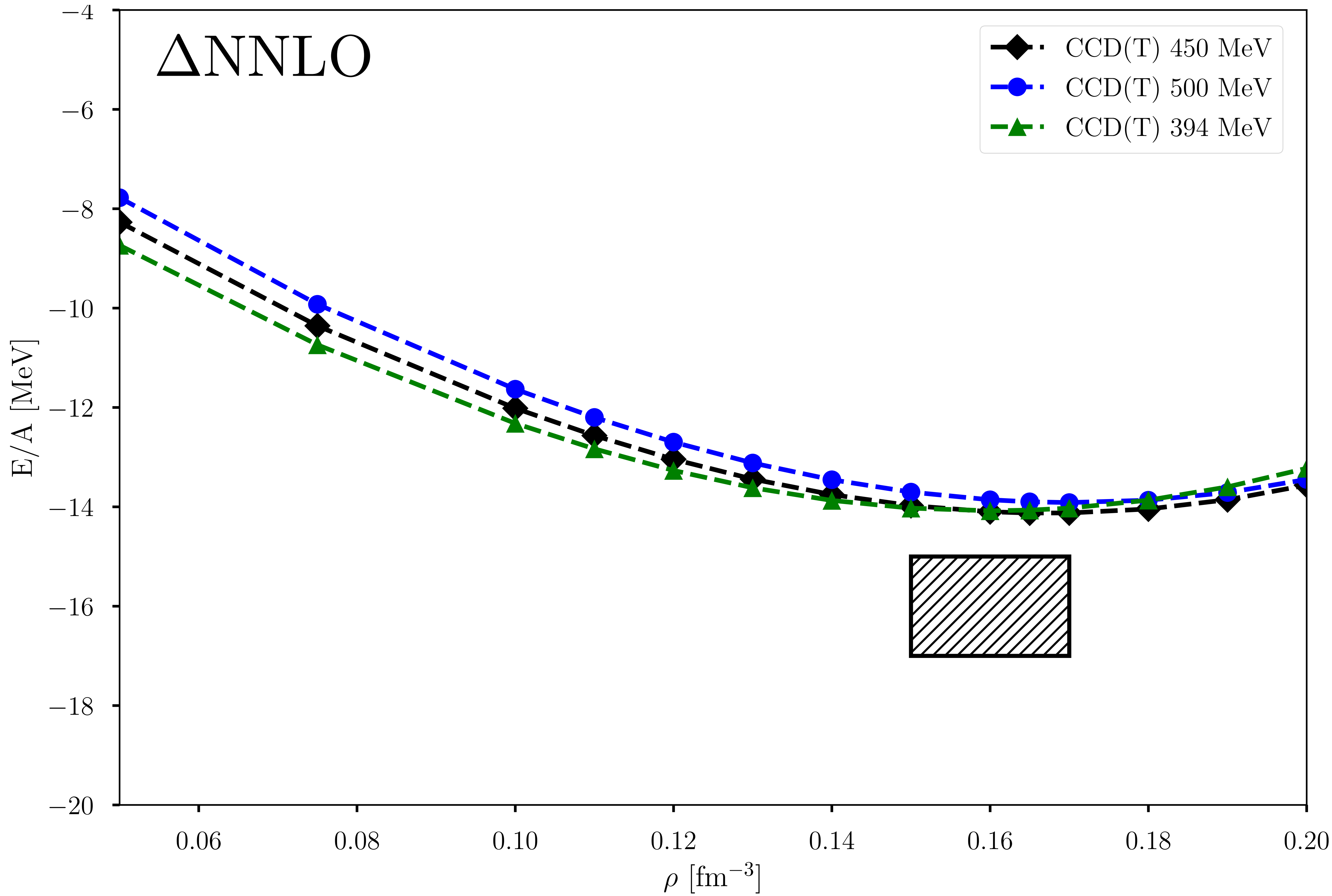
Nucleonic matter is interesting for several reasons:

- The equation of state (EoS) of neutron matter, for instance, determines properties of supernova explosions and of neutron stars.
- It largely determines neutron radii in atomic nuclei and the symmetry energy. Which in turn is related to the difference between proton and neutron radii in atomic nuclei.
- Likewise, the compressibility of nuclear matter is probed in giant dipole excitations.
- The saturation point of nuclear matter determines bulk properties of atomic nuclei, and is therefore an important constraint for nuclear energy-density functionals and mass models.



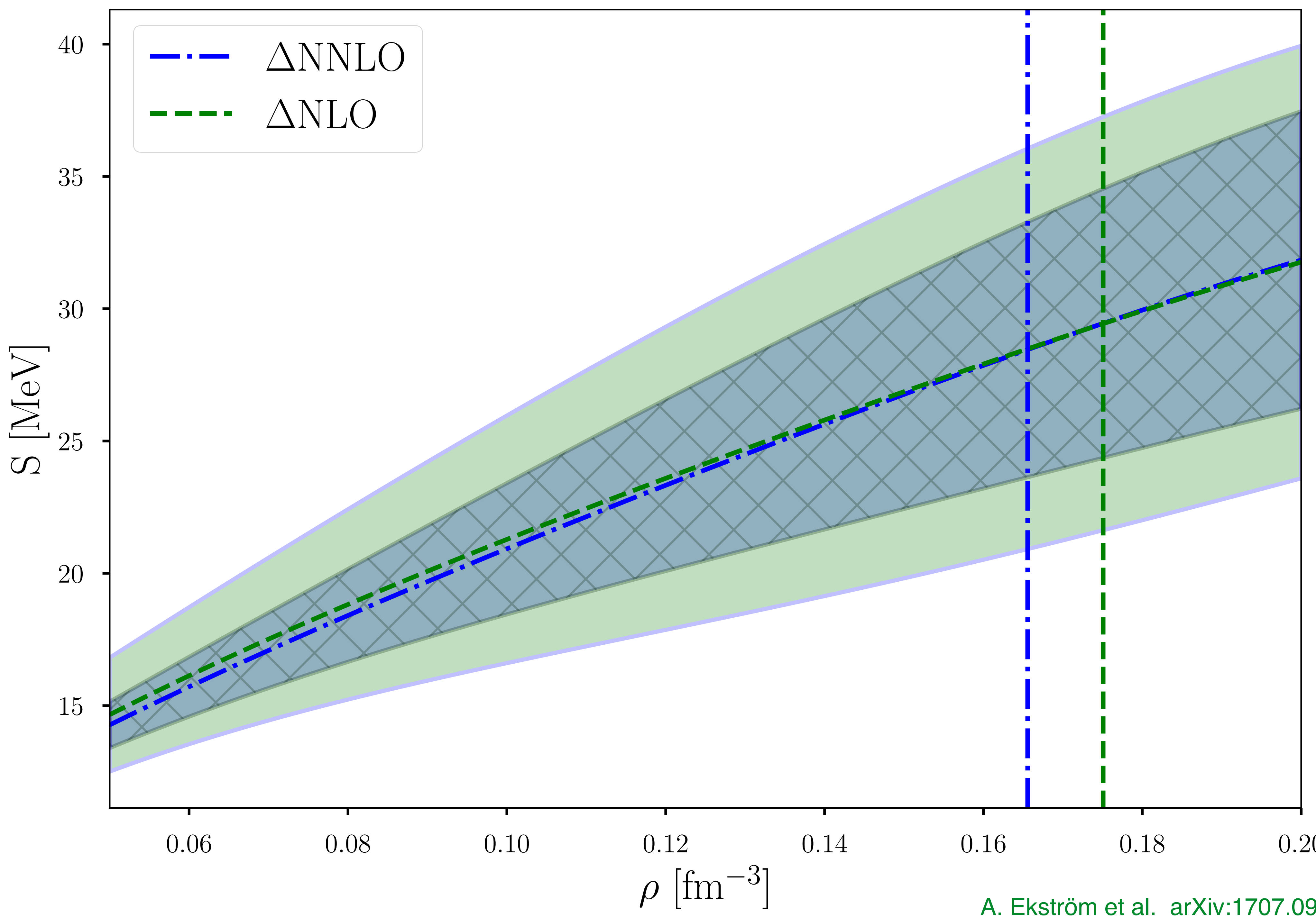

ΔNNLO(450)
NNLO(450)
NNLOsat
1.8/2.0(EM)
E/A [MeV]
ρ [fm^{-3}]
−6
−8
−10
−12
−14
−16
−18
−20
0.08
0.10
0.12
0.14
0.16
0.18
0.20

Varying the cutoff



Symmetry energy

$$22.3 \lesssim S \lesssim 33.3 \ \text{MeV}$$



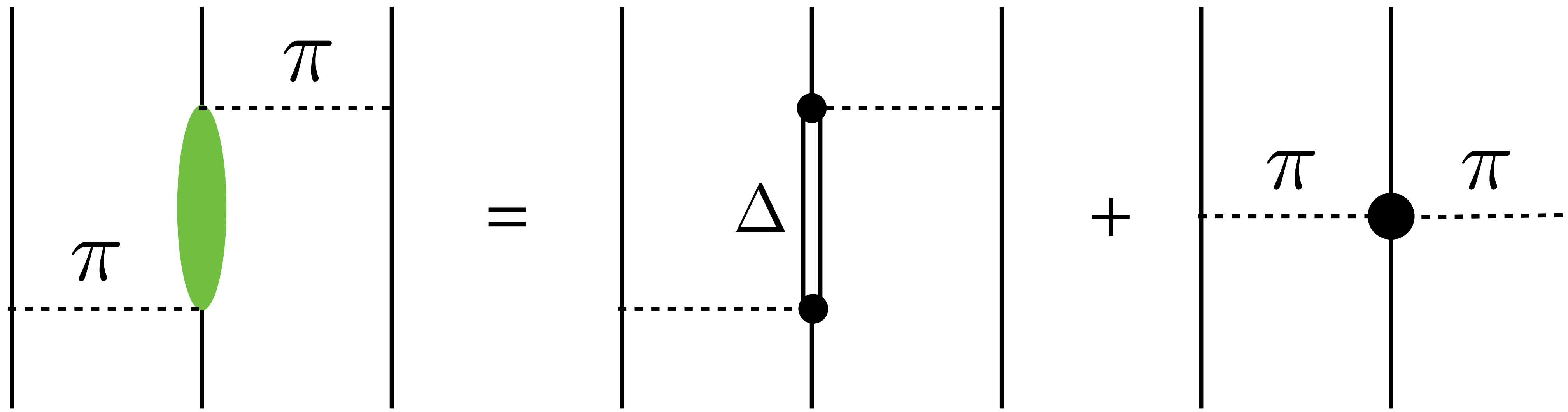
A. Ekström et al. arXiv:1707.09028 [nucl-th] (2017)

LECs: Numerical values

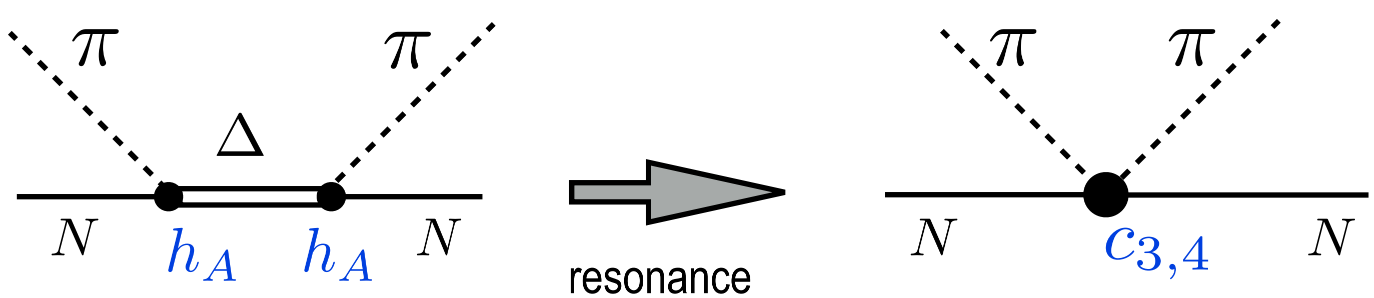
LEC	LO(450)	ΔNLO(450)	ΔNNLO(450)	LO(500)	ΔNLO(500)	ΔNNLO(500)
c_1	–	–	−0.74	–	–	−0.74
c_2	–	–	−0.49	–	–	−0.49
c_3	–	–	−0.65	–	–	−0.65
c_4	–	–	+0.96	–	–	+0.96
$\tilde{C}^{(nn)}_{^1S_0}$	−0.112927	−0.310511	−0.338023	−0.108522	−0.310256	−0.338223
$\tilde{C}^{(np)}_{^1S_0}$	−0.112927	−0.310712	−0.338139	−0.108522	−0.310443	−0.338320
$\tilde{C}^{(pp)}_{^1S_0}$	−0.112927	−0.309893	−0.337137	−0.108522	−0.309618	−0.337303
$\tilde{C}_{^3S_1}$	−0.087340	−0.197951	−0.229310	−0.068444	−0.191013	−0.221721
$C_{^1S_0}$	–	+2.391638	+2.476589	–	+2.395375	+2.488019
$C_{^3S_1}$	–	+0.558973	+0.695953	–	+0.539378	+0.675353
$C_{^1P_1}$	–	+0.004813	−0.028541	–	+0.015247	−0.012651
$C_{^3P_0}$	–	+0.686902	+0.645550	–	+0.727049	+0.698454
$C_{^3P_1}$	–	−1.000112	−1.022359	–	−0.951417	−0.937264
$C_{^3P_2}$	–	−0.808073	−0.870203	–	−0.793621	−0.859526
$C_{^3S_1-^3D_1}$	–	+0.362094	+0.358330	–	+0.358443	+0.354479
c_D	–	–	+0.790	–	–	−0.820
c_E	–	–	+0.017	–	–	−0.350

Three-nucleon forces

“The Fujita-Miyazawa”



