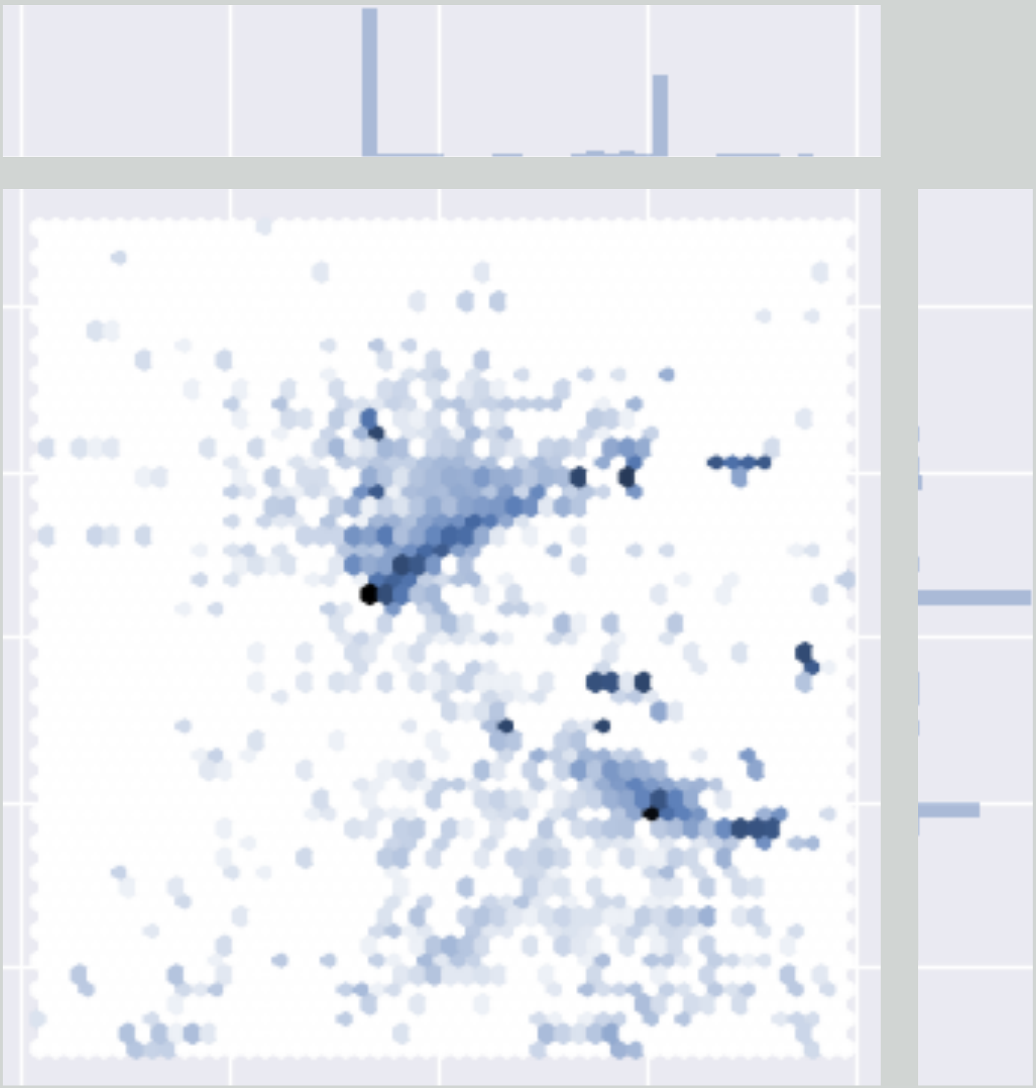

BAYESIAN POSTERIORS IN THE NUCLEON-NUCLEON SECTOR

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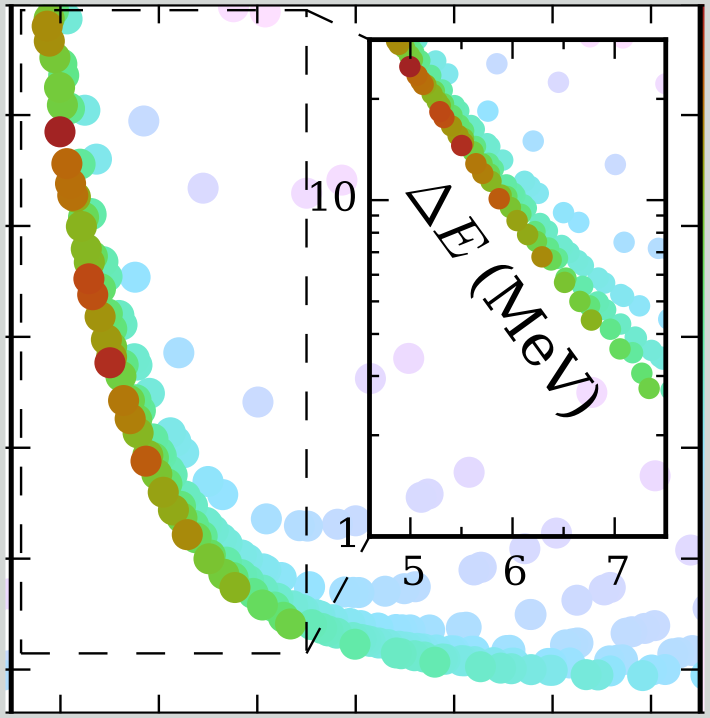
TRIUMF ab initio workshop,
Feb. 27 - Mar. 2, 2018

Outline

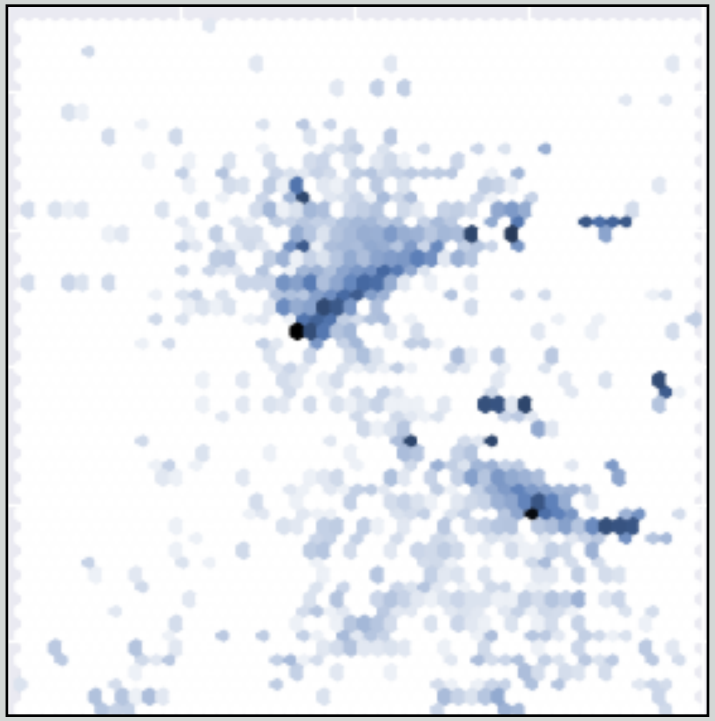
- Part 1:
  Many-body systems in finite oscillator spaces
  - IR extrapolations at fixed UV cutoff
  - Low-momentum scales of finite nuclei

