Uncertainty Quantification Challenges From Modern *Ab Initio* Nuclear Theory

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Bayesian Methods in Nuclear Physics
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The Modern *Ab Initio* Approach to Low Energy Nuclear Physics

Fundamental Description

QCD

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Fundamental Description

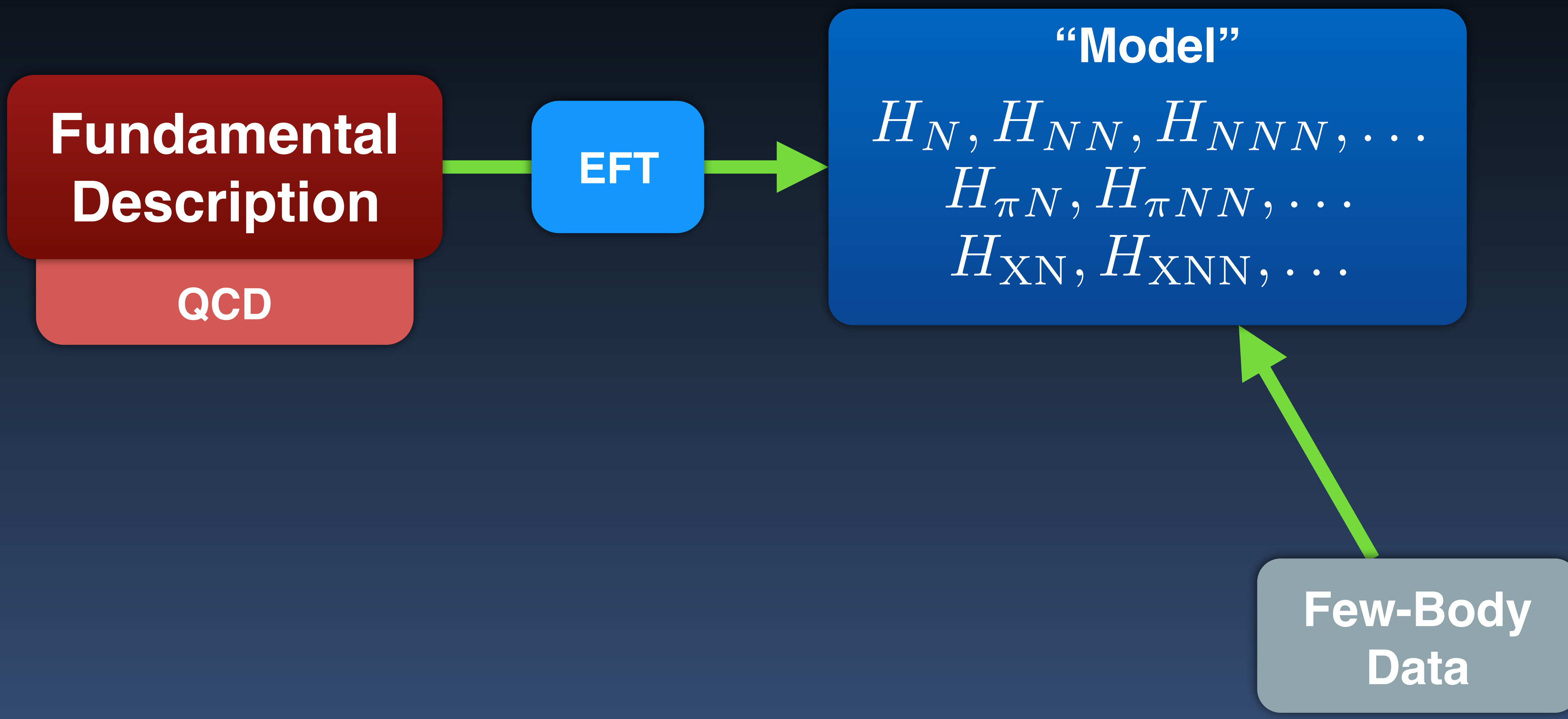
QCD

EFT

"Model"

$$H_N, H_{NN}, H_{NNN}, \ldots$$
$$H_{\pi N}, H_{\pi NN}, \ldots$$
$$H_{\mathrm{XN}}, H_{\mathrm{XNN}}, \ldots$$

The Modern *Ab Initio* Approach to Low Energy Nuclear Physics



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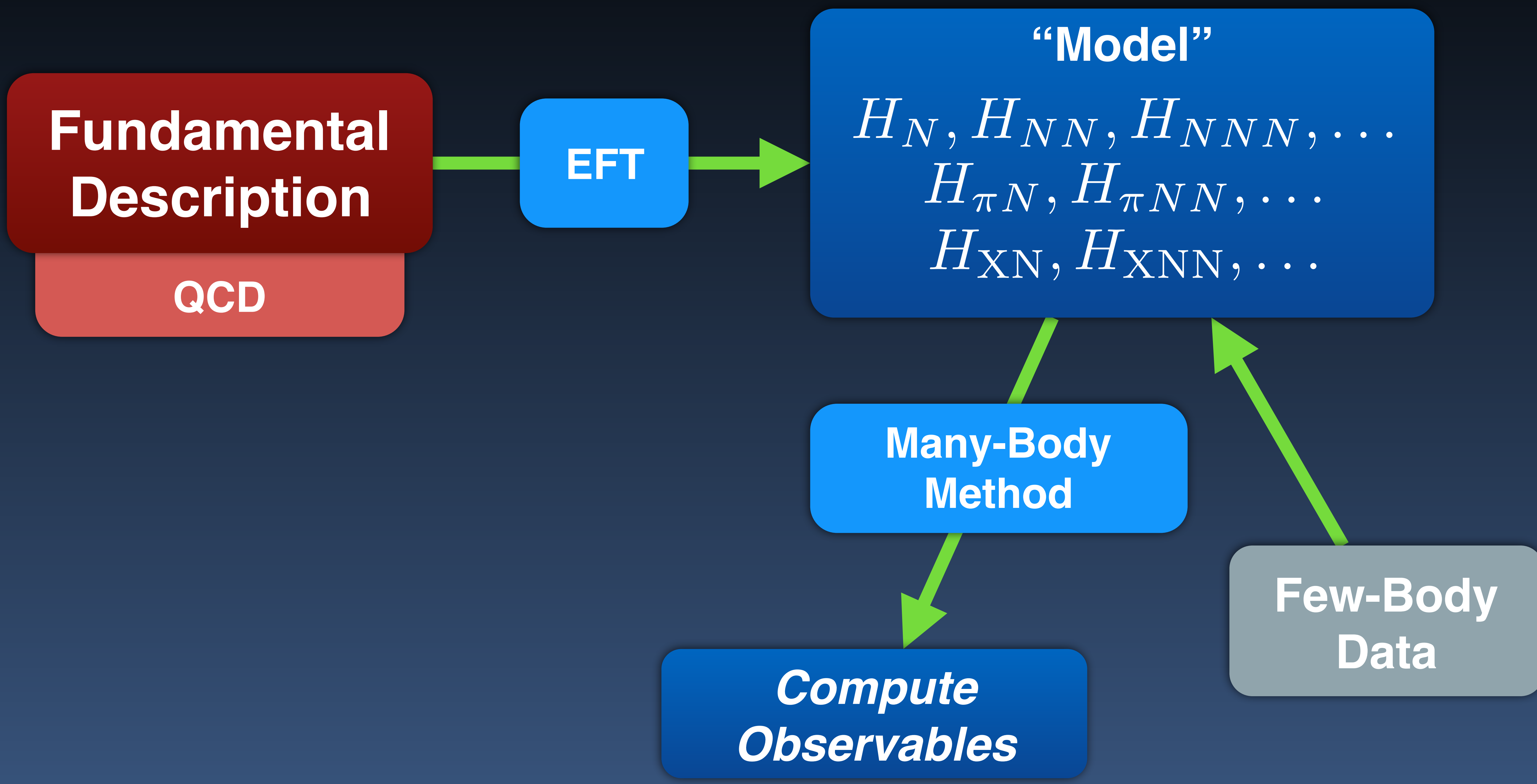

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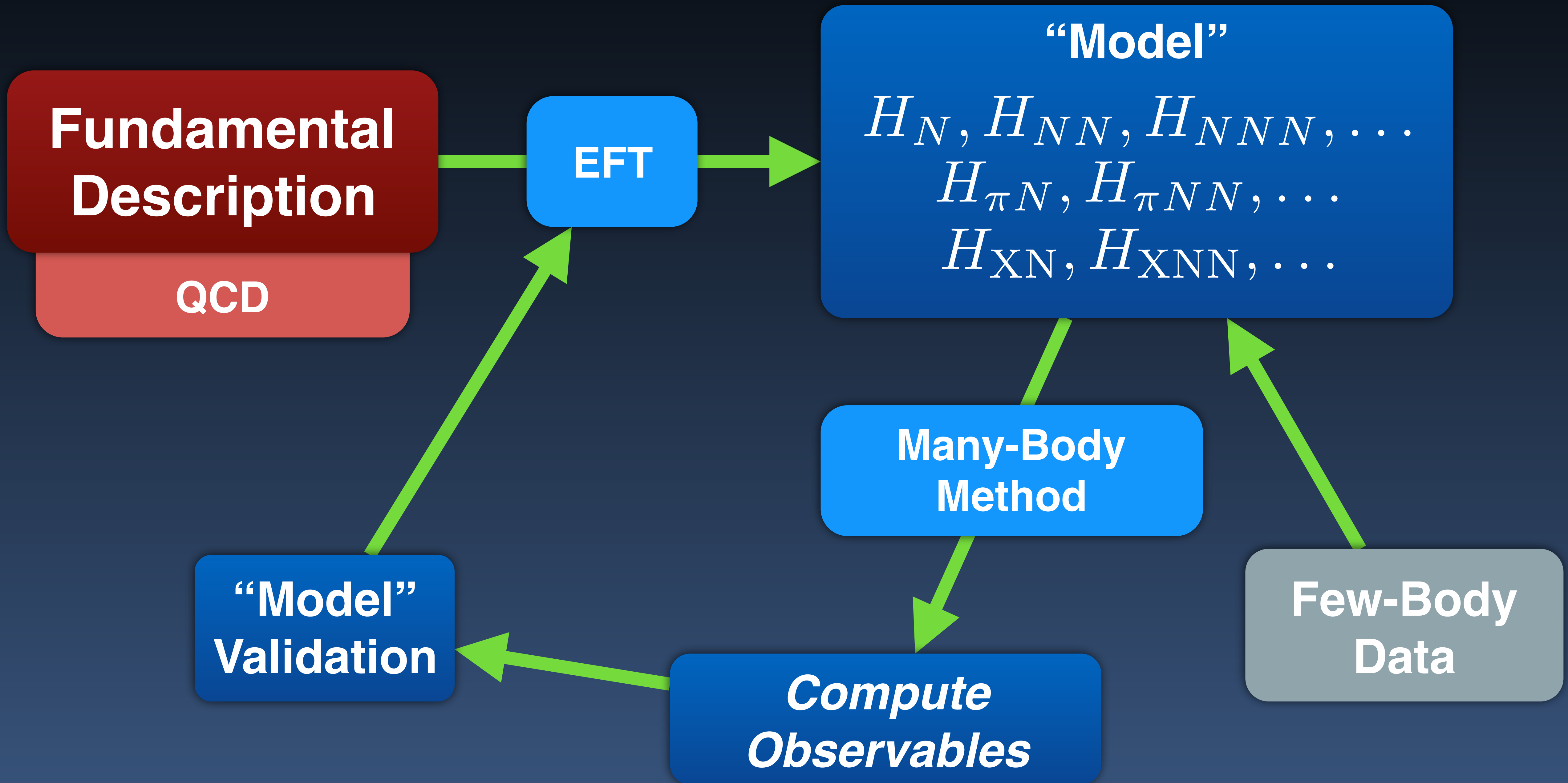

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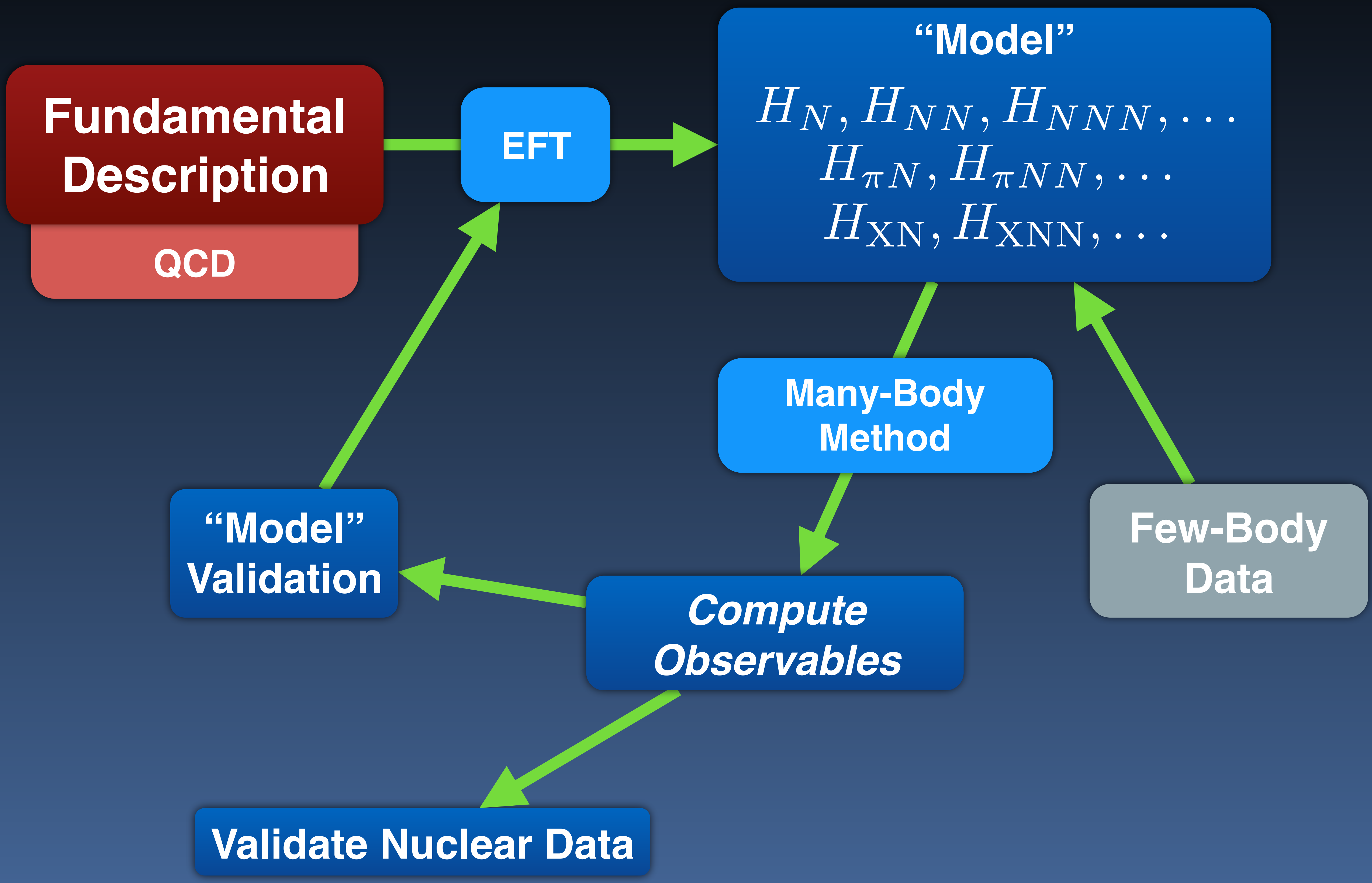

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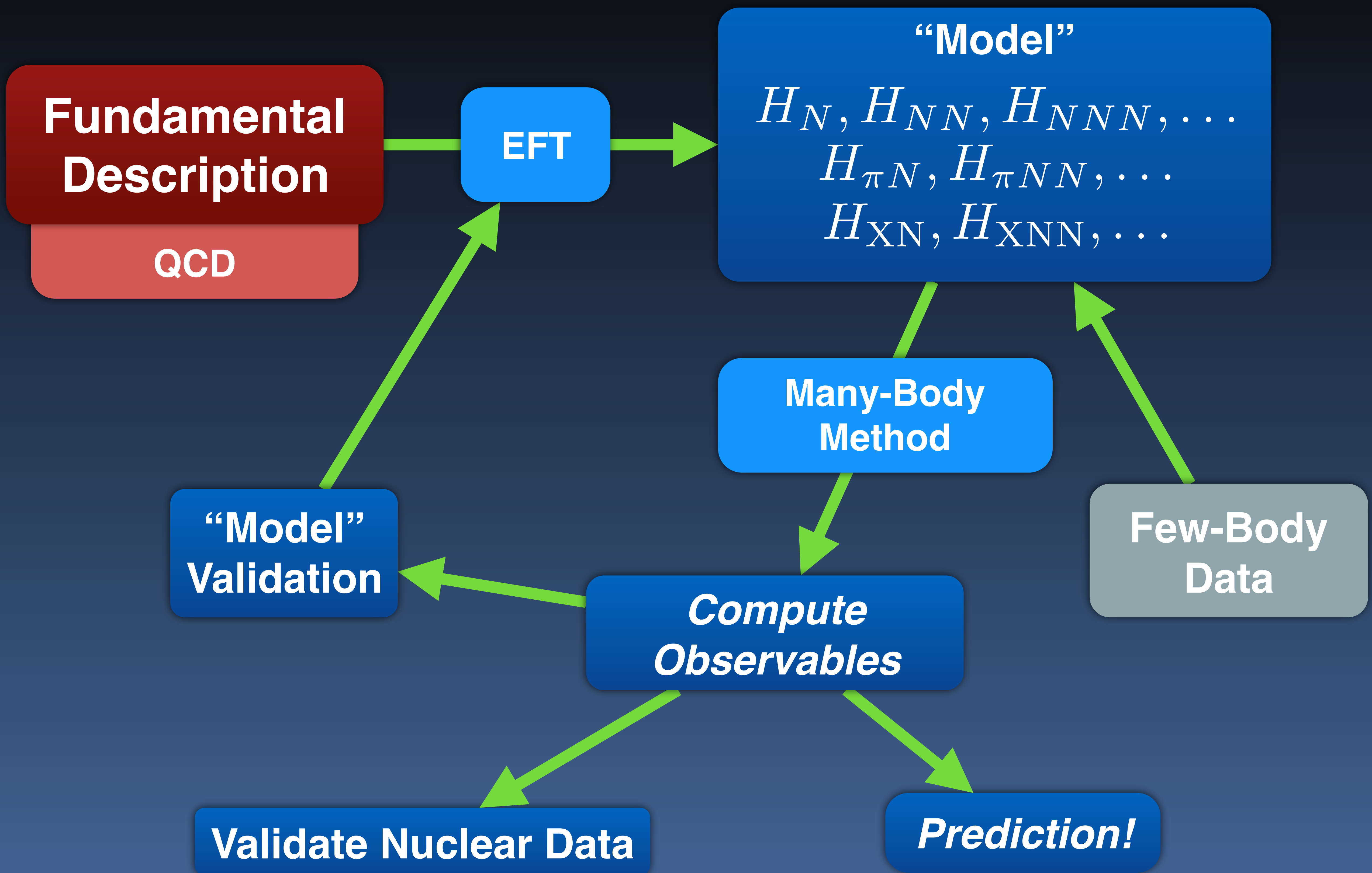


Nuclear forces from chiral effective field theory

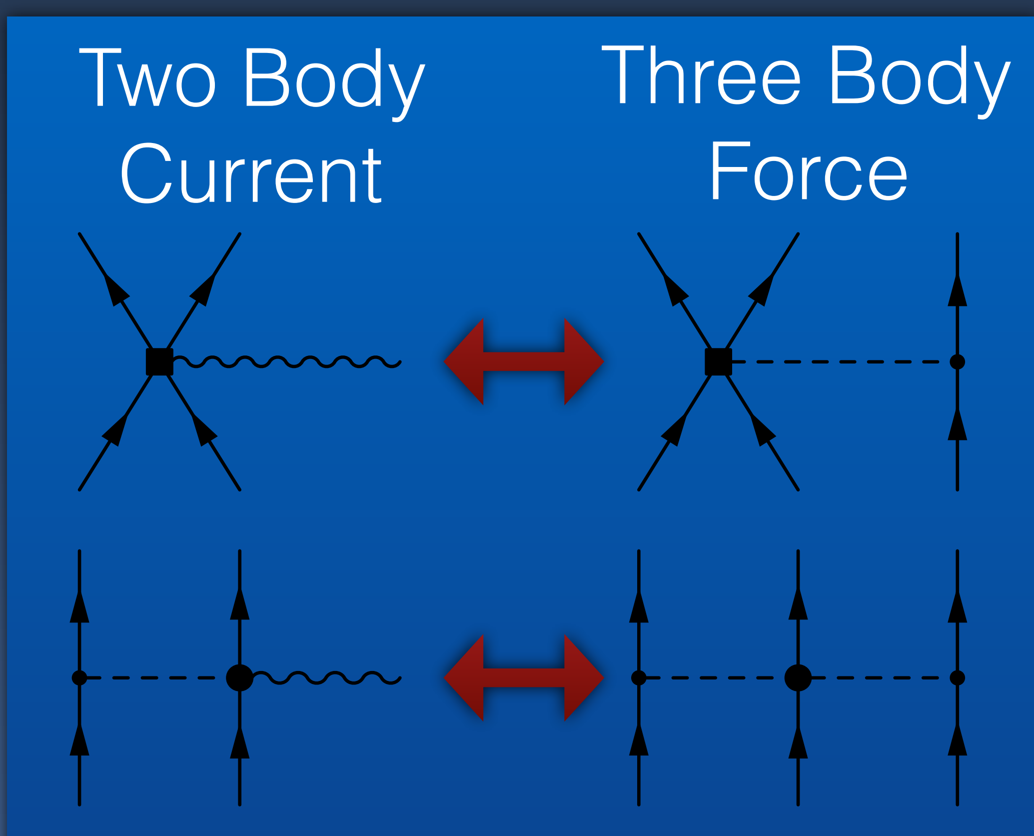
[Weinberg; van Kolck; Epelbaum et al.; Entem & Machleidt; …]

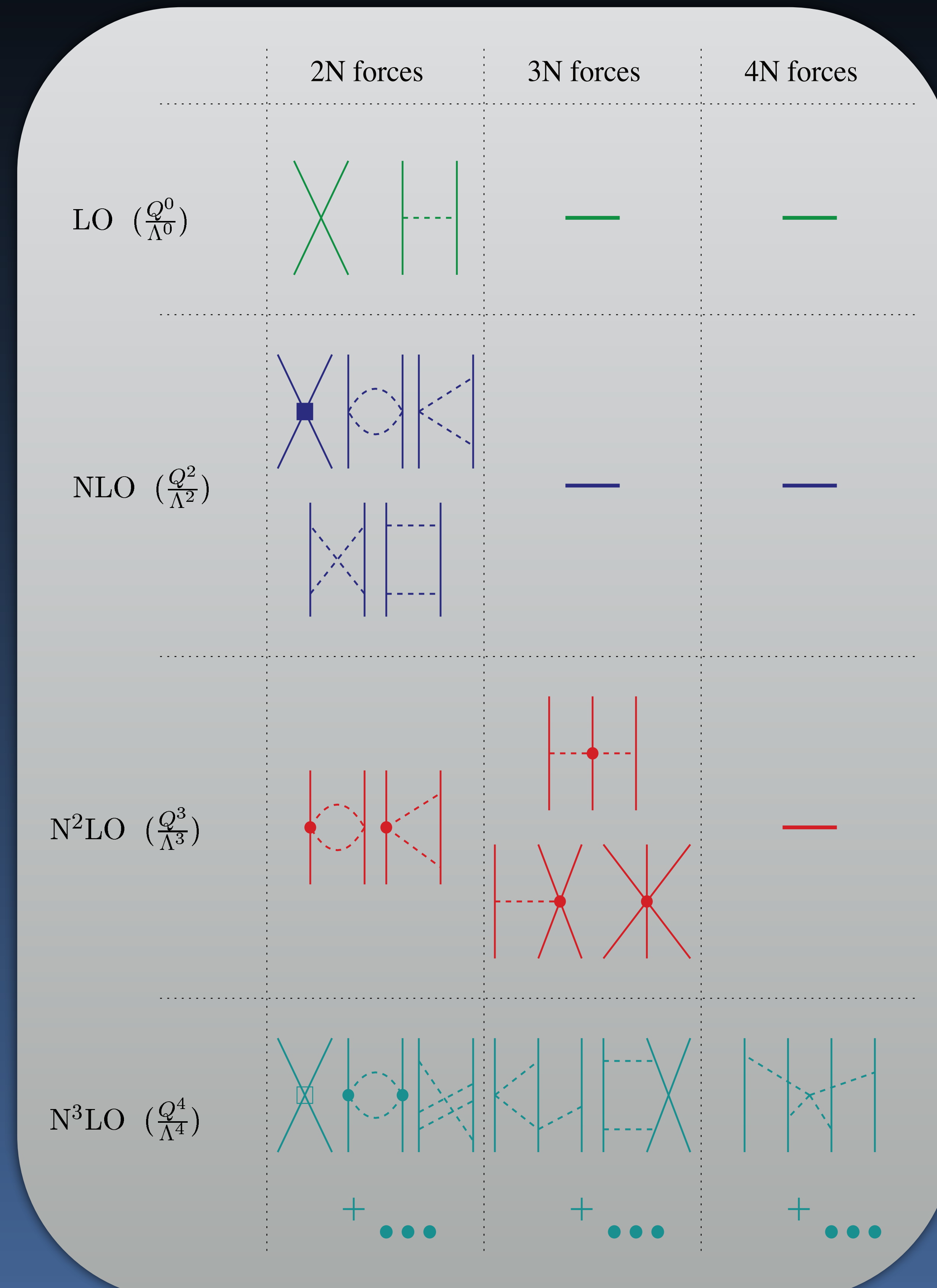
We can use EFT to build nuclear forces!

