

# Lattice QCD for Nuclear Physics (and maybe Nuclear Astro Physics)

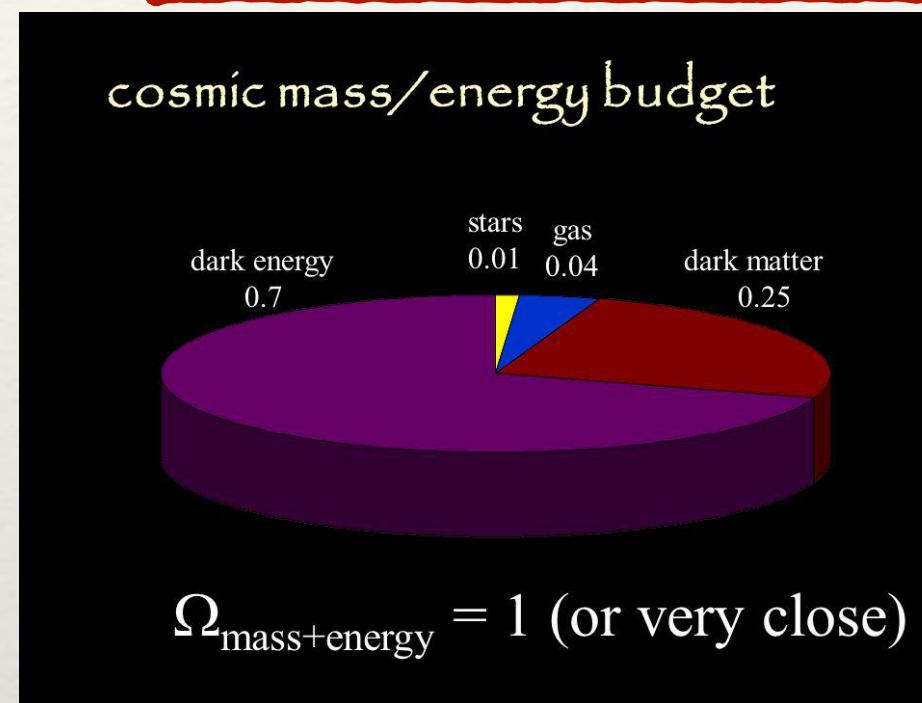
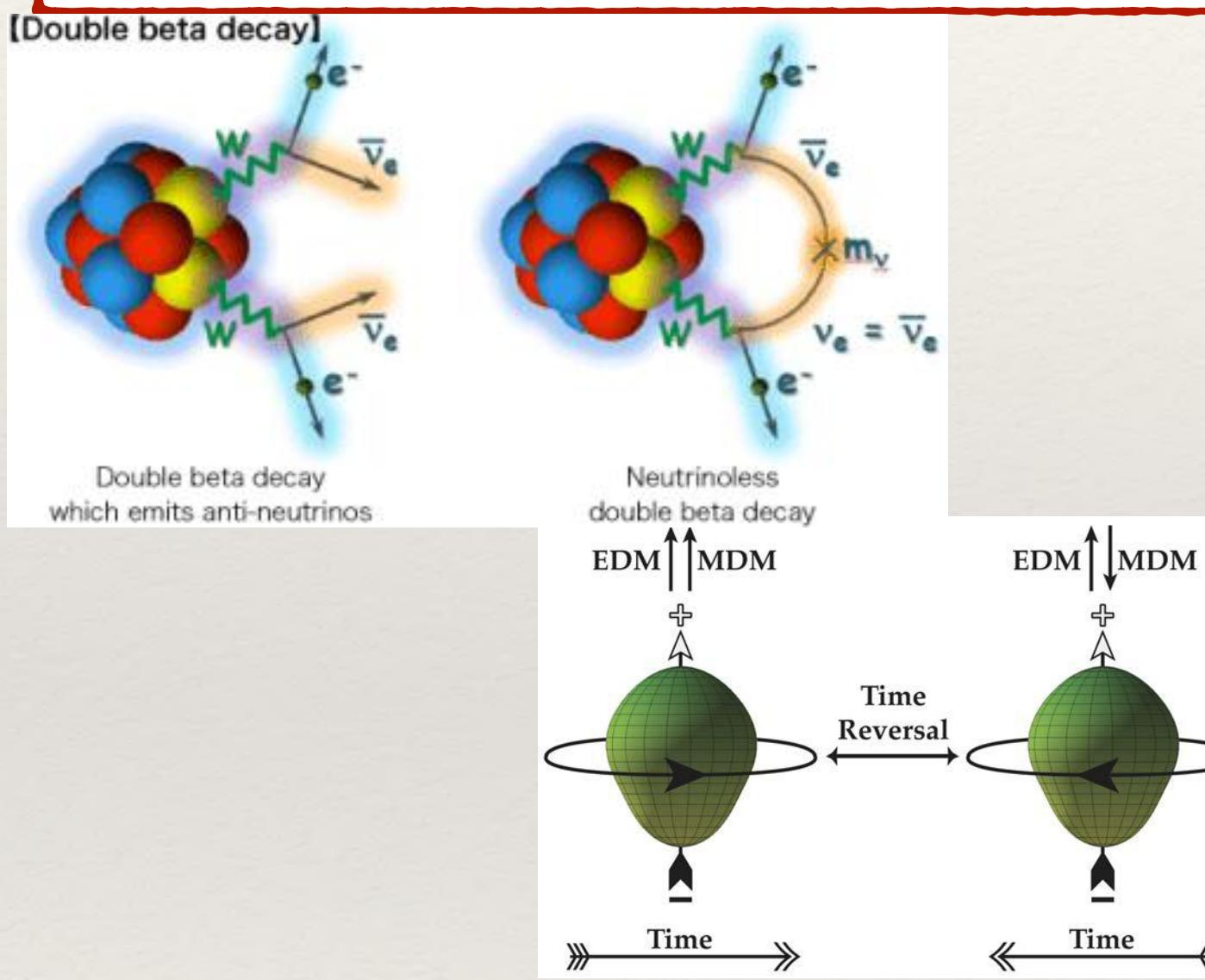
N3AS Seminar  
26th July, 2022