arXiv 1712:09951

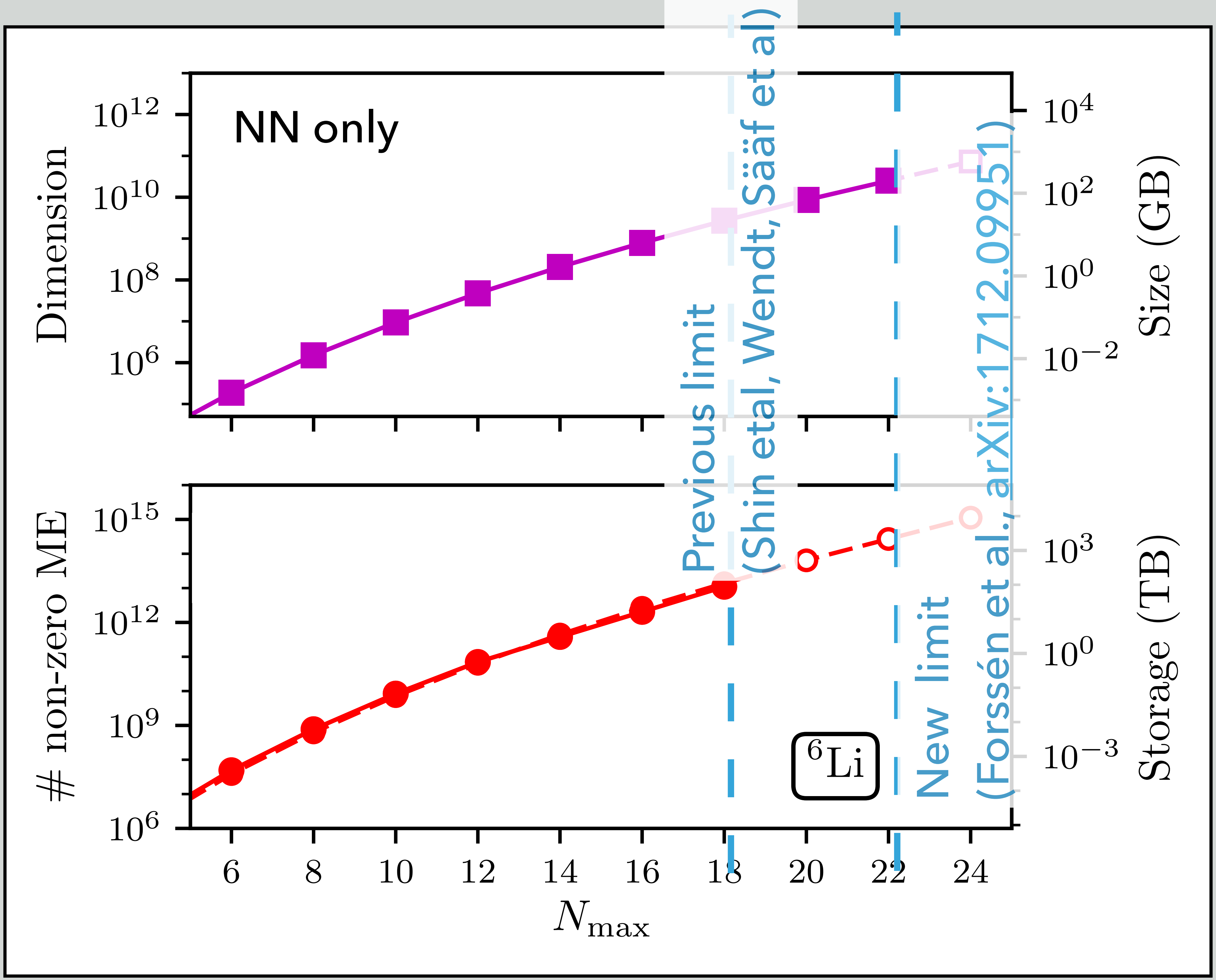


- Part 2:
  Bayesian data analysis in the nucleon-nucleon sector
  - Proof-of-principle demonstration with posterior sampling, error propagation.
  - Outlook

Progress report

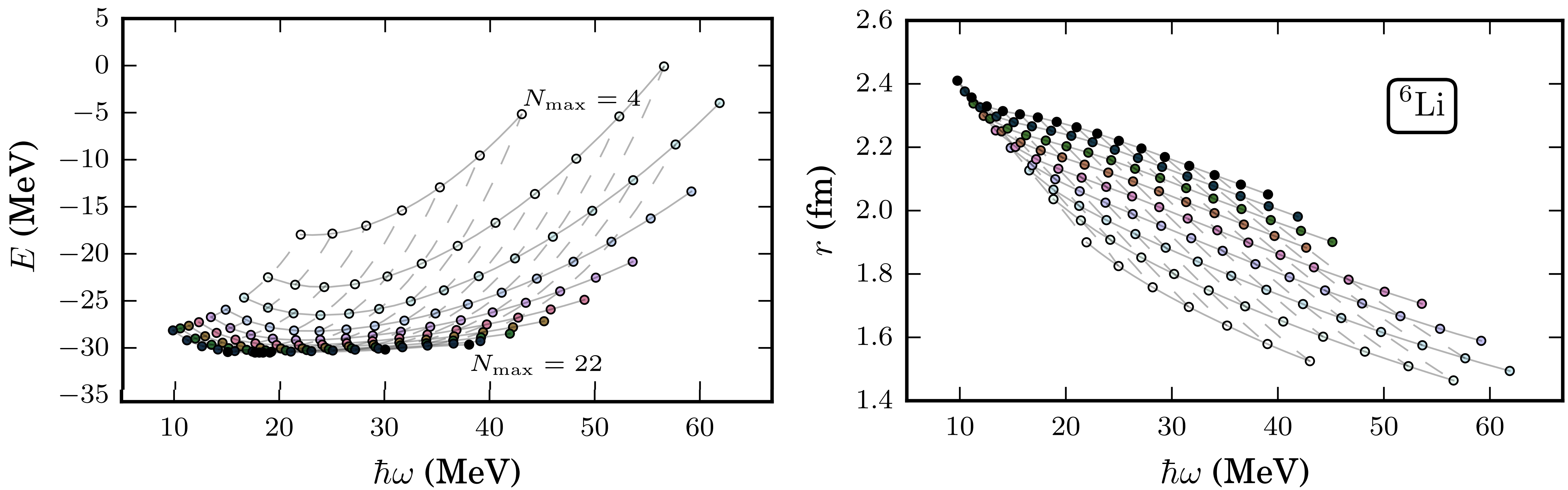


The NCSM curse of dimensionality - explicit matrix storage



6-Li ground-state observables

NN interaction: NNLOopt (Ekström et al, 2013)



From N_{max}=20 to 22 the variational minimum changes by < 90 keV

Convergence in finite oscillator spaces

- What is the equivalent of Lüscher's formula for the harmonic oscillator basis?
  [Lüscher, Comm. Math. Phys. 104, 177 (1986)]

- Convergence in momentum space (UV) and in position space (IR) needed
  [Stetcu et al. (2007); Coon et al. (2012); Furnstahl et al. (2012, 2015); König et al. (2014)]

- Choose regime (N, $\hbar\omega$) with negligible UV corrections.
- The infrared error term is universal for short range Hamiltonians.

- It can be systematically corrected and resembles error from putting system into an infinite well.

$$E(L) = E_\infty + Ae^{-2k_\infty L} + \mathcal{O}(e^{-4k_\infty L})$$

$$\langle r^2 \rangle_L \approx \langle r^2 \rangle_\infty [1 - (c_0\beta^3 + c_1\beta + c_2)e^{-\beta}]$$

What (precisely) is the IR scale L?

Key idea: compute eigenvalues of kinetic energy and compare with *corresponding* (hyper)spherical cavity to find L.

What is the corresponding cavity?

Single particle	A particles (product space)	A particles in No-core shell model
Diagonalize $T_{kin}=p^2$	Diagonalize A-body T_{kin}	Diagonalize A-body T_{kin}
3D spherical cavity	A fermions in 3D cavity	3(A-1) hyper-radial cavity
$L_2 = \sqrt{2(N+3/2+2)}b$	$L_{\rm eff} = \left(\frac{\sum_{nl}\nu_{nl}a_{l,n}^2}{\sum_{nl}\nu_{nl}\kappa_{l,n}^2}\right)^{1/2}$	$L_{\rm eff} = b\frac{X_{1,\mathcal{L}}}{\sqrt{T_{1,\mathcal{L}}(N_{\rm max}^{\rm tot})}}$

More, Ekström, Furnstahl, Hagen, Papenbrock, PRC 87, 044326 (2013)

Furnstahl, Hagen, Papenbrock, Wendt, J. Phys. G 42, 034032 (2015)

Wendt, Forssén, Papenbrock, Sääf, PRC 91, 061301(R) (2015)

A practical approach to IR extrapolations

- In practice it is often challenging to fulfill:

  1. … being UV converged

  2. … reaching asymptotically large values of $k_\infty L$

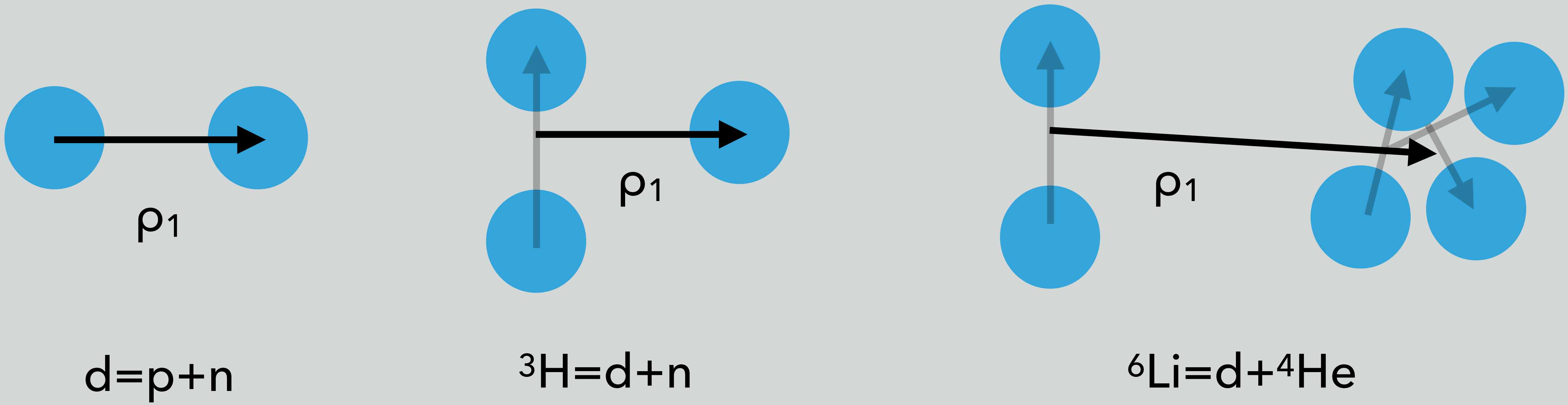
- Moreover, we lack a physical interpretation of k_∞ for many-body systems.