- Systematically improvable

$$\langle O(Q) \rangle = \left\langle O^{(\nu)}_{\mathrm{EFT}}(Q) \right\rangle + \mathcal{O}\left(\frac{Q}{\Lambda}\right)^{\nu+1}$$

- Connects different sets of strong-interaction phenomena: πN, NN, NNN





Nuclear forces from chiral effective field theory

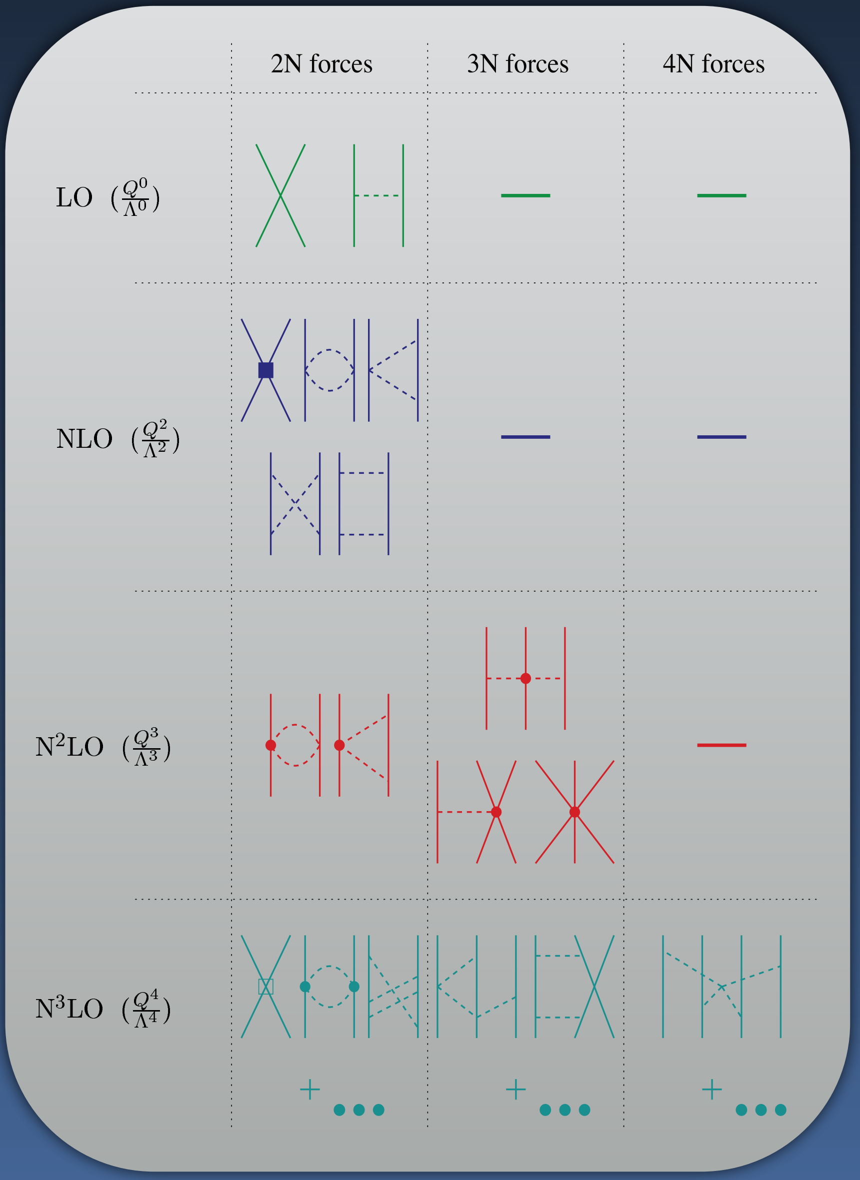
[Weinberg; van Kolck; Epelbaum et al.; Entem & Machleidt; …]

$$P(\theta;\Lambda,\mathrm{Data}) \propto \exp\left[-\frac{1}{2}\sum_i \frac{\left(y_i^{(\mathrm{data})} - y_i^{(\mathrm{EFT})}(\theta,\Lambda)\right)^2}{\sigma_i^2}\right]$$

$$y_{i,2\mathrm{B}/3\mathrm{B}}^{(\mathrm{EFT})}(\theta,\Lambda) = m(\theta,\Lambda) + u_{\mathrm{EFT}}$$

$$\theta = \text{Set of Parameters (LECs)}$$

$$\Lambda = \text{Regularization Specification}$$



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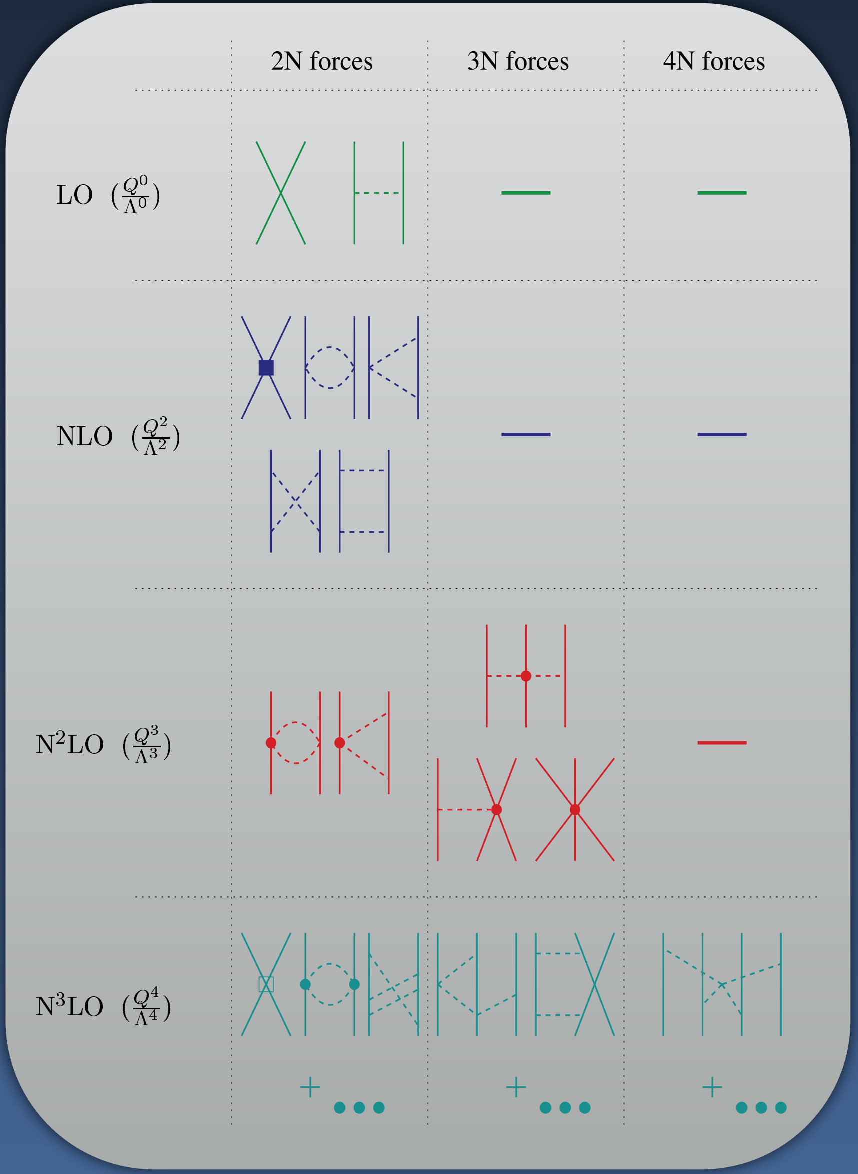


Open Problems

- How to choose regularization?
- How to correctly order power counting?
- What data should we fit?

Two Main Classes of Ab Initio Many-Body Methods

Quasi Exact	***Reference State***
Quantum Monte Carlo	Coupled Clusters Expansion
Direct Basis Expansion	In-medium SRG
	(Indirect Basis Expansion)
Exact many-body correlations	Approximate many-body correlations
Scale factorially in number of particles	Scale polynomially in number of particles

Two Main Classes of Ab Initio Many-Body Methods

Quasi Exact

~~Quantum Monte Carlo~~

Direct Basis Expansion

Exact many-body correlations

Scale factorially in number of particles

Reference State

Coupled Clusters Expansion

In-medium SRG

(Indirect Basis Expansion)

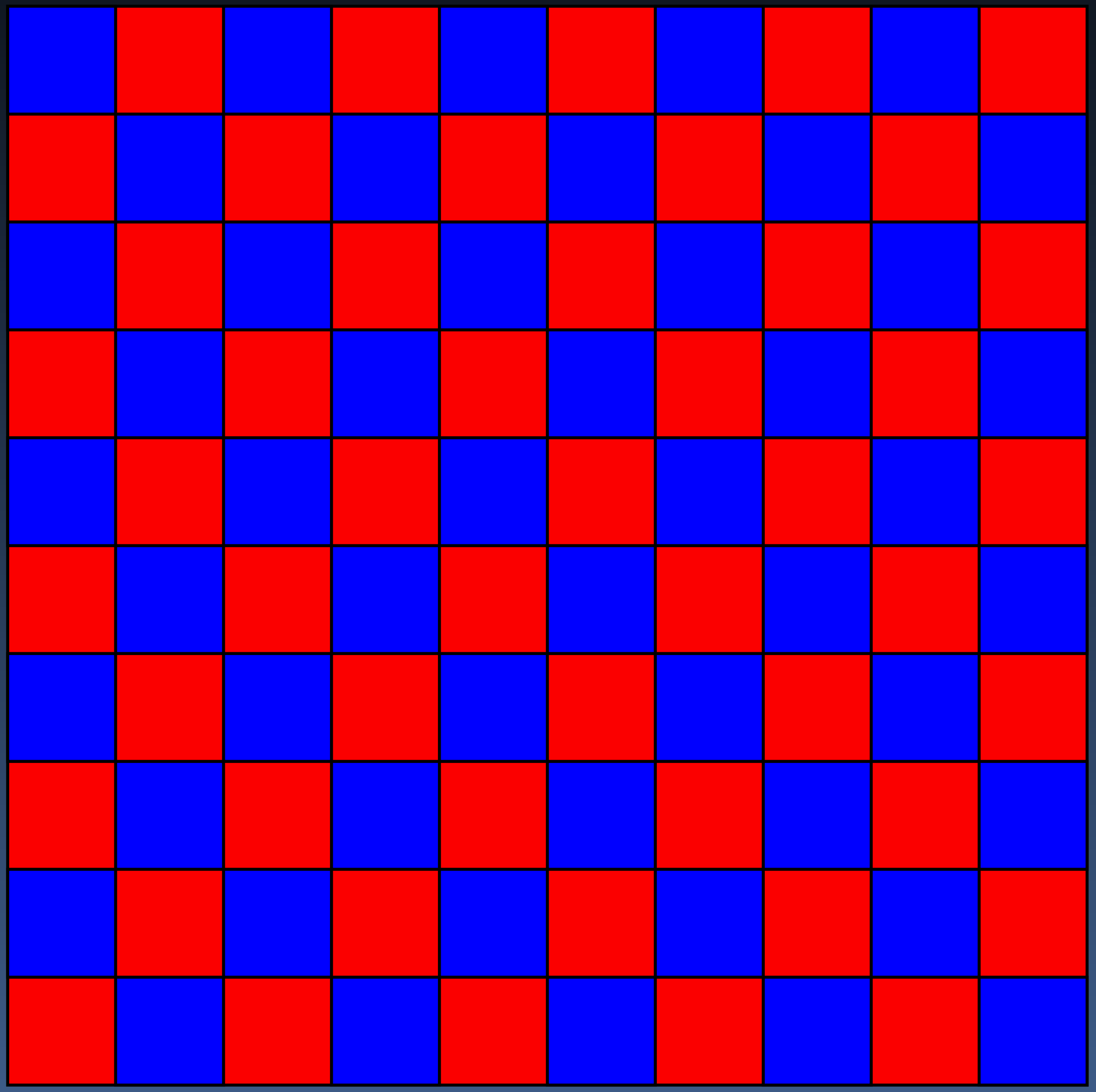
Approximate many-body correlations

Scale polynomially in number of particles

Direct Basis Expansion

For only a few (< 12) particles, one can construct the many-body Hamiltonian as a large matrix

Many-body correlations are included exactly!



Quasi-Exact Many-Body Methods

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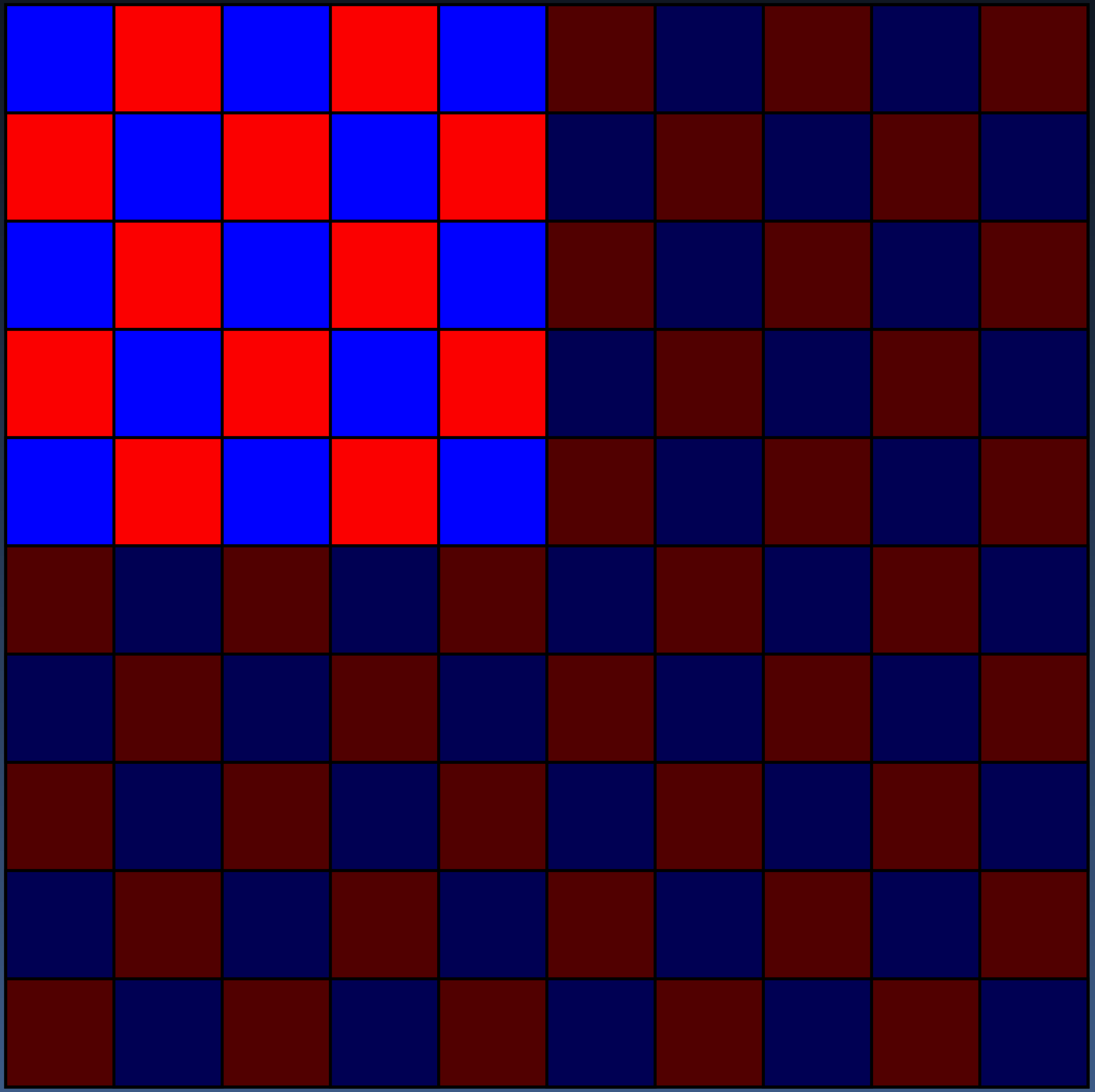
Uncertainty enters from the basis truncation



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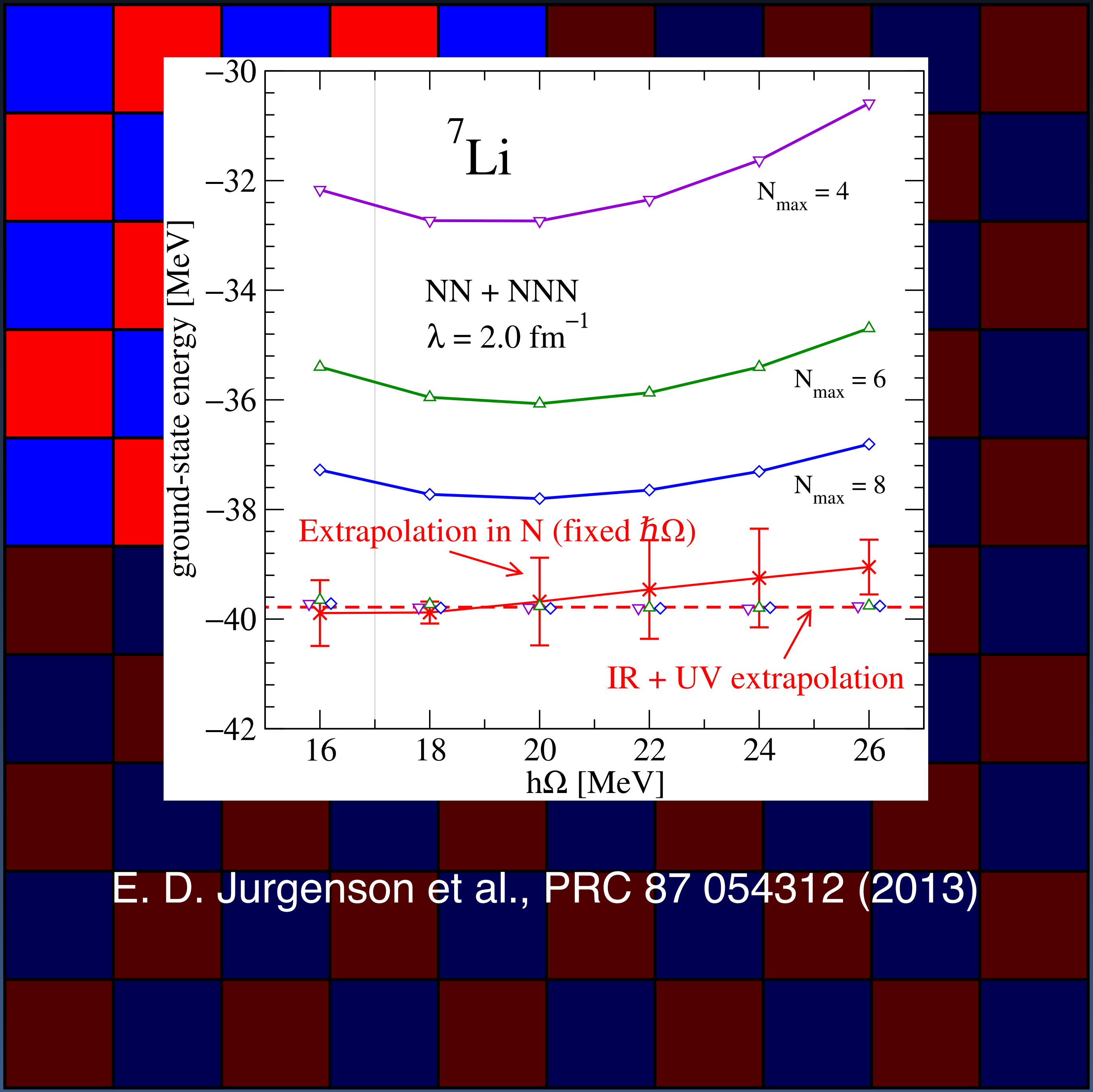