Appears already at NLO in Δ-full theory



resonance saturation

$$c_4^\Delta = +1.49$$
$$c_3^\Delta = -2.97$$

A=2,3,4 energies & radii

$\Lambda = 450$ MeV

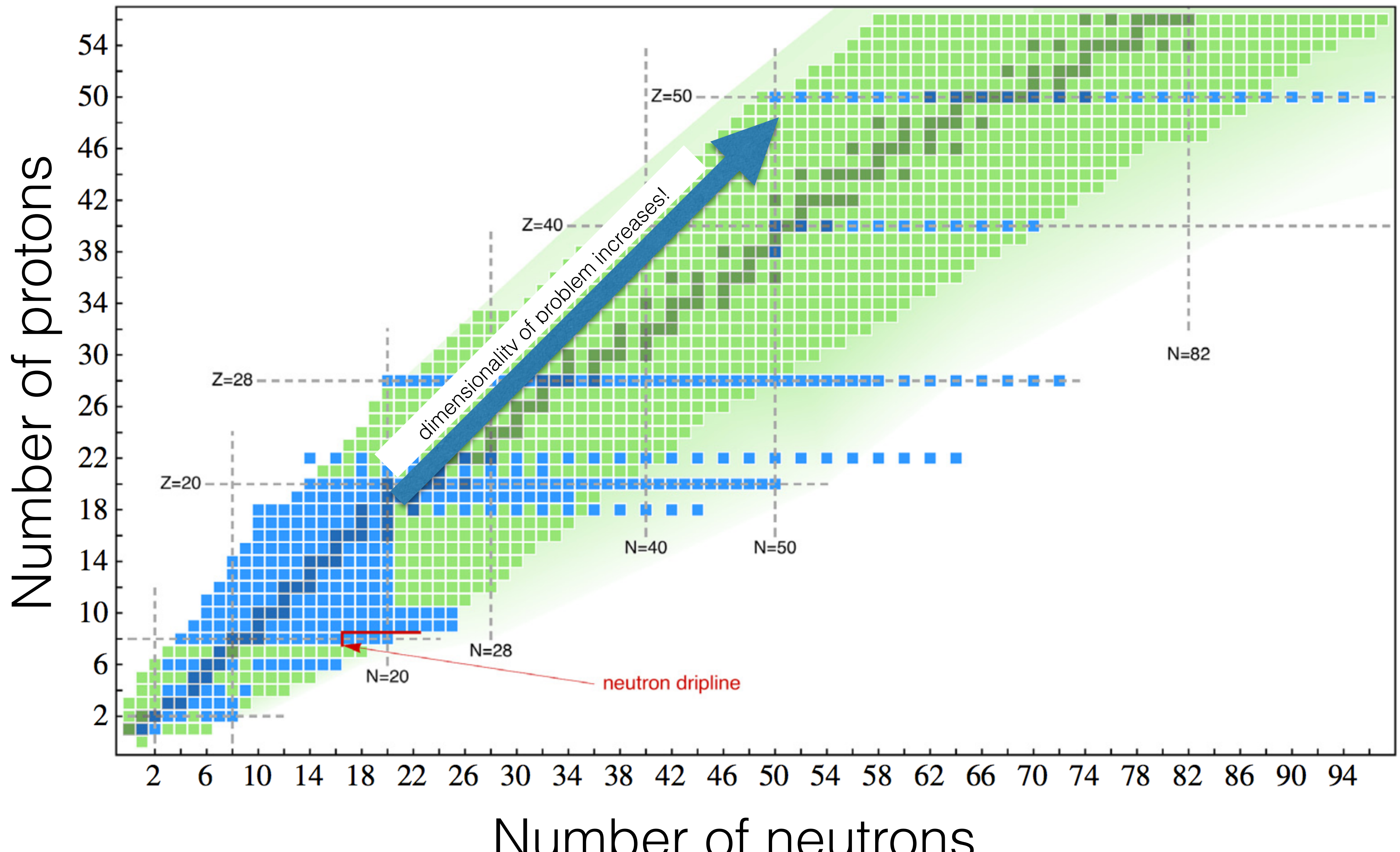
	LO	ΔNLO	ΔNNLO	Exp.
$E(^2\mathrm{H})$	2.01(15)	2.10(5)	2.16(2)	2.2245
$R_{\mathrm{ch}}(^2\mathrm{H})$	2.16(16)	1.157(7)	2.1486(21)	2.1421(88)
$P_{\mathrm{D}}(^2\mathrm{H})$	7.15(3.51)	3.63(97)	3.74(27)	–
$Q(^2\mathrm{H})$	0.322(41)	0.277(11)	0.277(3)	0.27[a]
$E(^3\mathrm{H})$	10.91(2.38)	8.65(62)	8.53(17)	8.48
$R_{\mathrm{ch}}(^3\mathrm{H})$	1.52(23)	1.72(6)	1.74(2)	1.7591(363)
$E(^3\mathrm{He})$	9.95(2.21)	7.85(58)	7.73(16)	7.72
$R_{\mathrm{ch}}(^3\mathrm{He})$	1.66(32)	1.94(8)	1.97(2)	1.9661(30)
$E(^4\mathrm{He})$	39.60(11.3)	29.32(2.83)	28.29(78)	28.30
$R_{\mathrm{ch}}(^4\mathrm{He})$	1.37(30)	1.63(7)	1.67(2)	1.6755(28)

$\Lambda = 500$ MeV

	LO	ΔNLO	ΔNNLO	Exp.
$E(^2\mathrm{H})$	2.04(16)	2.12(5)	2.18(2)	2.2245
$R_{\mathrm{ch}}(^2\mathrm{H})$	2.15(16)	2.153(7)	2.1459(19)	2.1421(88)
$P_{\mathrm{D}}(^2\mathrm{H})$	7.80(3.97)	3.82(1.09)	3.97(30)	–
$Q(^2\mathrm{H})$	0.317(42)	0.276(11)	0.276(3)	0.27[a]
$E(^3\mathrm{H})$	10.47(1.97)	8.91(43)	8.50(12)	8.48
$R_{\mathrm{ch}}(^3\mathrm{H})$	1.54(21)	1.71(5)	1.75(1)	1.7591(363)
$E(^3\mathrm{He})$	9.50(1.80)	8.11(40)	7.70(11)	7.72
$R_{\mathrm{ch}}(^3\mathrm{He})$	1.68(30)	1.92(7)	1.98(2)	1.9661(30)
$E(^4\mathrm{He})$	37.00(8.69)	30.70(2.38)	28.31(65)	28.30
$R_{\mathrm{ch}}(^4\mathrm{He})$	1.39(28)	1.62(6)	1.67(2)	1.6755(28)

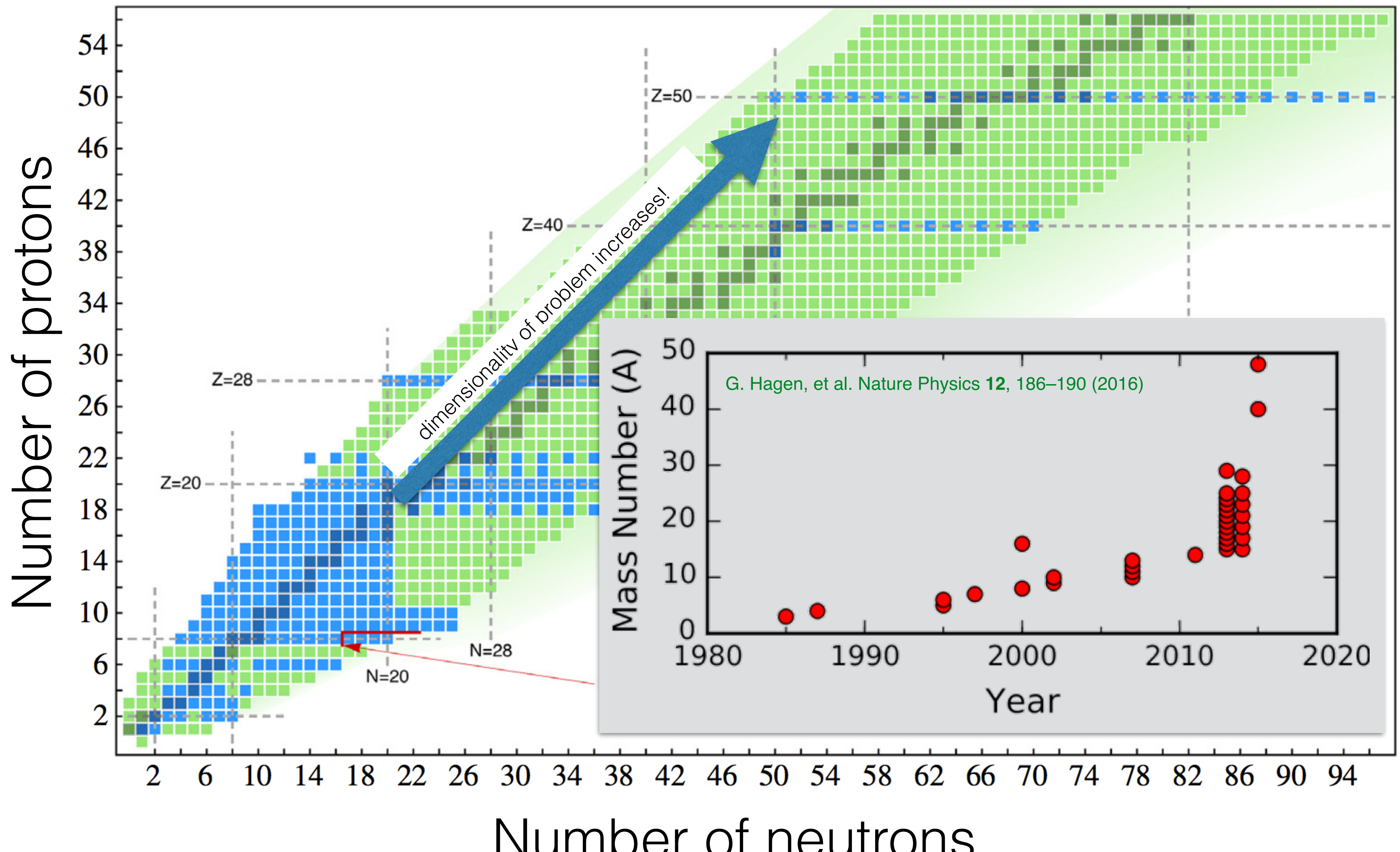
[a] CD-Bonn value [3]