- Perform instead the extrapolation at a fixed (not necessarily UV converged) value of Λ

- The LO IR extrapolation becomes

$$E(L,\Lambda) = E_\infty(\Lambda) + a(\Lambda)\exp\left[-2k_\infty(\Lambda)L\right]$$

Hyperradial well, explains low-momentum scale

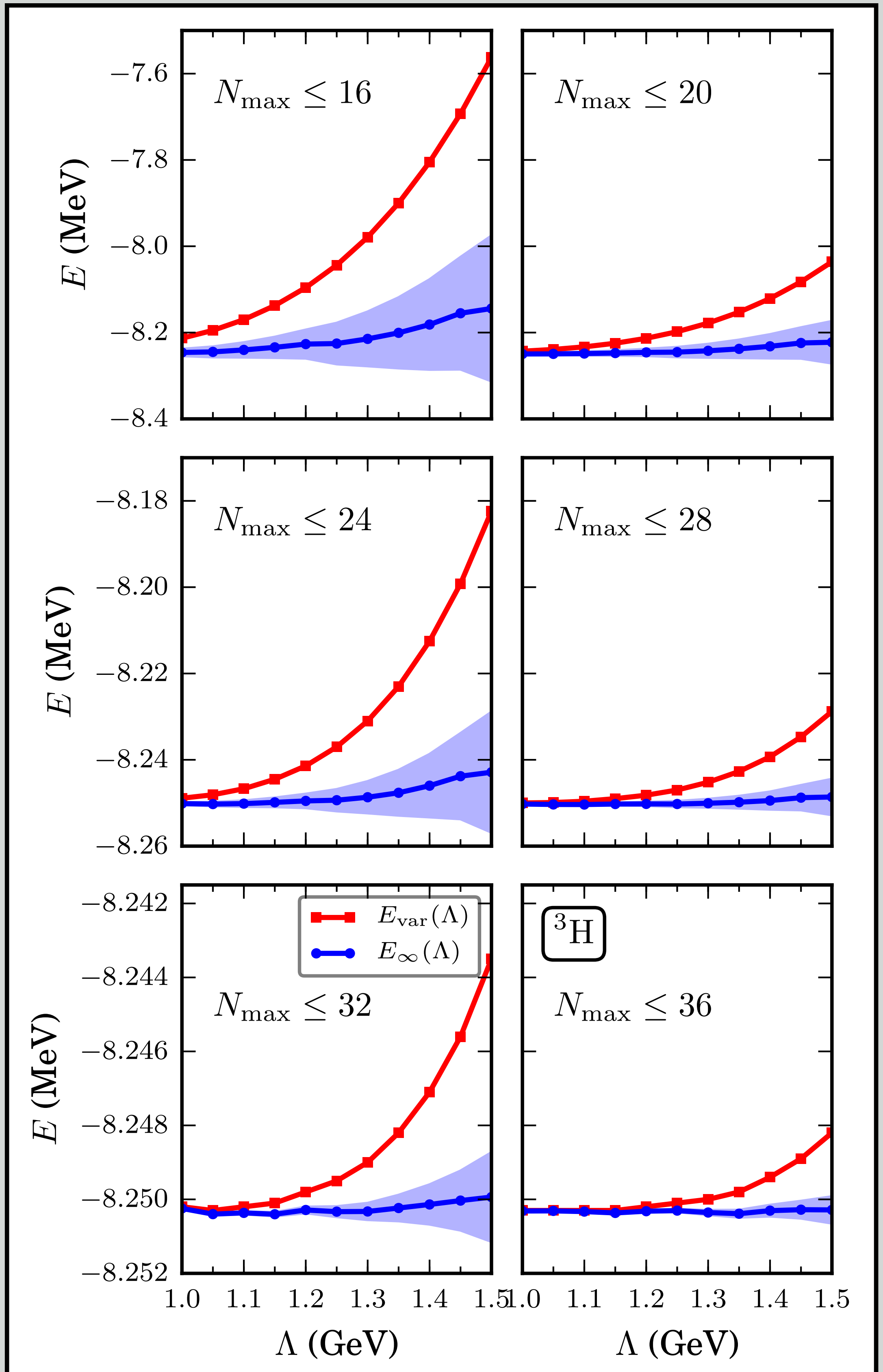


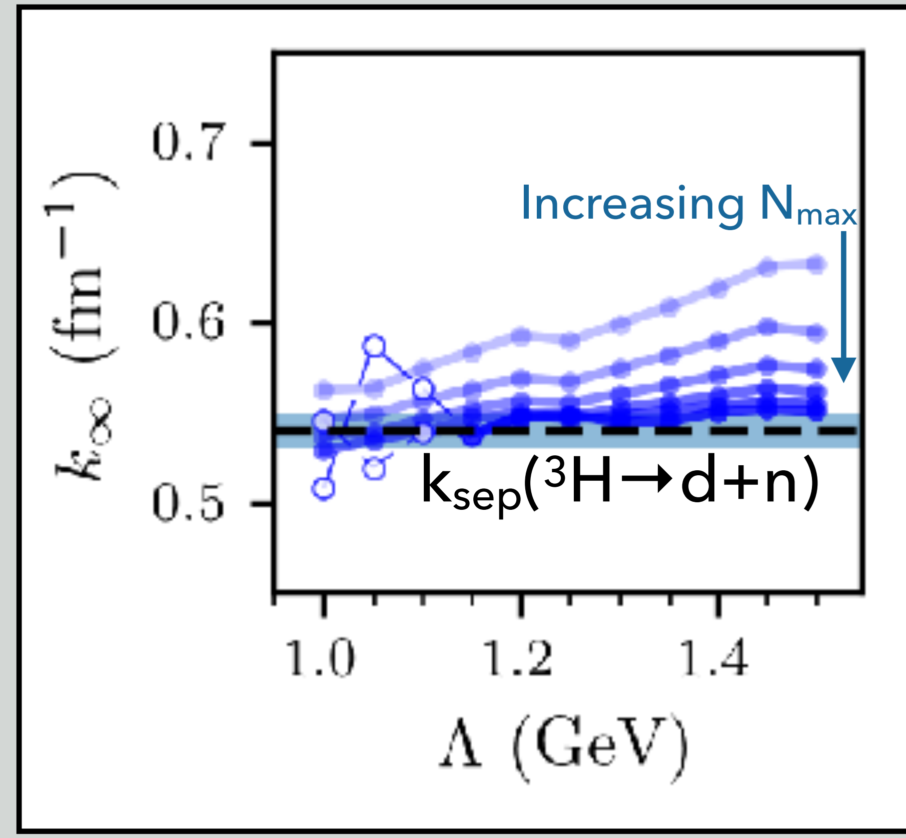
NCSM: hyper-radial well $\boxed{\vec{\rho}^{\,2} = \sum_{j=1}^{A-1} \vec{\rho}_j^{\,2}.}$ $e^{-k_1|\vec{\rho}_1|}$

Separation energy for lowest threshold $S = \frac{\hbar^2 k_\infty^2}{2m}$

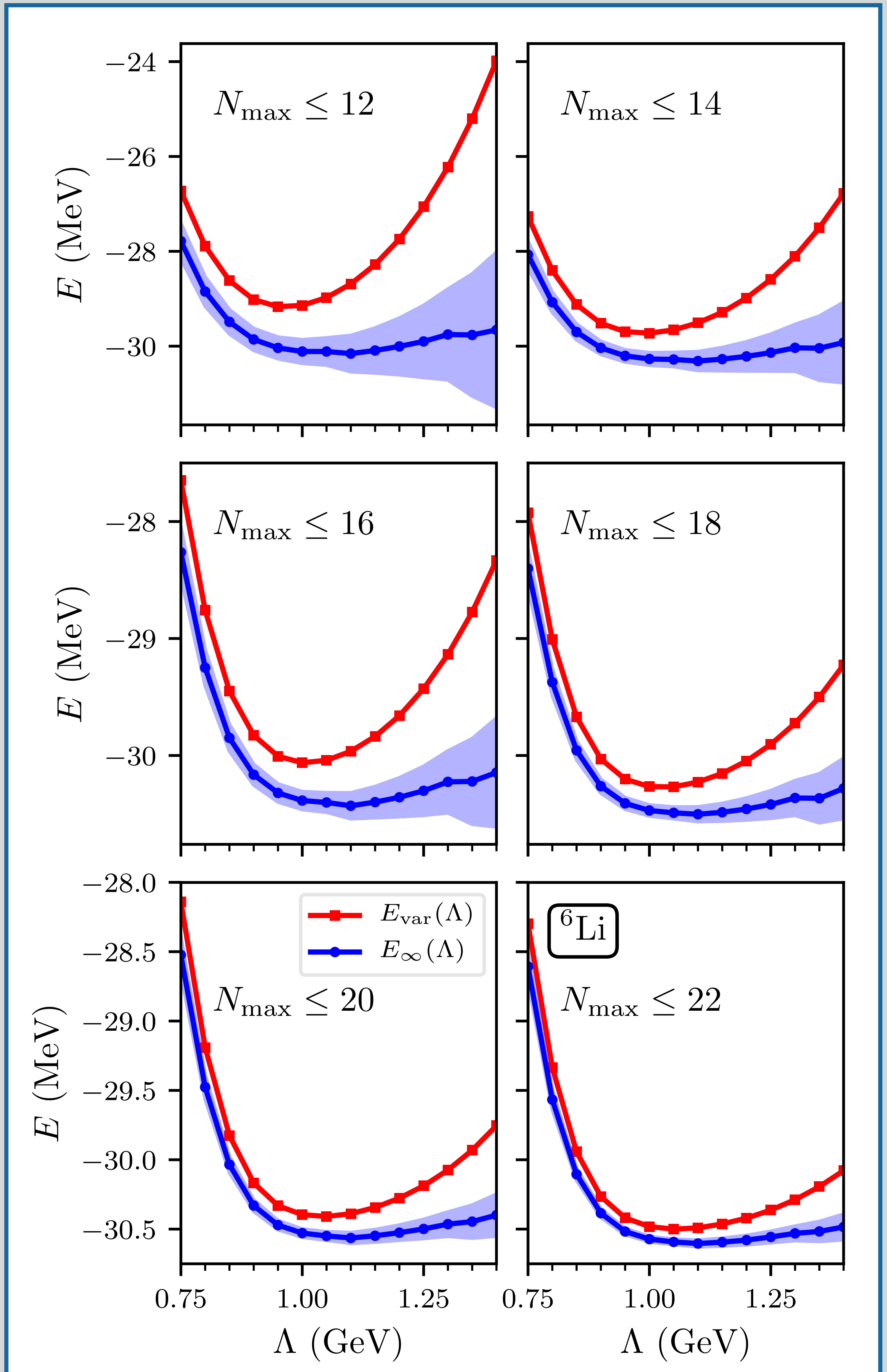
See also König and Lee, arXiv:1701.00279 for volume dependence of N-Body Bound States in lattice calculations.