E. D. Jurgenson et al., PRC 87 054312 (2013)

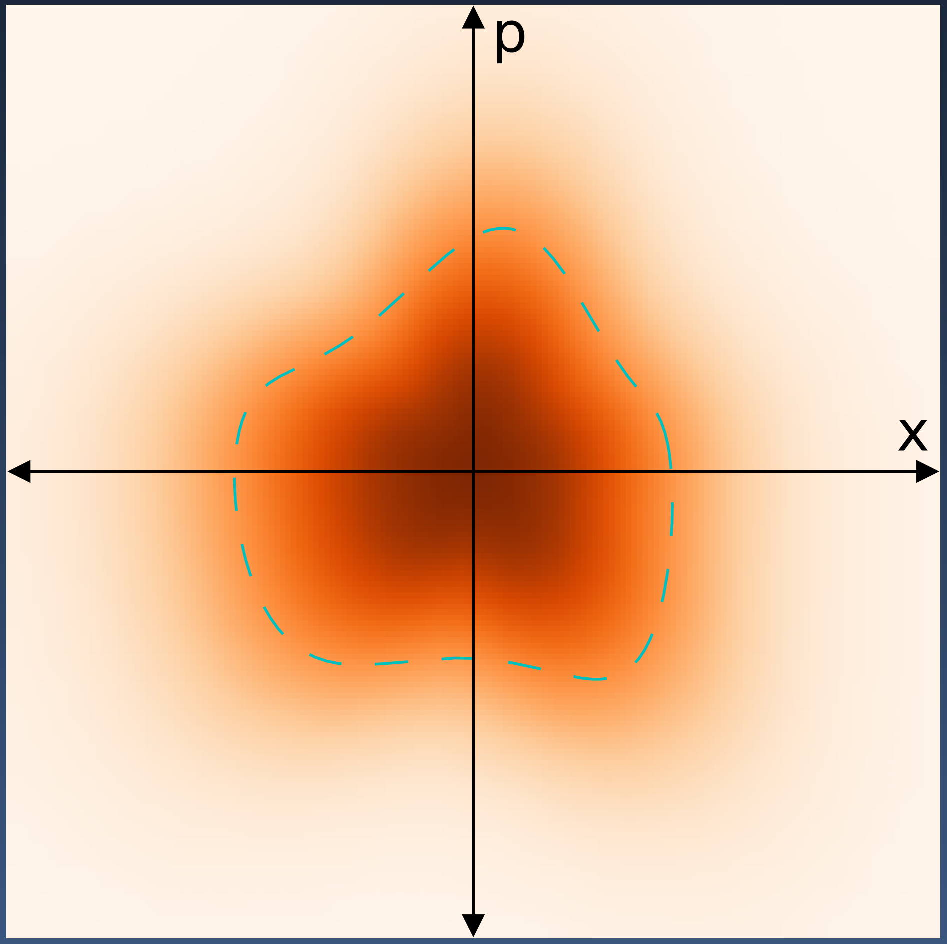
Quantifying Errors in Finite Oscillator Basis

R. J. Furnstahl et al., PRC 86 031301(R)
S. A. Coon et al. PRC 86 054002

$$E - E_{\text{exact}} = \Delta E =$$

$$\Delta E_{\text{IR}}(L) + \Delta E_{\text{mix}}(L, \Lambda) + \Delta E_{UV}(\Lambda)$$

$$u_i(r) = \sum_{n=0}^{N_{\max}} c_{i,n} \phi_n(r)$$



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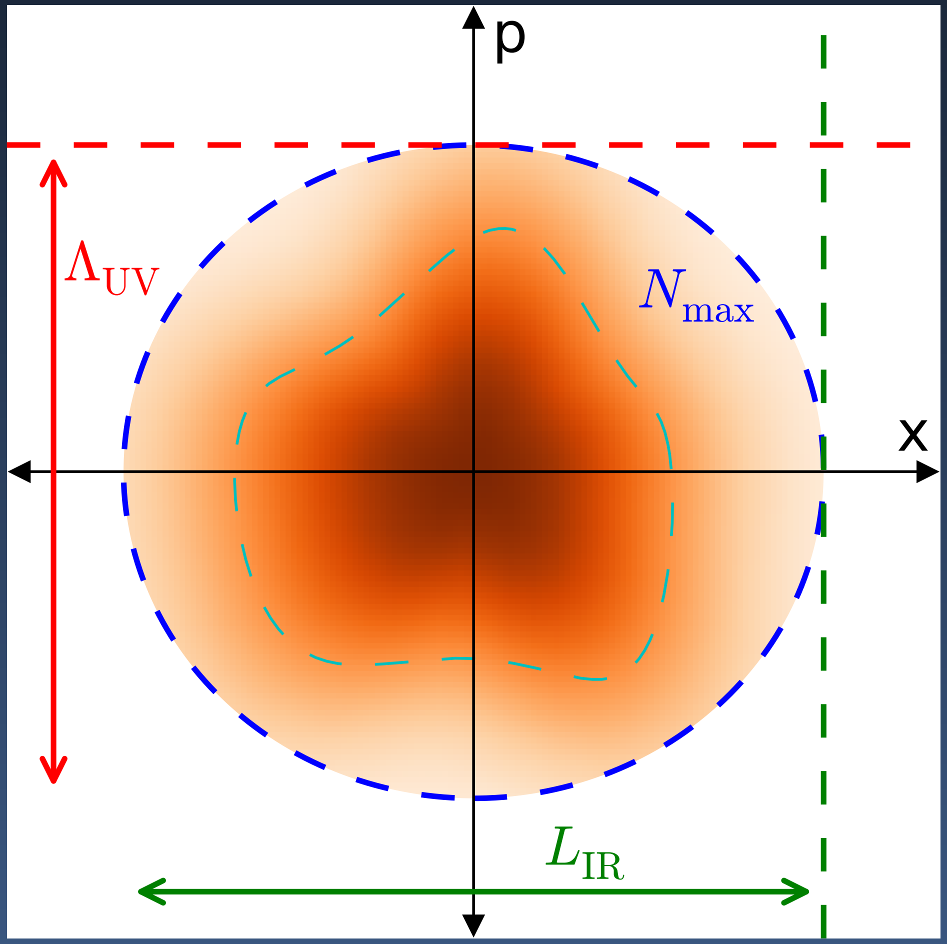

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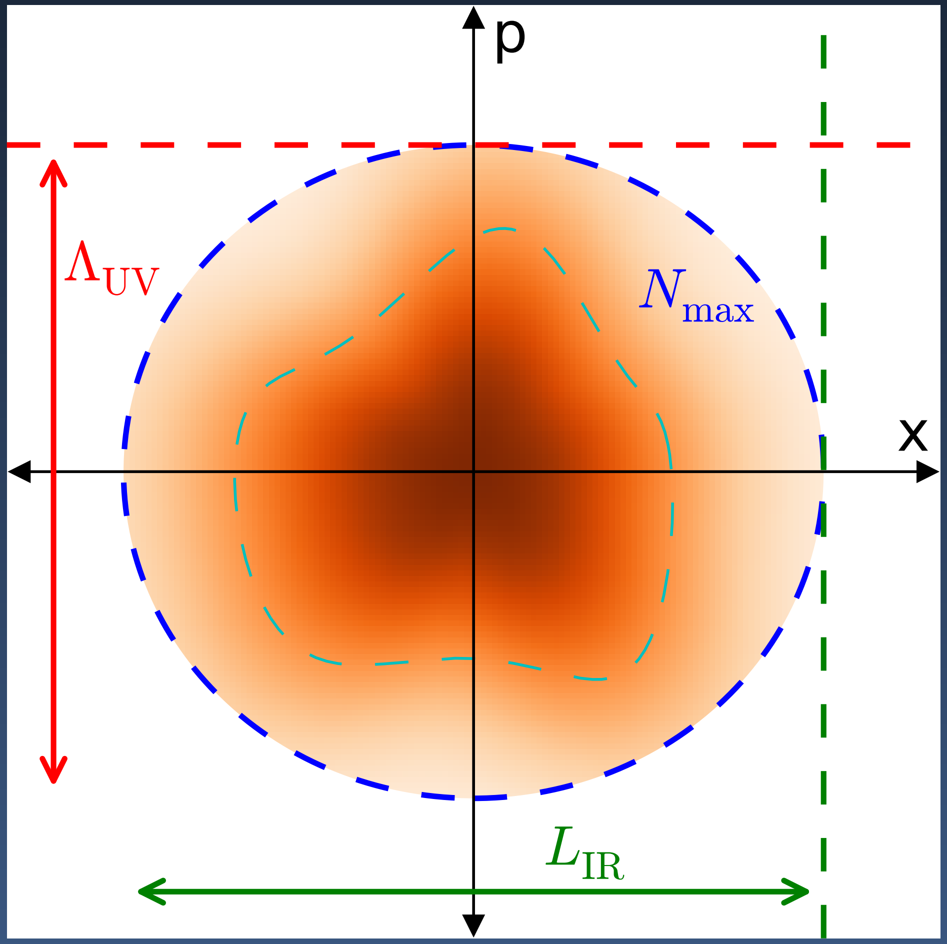
The Infrared Error Term:



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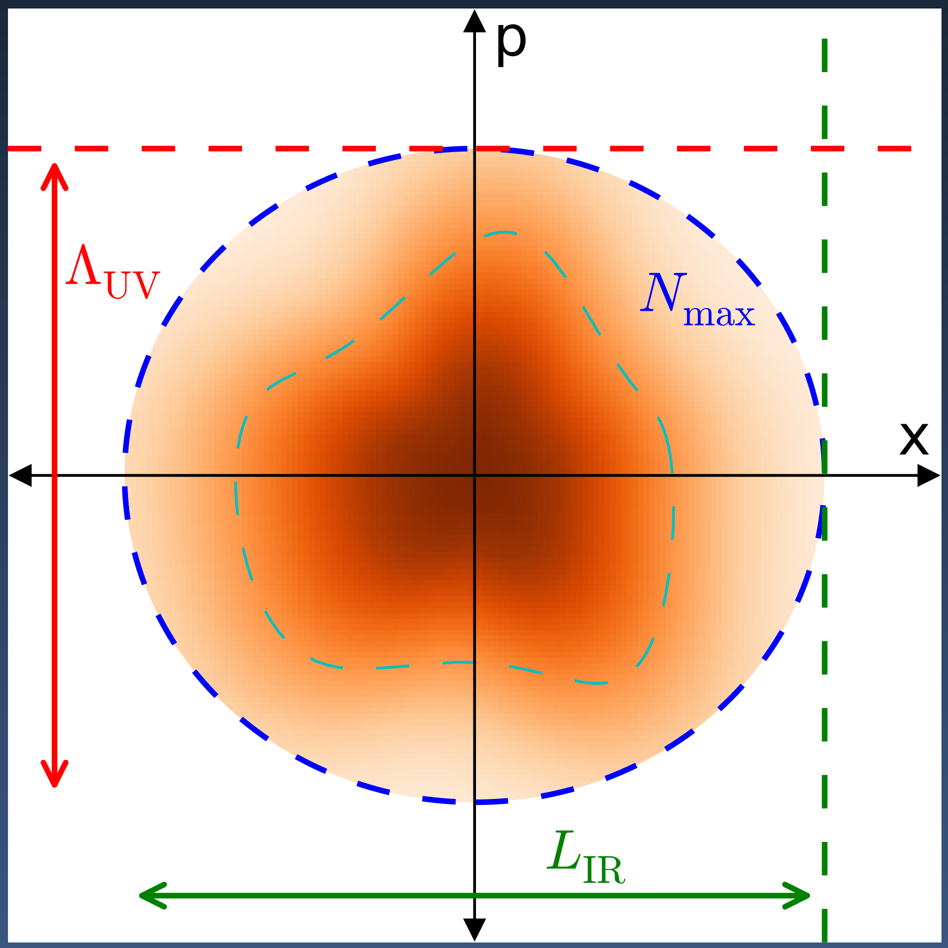
The Infrared Error Term:

- Universal for short range Hamiltonians



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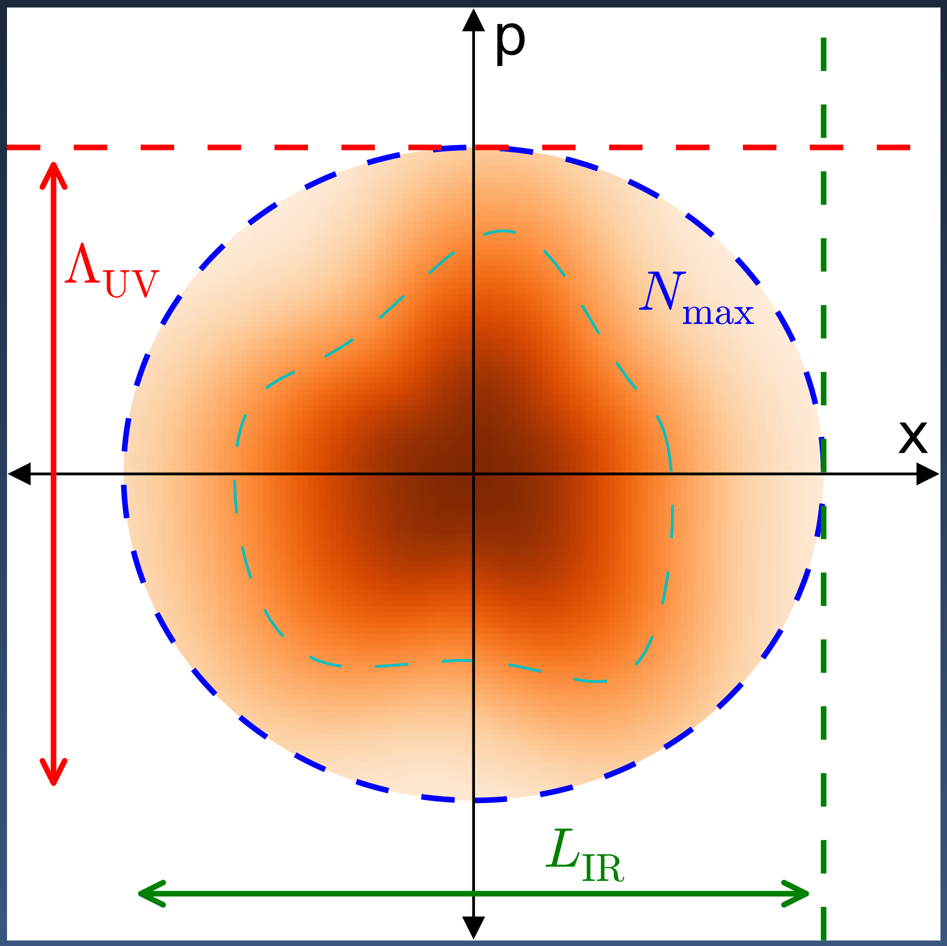

The Infrared Error Term:

- Universal for short range Hamiltonians
- Can be systematically corrected

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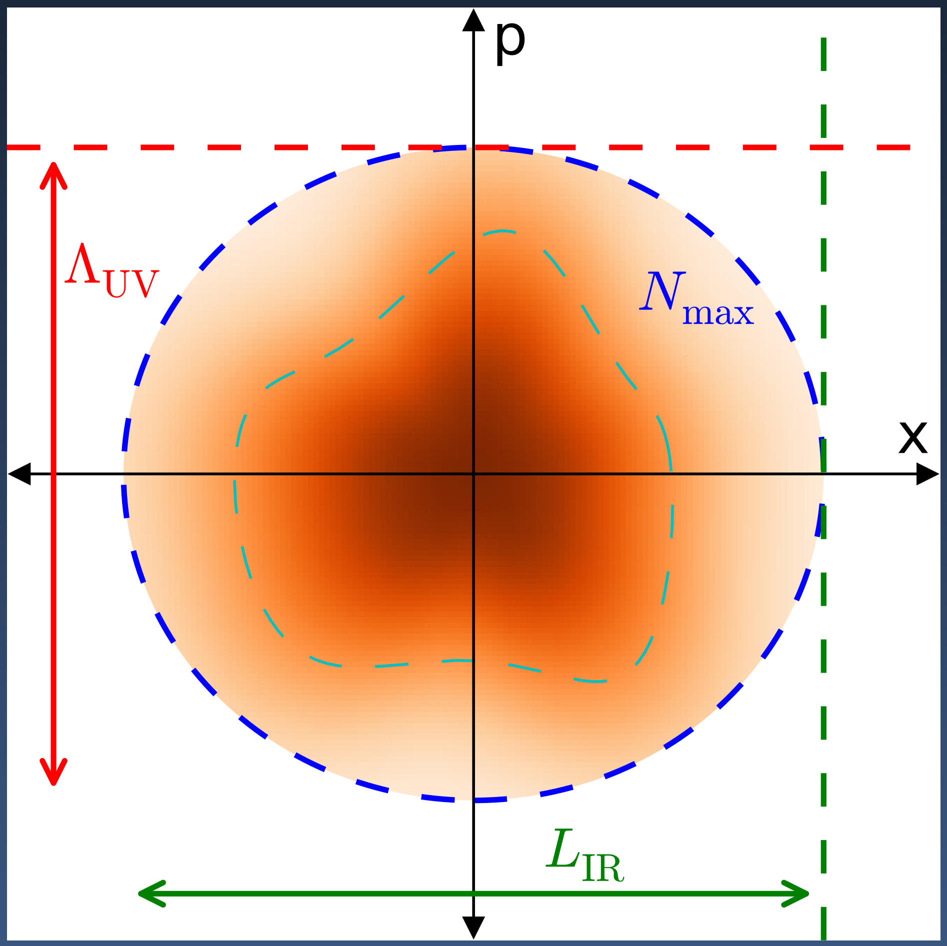

The Infrared Error Term:

- Universal for short range Hamiltonians
- Can be systematically corrected
- Resembles error from putting system into a infinite well

Quantifying Errors in Finite Oscillator Basis

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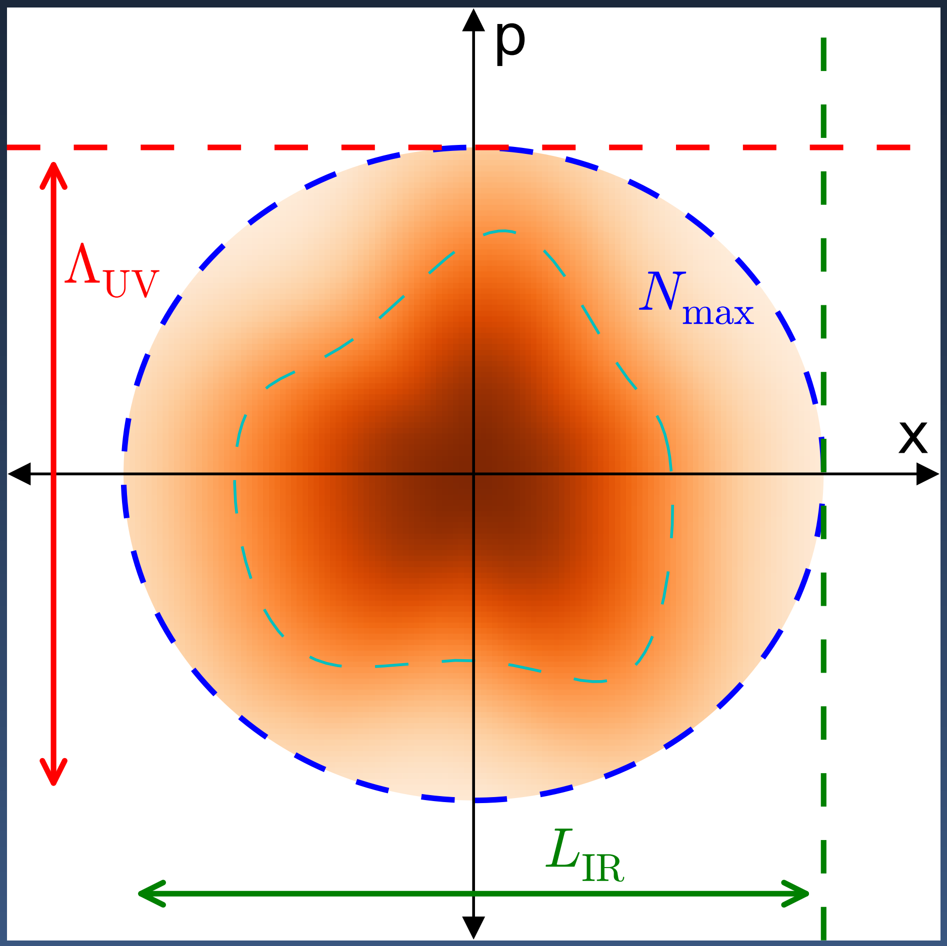

The Infrared Error Term:

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Requires Calculation to be UV converged

Quantifying Errors in Finite Oscillator Basis

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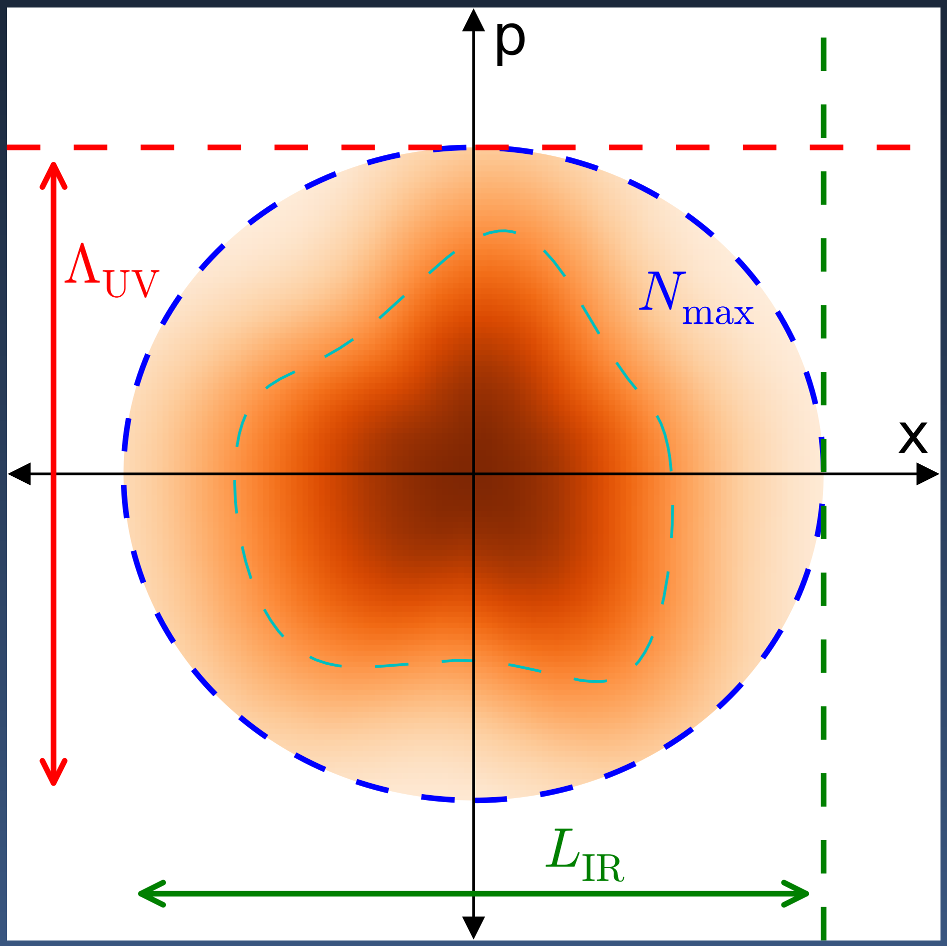
S. N. More et al., PRC 87 044326
R. J. Furnstahl et al., PRC 89 044301

$$\langle r\rangle / \langle r\rangle_\infty = 1 + \sum_{m=1}^{\infty} P_m(\beta) e^{-m\beta}$$

$$\langle E\rangle / \langle E\rangle_\infty = 1 + \sum_{m=1}^{\infty} a_m \frac{p_m(\beta)}{p_m(-\beta)} e^{-m\beta}$$



This is only one part of the Basis Truncation Error!!!