Progress in ab initio calculations



H. Hergert et al. Phys. Rep. **621**, 165-222 (2016)

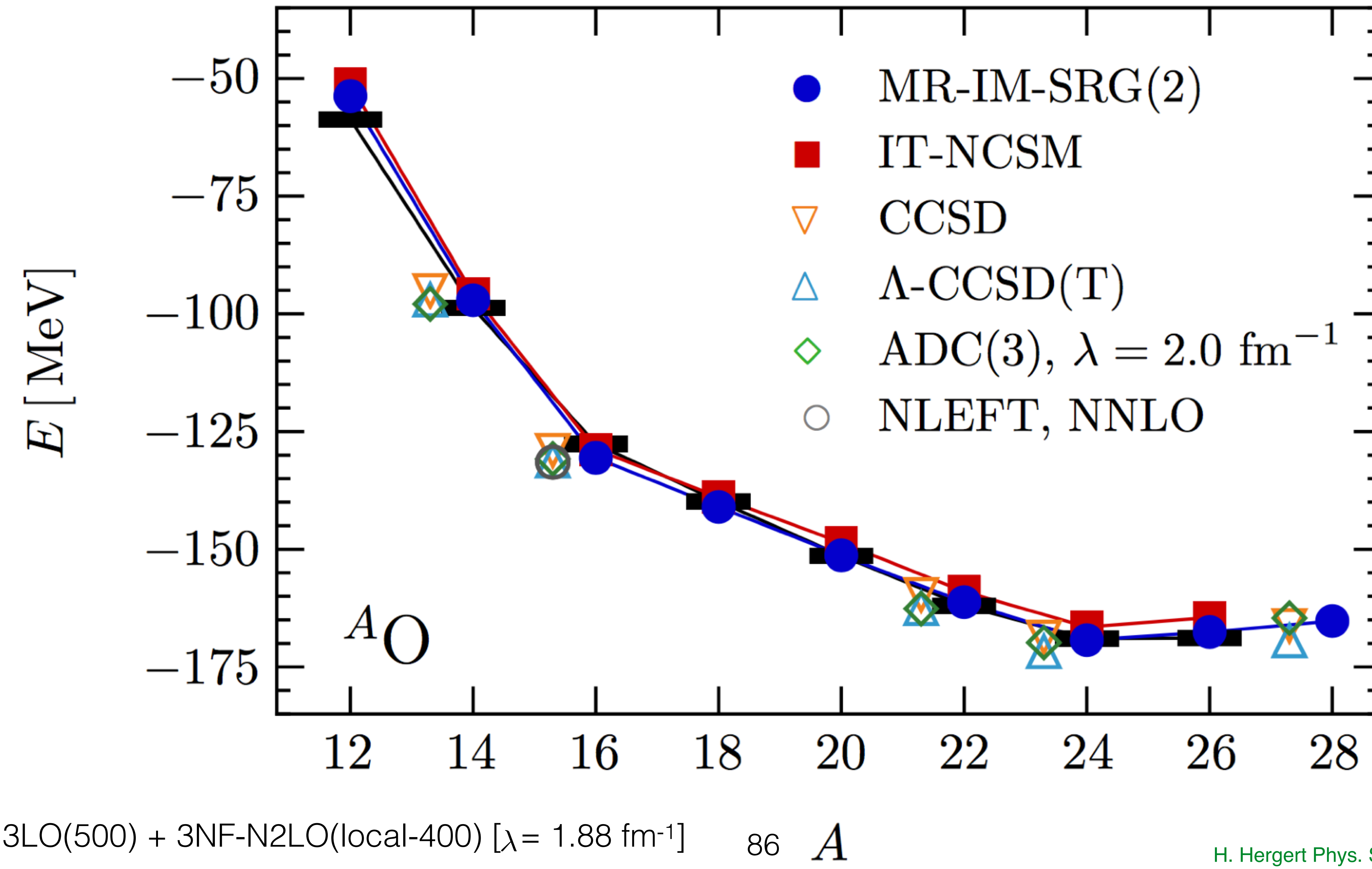
Progress in ab initio calculations



H. Hergert et al. Phys. Rep. **621**, 165-222 (2016)

Complementary methods agree

Same chiral interaction, but **different** many-body methods

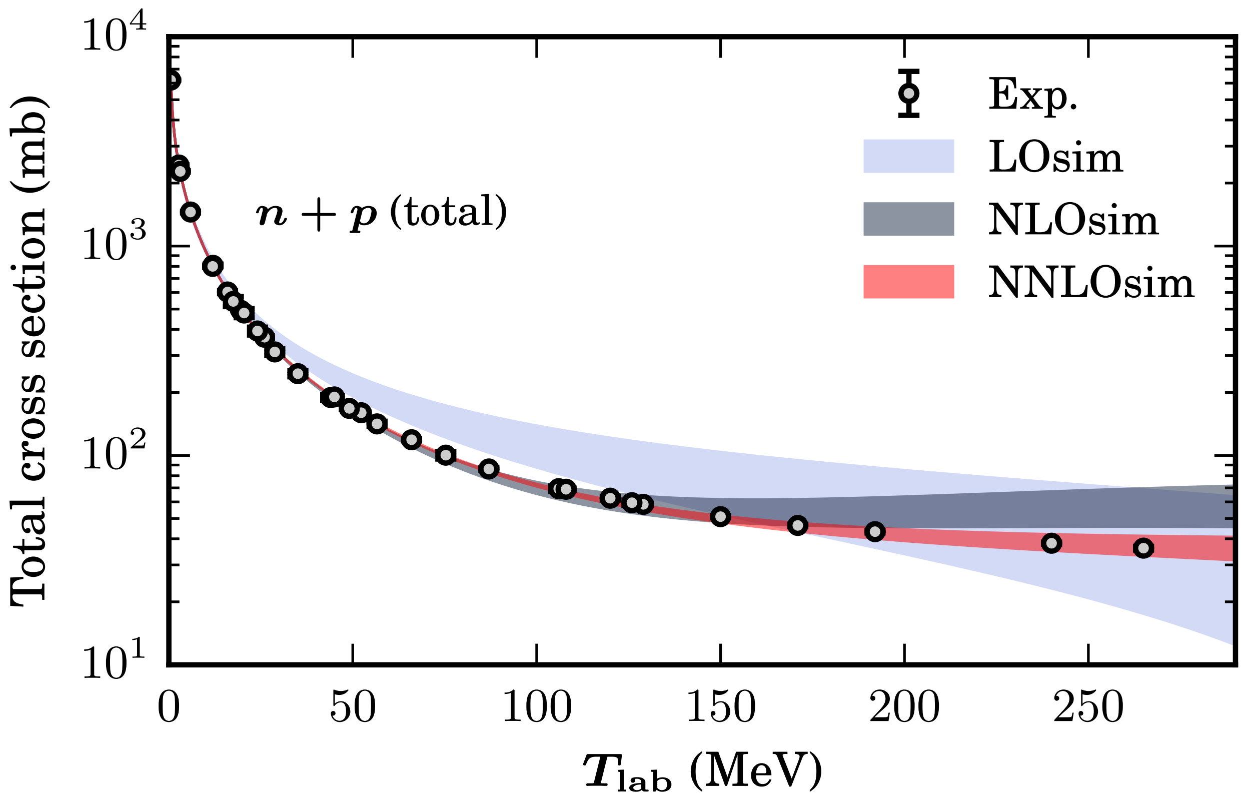


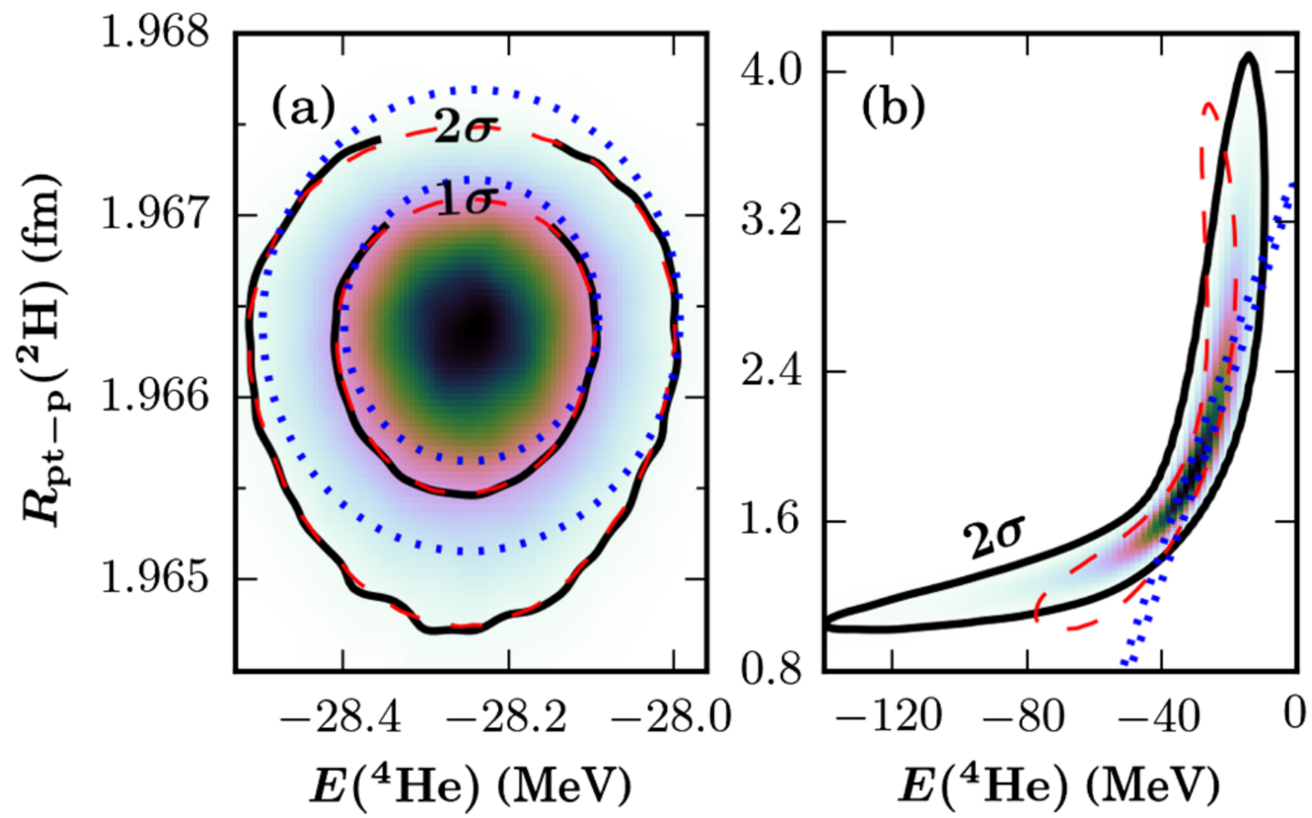
NN-N3LO(500) + 3NF-N2LO(local-400) [λ= 1.88 fm^{-1}]

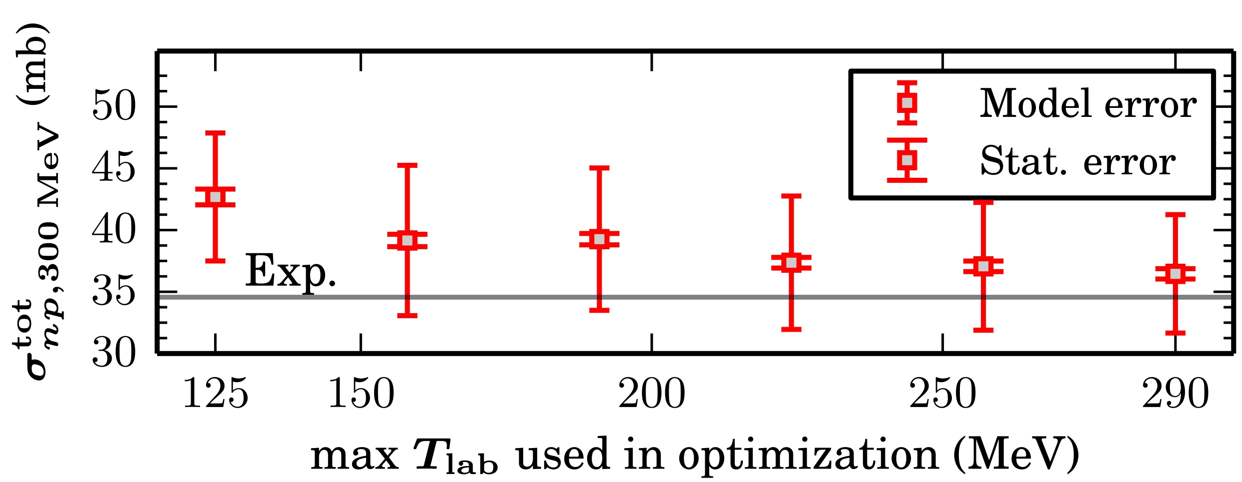
H. Hergert Phys. Scripta **92**, 023002 (2017)

Uncertainty in the interaction

“Calculations are only as good as their input”







$$\chi^2(\boldsymbol{\alpha}) \equiv \sum_{i \in \mathbb{M}} \left(\frac{\mathcal{O}_i^{\text{theo}}(\boldsymbol{\alpha}) - \mathcal{O}_i^{\text{exp}}}{\sigma_i} \right)^2 \equiv \sum_{i \in \mathbb{M}} r_i^2(\boldsymbol{\alpha}),$$

$$\begin{aligned} \sigma^2 &= \sigma_{\text{exp}}^2 + \sigma_{\text{theo}}^2 \\ &= \sigma_{\text{exp}}^2 + \sigma_{\text{numerical}}^2 + \sigma_{\text{method}}^2 + \sigma_{\text{model}}^2 \end{aligned}$$

$$\sigma_{\text{model,x}}^{(\text{amp})} = C_{\text{x}} \left(\frac{Q}{\Lambda_\chi} \right)^{\nu_{\text{x}}+1}, \qquad \text{x} \in \{NN, \pi N\}$$

B. D. Carlsson et al. Phys. Rev. X **6**, 011019 (2016)
A. Ekström et al J. Phys. G: Nucl. Part. Phys. **42** 034003 (2015)

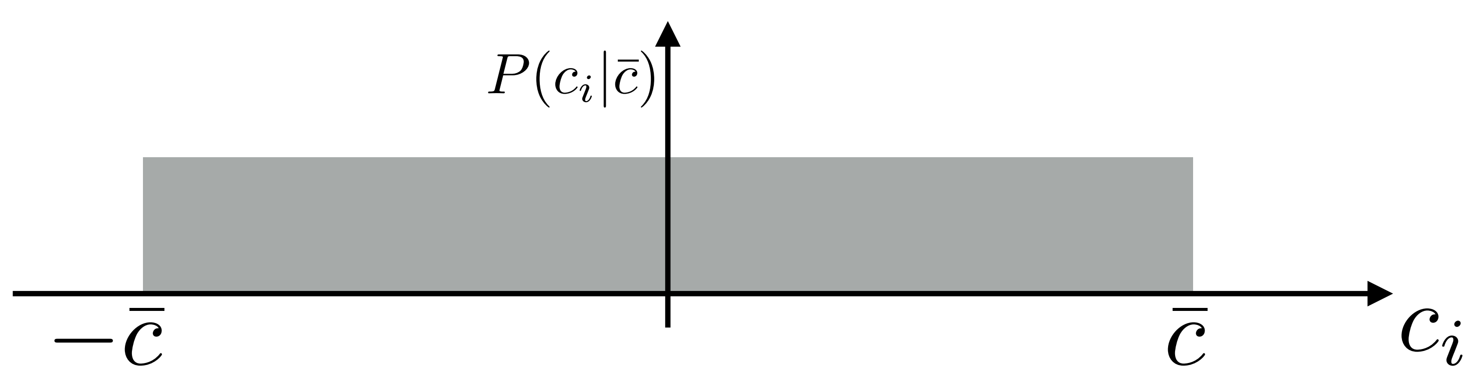
assumptions, assumptions, ….

1) Independence: $P(c_0,\ldots,c_k|\bar{c}) = \prod_{i=0}^{k} P(c_i|\bar{c})$

where $\bar{c}$ is a common upper bound, and
$P(c_i|\bar{c}) = P(c_j|\bar{c})\ \ \forall(i,j)$

2) Priors for the expansion coefficients: $P(c_i|\bar{c})$

Maximum entropy dictates that the
least informative distribution is uniform.



3) Prior on $\bar{c}$

$$P(\bar{c}) = \frac{1}{\ln(\bar{c}_>/\bar{c}_<)}\frac{1}{\bar{c}}\theta(\bar{c}-\bar{c}_<)\theta(\bar{c}_>-\bar{c})$$

$$\bar{c}_< = \varepsilon, \quad \bar{c}_> = 1/\varepsilon$$

R. J. Furnstahl et al, PRC **92**, 024005 (2015)

$$P(\Delta_k|c_0,\ldots,c_k) = \int_{-\infty}^{+\infty} P(\Delta_k|c_{k+1},\ldots)P(c_{k+1},\ldots|c_0,\ldots,c_k)\, dc_{k+1}dc_{k+2}\ldots$$

Following R. J. Furnstahl et al, PRC **92**, 024005 (2015) gives
(Integrating in, marginalizing, and exploiting Bayes' theorem, …)

Leading-term approximation: $\Delta_k \approx c_{k+1}Q^{k+1} \equiv \Delta_k^{(1)}$

$$P(\Delta_k^{(1)}|c_0,\ldots,c_k) = \frac{\int_0^\infty P(c_{k+1}|\bar{c})\prod_{i=0}^{k} P(c_i|\bar{c})P(\bar{c})d\bar{c}}{Q^{k+1}\prod_{i=0}^{k} P(c_i|\bar{c}')P(\bar{c}')d\bar{c}'}$$

Which can be evaluated explicitly for uniform priors.
In fact, so can also the degree of belief integral

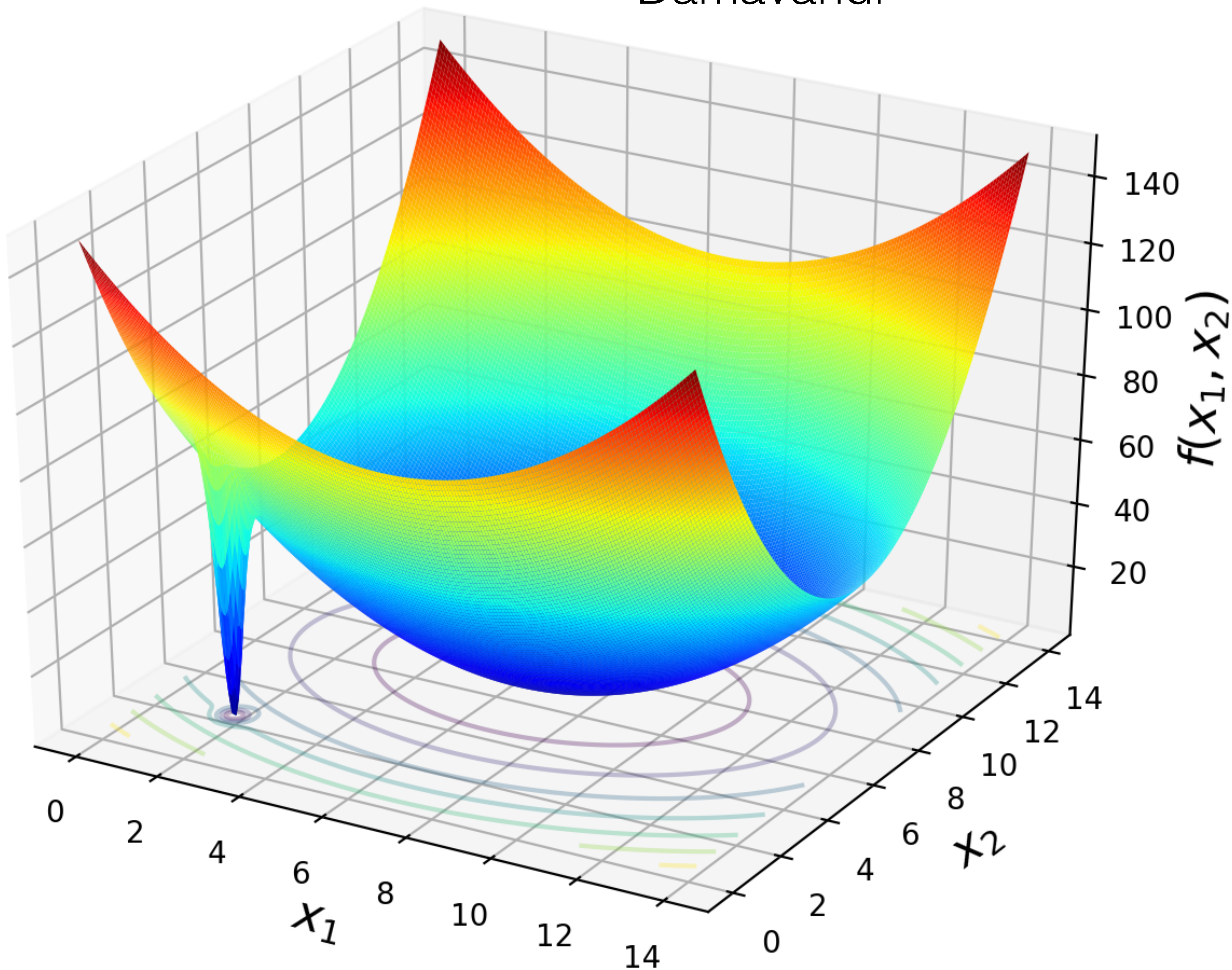
$$p\% = \int_{-d_k^{(p)}}^{+d_k^{(p)}} = P(\Delta_k^{(1)}|c_0,\ldots,c_k)d\Delta_k^{(1)}$$