Results: A=3 — ground-state energy





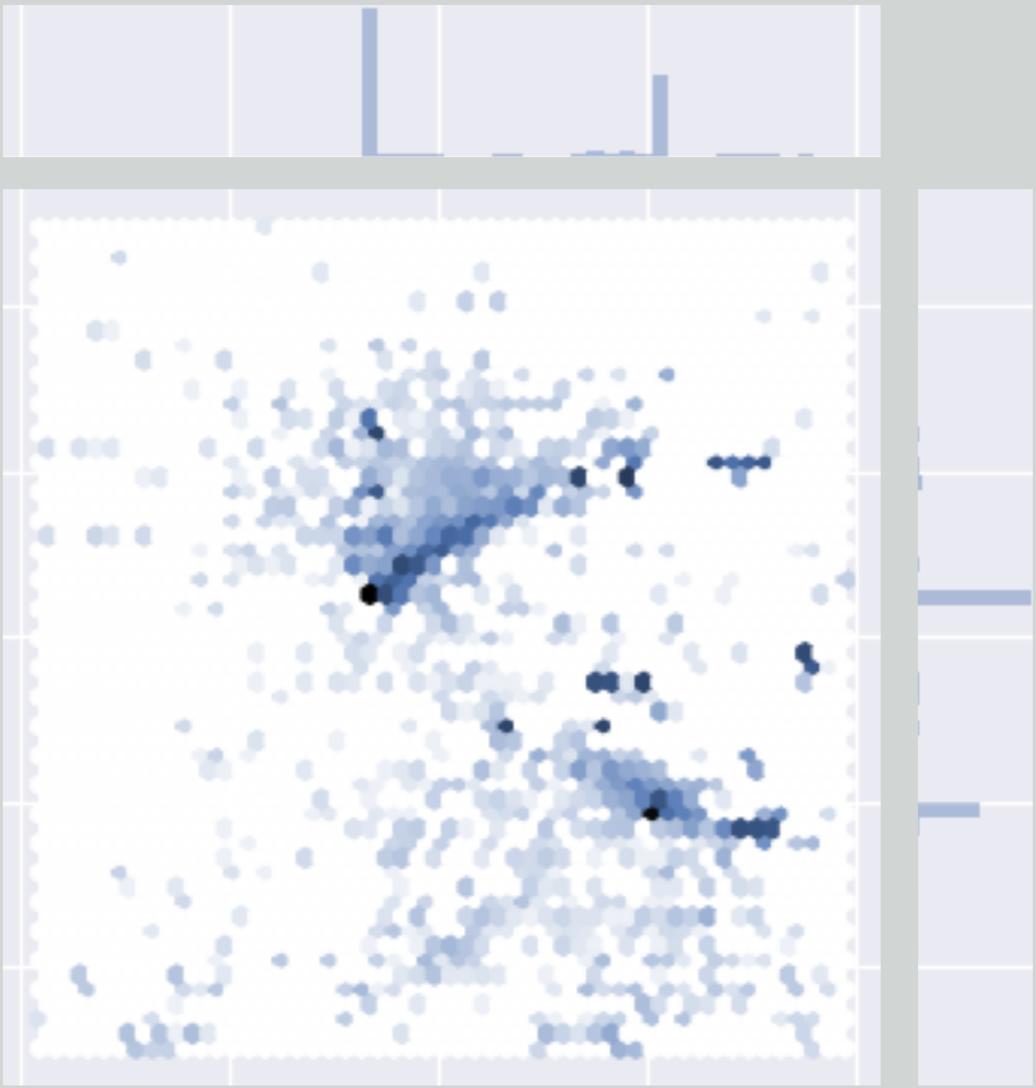
Results: ^{6}Li —— ground-state energy



From extrapolation

From extracted threshold

Nucleus	Channel	k_∞	k_{sep}
^{3}H	d+n	0.54(1)	0.54(1)
^{3}He	d+p	0.51(2)	0.51(1)
^{4}He	^{3}H+p	0.84(5)	0.97(3)
^{6}Li	^{4}He+d	0.44(5)	0.19(8)



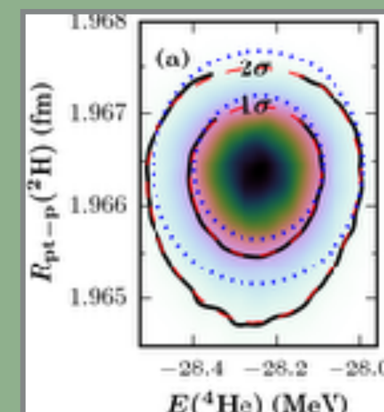
BAYESIAN POSTERIORS IN THE NUCLEON-NUCLEON SECTOR

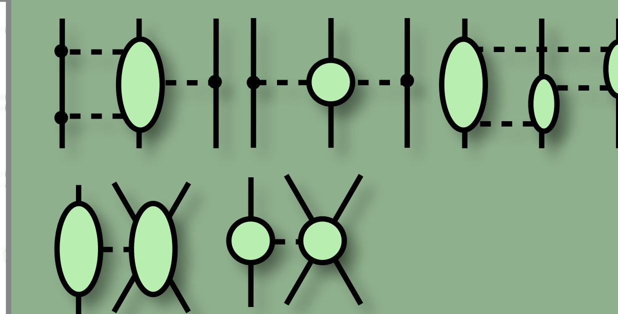
Overview of our research efforts

We aim to develop the technology and ability to:

- **Does nuclear-physics phenomena emerge in a "from few to many" ab initio approach?**
- **Is available few-body data sufficient to constrain this model? Does the model become fine-tuned?**

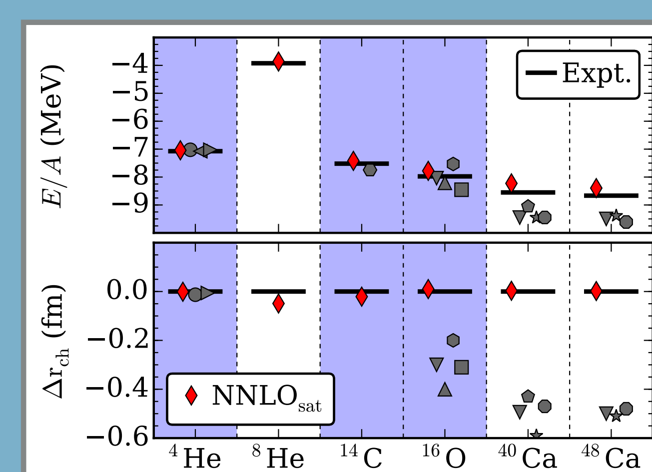
Diversify and extend the **statistical analysis** of chiral-EFT based nuclear interactions in a **data-driven** approach.





- **Can/should emergent phenomena be used to constrain the model?**
- **How to quantify systematic uncertainties in such an approach?**

Explore **alternative strategies of informing** the model about low-energy many-body observables.



Inference

"the act of passing from one proposition, statement, or judgment considered as true to another whose truth is believed to follow from that of the former" (Webster)

Do premises $A, B, \ldots \rightarrow$ hypothesis, H?

- **Inductive inference**: Premises bear on truth/falsity of H, but don't allow its definite determination
- **Statistical Inference**: Quantify the strength of inductive inferences from data and other premises to hypotheses about the phenomena producing the data.
- Quantify via **probabilities**, or averages calculated using probabilities. *Frequentists* and *Bayesians* use probabilities very different for this.

Parametric models

- Assume that hypothesis H_i is a model M_i with parameters $\boldsymbol{\alpha}_i$.
- In **frequentist statistics** we devise a procedure to choose among H_i using data D. Apply this procedure to D_{obs}.
- Report long-run performance (e.g., how often it is correct, how “far” the choice is from the truth on average).

FREQUENTIST CHI-SQUARED MINIMZATION

Low-energy constants (LECs) need to be fitted to experimental data.

$$\chi^2(\vec{p}) \equiv \sum_i r_i^2(\vec{p}) = \sum_{j \in NN} r_j^2(\vec{p}) + \sum_{k \in \pi N} r_k^2(\vec{p}) + \sum_{l \in 3N} r_l^2(\vec{p})$$

FIT πN-SECTOR TO πN DATA → FIT NN CONTACTS TO NN PHASE SHIFTS → FIT NN CONTACTS TO NN DATA → FIT C_D,C_E (+ Ct^{nn}_{1S0}) TO A=3 DATA → SIMULTANEOUS OPTIMIZATION

- Efficient minimization algorithms (Levenberg-Marquardt, Newton), and statistical error analysis require **derivatives.** We use Automatic Differentiation (AD) for this purpose.

- There is a possibility to find several minima in the various channels; They will then multiply into many **local minima** that don't necessarily disappear when doing simultaneous optimisation of all parameters to all data.