Quantifying Errors in Finite Oscillator Basis

$$u_i(r) = \sum_{n=0}^{N_{\max}} c_{i,n}\phi_n(r)$$

$$y_i^{(\mathrm{thy})} = m(\theta, \Lambda) + u_{\mathrm{EFT}} + v_{\mathrm{Basis}}$$

$$v_{\mathrm{Basis}} = v_{\mathrm{IR}} + v_{\mathrm{UV}} + v_{\mathrm{mixed}}$$

$$v_{\mathrm{IR}}$$

$$\langle r\rangle/\langle r\rangle_\infty = 1 + \sum_{m=1}^{\infty} P_m(\beta)e^{-m\beta}$$

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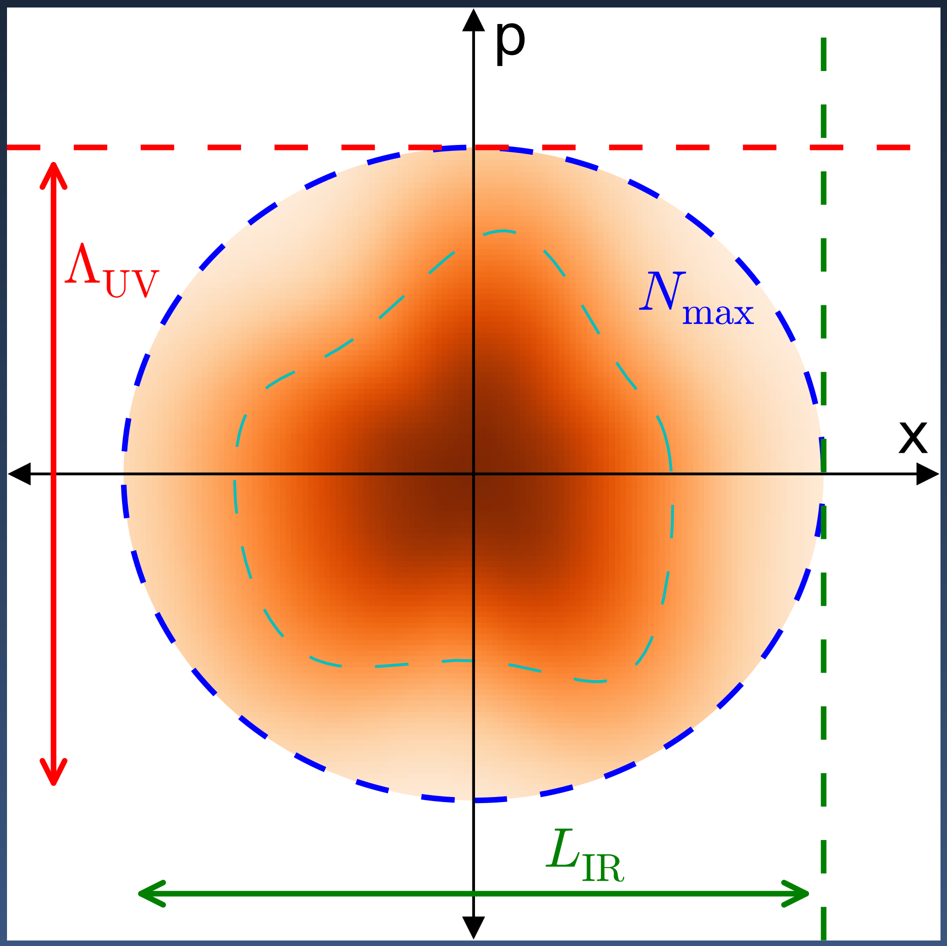
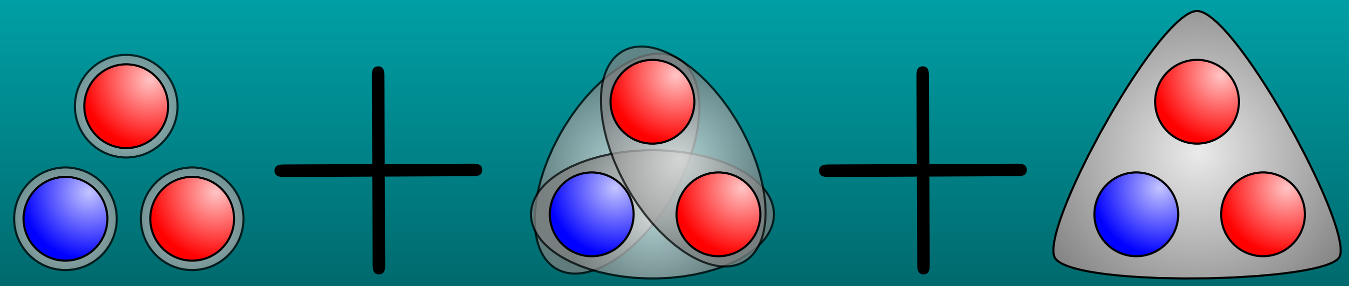


Coupled Clusters Expansion

$$\hat{T} = $$



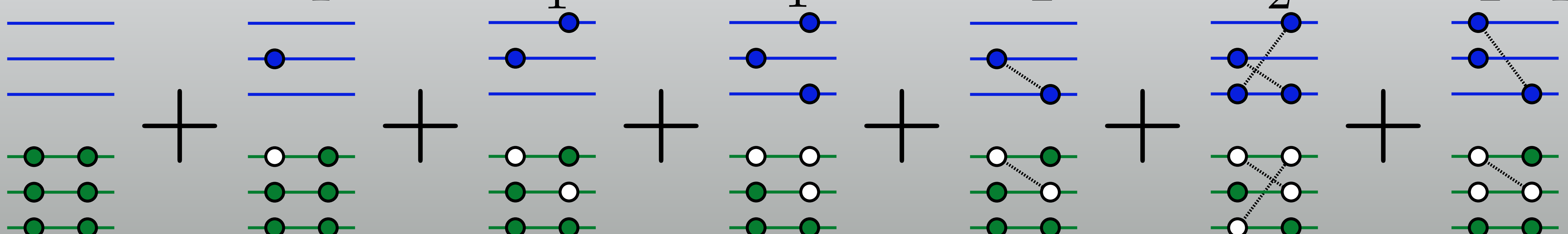
$$+ \dots$$

$$|\Psi\rangle = e^{\hat{T}} |\Phi\rangle$$

$$0 = \langle \Phi_i^a | e^{-\hat{T}} \hat{H} e^{\hat{T}} | \Phi \rangle$$

$$0 = \langle \Phi_{ij}^{ab} | e^{-\hat{T}} \hat{H} e^{\hat{T}} | \Phi \rangle$$

$$1 + \hat{T}_1 + \hat{T}_1^2 + \hat{T}_1^3 + \hat{T}_2 + \hat{T}_2^2 + \hat{T}_2 \hat{T}_1$$



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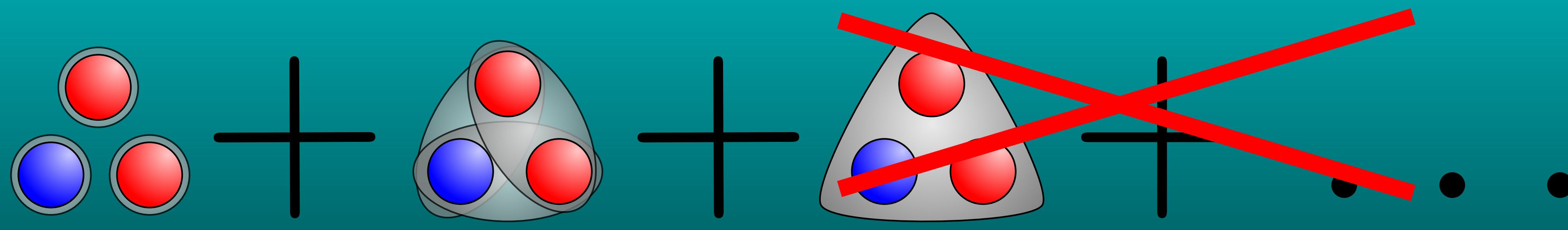

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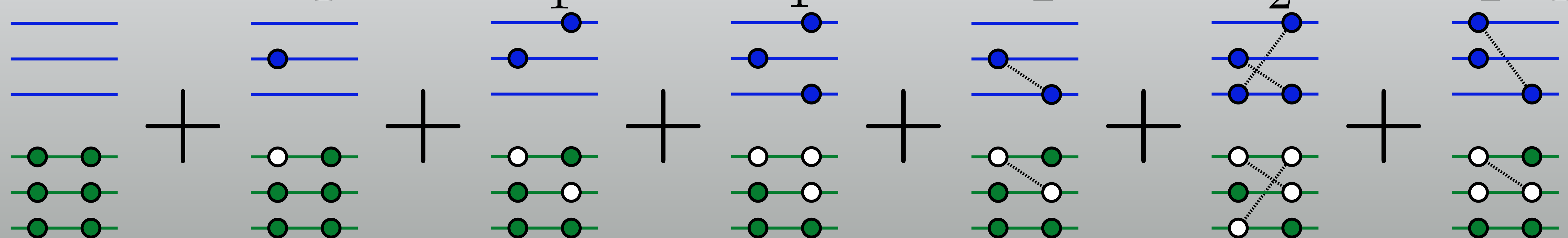

Reference State Methods (Coupled Clusters)

$$y_i^{(\mathrm{thy})} = m(\theta, \Lambda) + u_{\mathrm{EFT}} + v_{\mathrm{Basis}} + w_{\mathrm{M.B.\ corr}}$$

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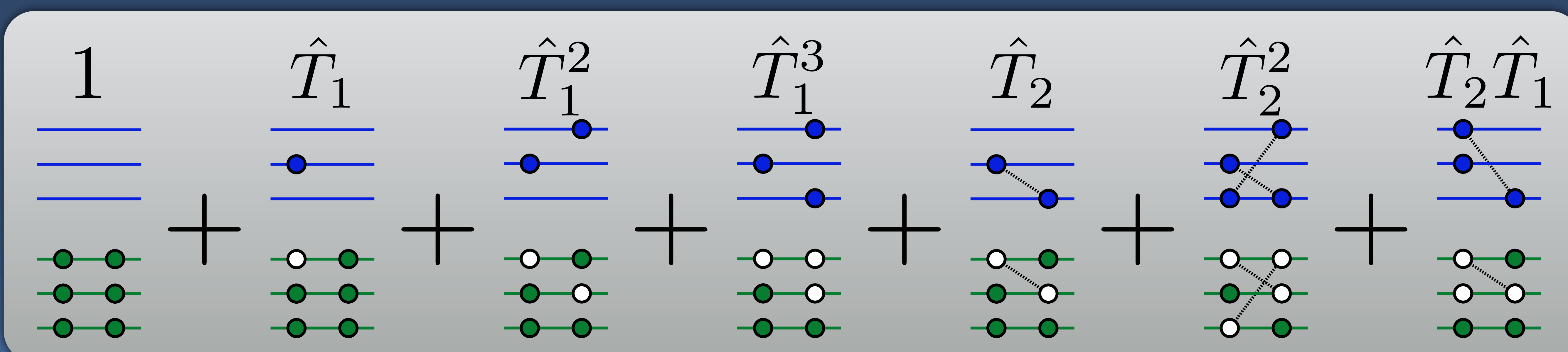
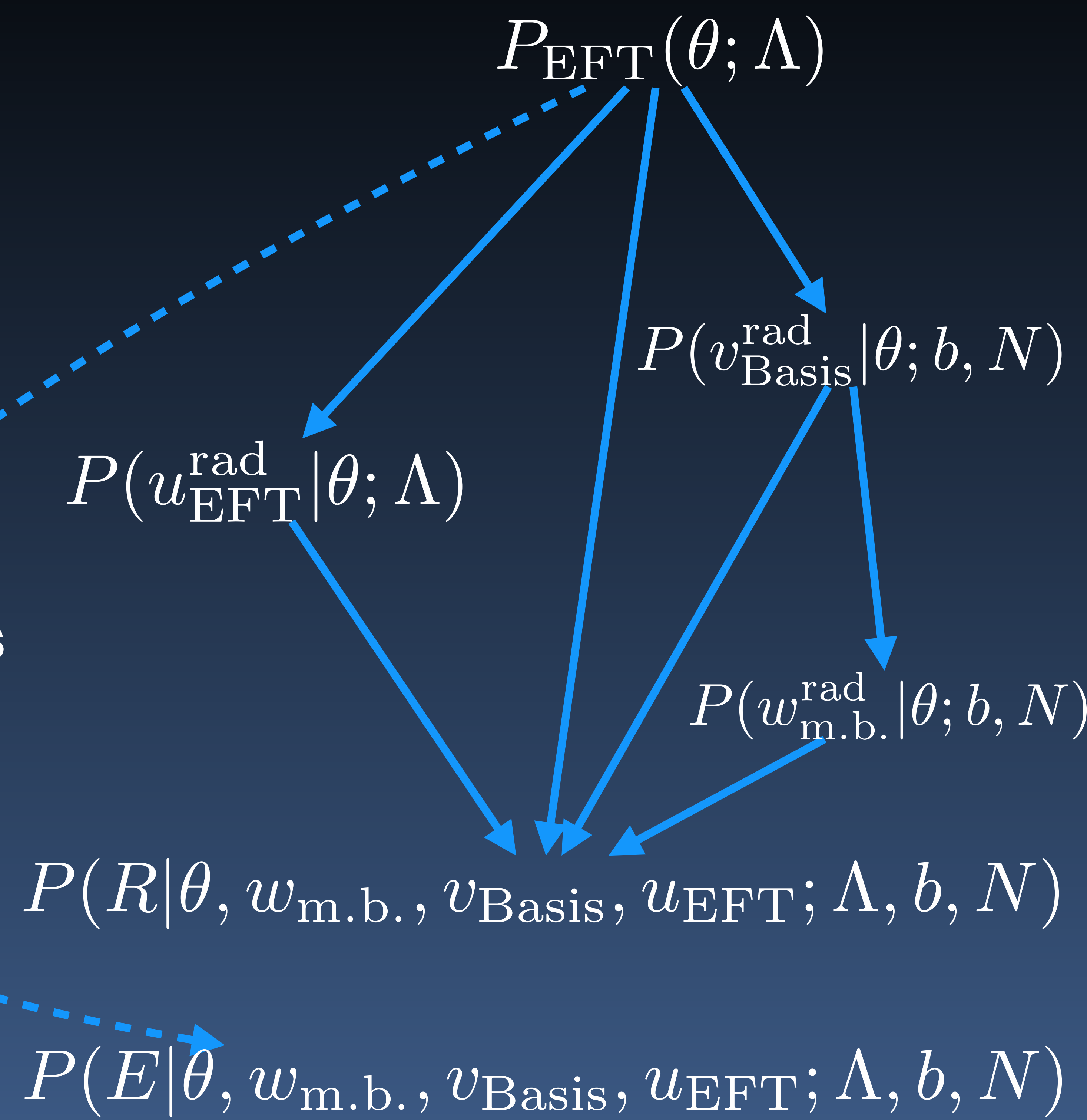


Sub Conclusions

Uncertainty enters in many places modern *ab initio* calculations

Underlying interactions model
Basis systematics
Missing many-body correlations

The relative sizes of each contribution can be observable dependent



Neutron and weak-charge distributions of the ^{48}Ca nucleus

Nature Physics 12, 186–190 (2016) 10.1038/nphys3529

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T. Papenbrock[1,2]
KAW[11(1,2)]
S. Bacca[6,7]
N. Barnea[8]
B. Carlsson[4]
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K. Hebeler[11,12]
M. Hjorth-Jensen[3,5]
M. Miorelli[6,9]
G. Orlandini[10]
A. Schwenk[11,12]
J. Simonis[11,12]

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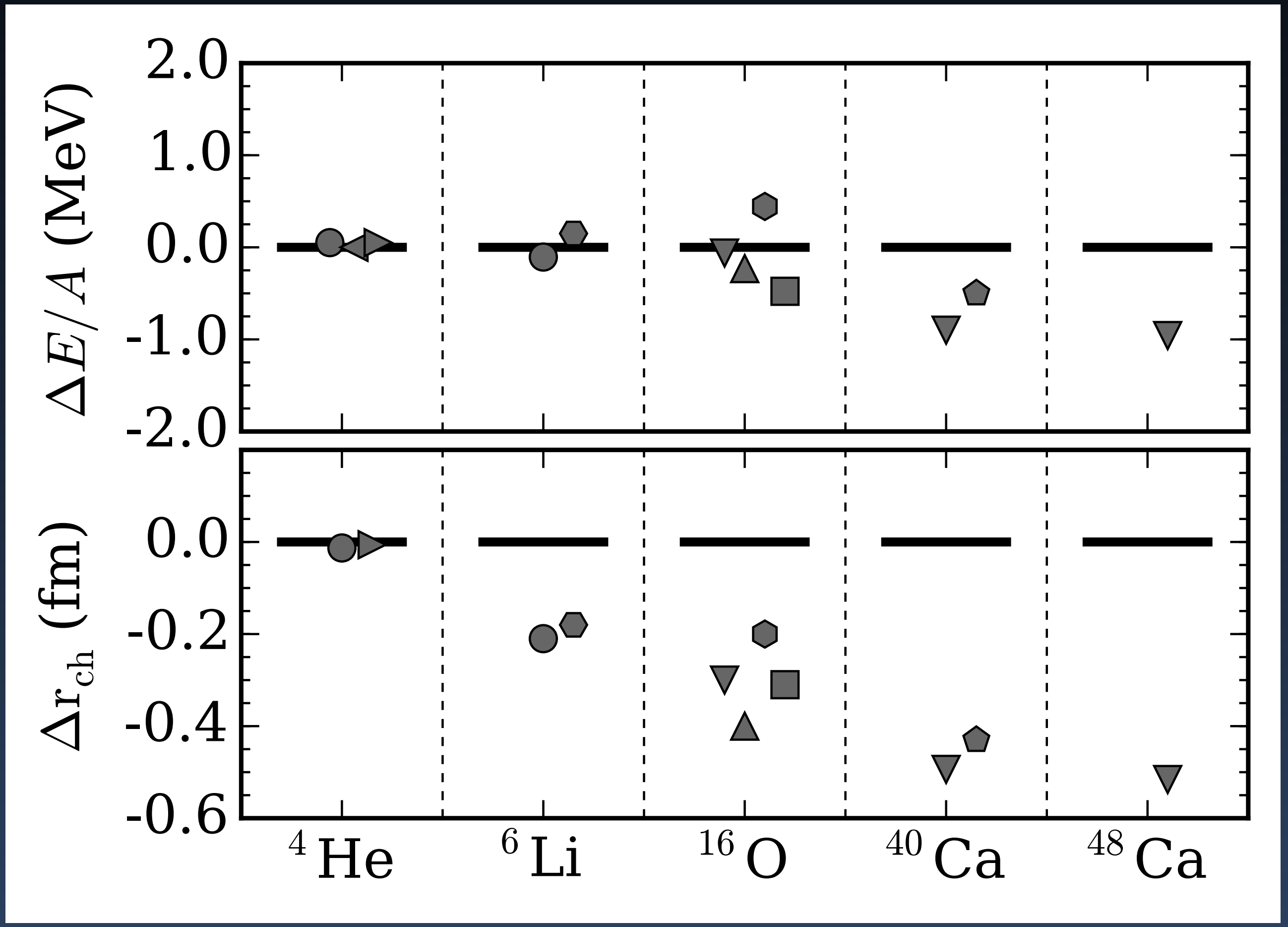
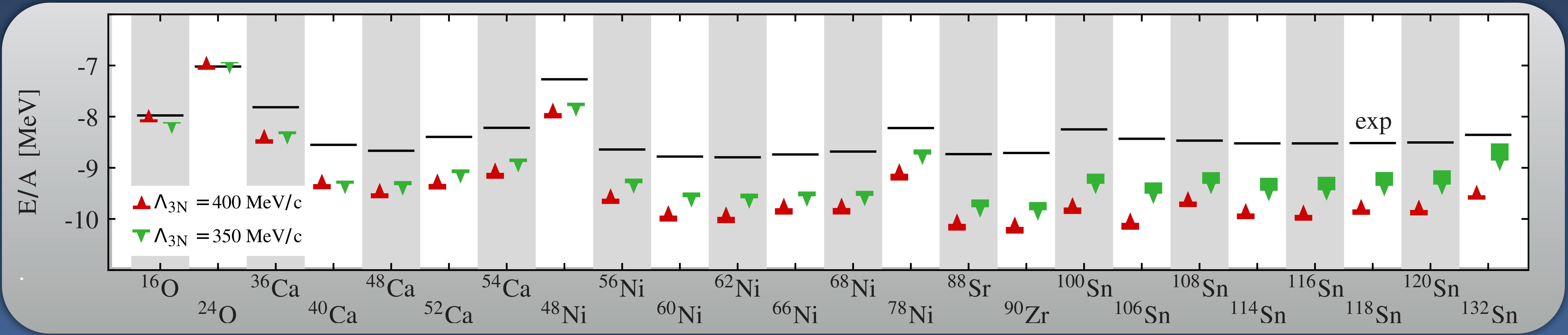
Problems in Many-body Systems

Effective Field Theory fit to A=2, 3, 4 body systems.