(not a Gaussian)

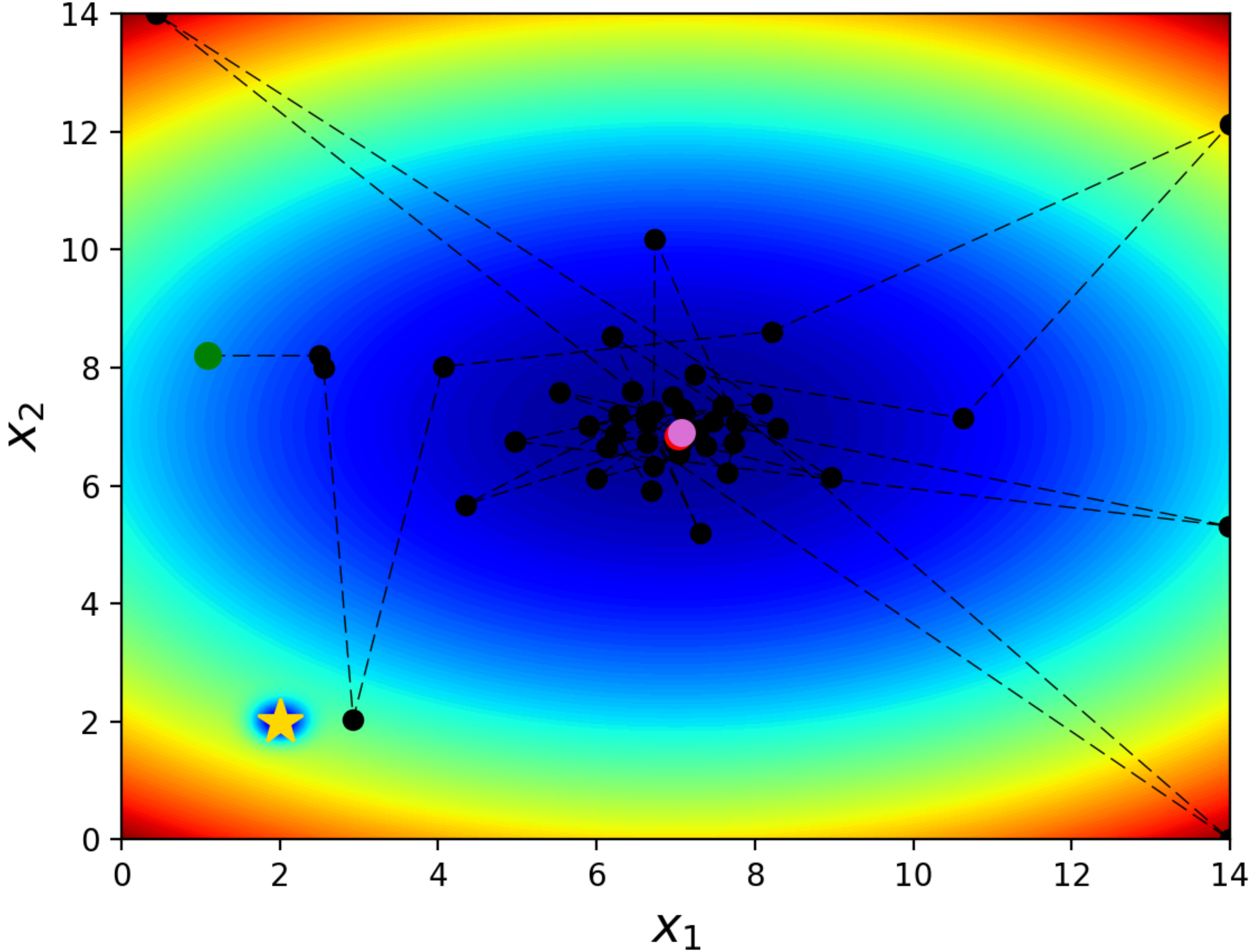
R. J. Furnstahl et al, PRC **92**, 024005 (2015)

Interaction	BE	S_n	Δ	R_{ch}	R_W	S_v	L
$NNLO_{sat}$	404(3)	9.5	2.69	3.48	3.65	26.9	40.8
1.8/2.0 (EM)	420(1)	10.1	2.69	3.30	3.47	33.3	48.6
2.0/2.0 (EM)	396(2)	9.3	2.66	3.34	3.52	31.4	46.7
2.2/2.0 (EM)	379(2)	8.8	2.61	3.37	3.55	30.2	45.5
2.8/2.0 (EM)	351(3)	8.0	2.41	3.44	3.62	28.5	43.8
2.0/2.0 (PWA)	346(4)	7.8	2.82	3.55	3.72	27.4	44.0
Experiment	415.99	9.995	2.399	3.477			