André Walker-Loud

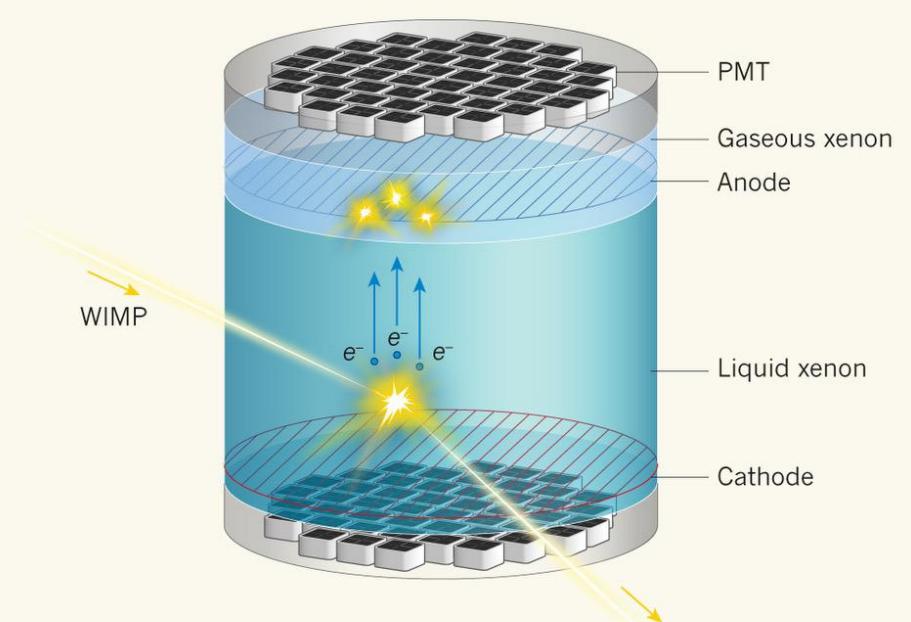


# Science Questions

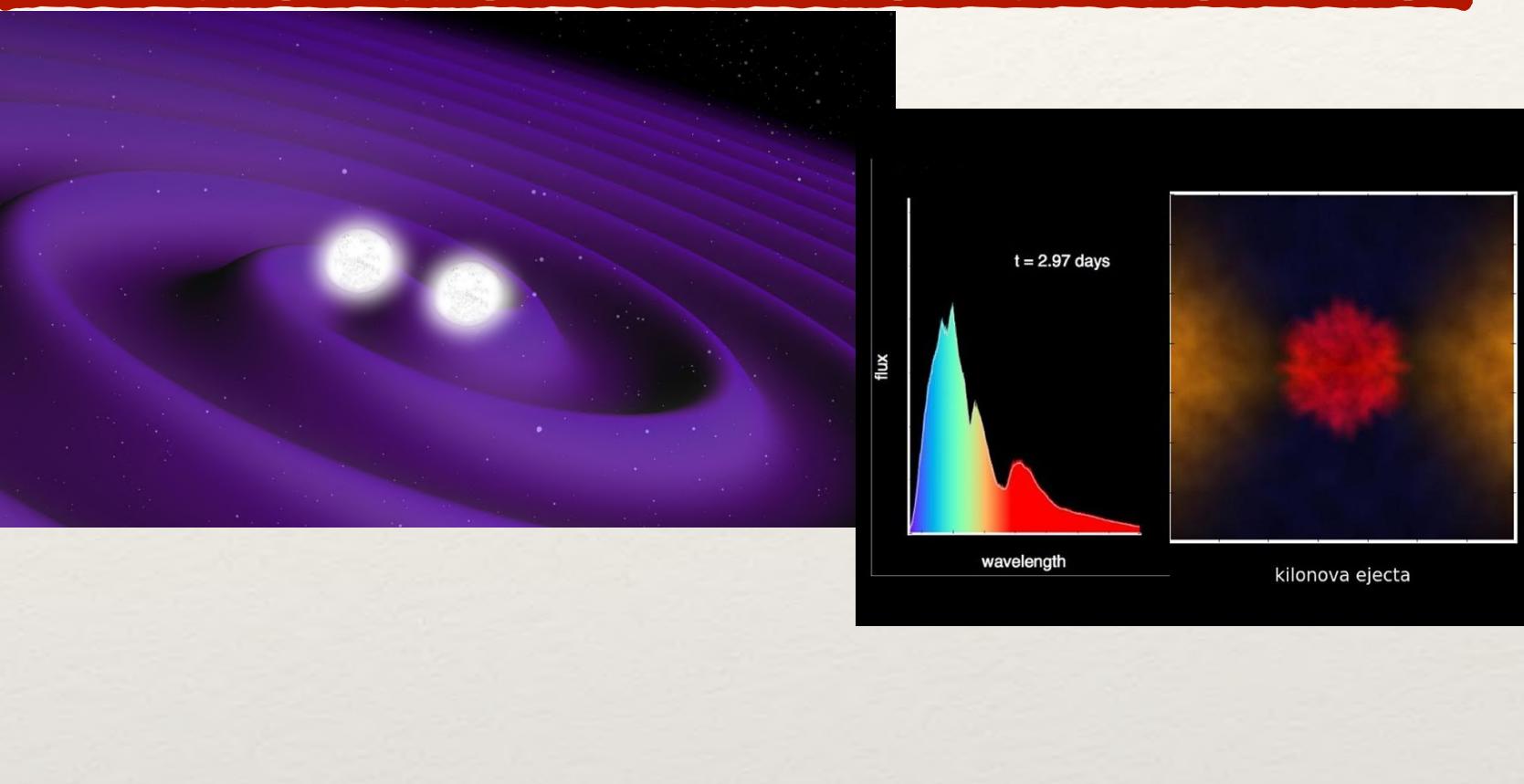
Why is the universe composed of matter? (and not anti-matter)