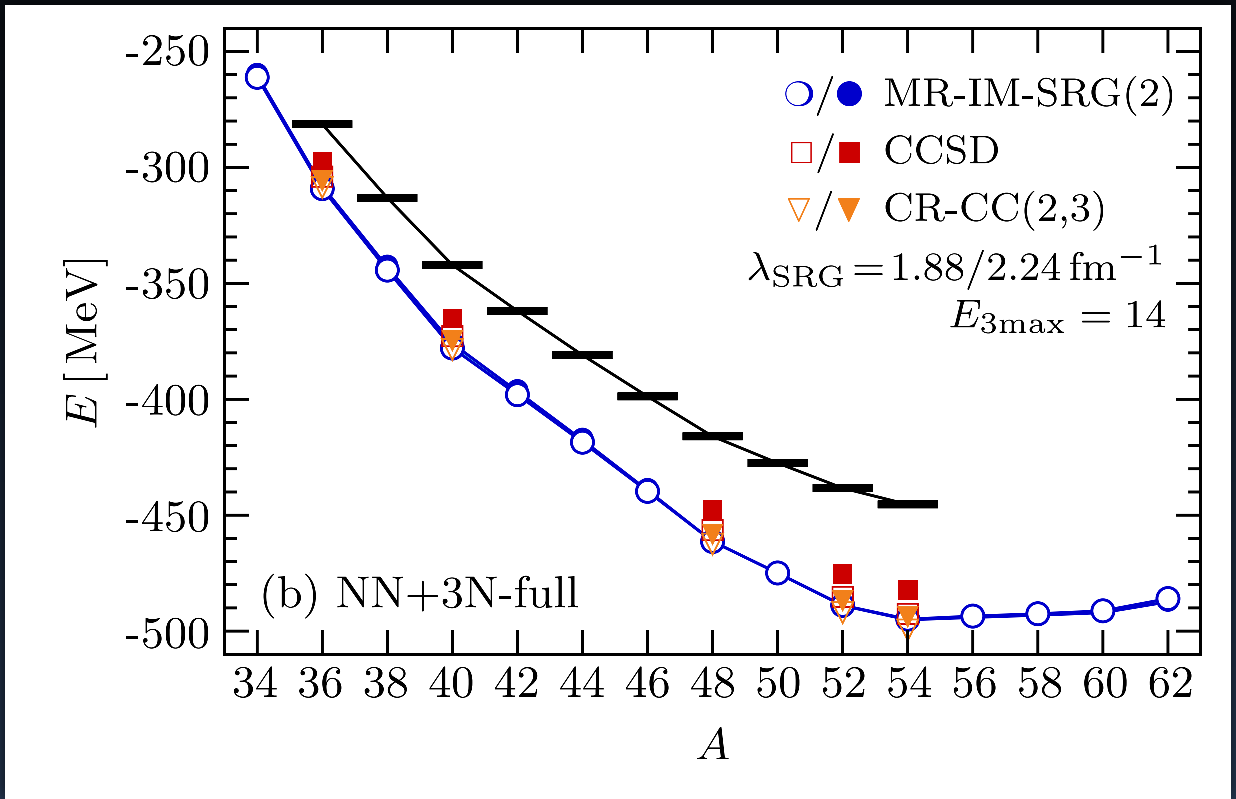
Large extrapolations do not go hand in hand with predictive power!





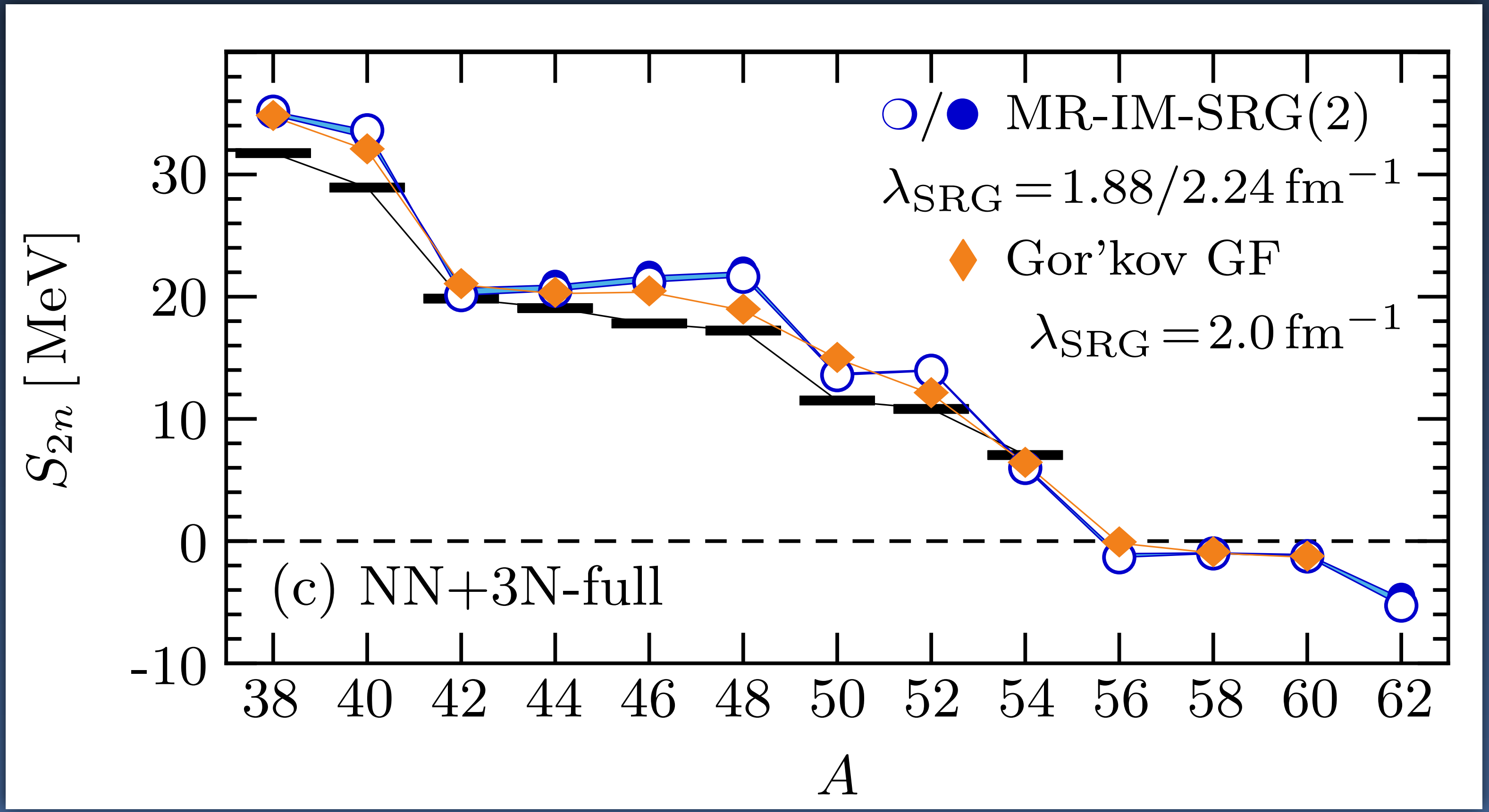
Binder, Langhammer, Calci, Roth, Phys. Lett. B. 736 (2014) 119-123

Catastrophic Errors?



EFT potentials have a catastrophic systematic error as the size of the nucleus increases

$$S_{2N}(N,Z) = E(N-2,Z) - E(N,Z)$$



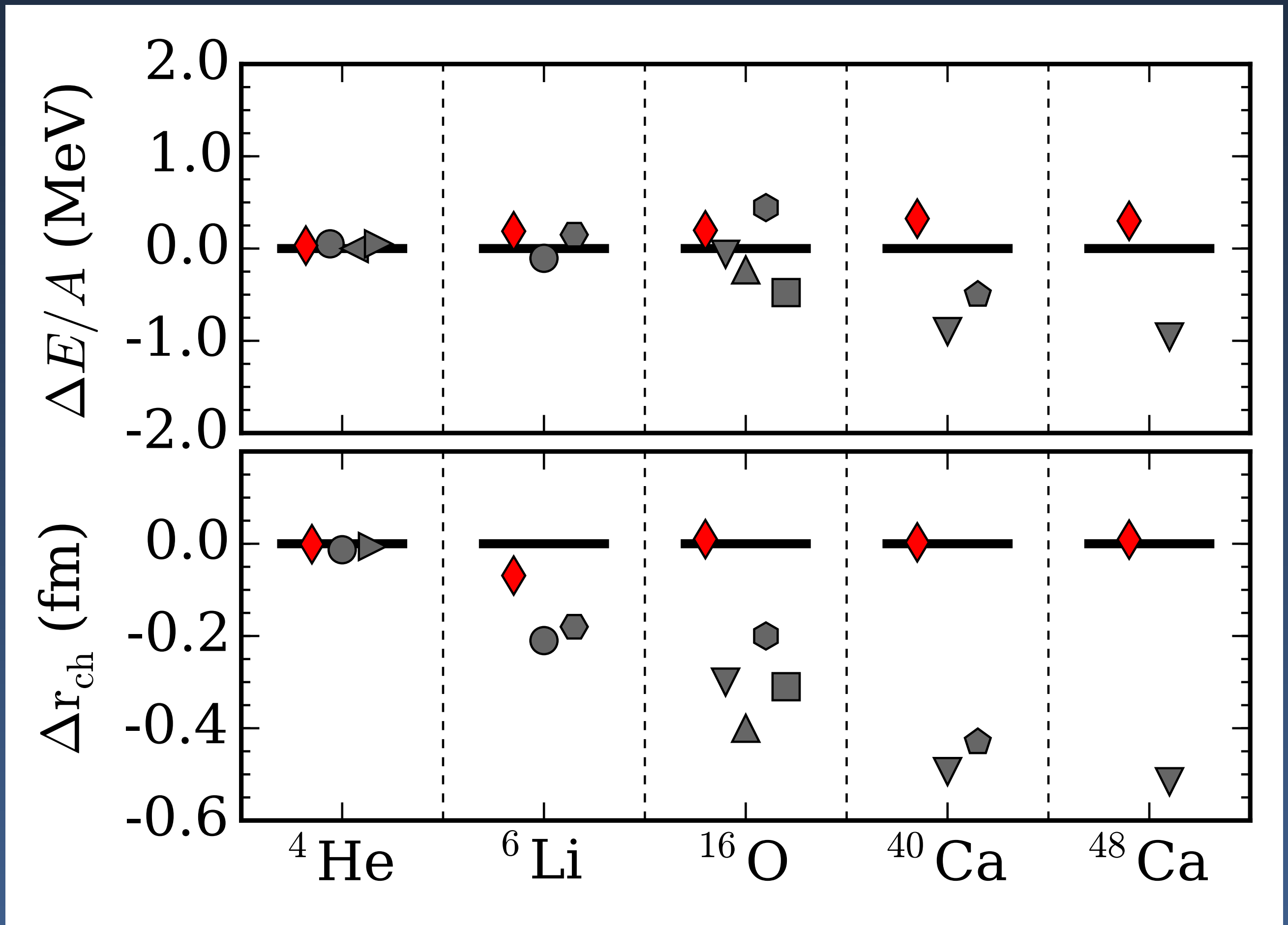
Differential Quantities seem unaffected by this systematic error!

H. Hergert et. al., Phys. Rev. C 90, 041302(R) (2014)

How to Address This Issue?

Fit effective field theory to light nuclei and very low energy scattering data.

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



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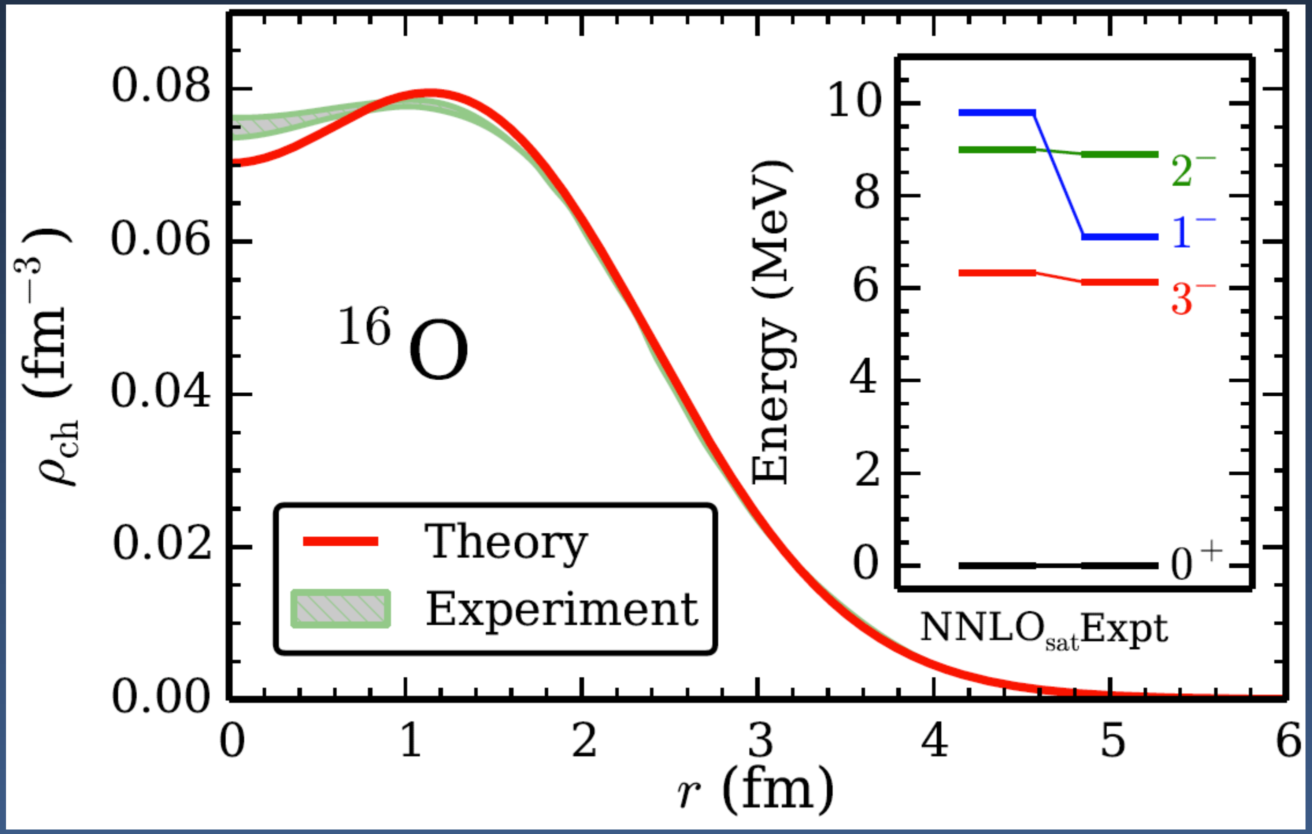

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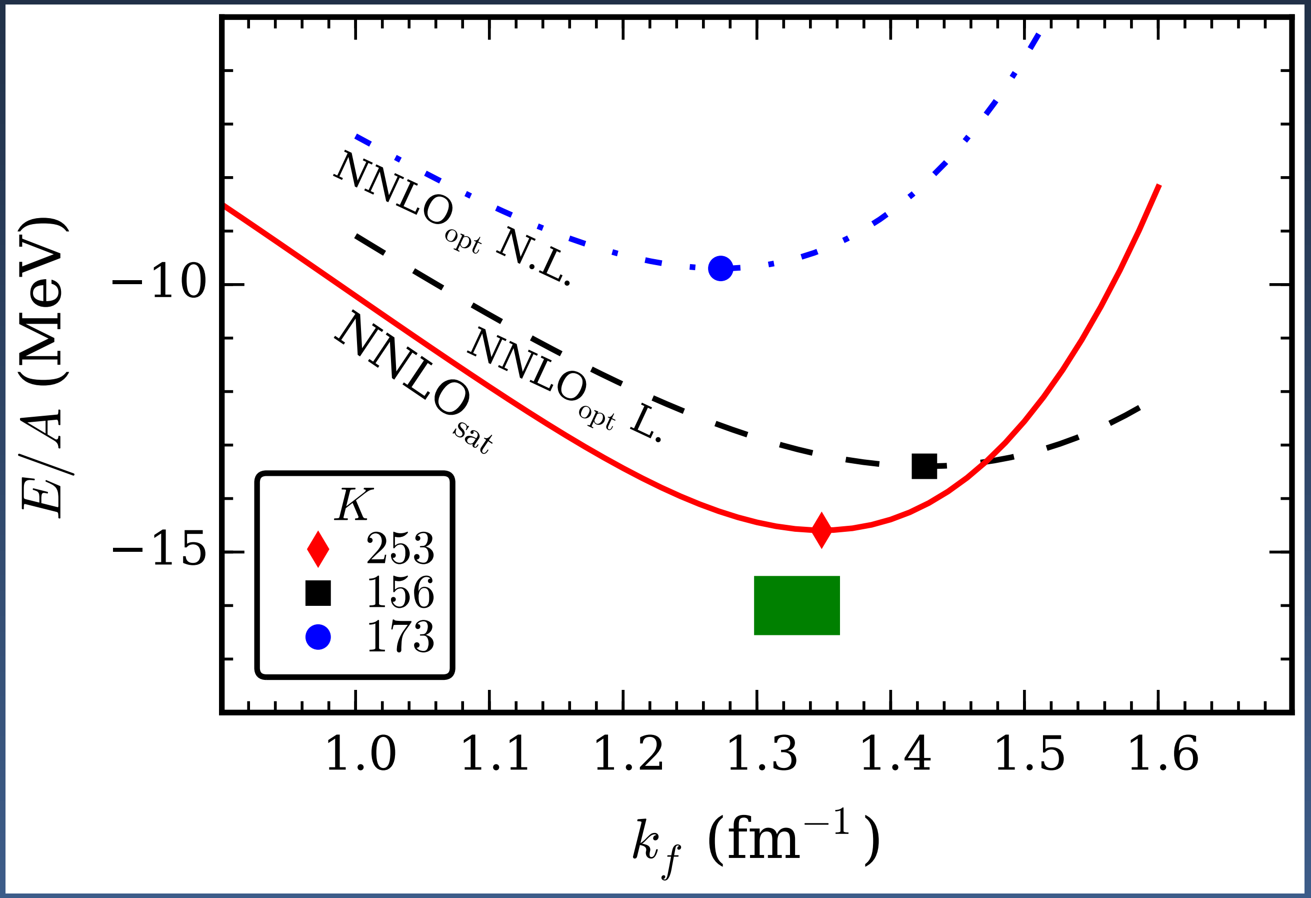

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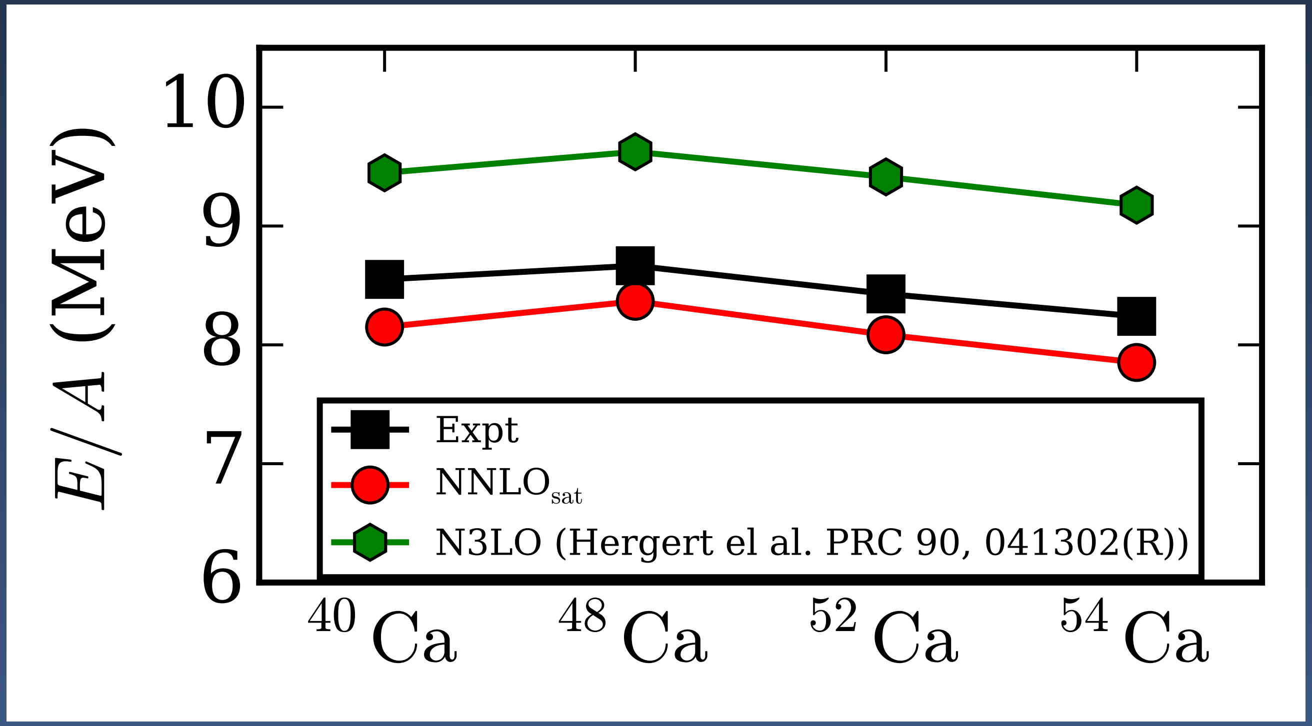