Damavandi

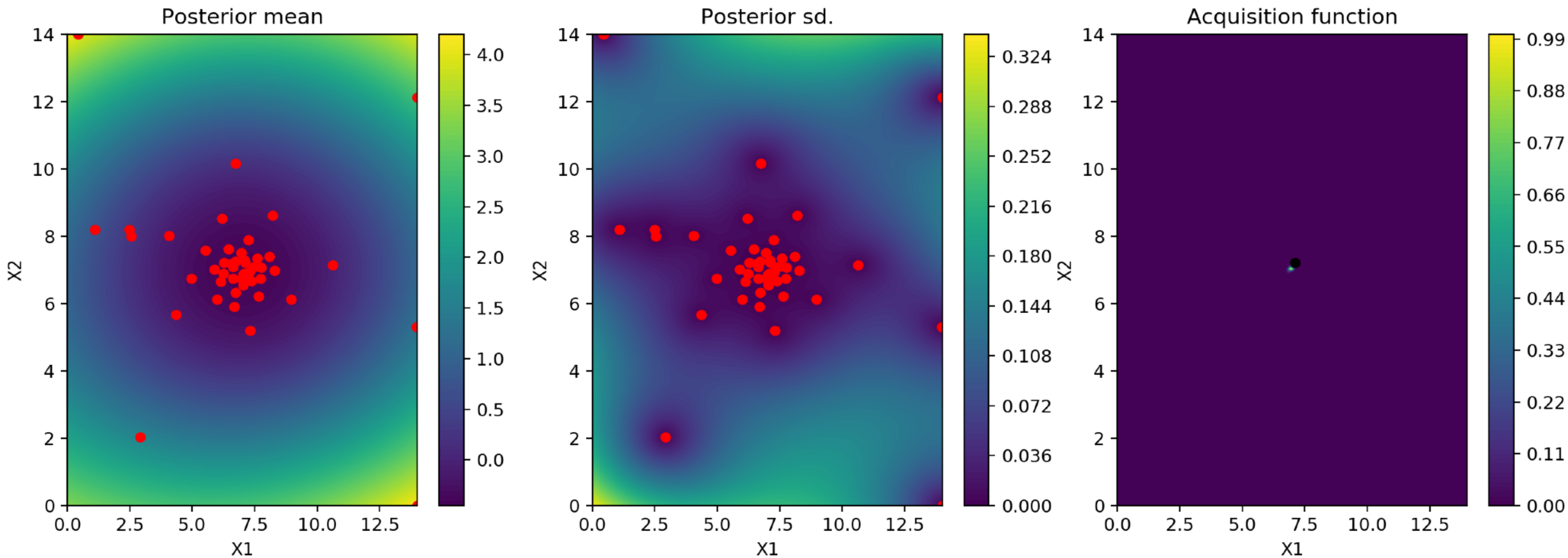


100

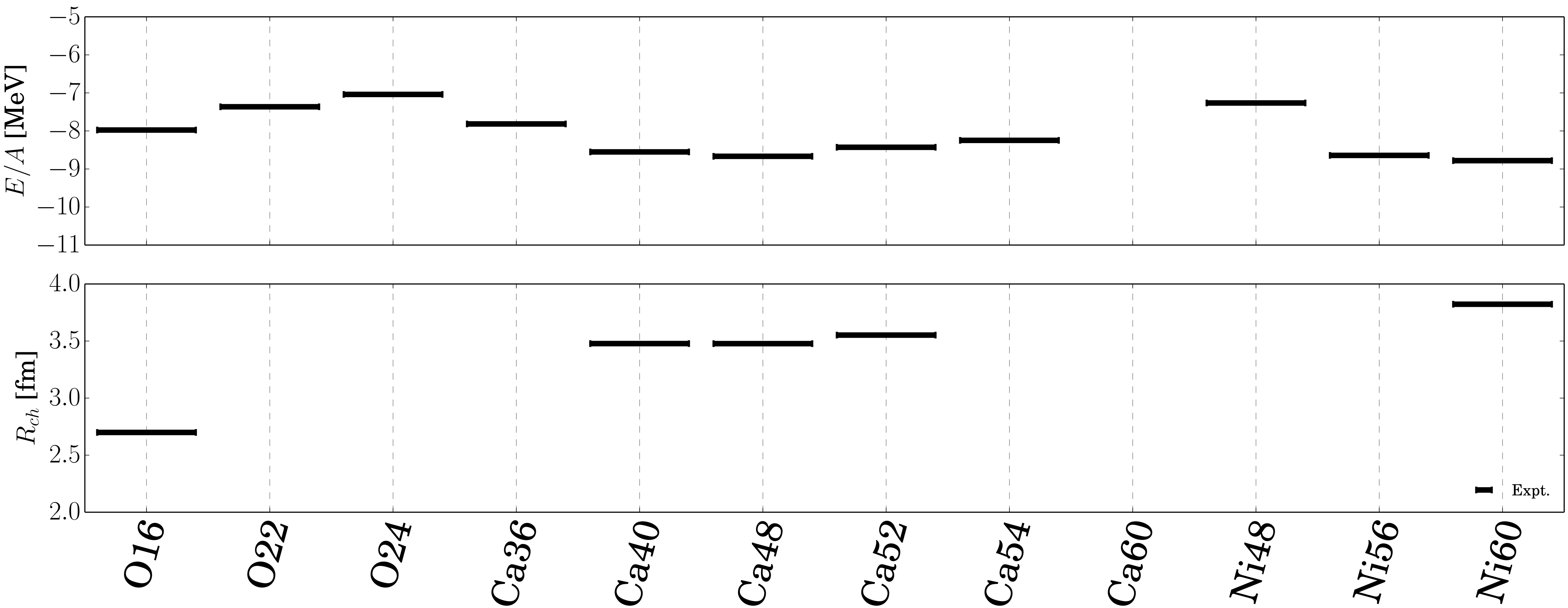


100

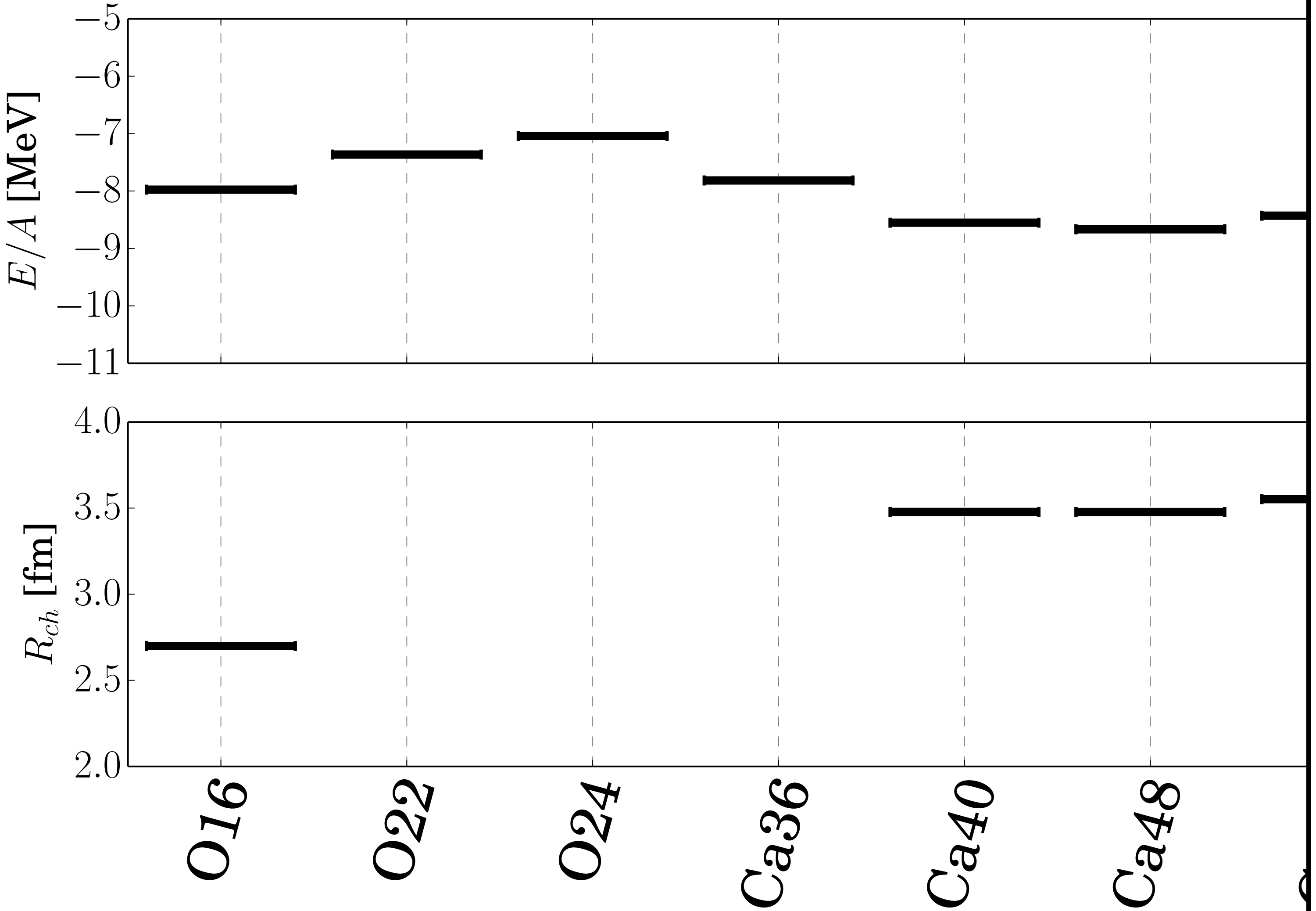
Damavandi



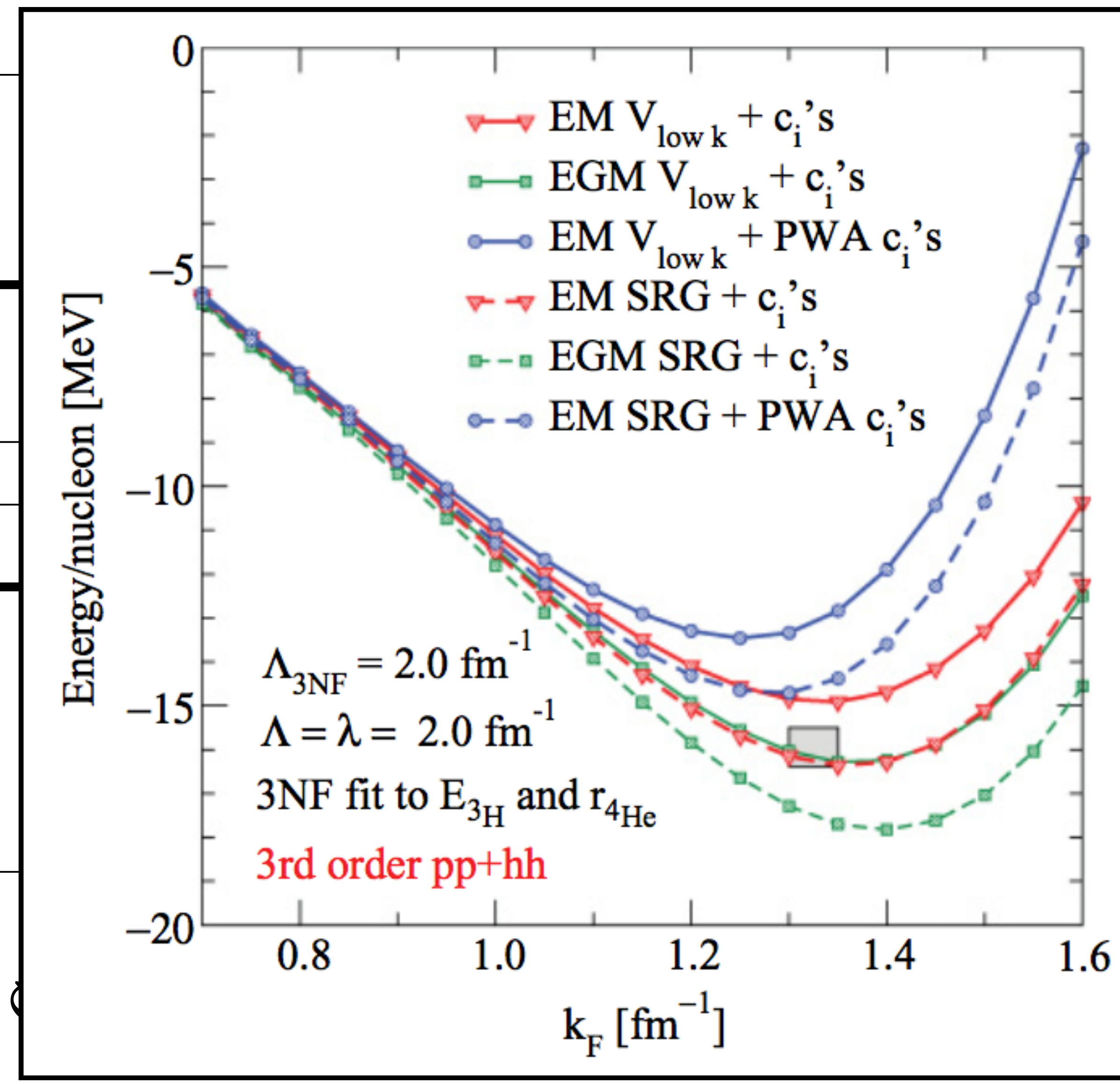
Energy & charge radius

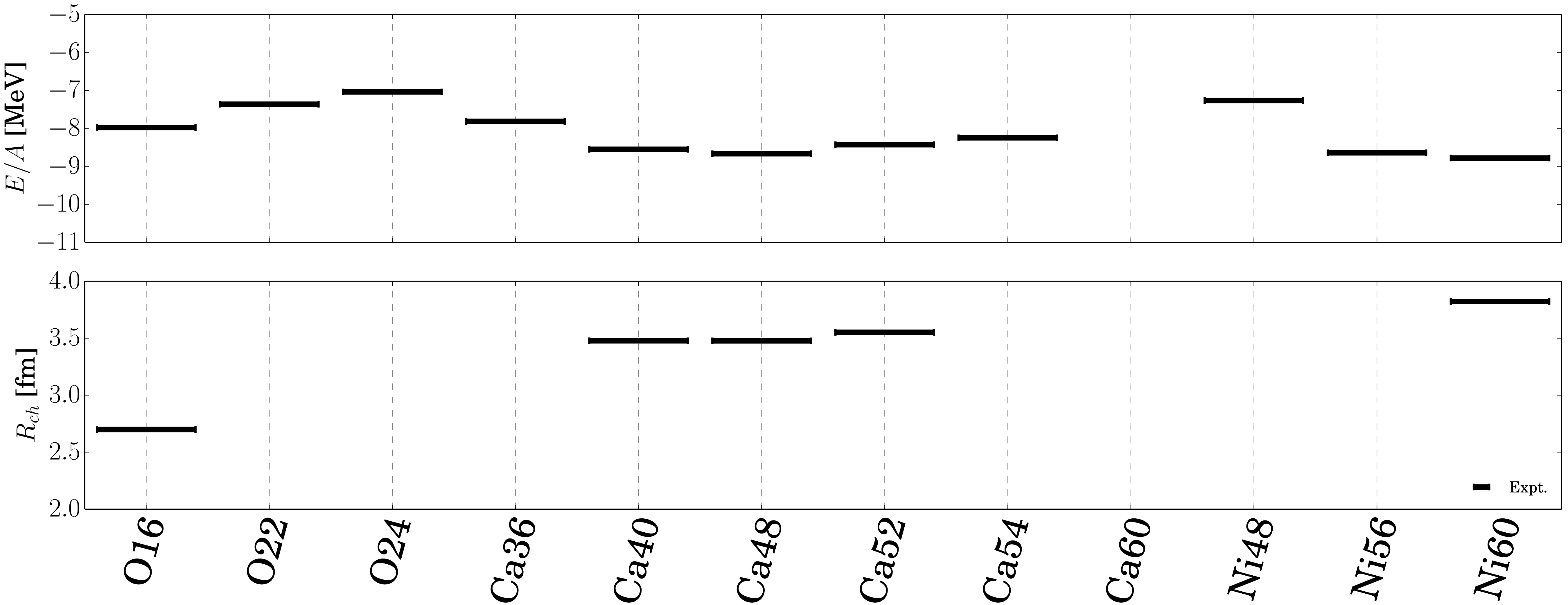


Energy & charge radius

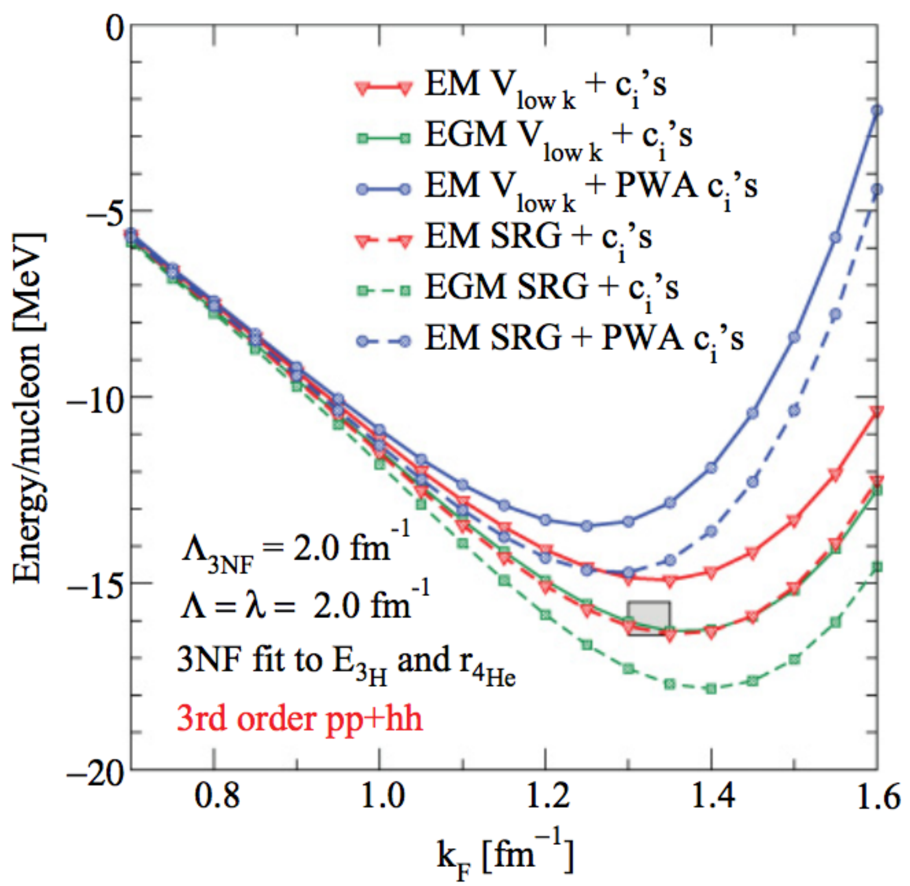


K. Hebeler, et al. PRC **83**, 031301(R) (2011)

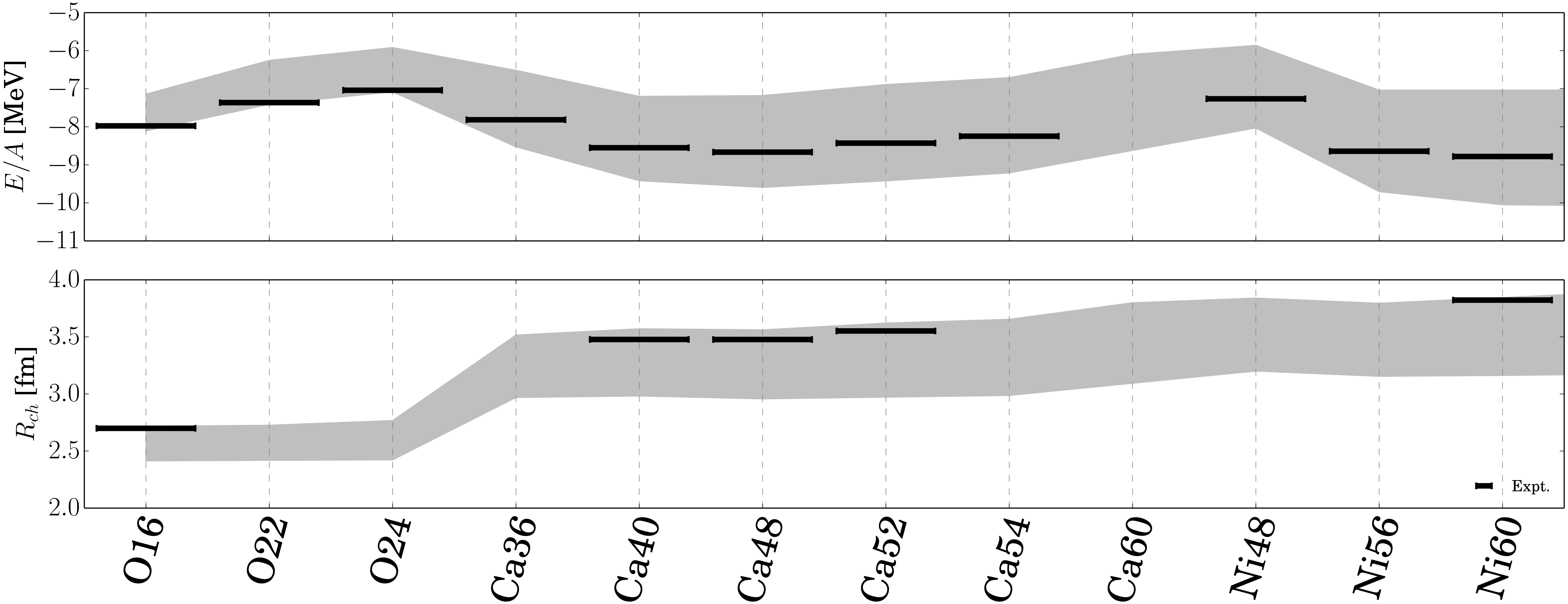


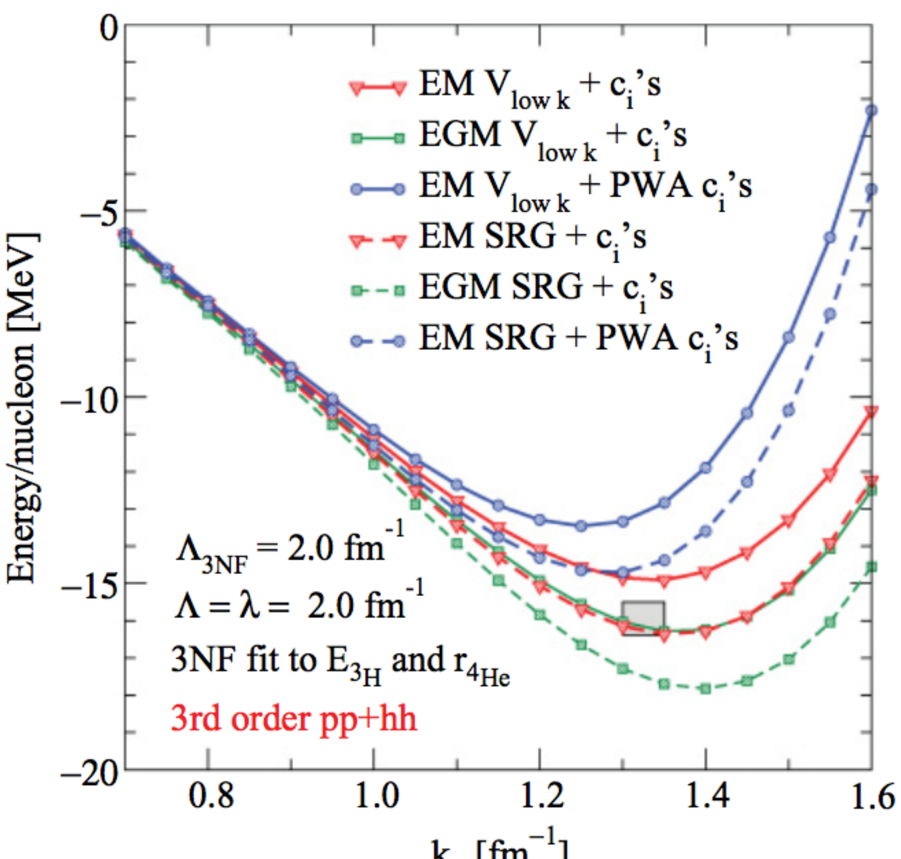


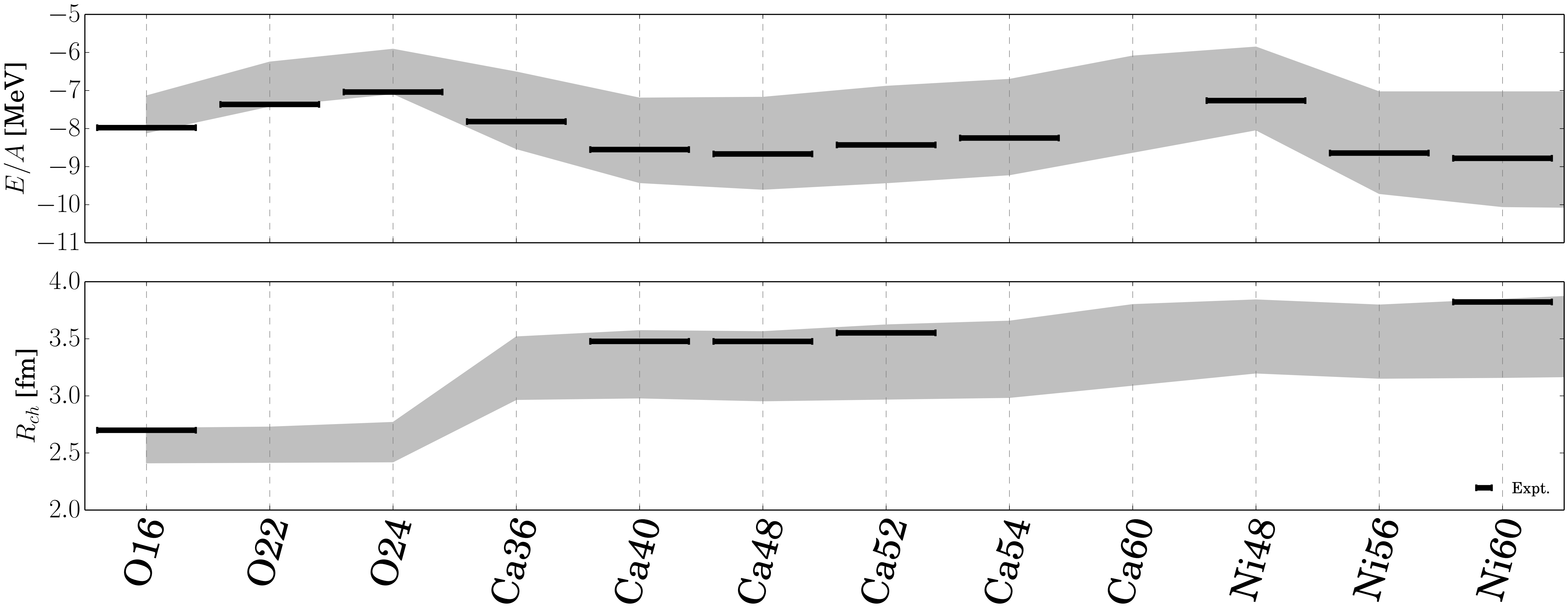
E/A [MeV]
R_ch [fm]
Expt.
O16
O22
O24
Ca36
Ca40
Ca48
Ca52
Ca54
Ca60
Ni48
Ni56
Ni60