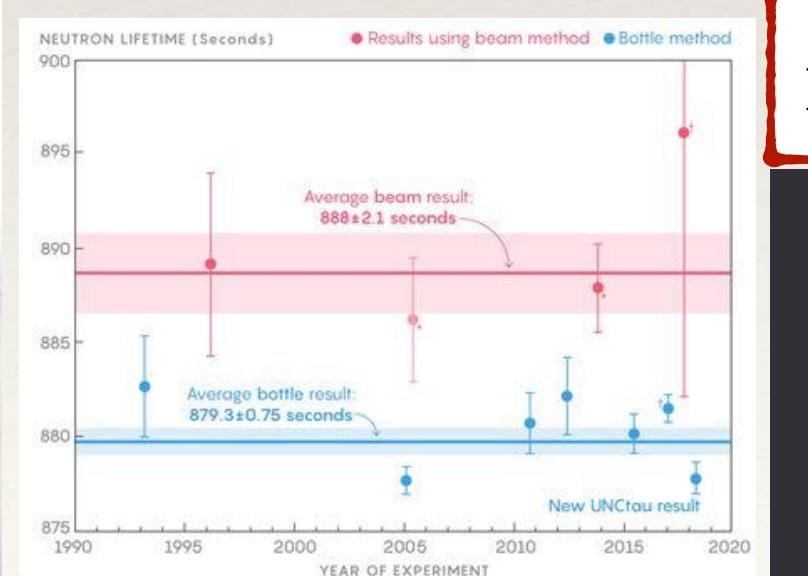
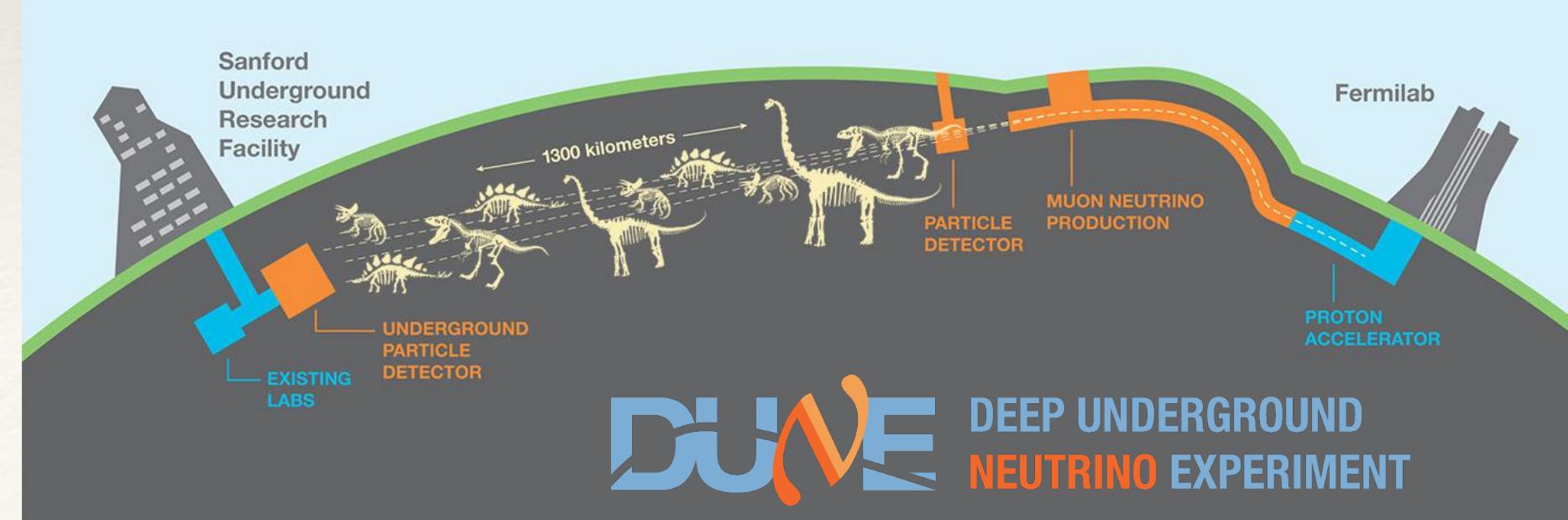
Does dark matter interact with matter? (beyond gravitationally)



What are the properties of dense nuclear matter?