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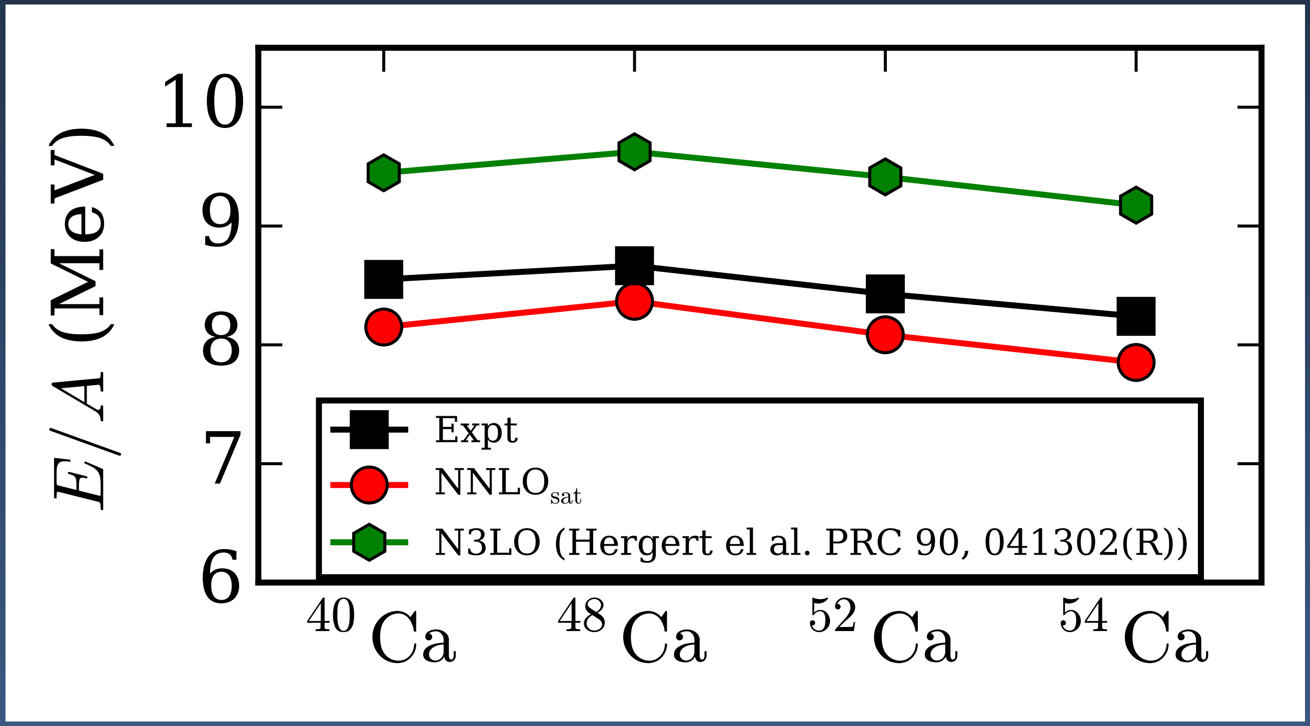
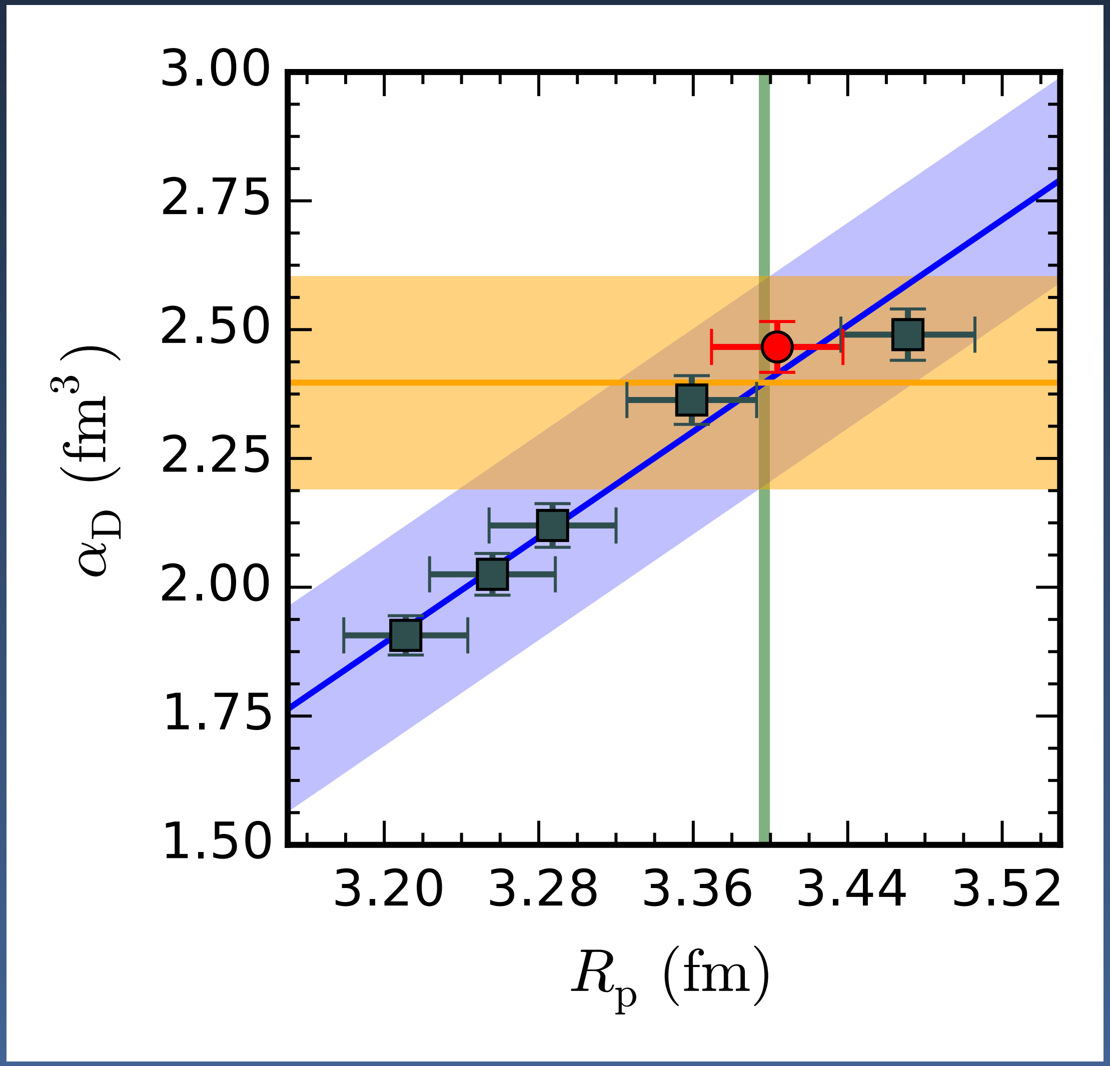


Exploit correlations between predictions!

Differential quantities seem unaffected by this systematic error!



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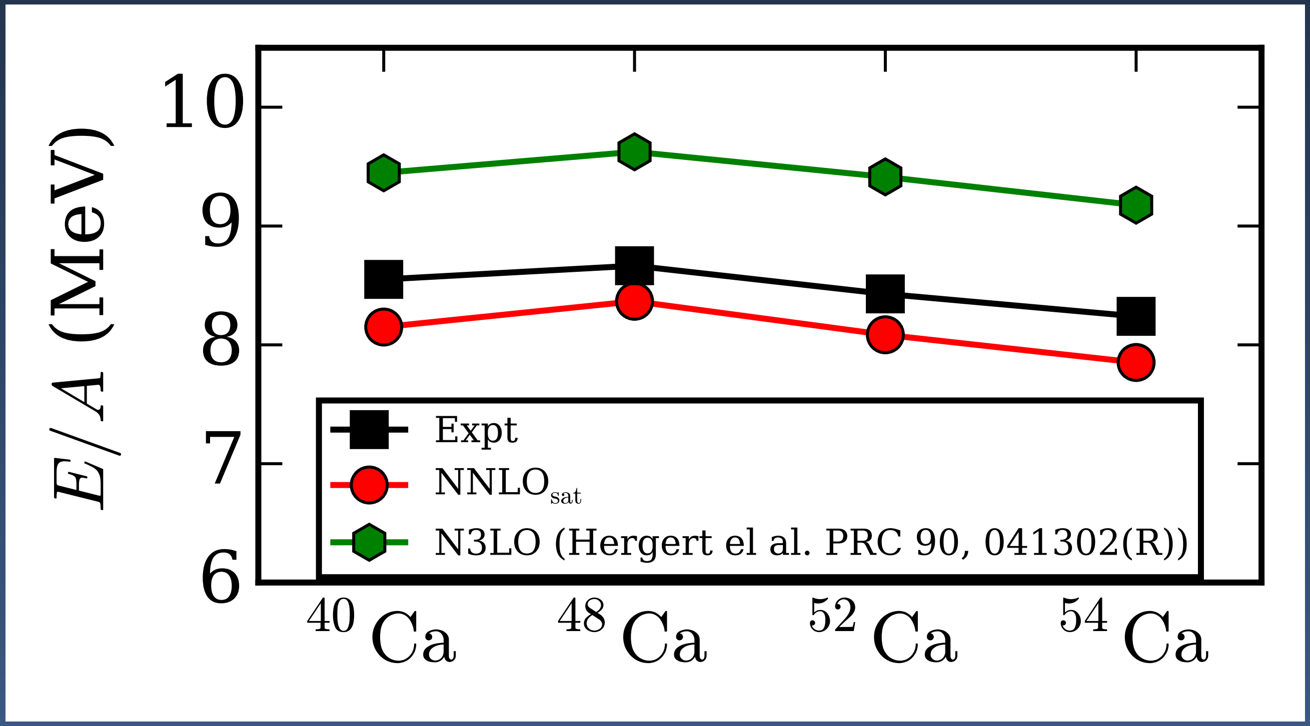
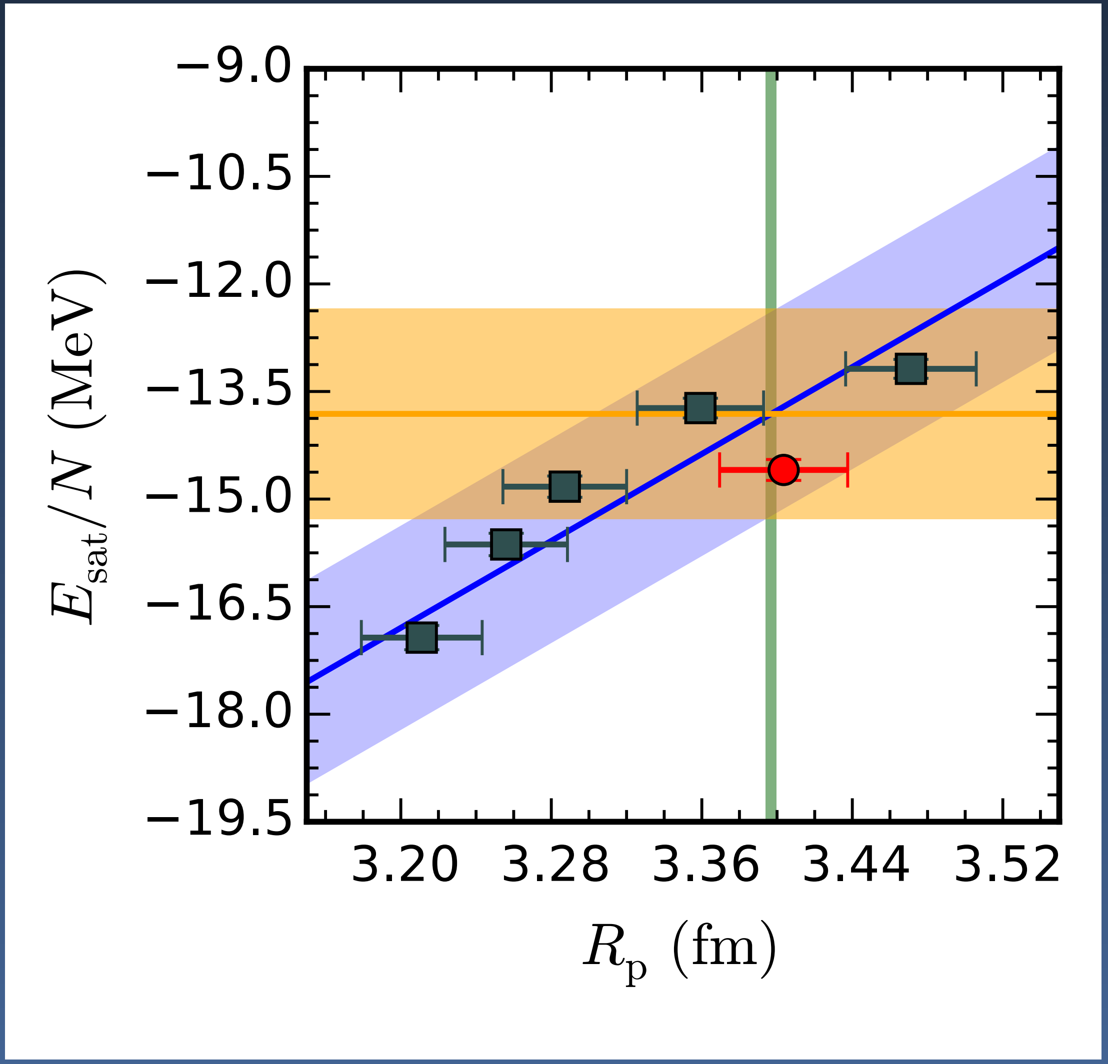


Exploit correlations between predictions!

Differential quantities seem unaffected by this systematic error!



Exploiting Correlations Between Observables

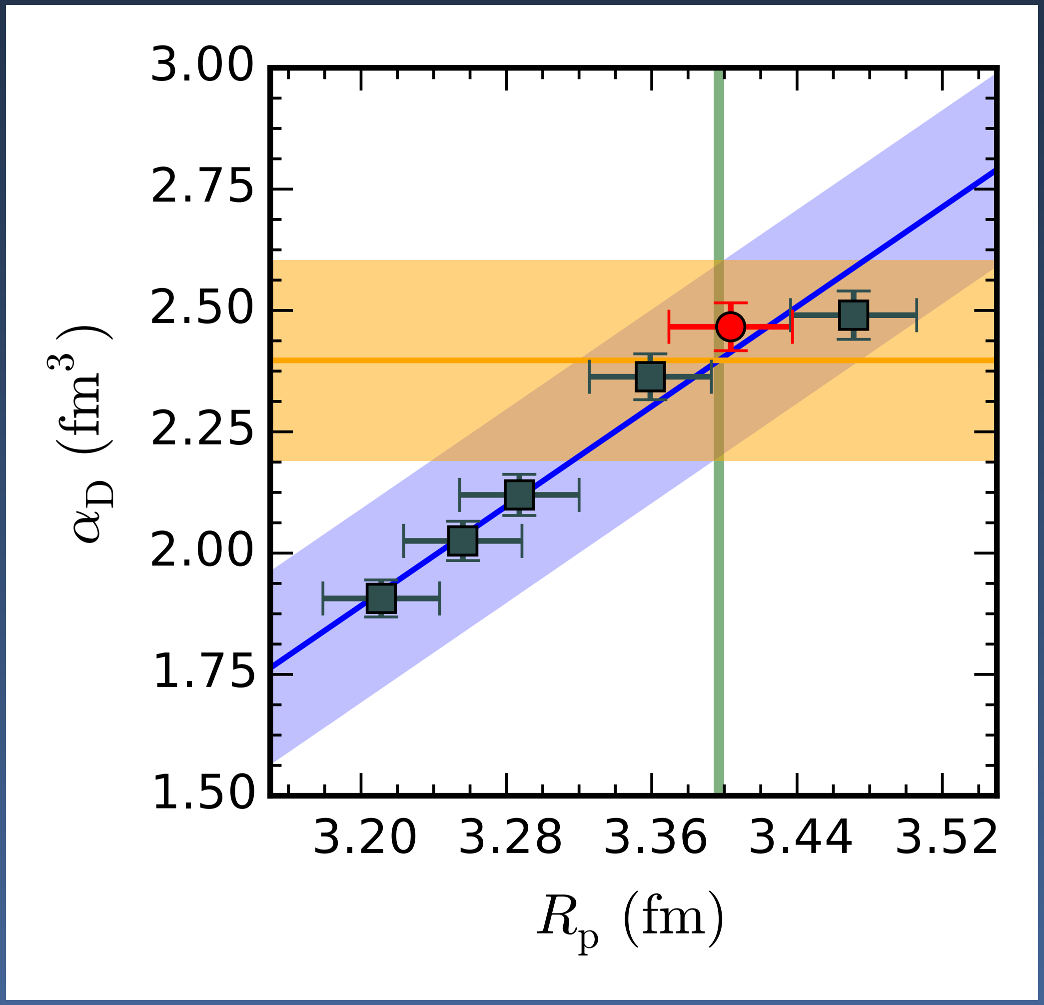
Observables are correlated in heavy systems

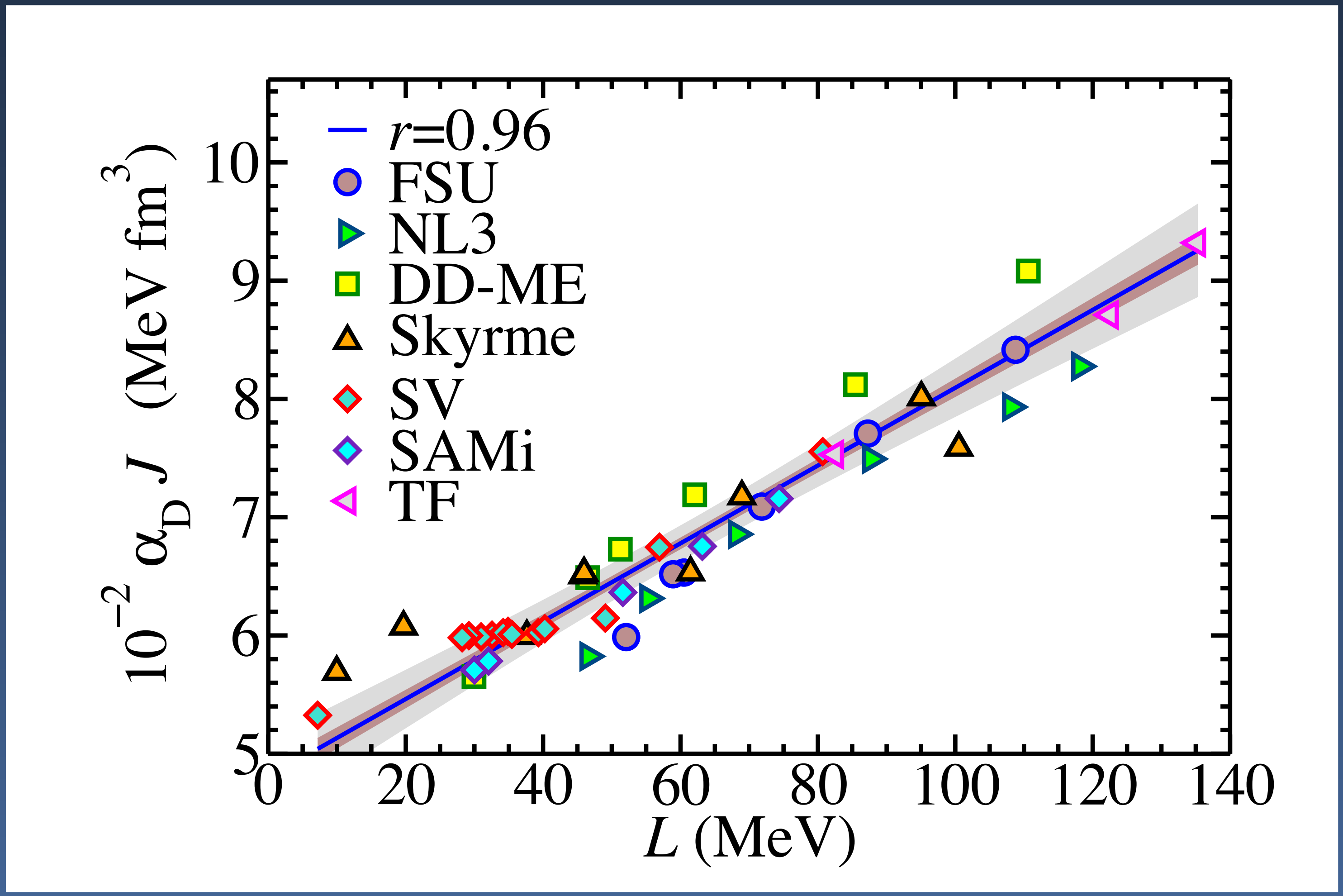
(e.g. droplet model)

X. Roca-Maza, et. al., PRC 88, 024316 (2013)

What about lighter systems?

$$\alpha_{\mathrm{D}} J = \frac{\pi e^2 A}{54} R^2 \left(1 + \frac{5}{3}\frac{L}{J}\epsilon_A\right)$$



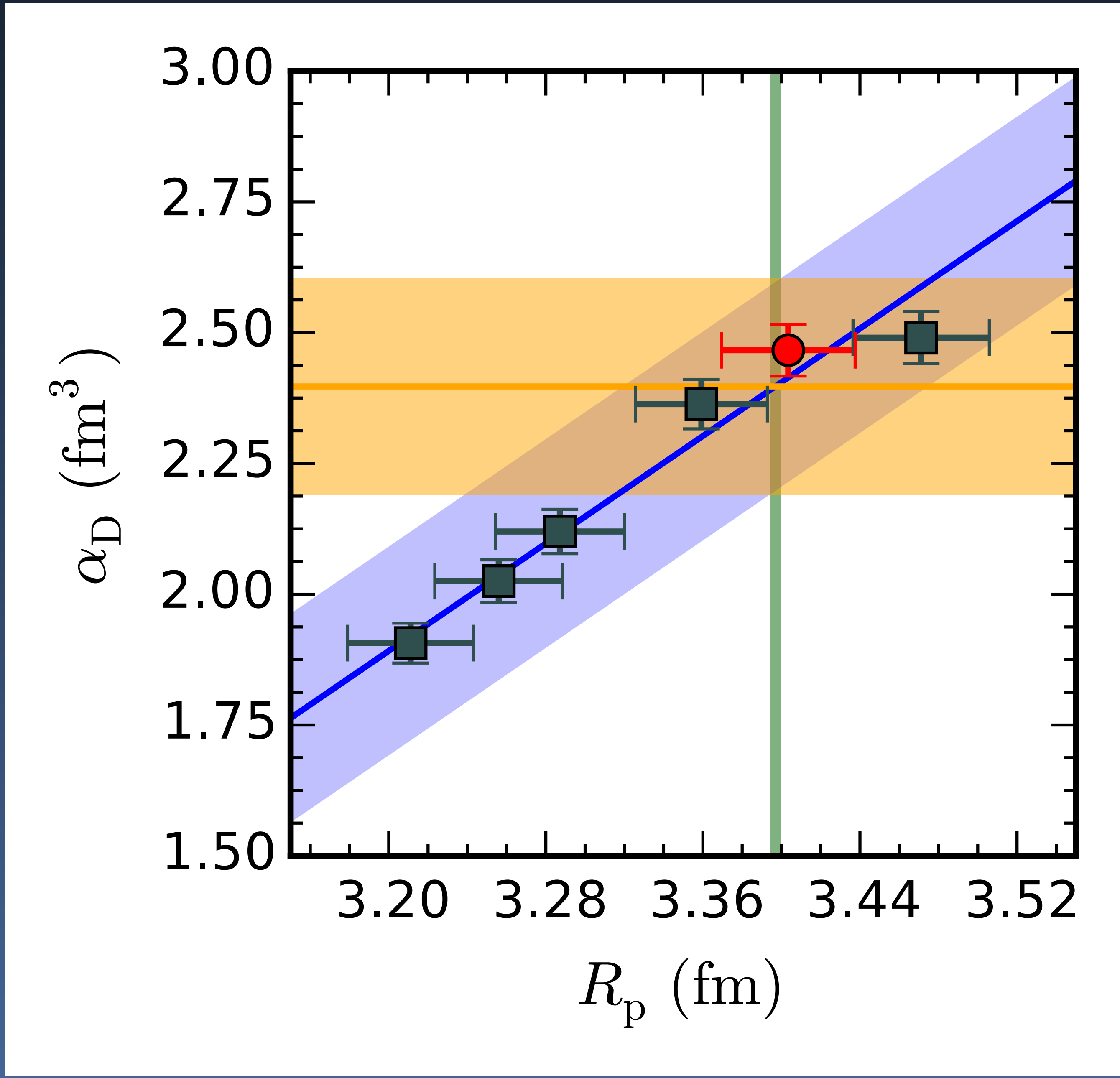


Exploiting Correlations Between Observables

Observables are correlated in heavy systems

(e.g. droplet model)

$$\alpha_{\mathrm{D}} J \approx (aR^2 + b) \approx (a_{\alpha_{\mathrm{D}}} R + b_{\alpha_{\mathrm{D}}})(a_J R + b_J) + \ldots$$