Parametric models

- Assume that hypothesis H_i is a model M_i with parameters $\boldsymbol{\alpha}_i$.
- In **frequentist statistics** we devise a procedure to choose among H_i using data D. Apply this procedure to D_{obs}.
- Report long-run performance (e.g., how often it is correct, how "far" the choice is from the truth on average).
- In **Bayesian statistics** we assess the hypotheses by calculating their probabilities $p(H_i | \ldots)$ conditional on known and/or presumed information using the rules of probability theory.
- **Parameter estimation**: Assume that the model M_i is true; Compute: $p(\boldsymbol{\alpha}_i \,|\, D_{\mathrm{obs}}, M_i, I)$
- **Model comparison**: Compute ratio: $p(M_i \,|\, D_{\mathrm{obs}}, I) \,/\, p(M_j \,|\, D_{\mathrm{obs}}, I)$

Bayesian parameter estimation

Bayes' theorem (follows from probability product rule):

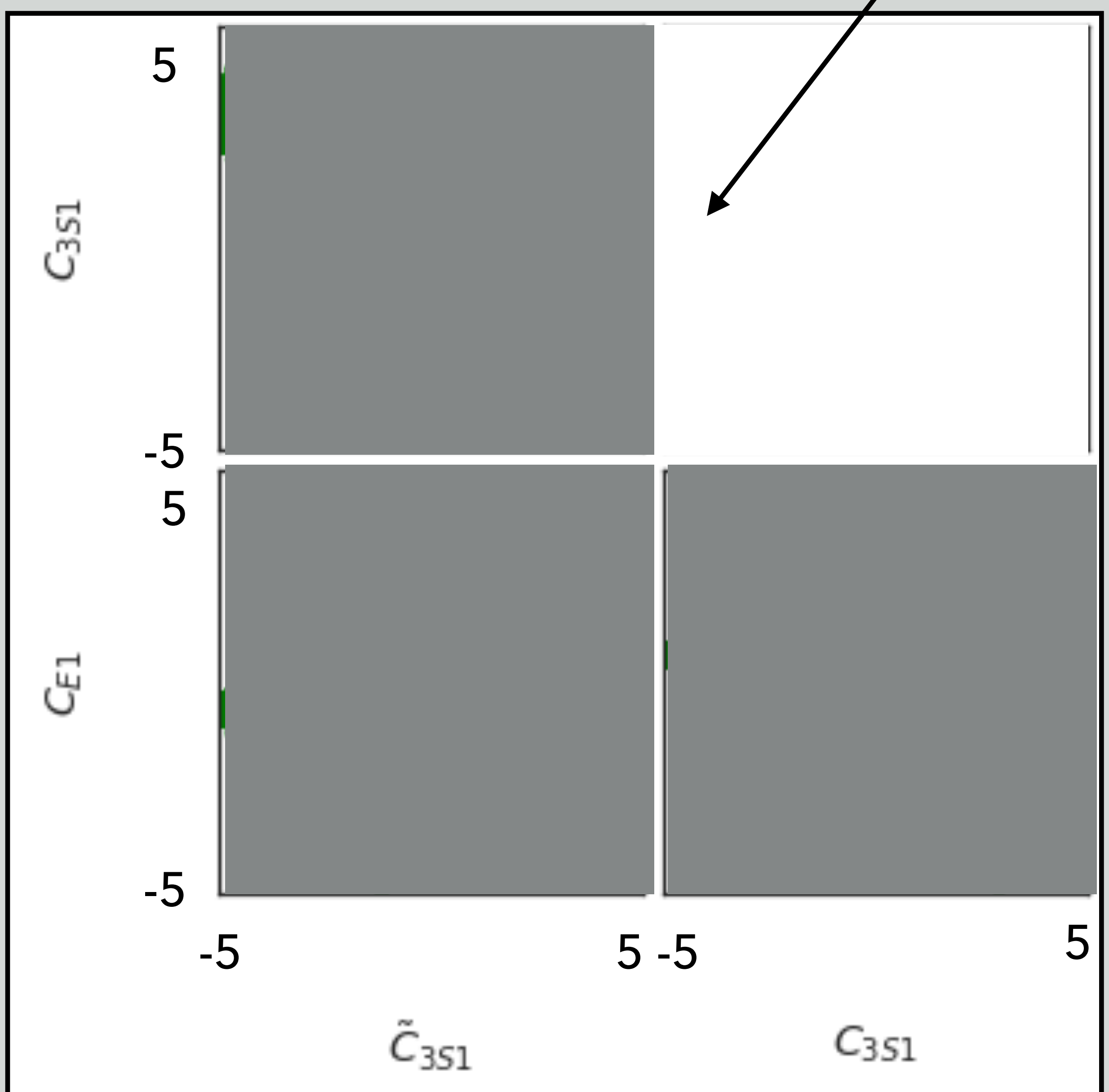
$$\underbrace{p(\boldsymbol{\alpha}|D,I)}_{\text{posterior}} = \frac{\overbrace{p(D|\boldsymbol{\alpha},I)}^{\text{likelihood}}\overbrace{p(\boldsymbol{\alpha}|I)}^{\text{prior}}}{\underbrace{p(D|I)}_{\text{normalization}}}$$

Marginalization: $$p(\alpha_1|D,I) = \int d\alpha_2 \ldots d\alpha_k p(\boldsymbol{\alpha}|D,I)$$

- For many lessons and suggestions on the use of Bayesian methods in Effective Field Theories, see work by the BUQEYE collaboration (and talks by Daniel and Sarah).
- Here we report on progress in implementing Bayesian methods for parameter estimation in Chiral EFT (up to N3LO) using NN scattering data (phase shifts).

The deuteron channel

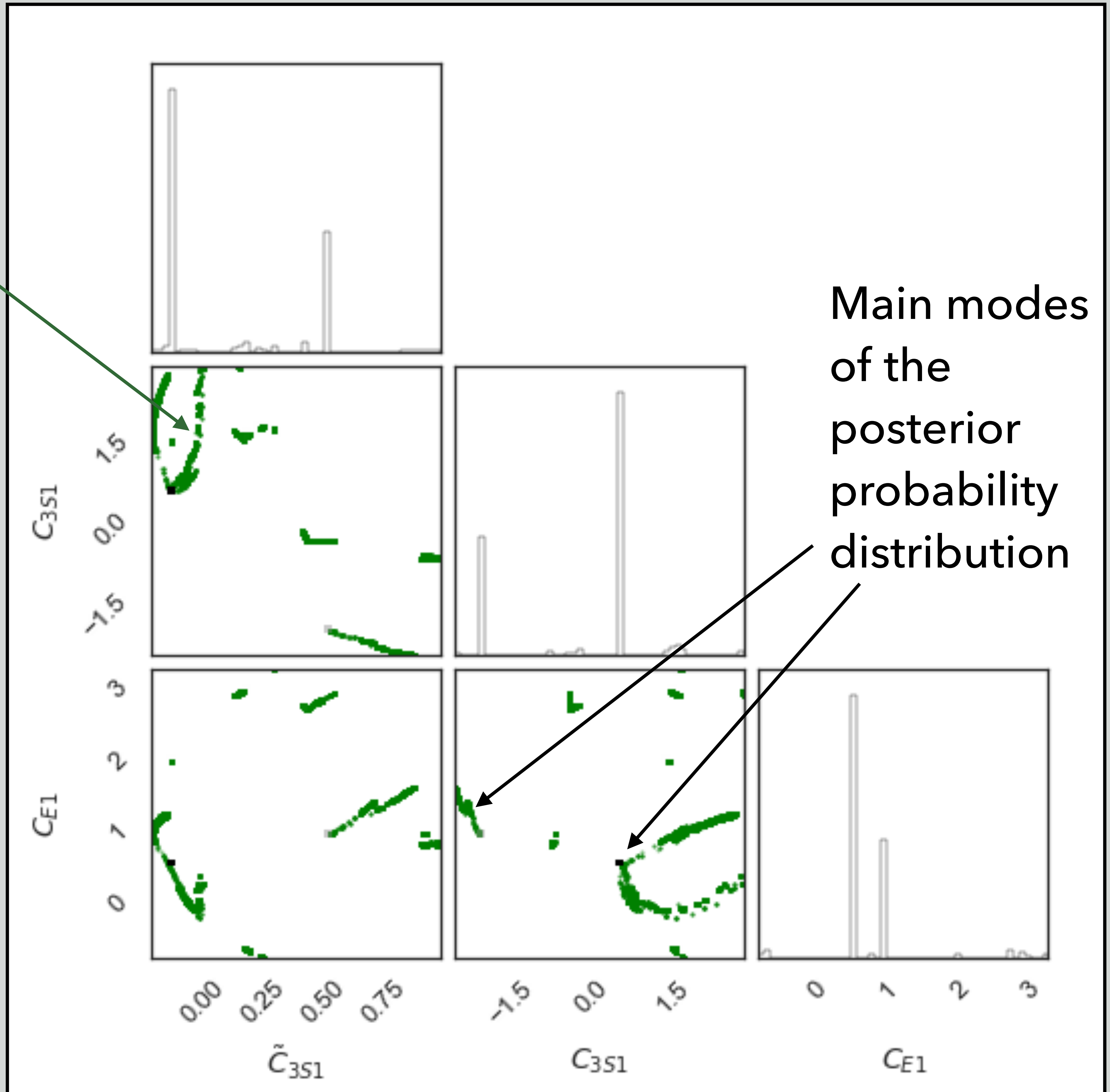
Projected
prior probability
distribution