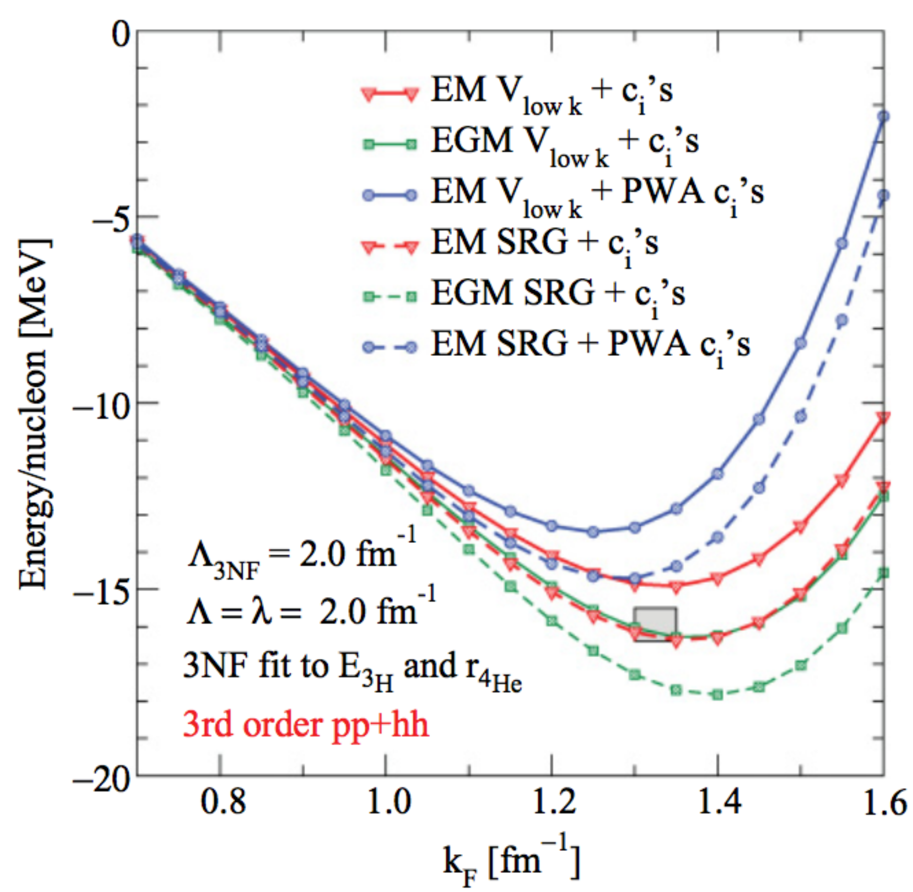
EM V_low k + c_i's
EGM V_low k + c_i's
EM V_low k + PWA c_i's
EM SRG + c_i's
EGM SRG + c_i's
EM SRG + PWA c_i's
Λ_3NF = 2.0 fm^-1
Λ = λ = 2.0 fm^-1
3NF fit to E_3H and r_4He
3rd order pp+hh
Energy/nucleon [MeV]
k_F [fm^-1]


E/A [MeV]
R_{ch} [fm]
Expt.
O16
O22
O24
Ca36
Ca40
Ca48
Ca52
Ca54
Ca60
Ni48
Ni56
Ni60

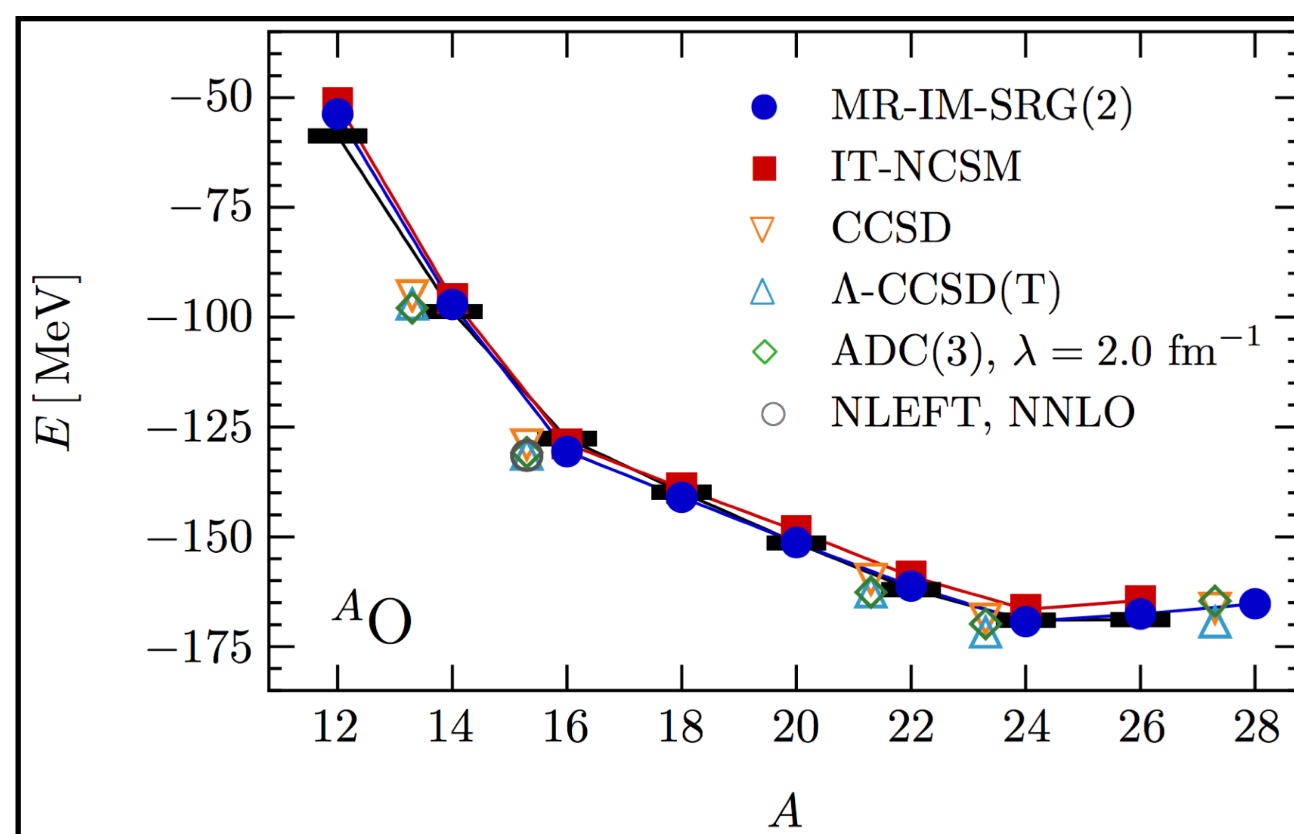

EM $V_{low\,k}$ + c_i's
EGM $V_{low\,k}$ + c_i's
EM $V_{low\,k}$ + PWA c_i's
EM SRG + c_i's
EGM SRG + c_i's
EM SRG + PWA c_i's
$\Lambda_{3NF} = 2.0$ fm^{-1}
$\Lambda = \lambda = 2.0$ fm^{-1}
3NF fit to E_{3H} and r_{4He}
3rd order pp+hh
Energy/nucleon [MeV]
k_F [fm^{-1}]



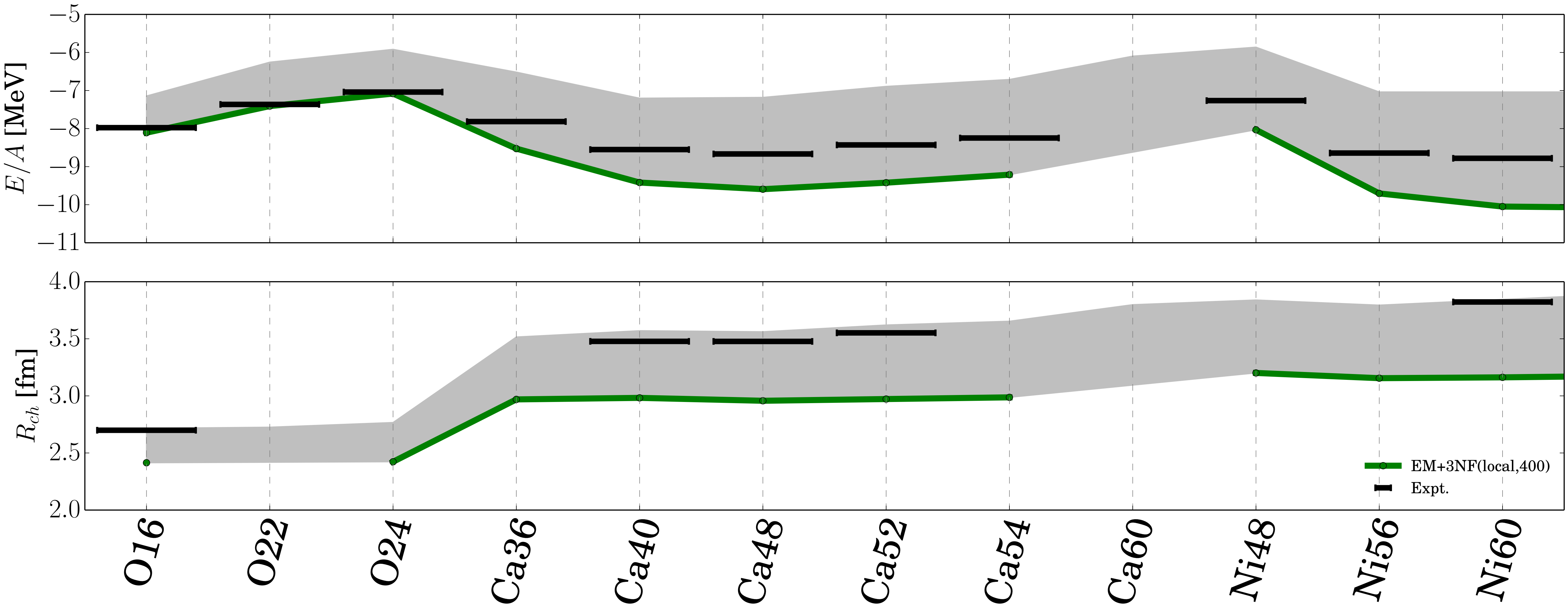
E/A [MeV]
R_{ch} [fm]
Expt.
O16
O22
O24
Ca36
Ca40
Ca48
Ca52
Ca54
Ca60
Ni48
Ni56
Ni60



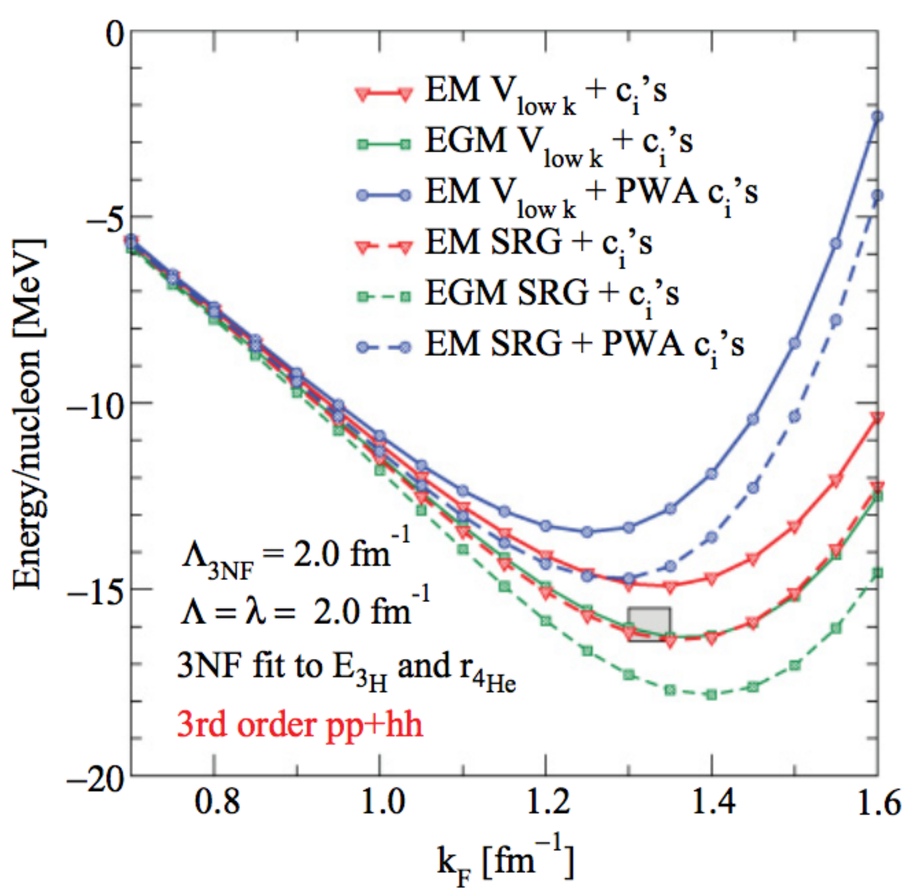
EM $V_{\mathrm{low\,k}}$ + c_i's
EGM $V_{\mathrm{low\,k}}$ + c_i's
EM $V_{\mathrm{low\,k}}$ + PWA c_i's
EM SRG + c_i's
EGM SRG + c_i's
EM SRG + PWA c_i's
$\Lambda_{3NF} = 2.0\ \mathrm{fm}^{-1}$
$\Lambda = \lambda = 2.0\ \mathrm{fm}^{-1}$
3NF fit to E_{3H} and r_{4He}
3rd order pp+hh
Energy/nucleon [MeV]
$k_F\ [\mathrm{fm}^{-1}]$