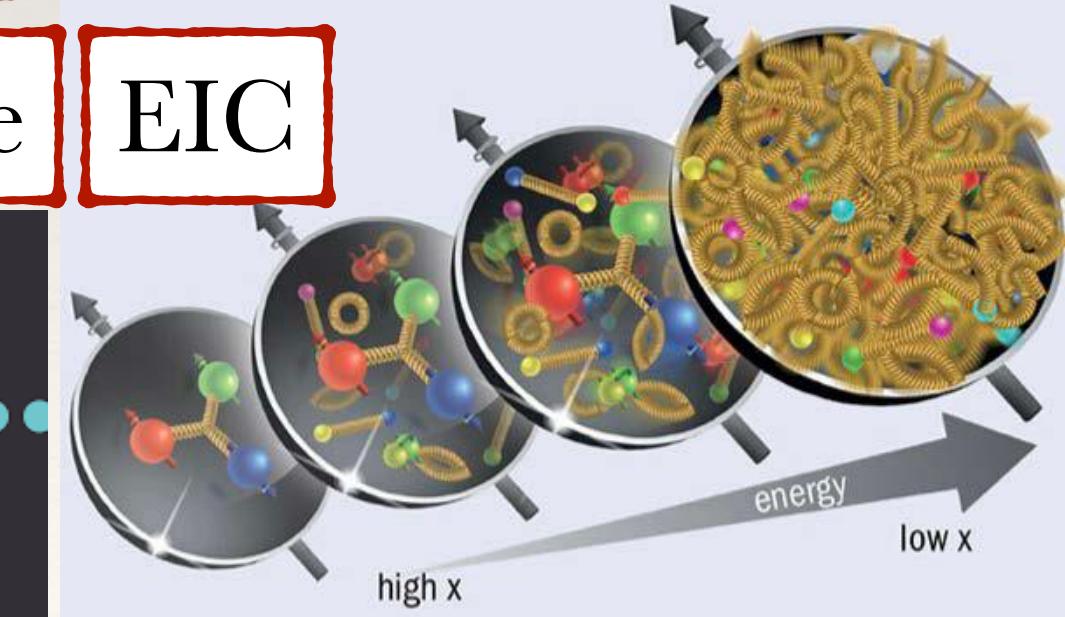


What are the properties of the proton?