N2LO: deuteron
channel

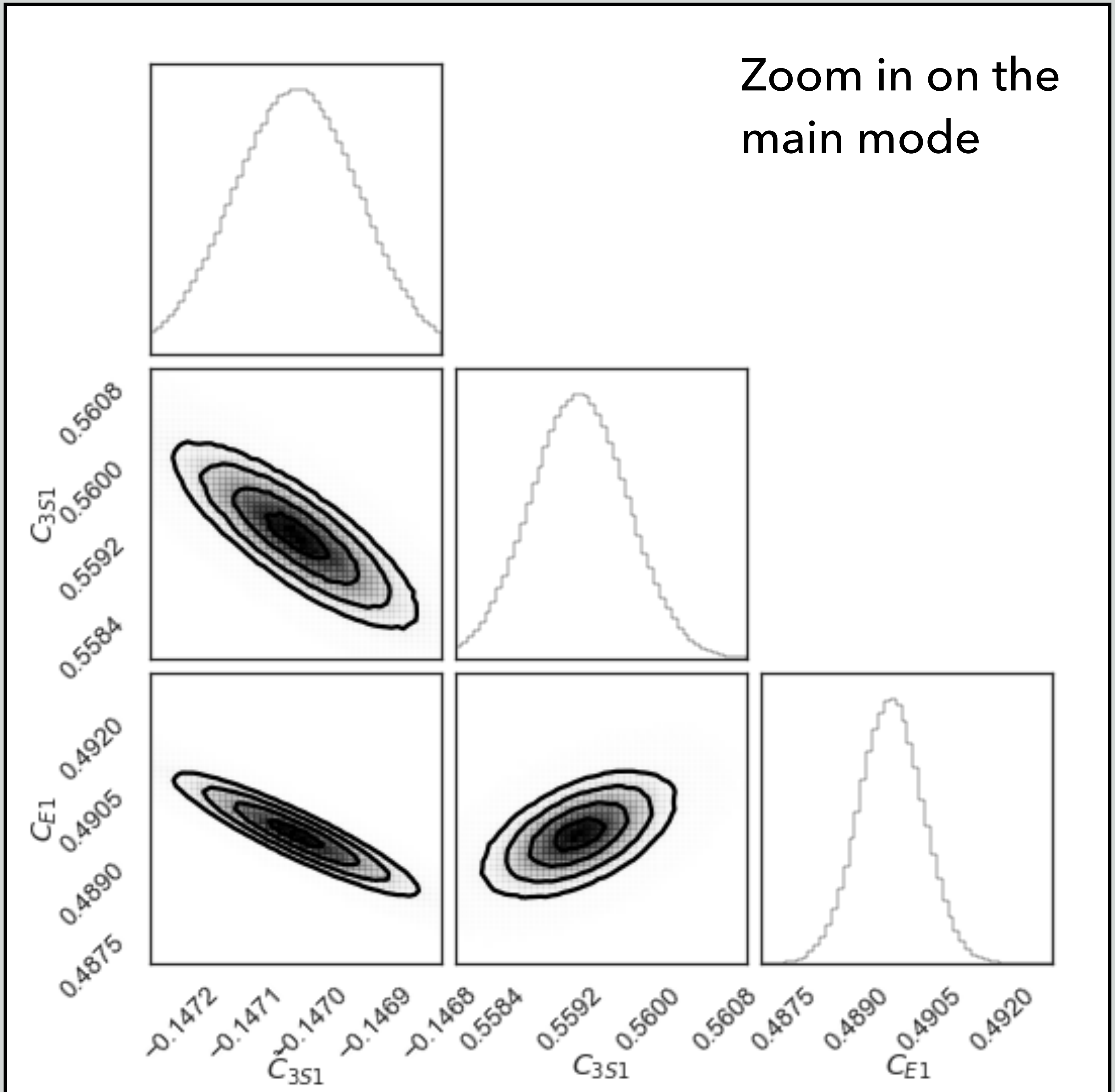
The deuteron channel

MCMC samples

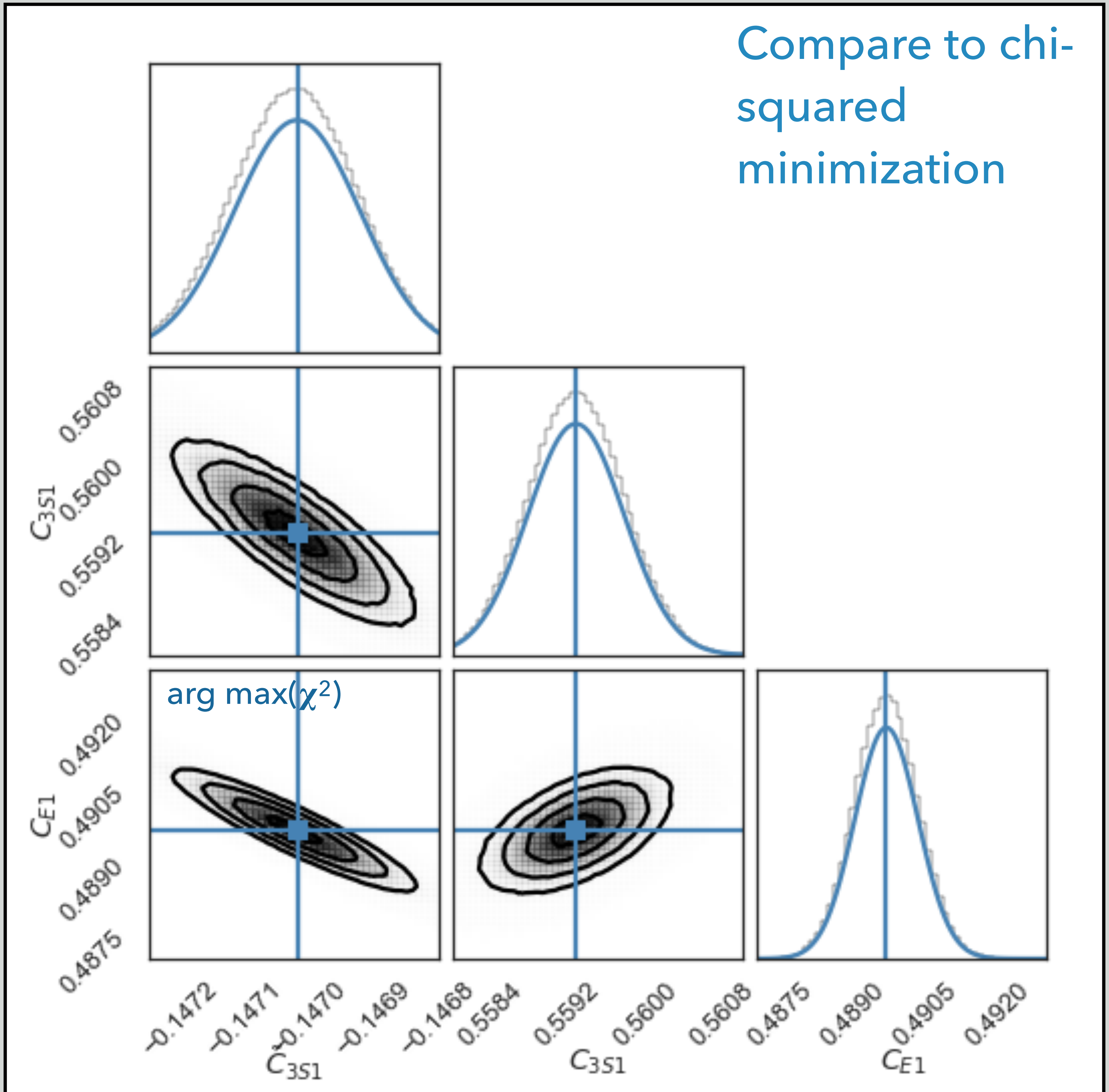


Main modes of the posterior probability distribution

The deuteron channel



The deuteron channel



Expectation integrals, error propagation

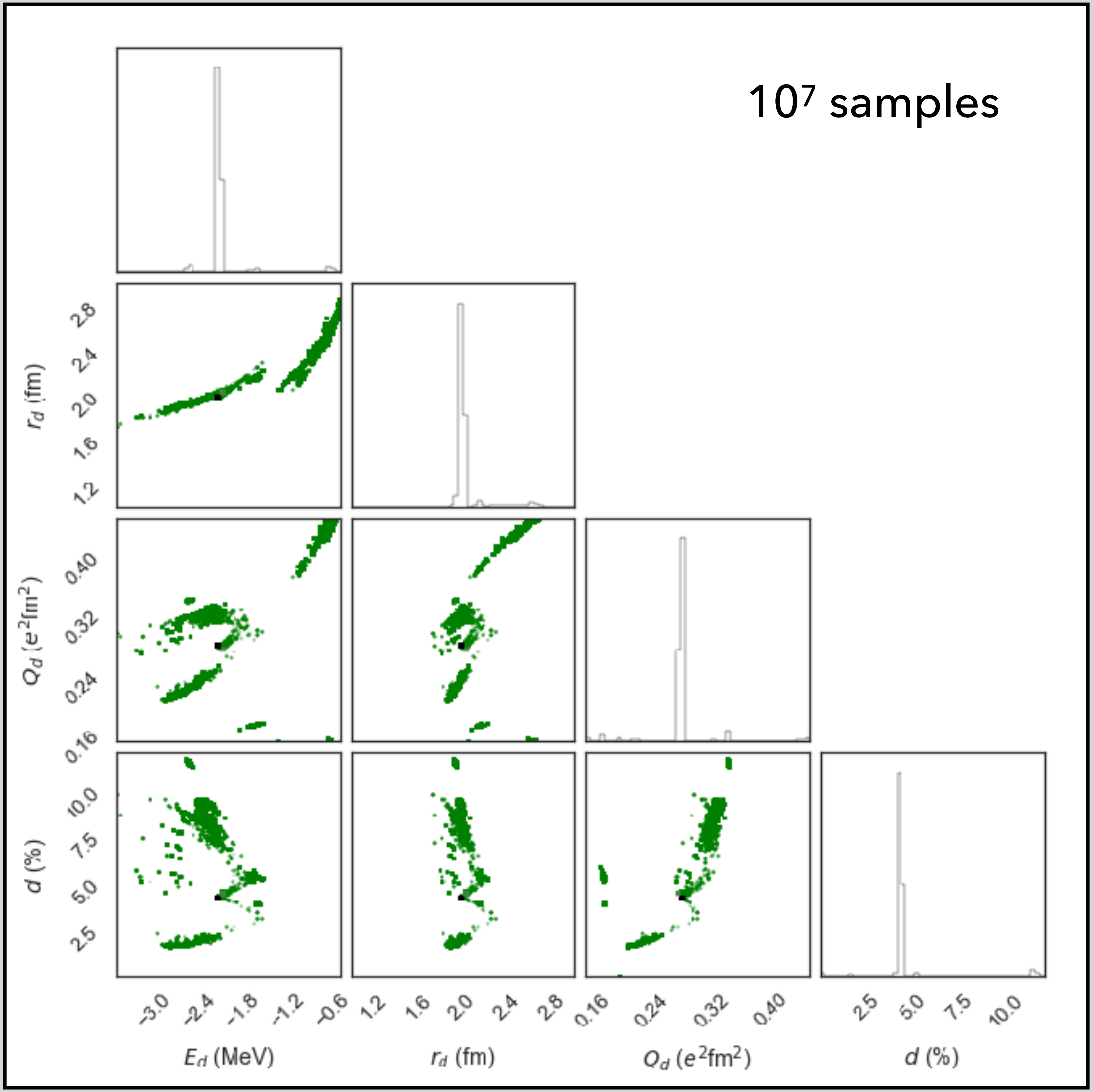
- Expectation integrals for observables can be performed using the posterior pdf