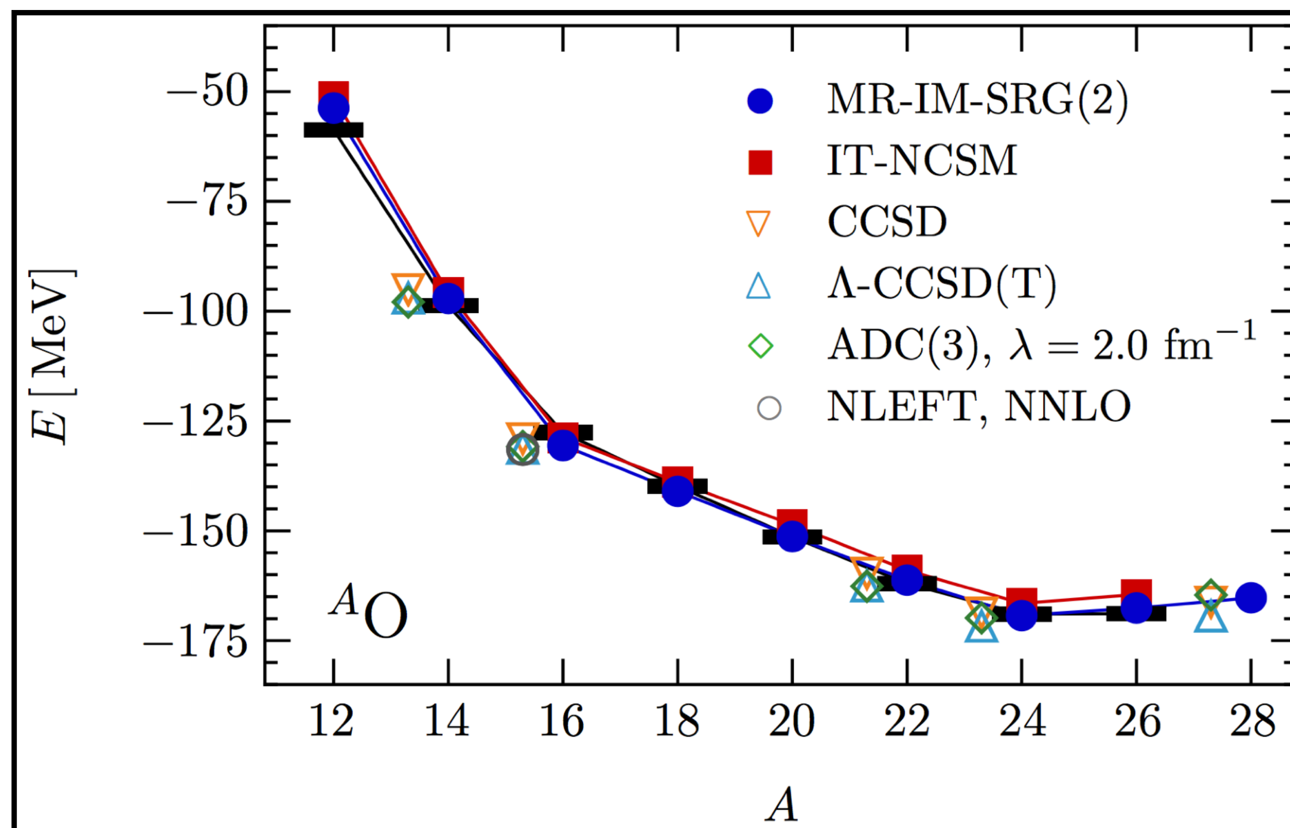
MR-IM-SRG(2)
IT-NCSM
CCSD
Λ-CCSD(T)
ADC(3), $\lambda = 2.0\ \mathrm{fm}^{-1}$
NLEFT, NNLO
^{A}O
E [MeV]
A



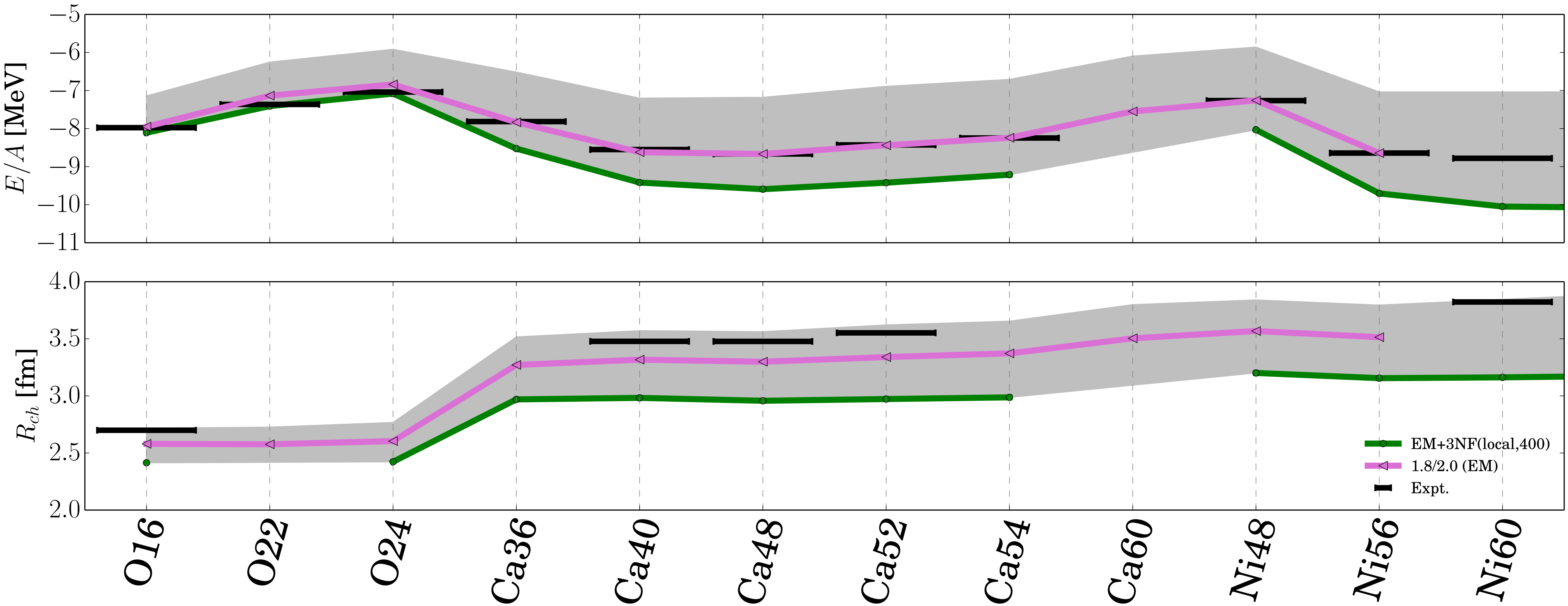
E/A [MeV]
R_ch [fm]
EM+3NF(local,400)
Expt.
O16
O22
O24
Ca36
Ca40
Ca48
Ca52
Ca54
Ca60
Ni48
Ni56
Ni60



EM V_low k + c_i's
EGM V_low k + c_i's
EM V_low k + PWA c_i's
EM SRG + c_i's
EGM SRG + c_i's
EM SRG + PWA c_i's
Λ_3NF = 2.0 fm^-1
Λ = λ = 2.0 fm^-1
3NF fit to E_3H and r_4He
3rd order pp+hh
Energy/nucleon [MeV]
k_F [fm^-1]

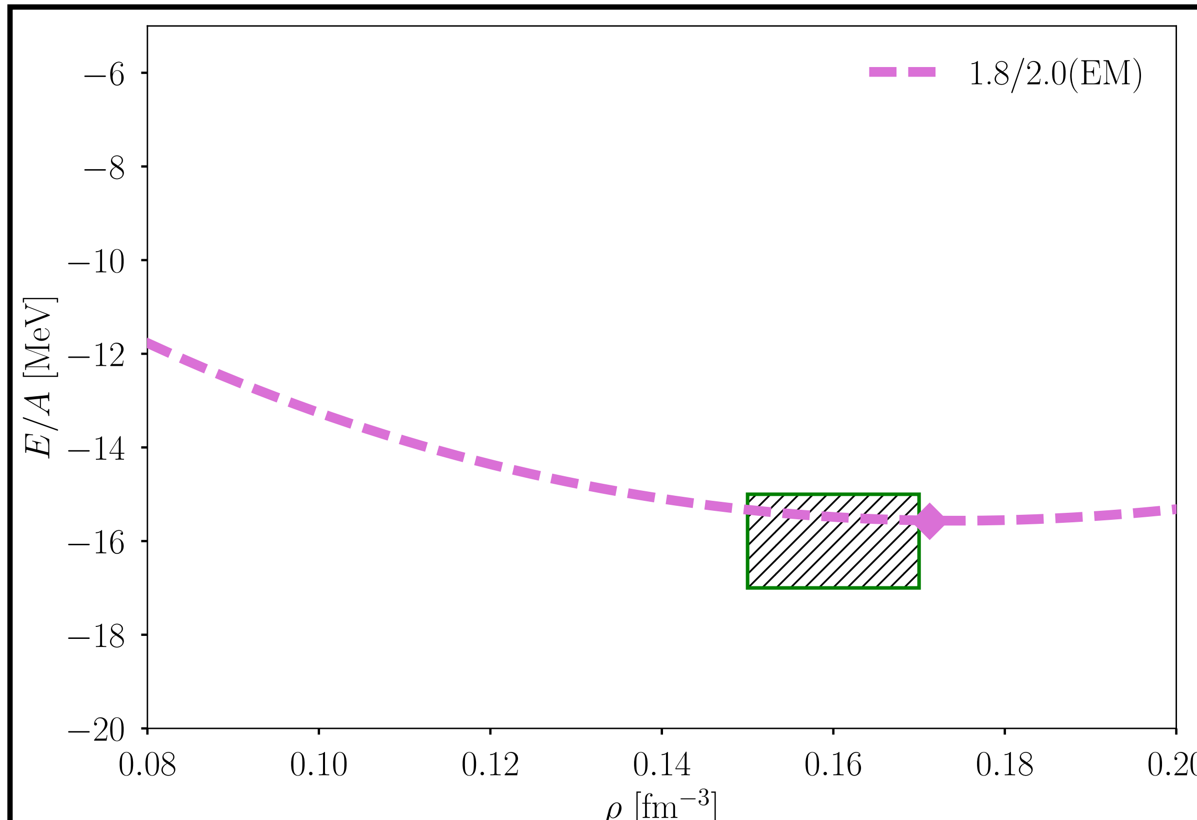


MR-IM-SRG(2)
IT-NCSM
CCSD
Λ-CCSD(T)
ADC(3), λ = 2.0 fm^-1
NLEFT, NNLO
^A O
E [MeV]
A



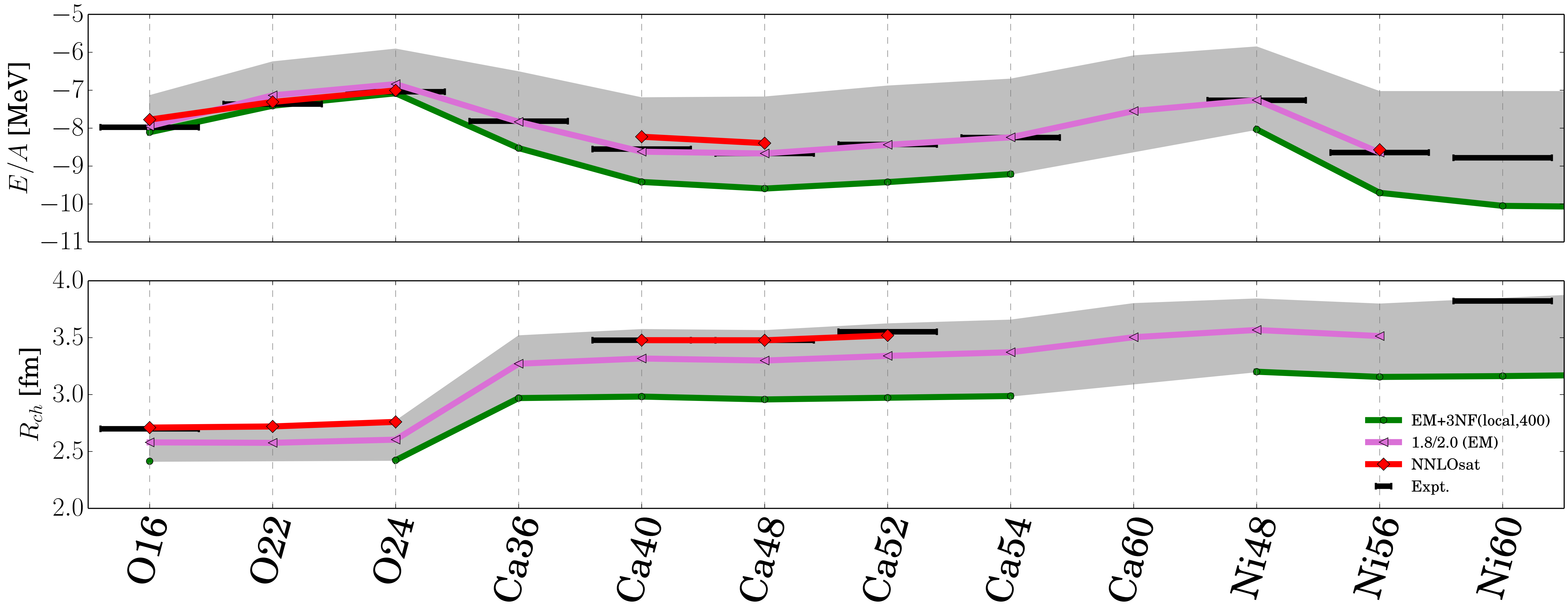
The **SRG-evolved (1.8/2.0)** EM-N3LO(500) + N2LO(2.0) reproduces energies very well!