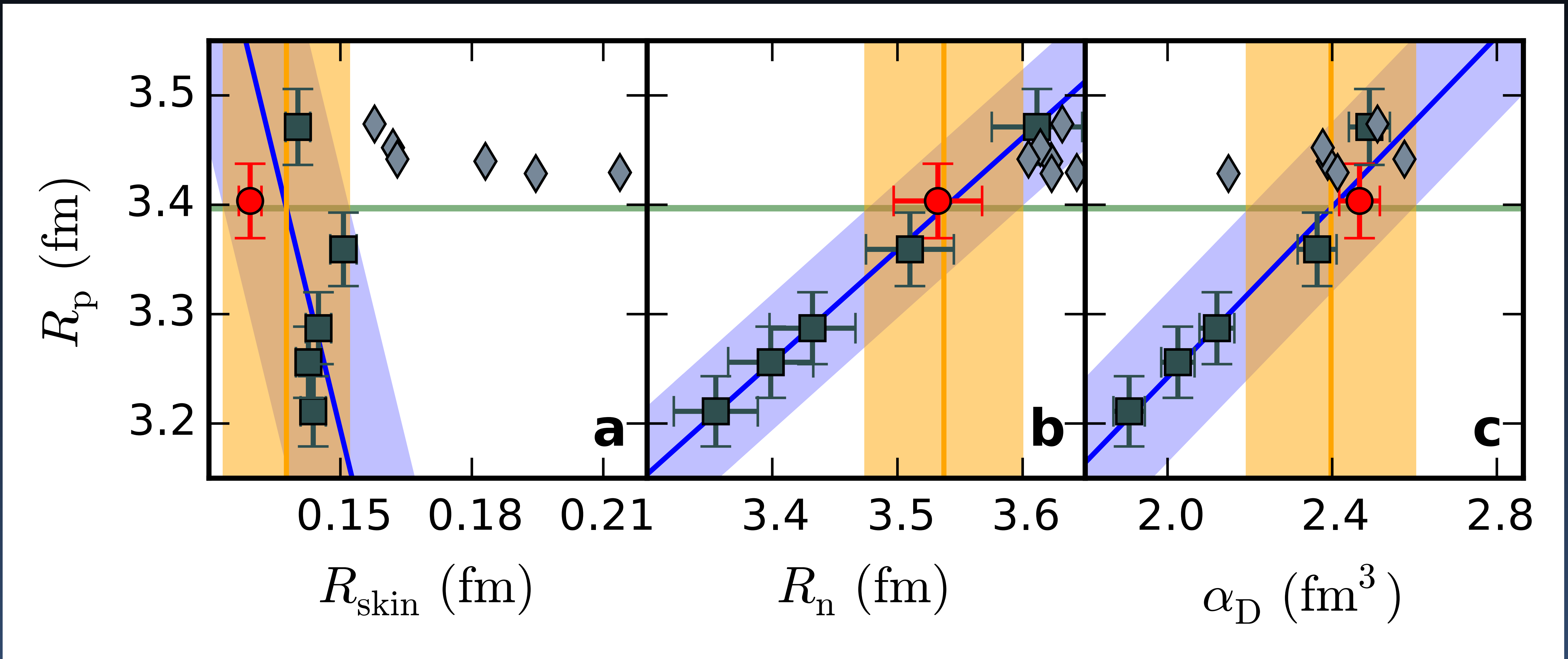


EFT in lighter systems has only a few parameters.

Many-body observables must be correlated.

Neutron Radius and Skin of ^{48}Ca

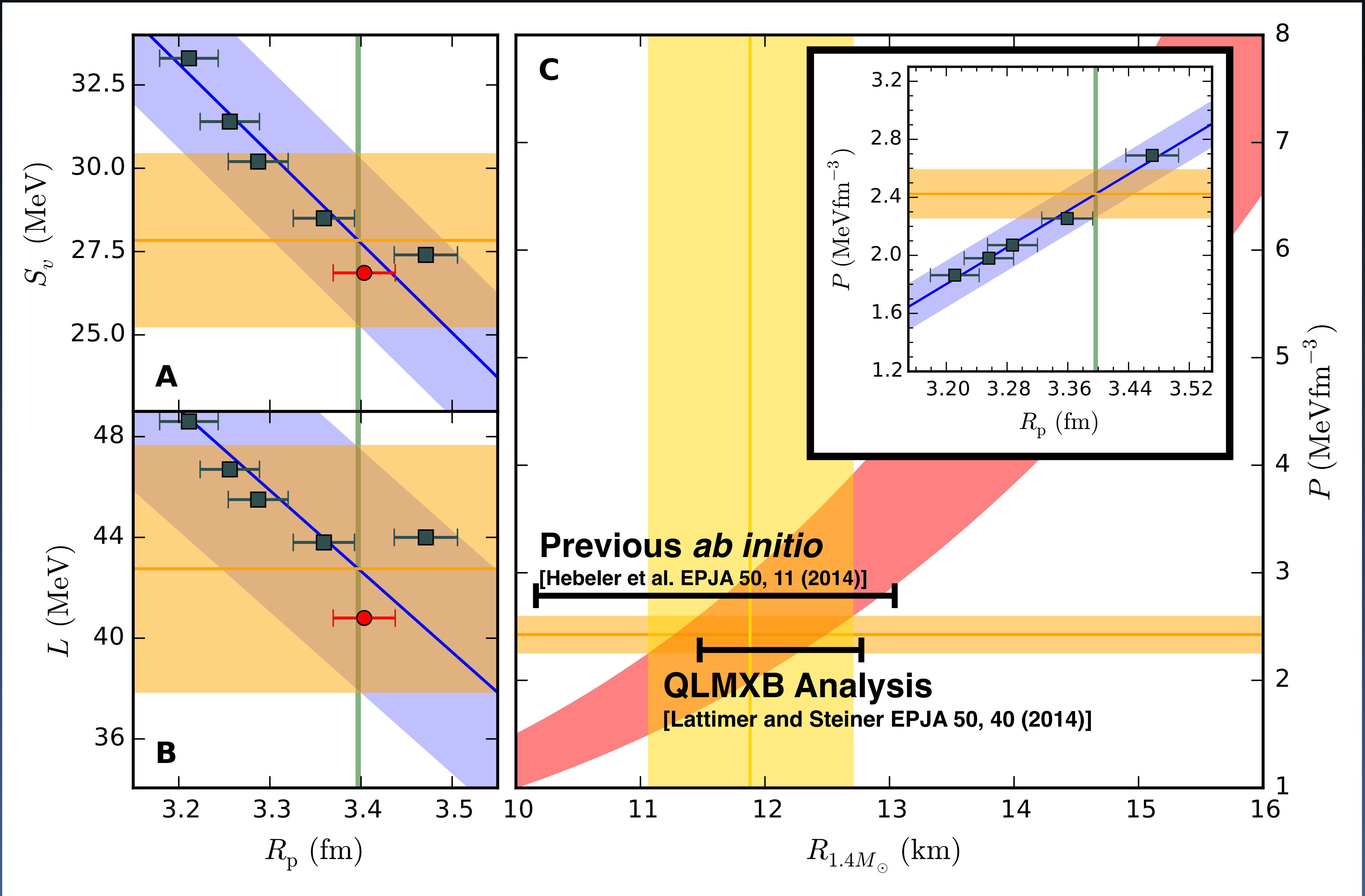
Hagen et al., Nature Physics 12, 186–190 (2016) 10.1038/nphys3529



Ab initio gives a a significantly thinner skin than DFT.
Ab initio and DFT give consistent prediction for α_D.

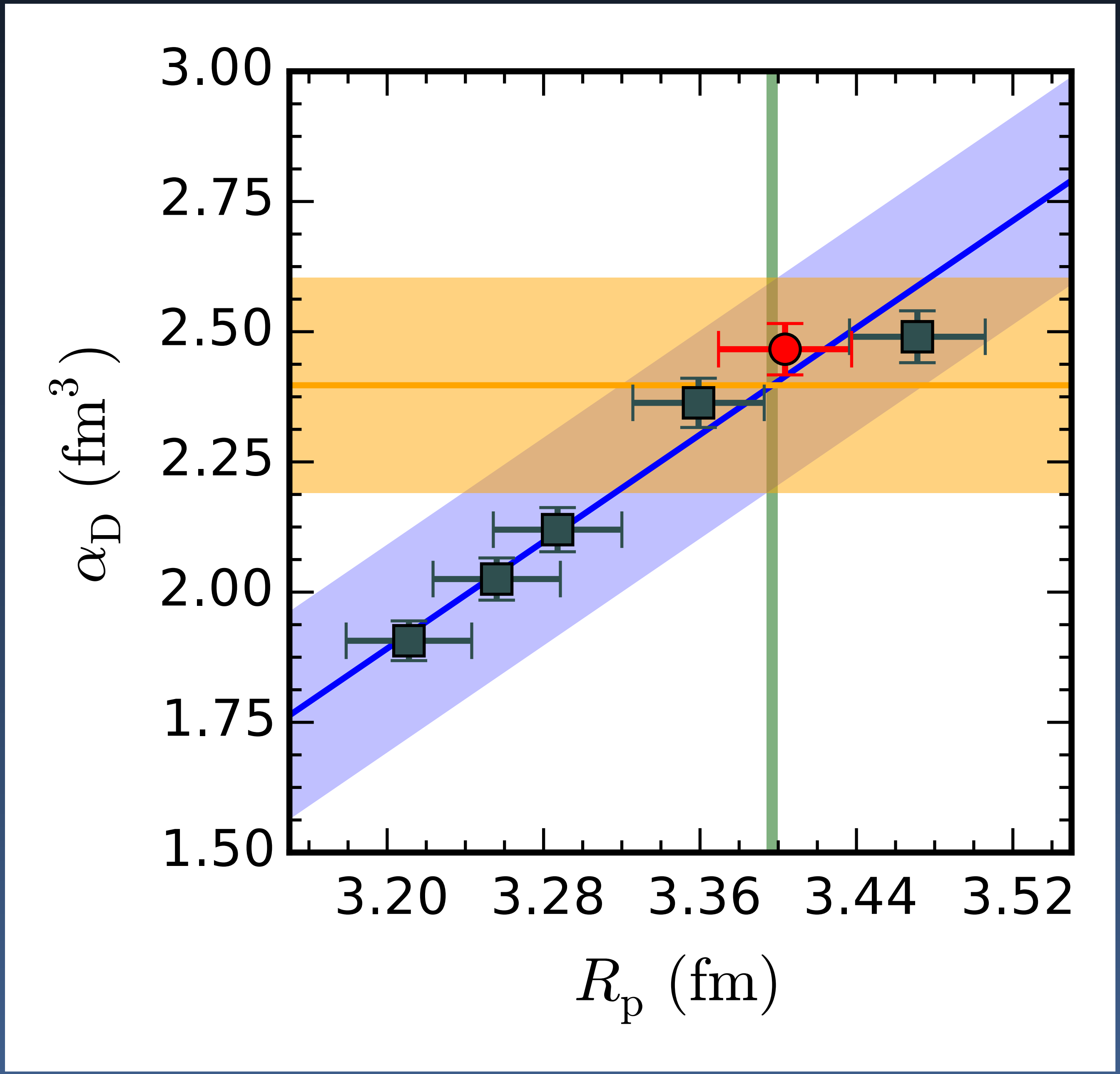
Implications for Neutron Stars

Hagen et al., Nature Physics 12, 186–190 (2016) 10.1038/nphys3529



Exploiting Correlations Between Observables

Observables are correlated in nuclear systems



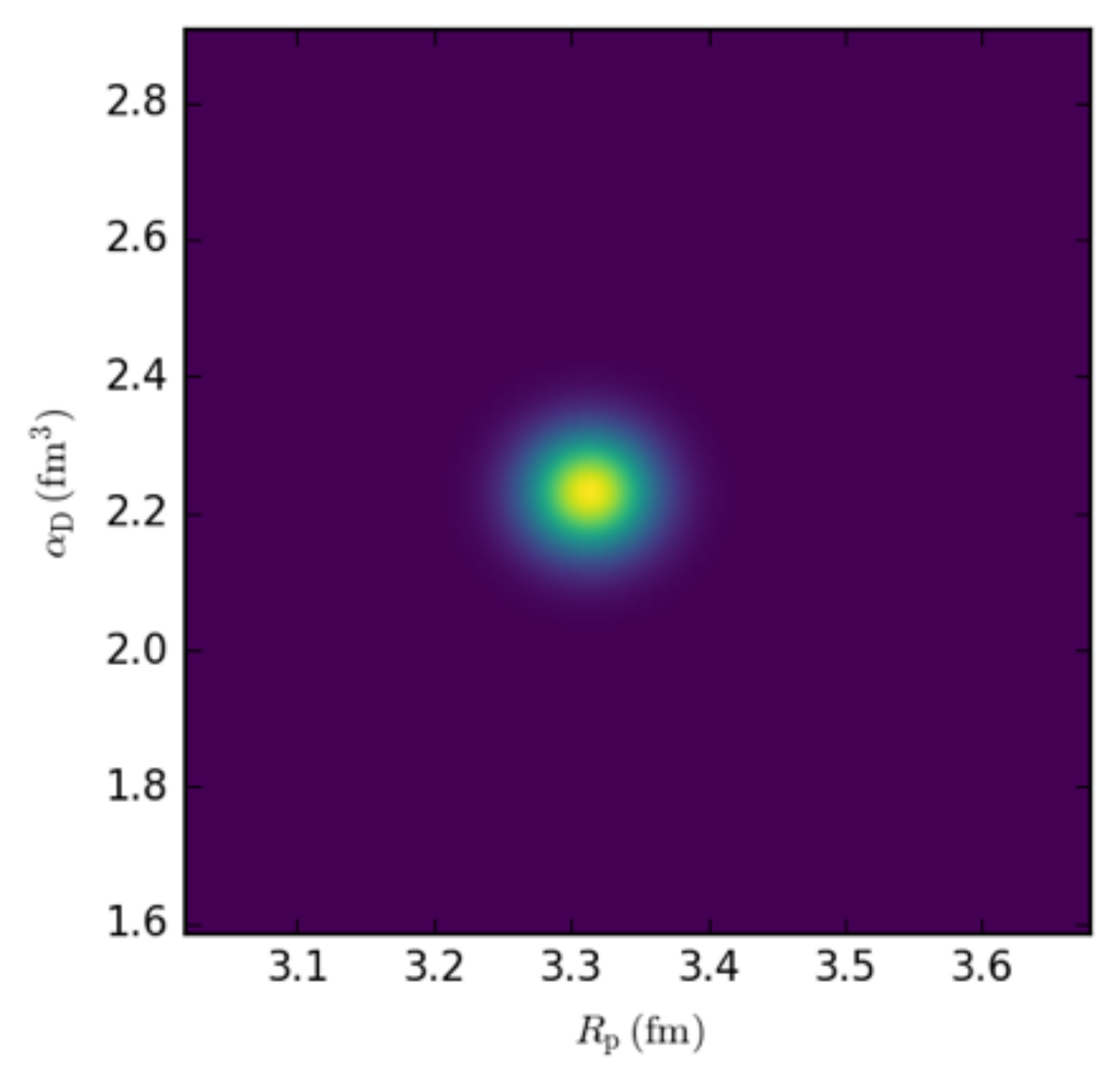
Explicit form of these correlations is unknown!

EFT in lighter systems has only a few parameters.

Many-body observables must be correlated.

But The Errors Are Correlated

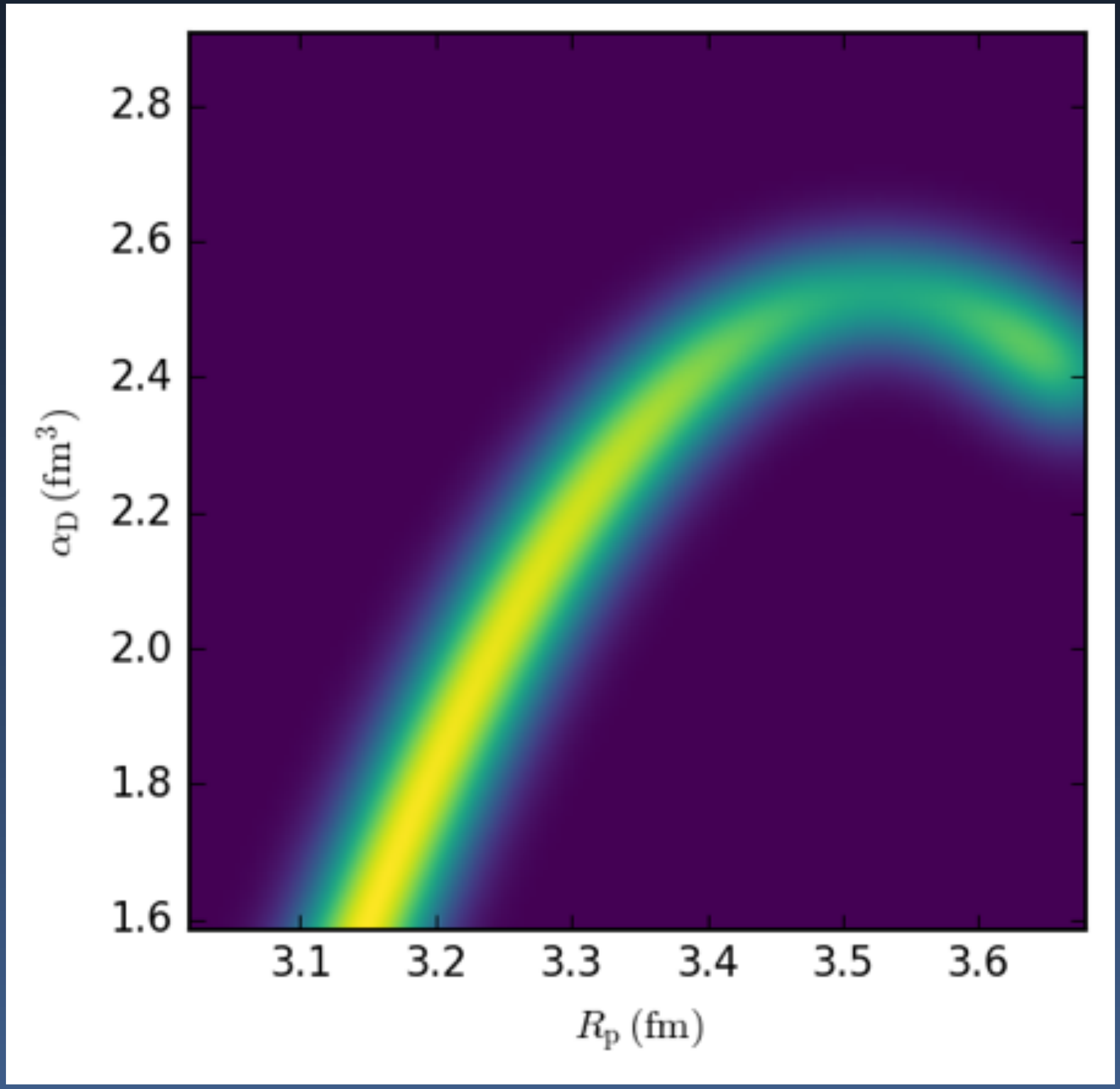
$$P_{\mathrm{thy}}(O, X|m)$$



A single model (potential) gives us limited information about the joint probability distribution of two many-body observables

But The Errors Are Correlated

$$P_{\rm thy}(O,X) = \int dm P(m) P_{\rm thy}(O,X|m)$$



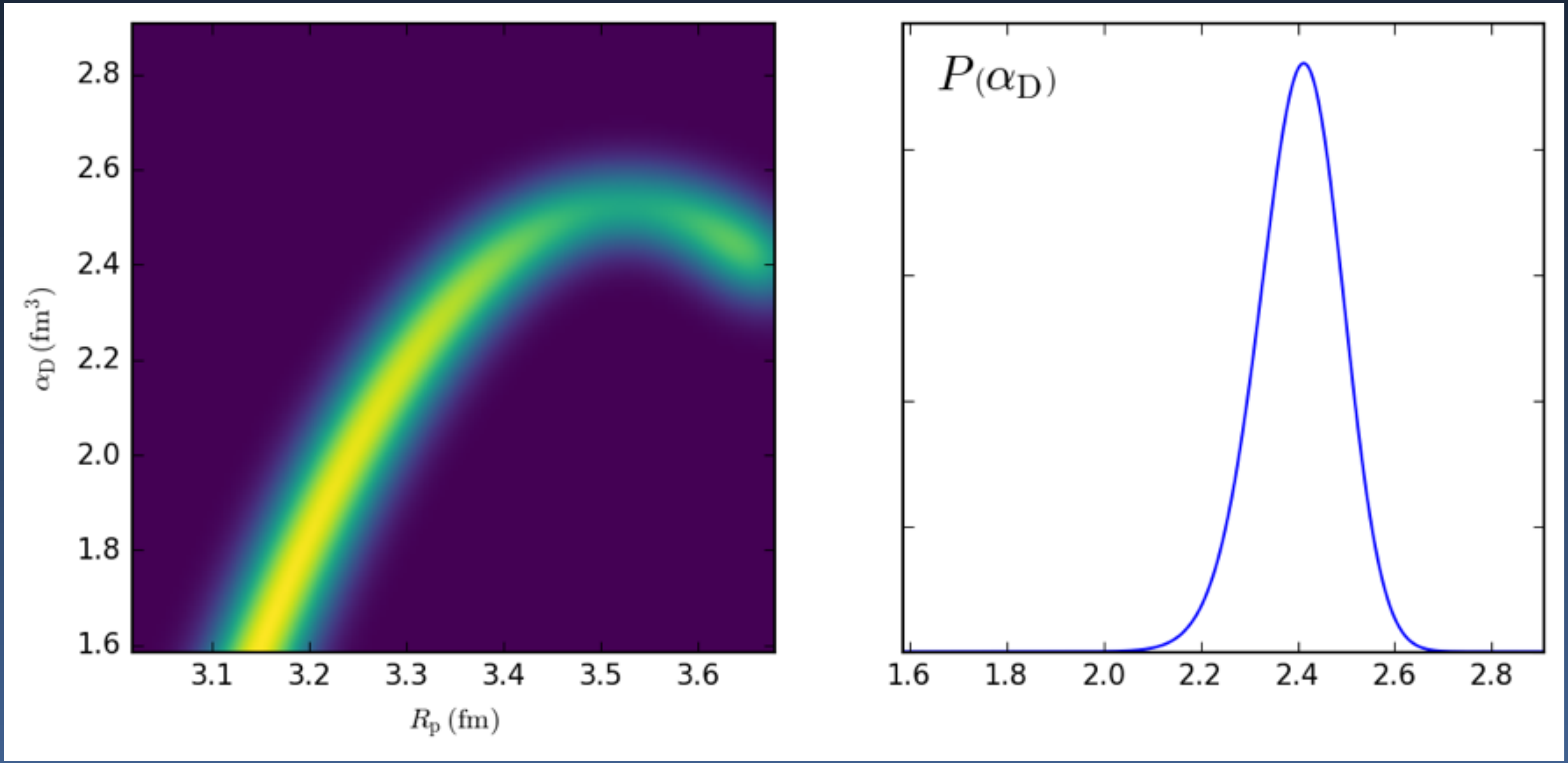
A single model (potential) gives us limited information about the joint probability distribution of two many-body observables

We can marginalize (integrate) over a family of models to better define our joint probability distribution.