$$\langle O(\boldsymbol{\alpha})\rangle = \int d\boldsymbol{\alpha} p(\boldsymbol{\alpha}|D,I)O(\boldsymbol{\alpha})$$

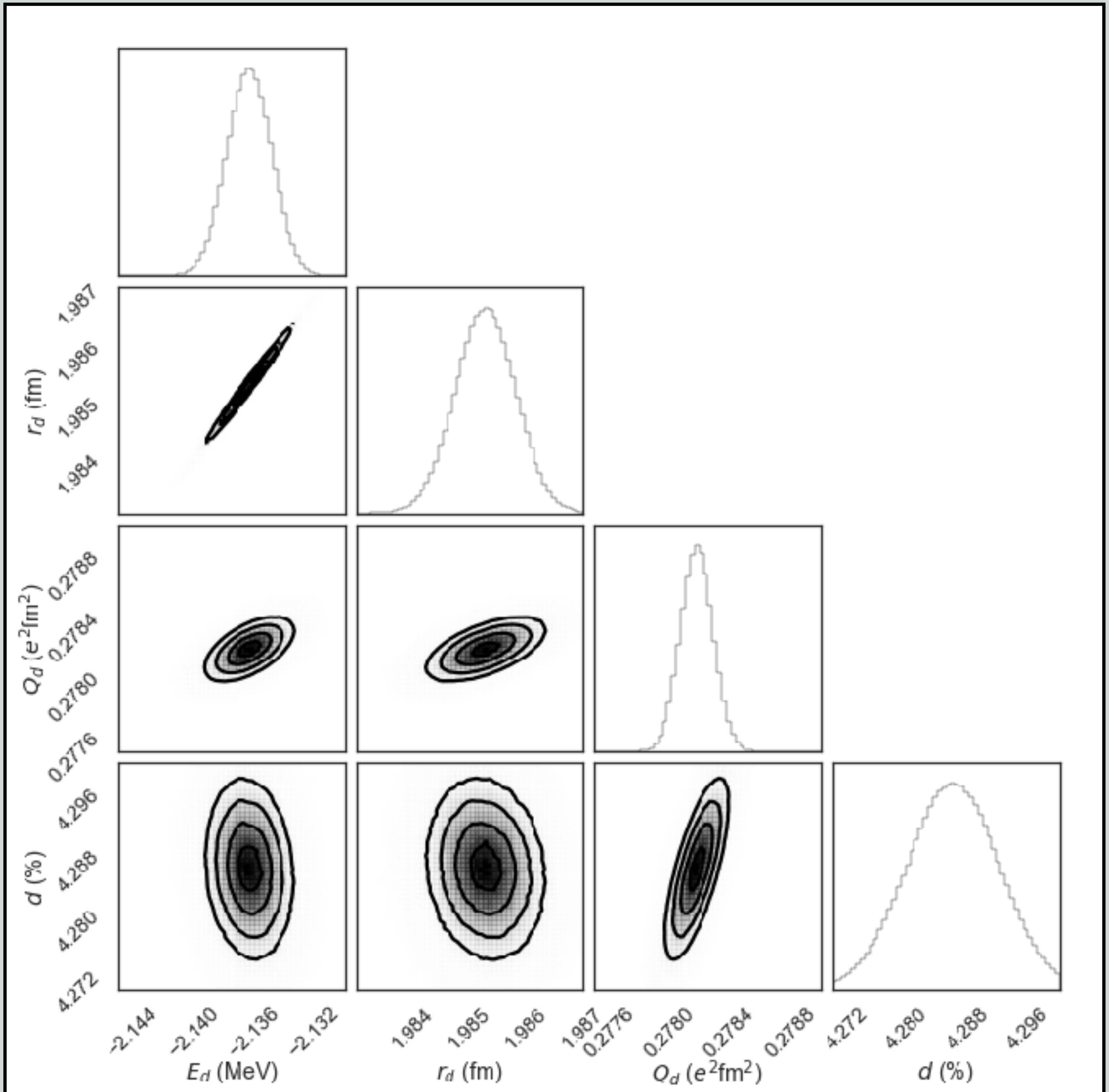
$$\approx \frac{1}{N}\sum_{j=1}^{N} O(\boldsymbol{\alpha}_j)$$

The MCMC algorithm generates *N* samples $\{\boldsymbol{\alpha}_j\}$ according to the posterior pdf

Deuteron observables

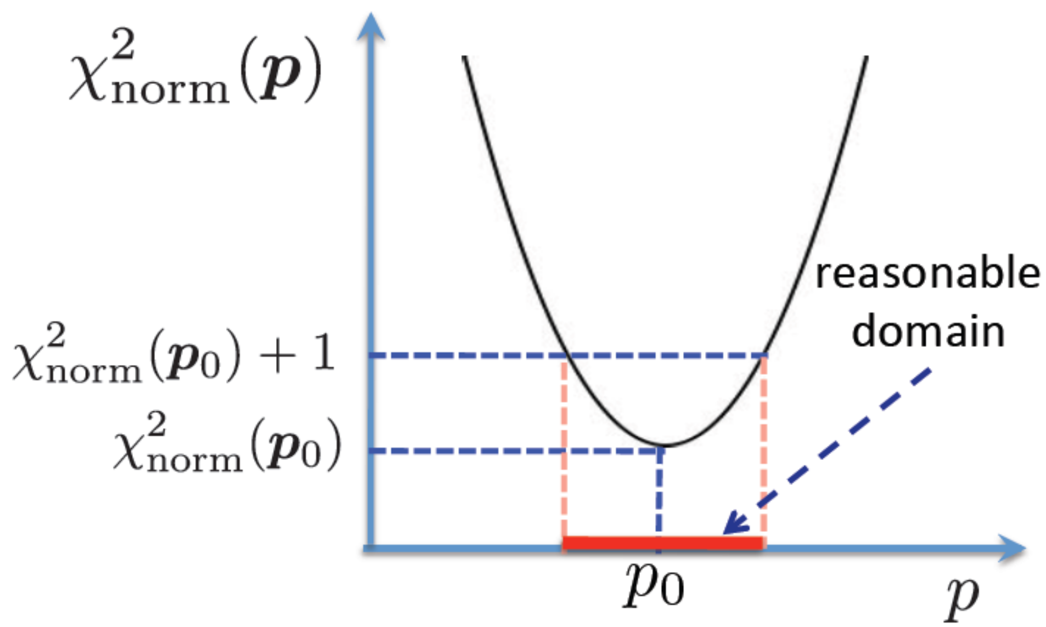


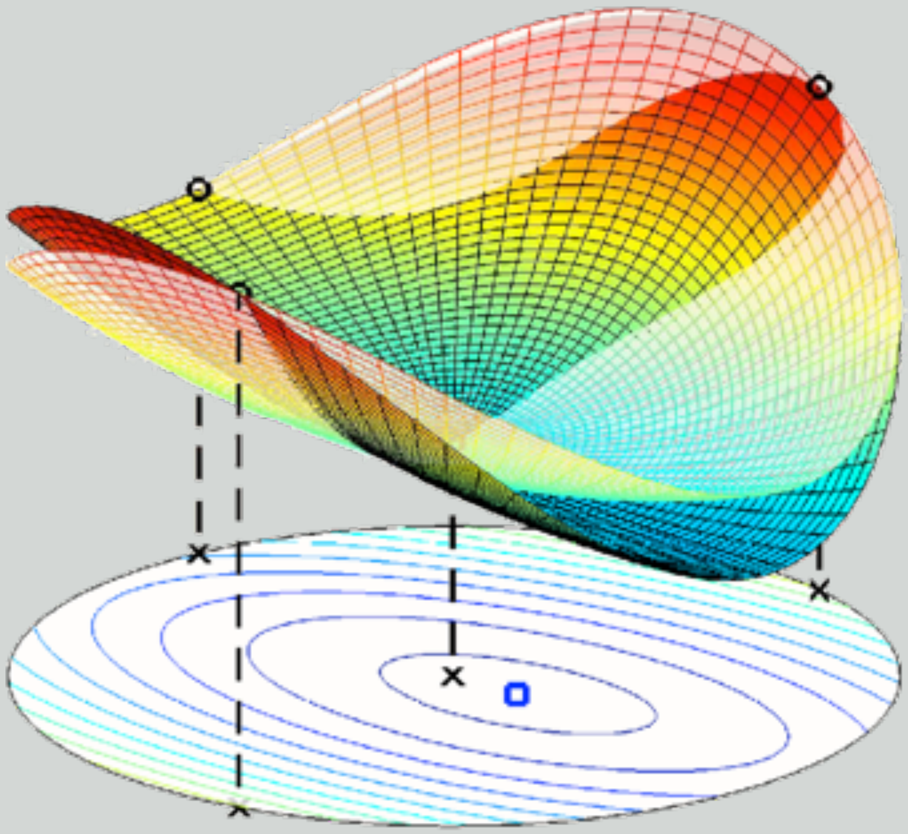
Deuteron observables



STATISTICAL ERROR ANALYSIS

- In a minimum there will be an **uncertainty in the optimal parameter values $\mathbf{p}_0$** given by the χ^2 surface.[1]





- Approximate the objective function with a quadratic form in the vicinity of the optimum. Compute the hessian matrix.