K. Hebeler, et al. PRC **83**, 031301(R) (2011)
J. Simonis, et al. PRC **96**, 014303 (2017)



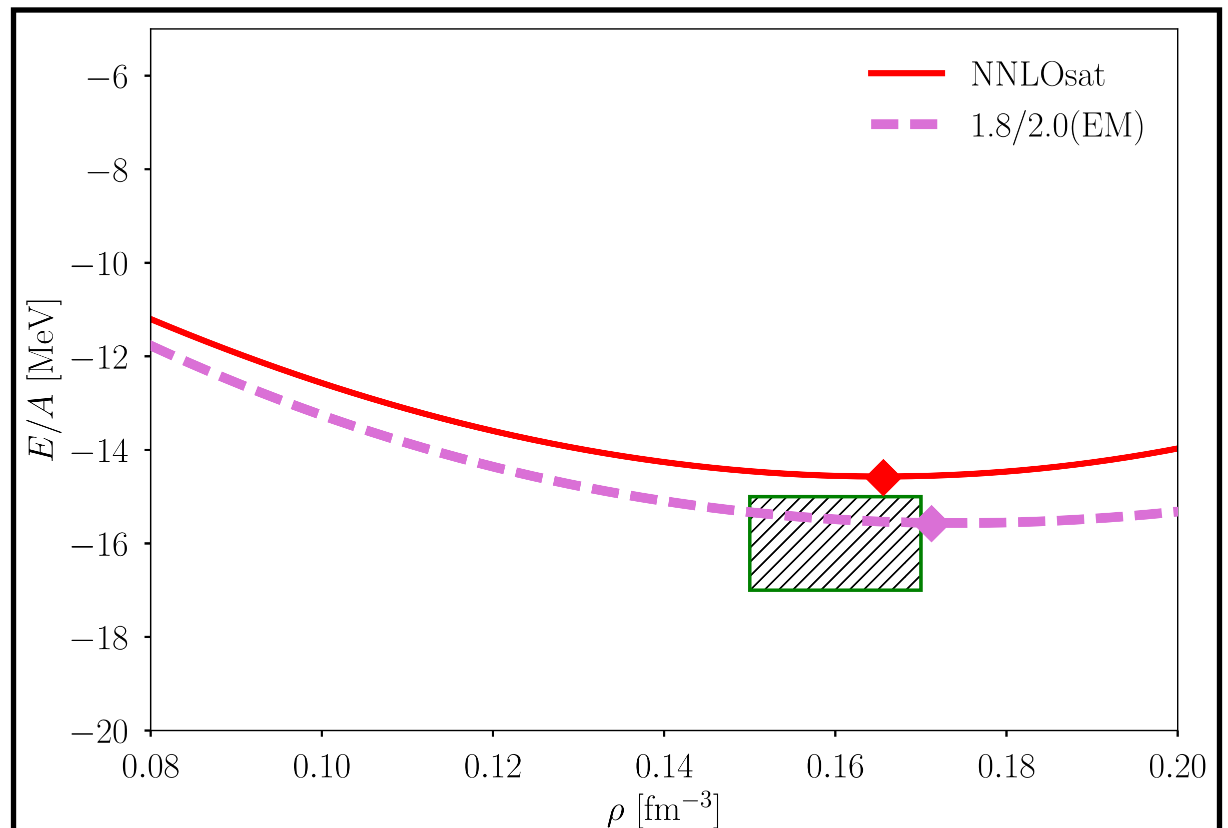
CC calculations in nuclear matter

G. Hagen, et al. PRC **89**, 014319 (2014)



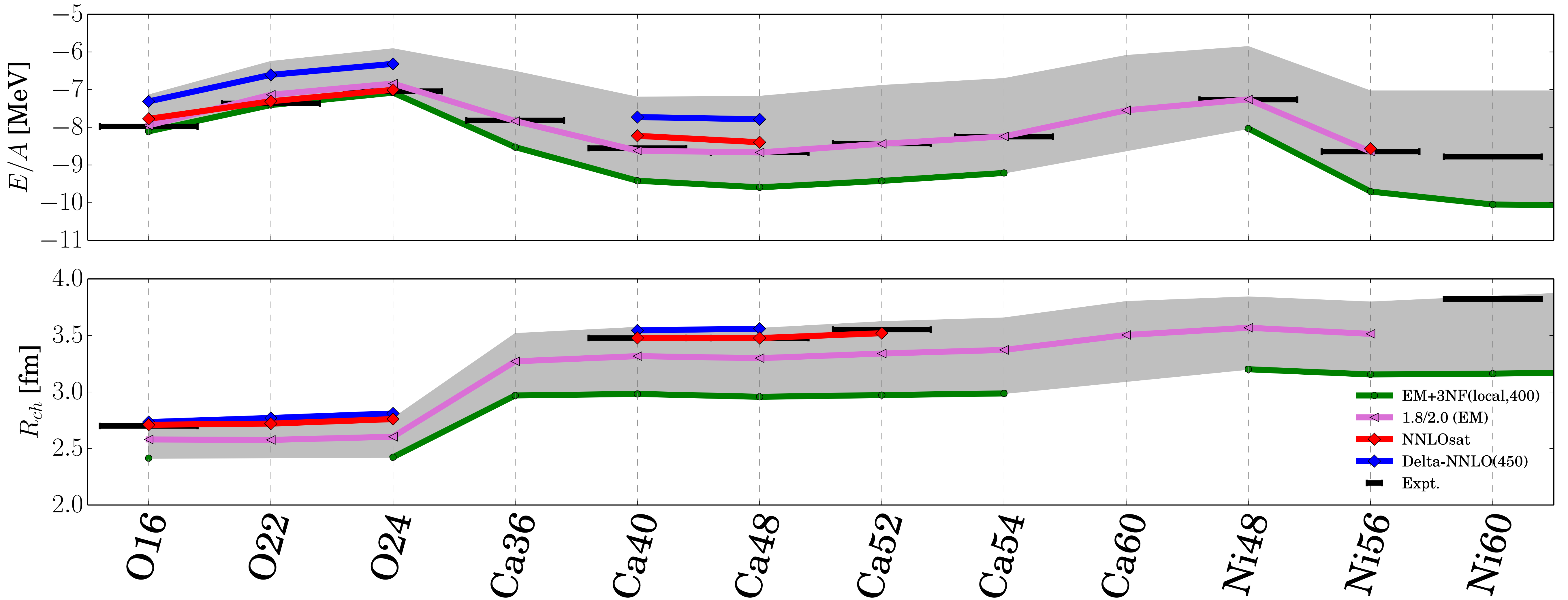
NNLOsat is designed to reproduce energies and radii of medium-mass nuclei very well!

A. Ekström, et al. PRC **91**, 051301(R) (2015)



CC calculations in nuclear matter

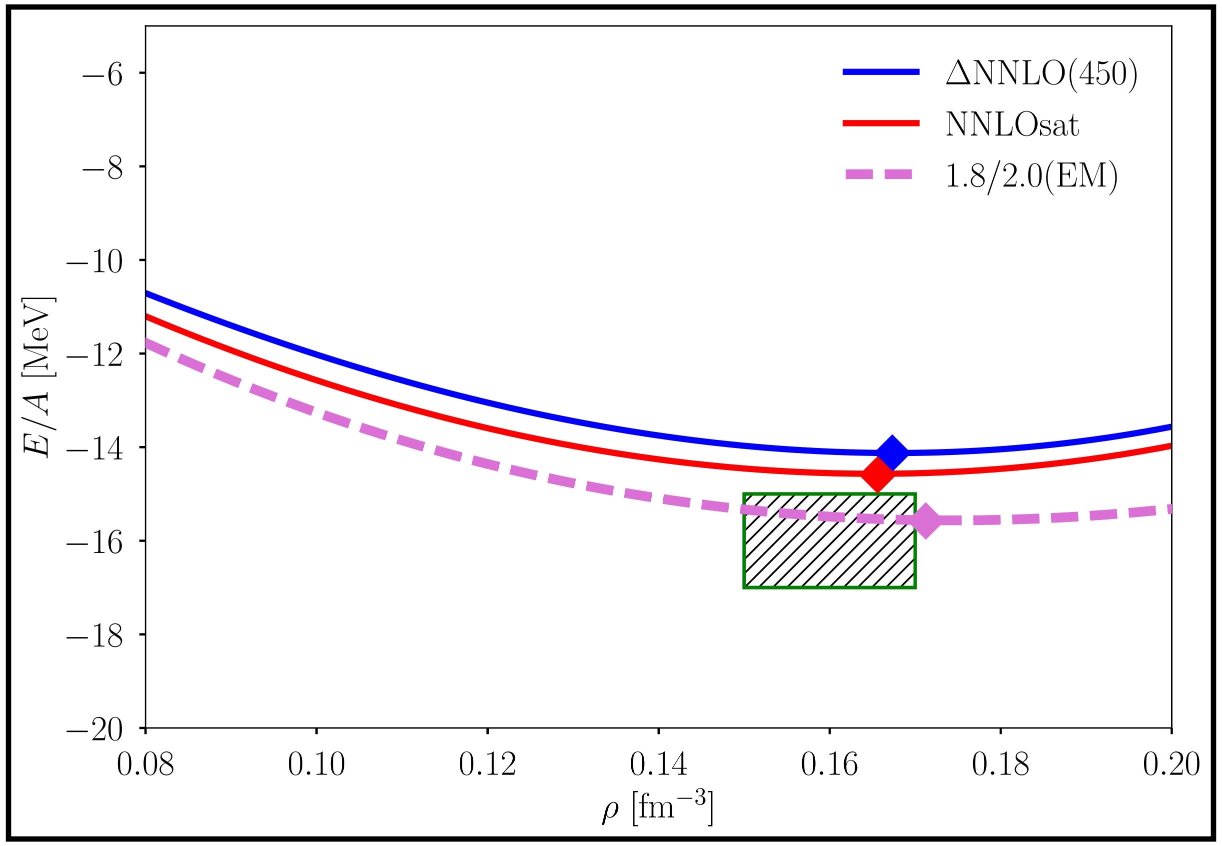
G. Hagen, et al. PRC **89**, 014319 (2014)



ΔNNLO(450) *predicts*

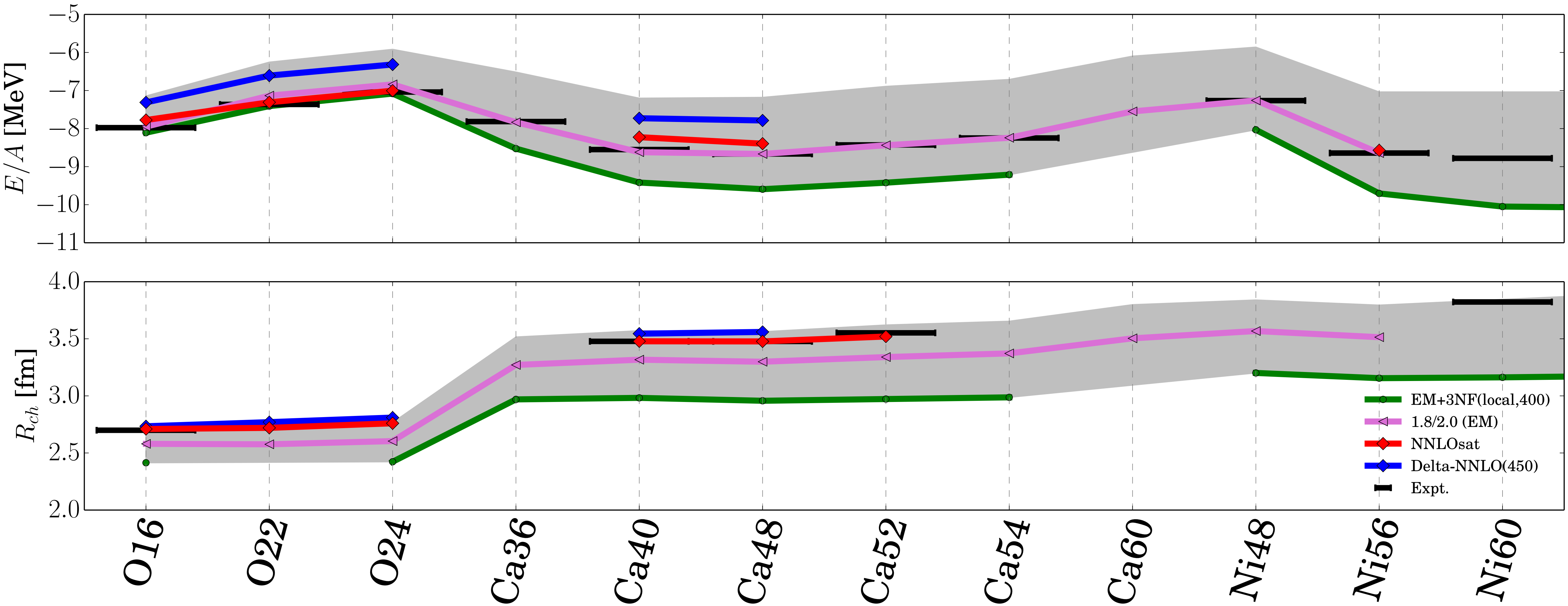
energies and radii of medium-mass nuclei rather well!

A. Ekström et al. arXiv:1707.09028 [nucl-th] (2017)



CC calculations in nuclear matter

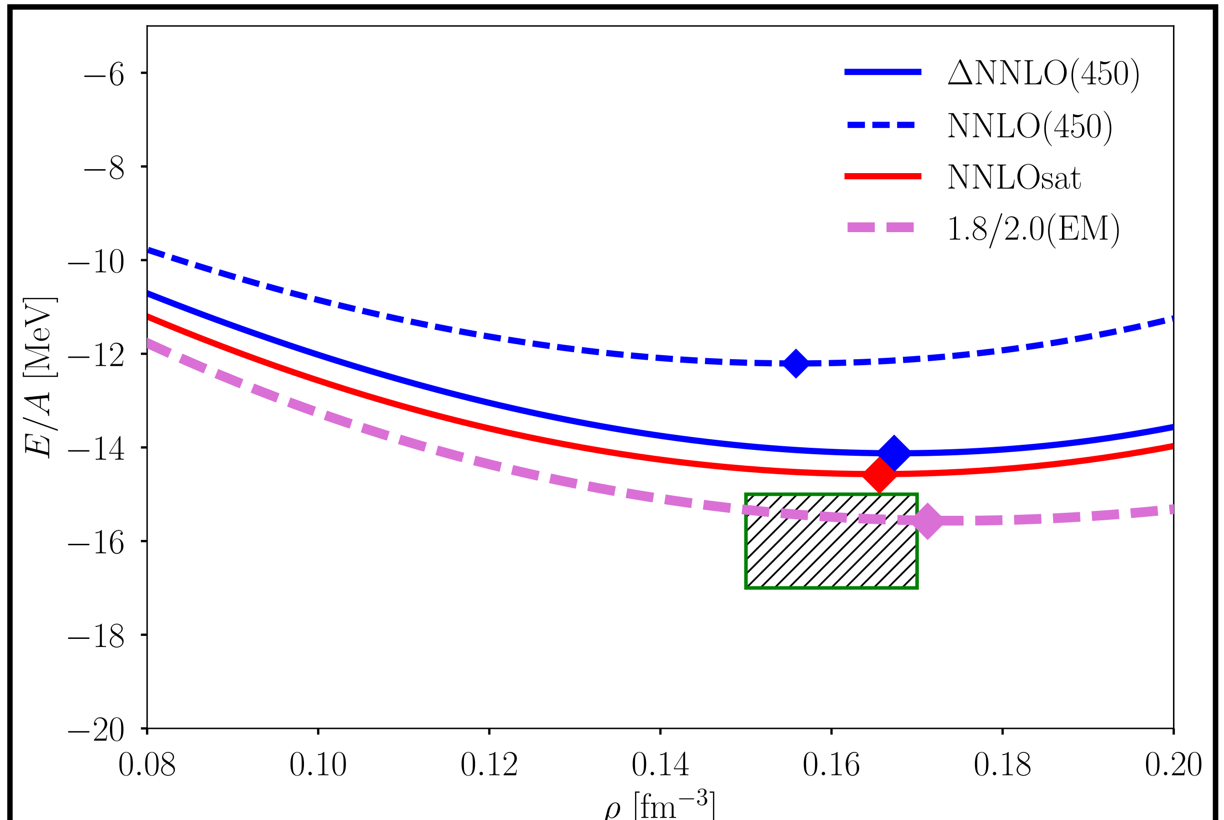
G. Hagen, et al. PRC **89**, 014319 (2014)



ΔNNLO(450) *predicts*
energies and radii of medium-mass nuclei rather well!

A. Ekström et al. arXiv:1707.09028 [nucl-th] (2017)

The ***Δ*** *is significant*



CC calculations in nuclear matter

G. Hagen, et al. PRC **89**, 014319 (2014)