But The Errors Are Correlated

We can marginalize (integrate) experimental data to further constrain our distribution.

$$P(O) = \int dX \, P_{\rm thy}(O|X) P_{\rm expt}(X)$$



Can we do this?

Can we compute:

$$P_{\text{thy}}(O, X|m)$$

$$P_{\text{thy}}(O, X) = \int dm P(m) P_{\text{thy}}(O, X|m)$$

$$P\left(O\right) = \int dX P_{\text{thy}}(O|X) P_{\text{expt}}(X)$$

Can we do this?

Can we compute:

$$P_{\text{thy}}(O, X|m) = \mathcal{N}(\{O_m, X_m\}, \Sigma_{O_m, X_m})$$ More or less

$$P_{\text{thy}}(O, X) = \int dm P(m) P_{\text{thy}}(O, X|m)$$

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$$P_{\text{thy}}(O, X|m) = \mathcal{N}\left(\{O_m, X_m\}, \Sigma_{O_m, X_m}\right)$$

More or less

$$P_{\text{thy}}(O, X) = \frac{1}{n}\sum_{m=1}^{n} P_{\text{thy}}(O, X|m)$$

Almost?

$$P\left(O\right) = \int dX P_{\text{thy}}(O|X) P_{\text{expt}}(X)$$

Can we do this?

Can we compute:

$$P_{\text{thy}}(O, X|m) \approx \mathcal{N}(O_m, \sigma_{O_m})\mathcal{N}(X_m, \sigma_{X_m})$$ More or less

$$P_{\text{thy}}(O, X) = \frac{1}{n}\sum_{m=1}^{n} P_{\text{thy}}(O, X|m)$$ Almost?

$$P(O) = \int dX P_{\text{thy}}(O|X) P_{\text{expt}}(X)$$

Can we do this?

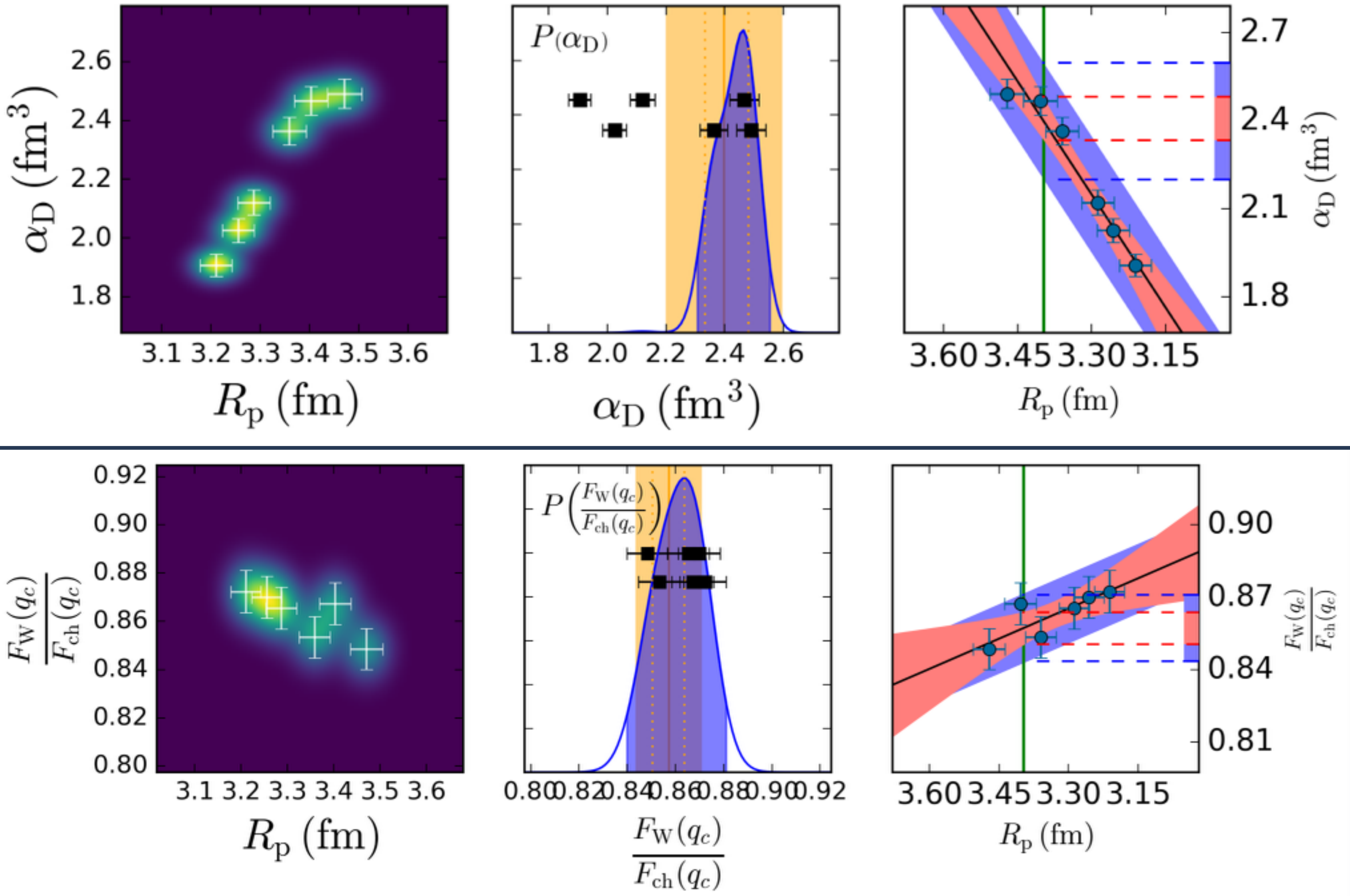
Can we compute:

$$P_{\text{thy}}(O, X|m) \approx \mathcal{N}(O_m, \sigma_{O_m})\mathcal{N}(X_m, \sigma_{X_m})$$ More or less

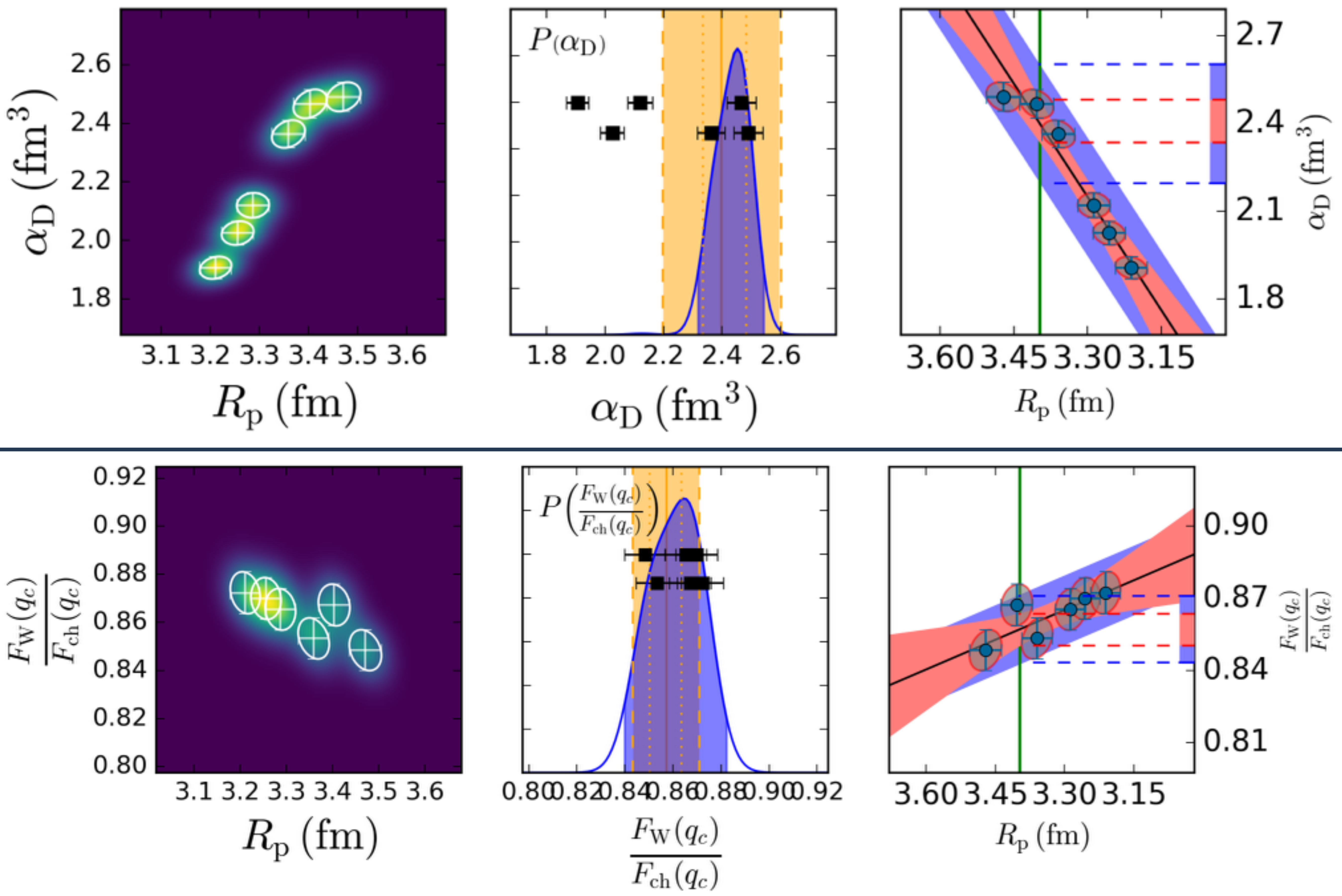
$$P_{\text{thy}}(O, X) = \frac{1}{n}\sum_{m=1}^{n} P_{\text{thy}}(O, X|m)$$ Almost?

$$P\left(O\right) = \int dX P_{\text{thy}}(O|X) P_{\text{expt}}(X)$$ Yes!

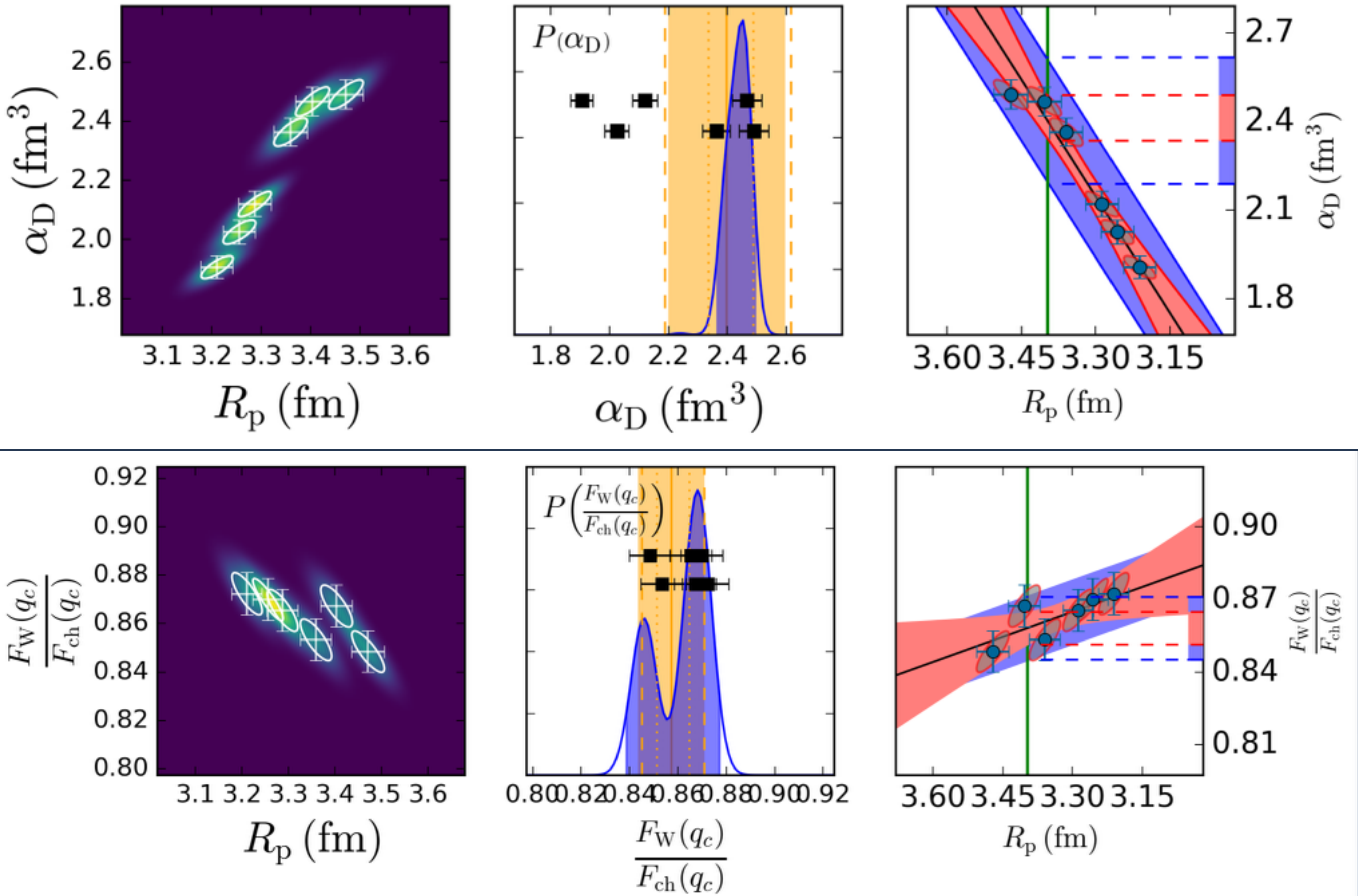
Dipole Polarizability and Weak Form Factor



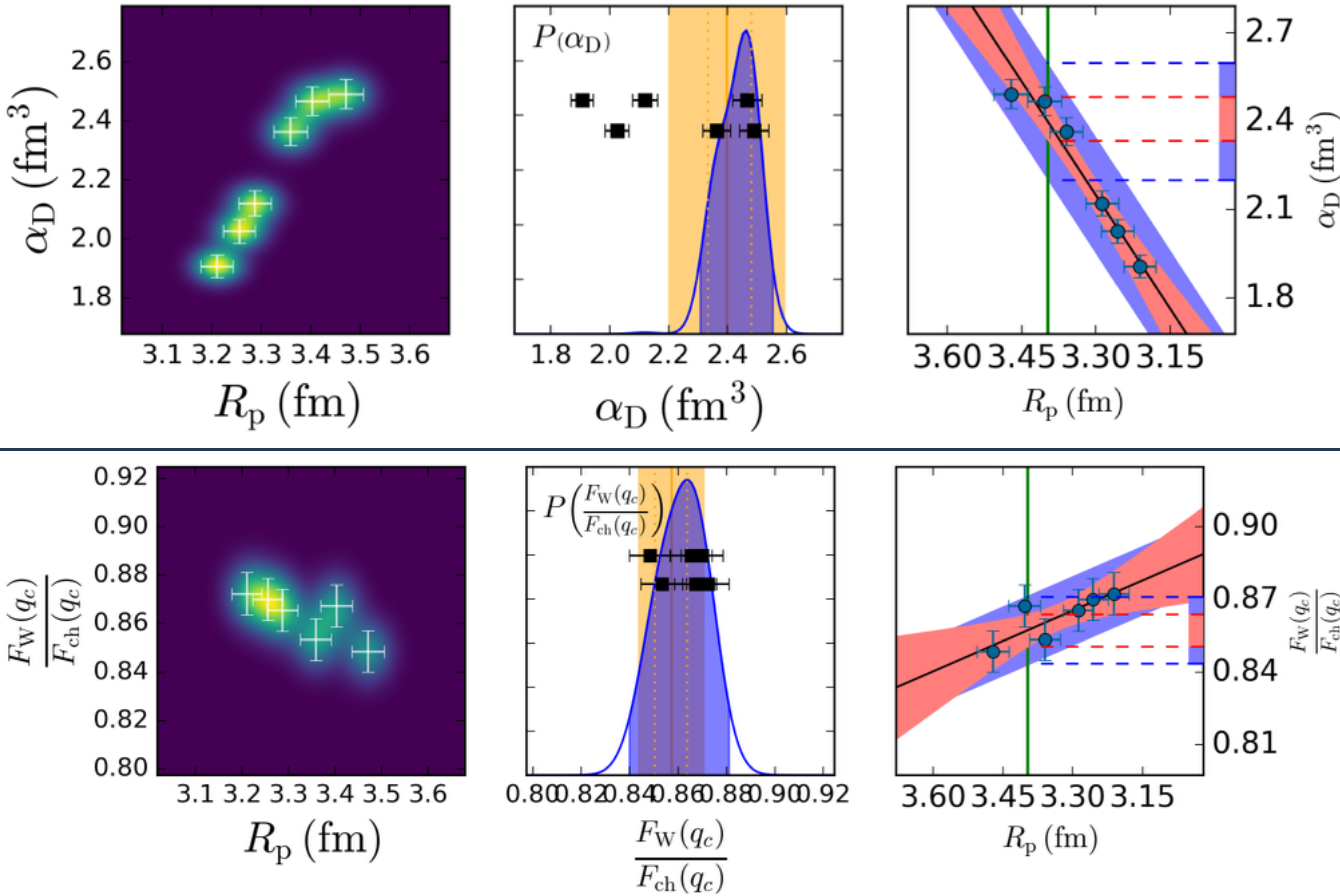
With Small Random Correlation Coefficient



With Large Random Correlation Coefficient



Dipole Polarizability and Weak Form Factor



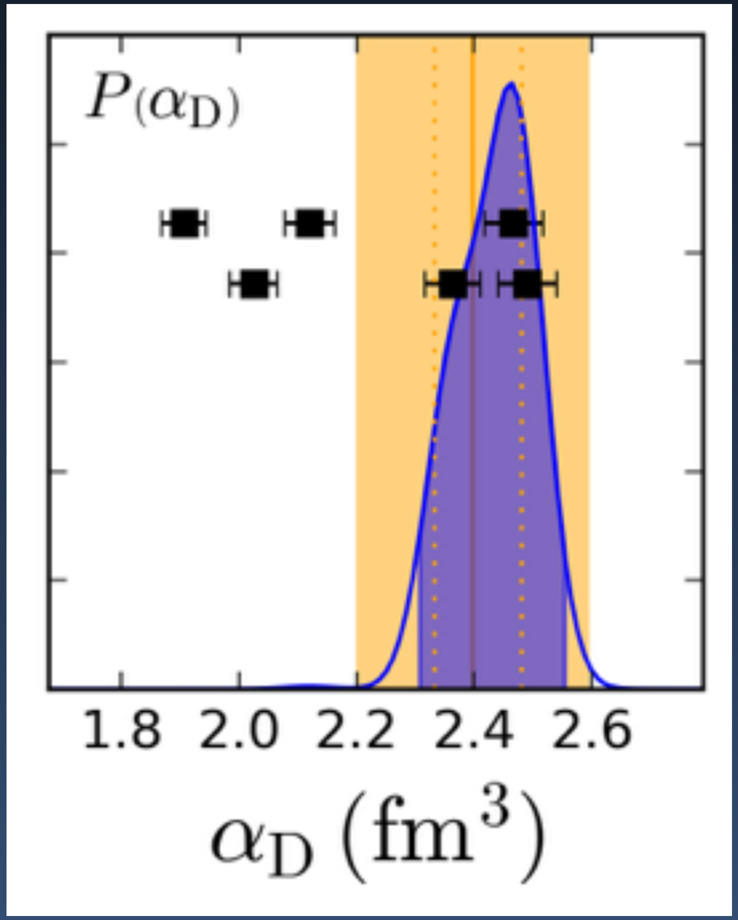
Summary

Chiral Effective Field Theory provides a tool for generating microscopic potentials.

Large systematic errors in many-body calculation tend to spoil this tool (EFT/model-independence)

Correlations between observables can be exploited to fix these issues

Need to exploit these correlations in as model independent manner as possible



Need to be able to fully propagate uncertainties from few-body input to many-body calculations (derivatives w.r.t model parameters)

Thank You