neutron lifetime

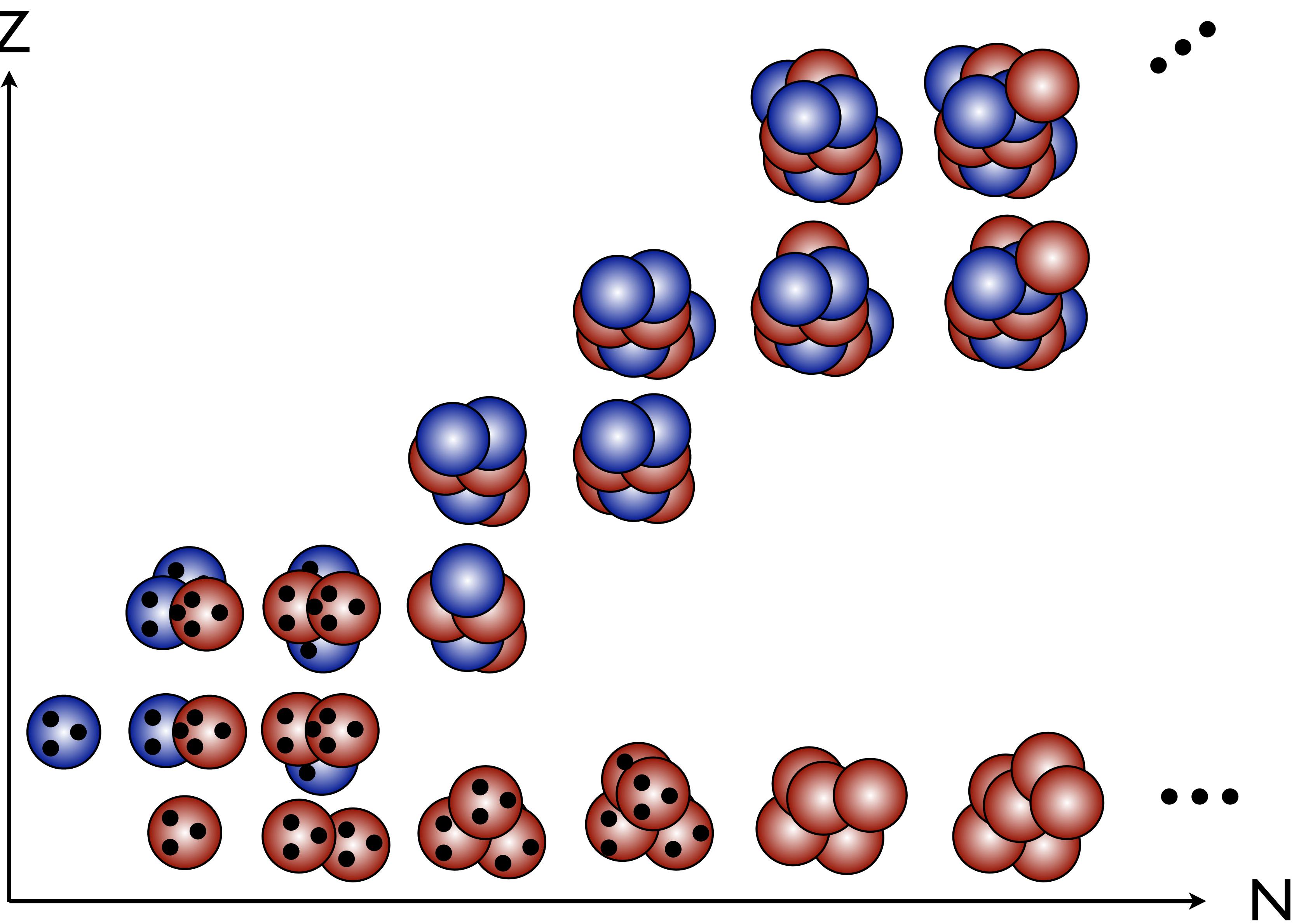
EIC

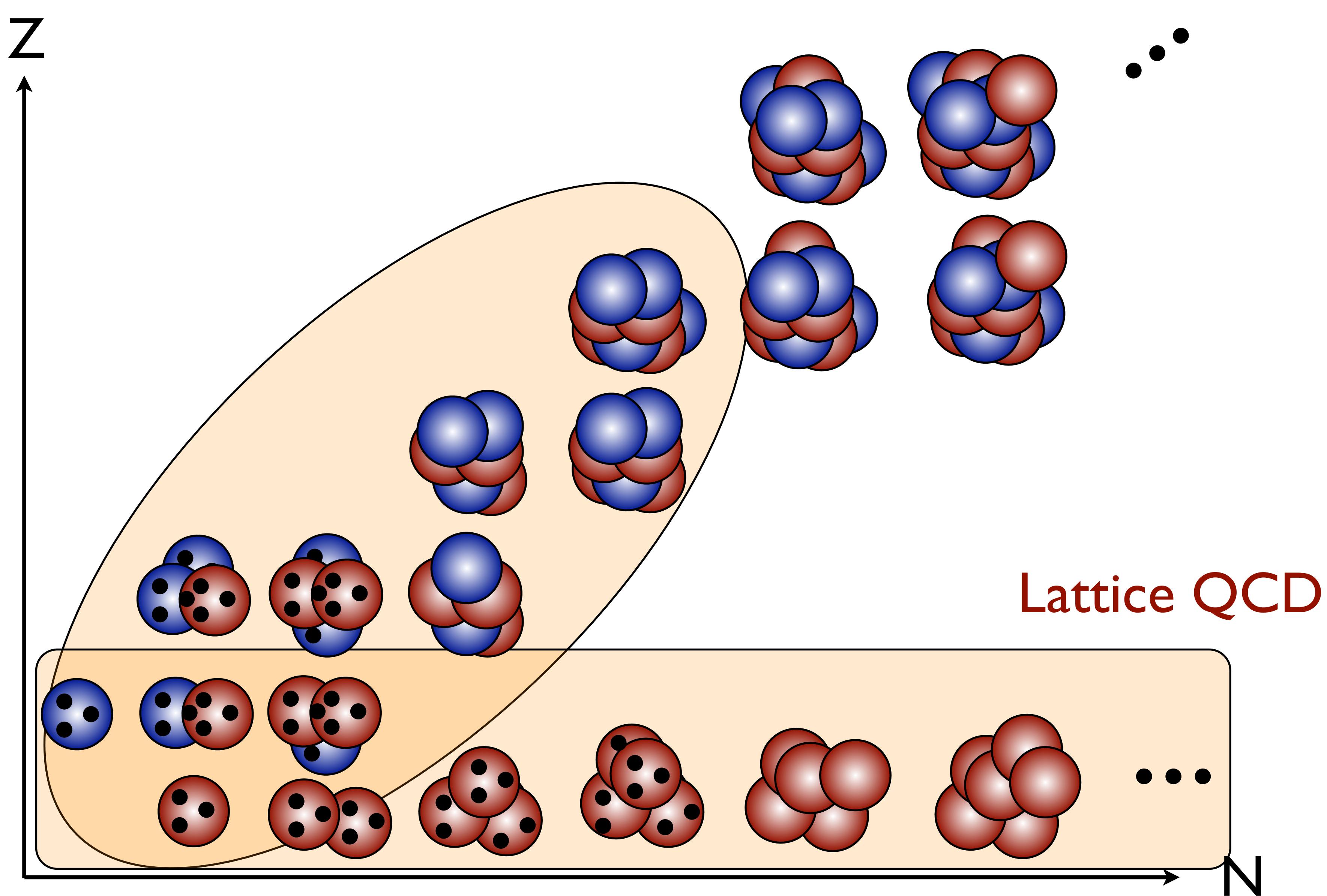


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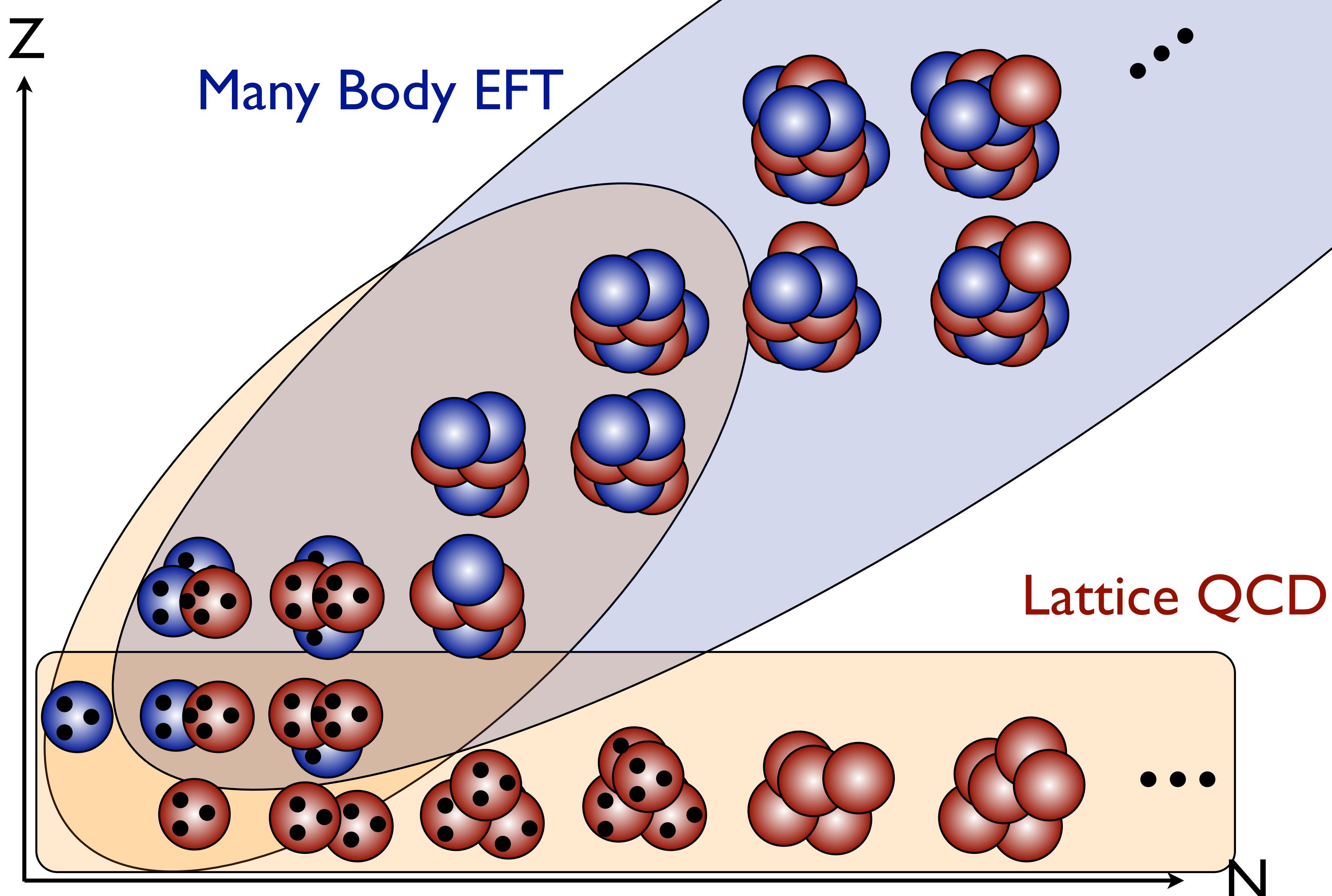
- Of course, we will not use LQCD to directly compute most of these processes
- In each case, there are key pieces of information that are challenging or impossible to determine from experimental information alone - and which we can address with LQCD
- Success requires a coordinated effort between
  - Lattice QCD
  - Effective Field Theory (EFT)
  - Theories of many body nuclear physics
- Allowing for the propagation of a quantitative theoretical uncertainty, rooted in the Standard Model, into theories of nuclear physics  
eg. Drischler et al, PPNP 121 (2021) 103888 [1910.07961]