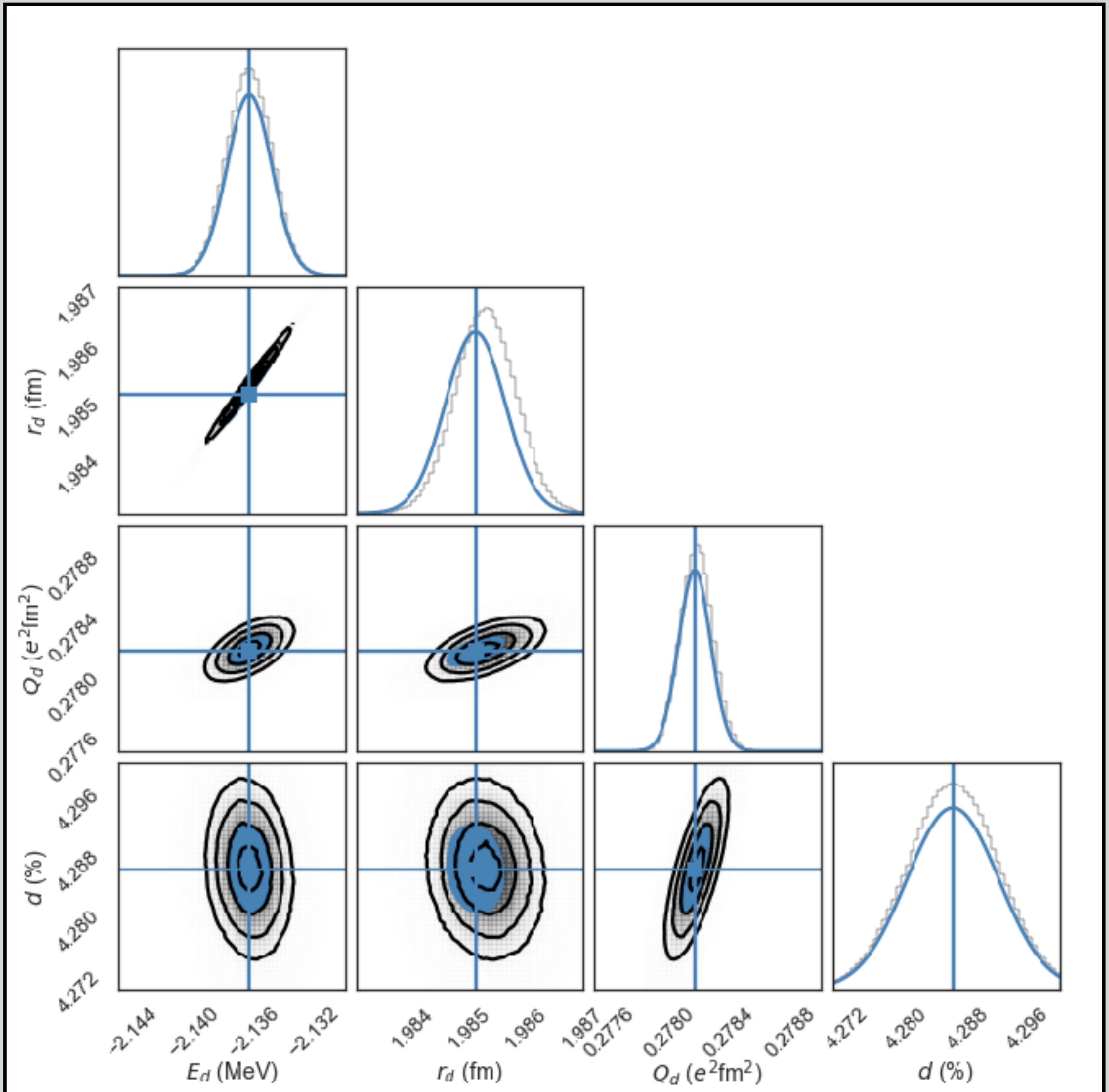
- Expand observables similarly, to second order

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

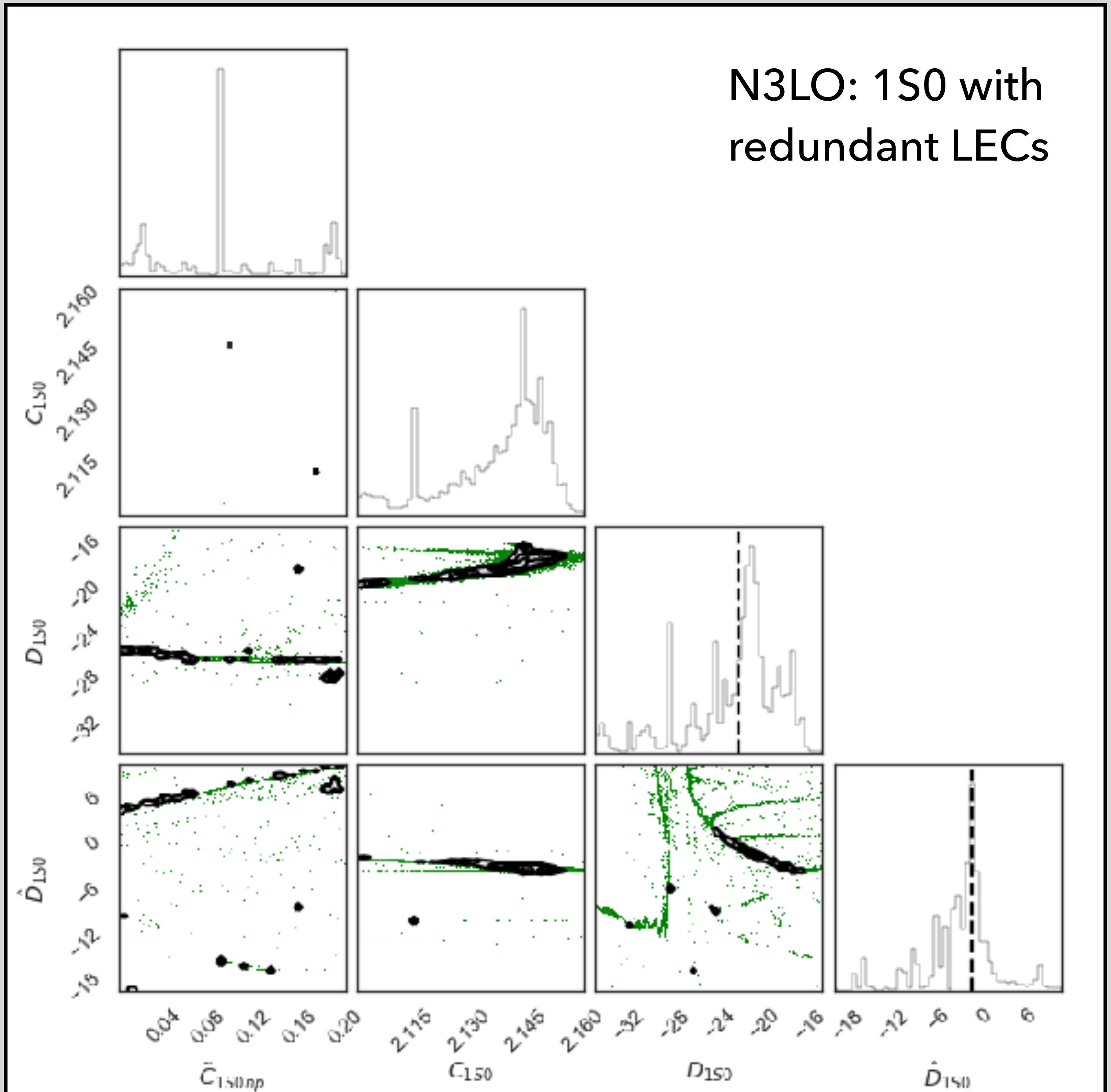
- The covariance between two observables is then

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

Deuteron observables



Redundant parameters



(see also
Sarah's talk)

Conclusion

CONCLUSION

Quantum many-body systems in finite oscillator spaces

- Demonstration how to profitably perform IR extrapolations in practice.
- Large-scale exact diagonalization reveals the relevant low-momentum scale of finite nuclei – related to the threshold energy for the first open decay channel.

Bayesian methods for uncertainty quantification

- Demonstrated successful sampling of Bayesian posterior pdfs in the nucleon-nucleon sector and the subsequent error propagation.
- Bayesian analysis will allow:
  - the incorporation of truncation errors using marginalisation
  - model validation
  - model checking.

see Daniels's and Sarah's talks

Many thanks to my collaborators

- Boris Carlsson, Andreas Ekström, Andreas Johansson, Håkan Johansson, Daniel Sääf (Chalmers)
- Aaina Bansal, Gaute Hagen, Thomas Papenbrock (ORNL/UT)

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