Determine 2, 3, 4 body forces directly from QCD

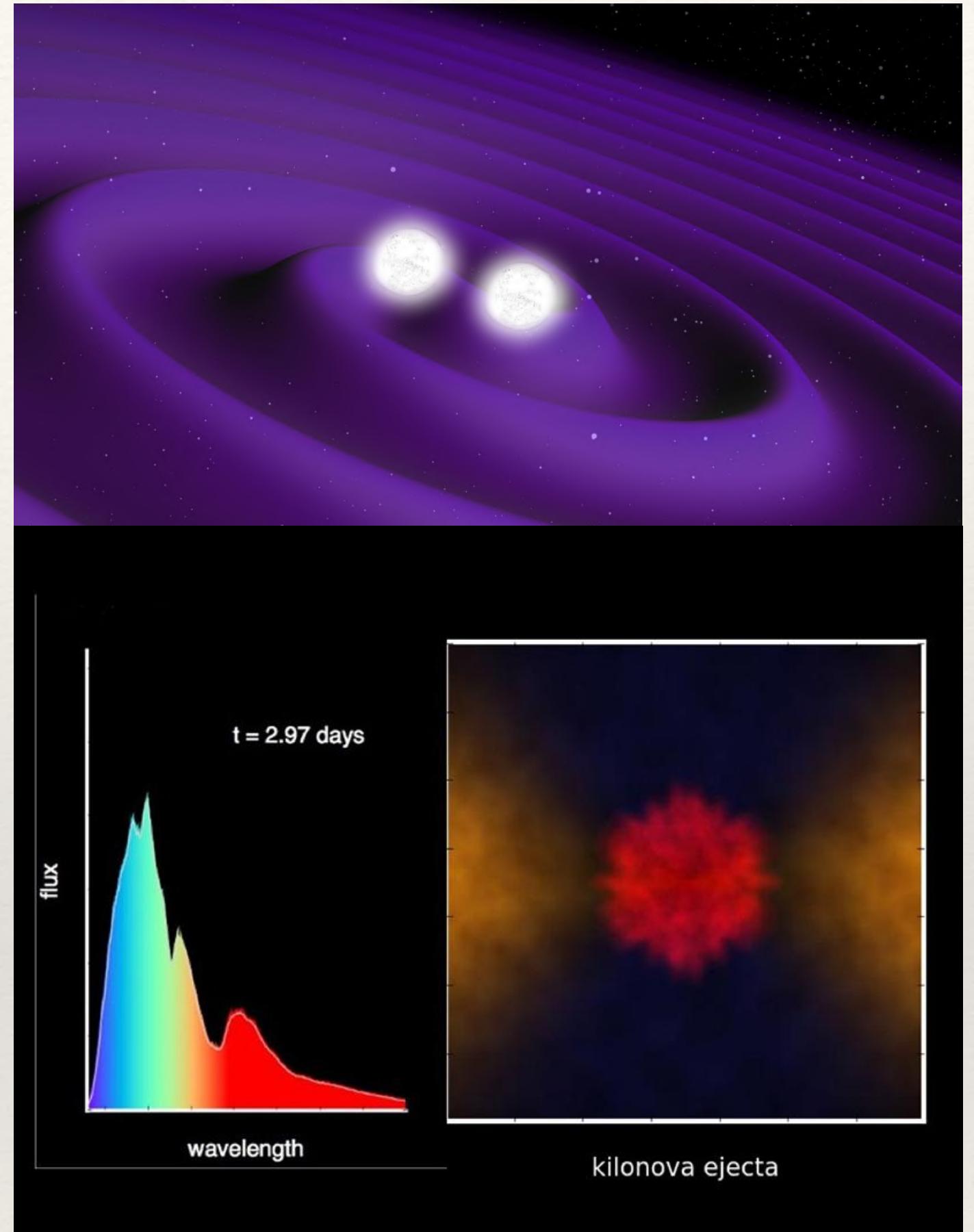


Determine 2, 3, 4 body forces directly from QCD  
match onto many body effective field theory

# Science Questions

## Multi-messenger era and neutron-star mergers

- The ability to measure neutron star mergers has brought to reality the possibilities of constraining the nuclear equation of state with much better precision than previously possible
- It is difficult to make models with hyperons that can support the heavy  $\sim 2M_\odot$  neutron stars
- It is difficult to imagine that hyperons are irrelevant in the core of neutron stars (based upon the anticipated energy/density)
- The three-neutron interaction plays an important role in stabilizing neutron stars - but it is challenging to constrain
- Hyperon-Nucleon (YN) interactions are challenging to measure (since hyperons decay rapidly)
- If hyperons exist in neutron stars - it is probable that YNN interactions are also important
- The NNN and YN and YNN are interactions in principle we can determine with Lattice QCD



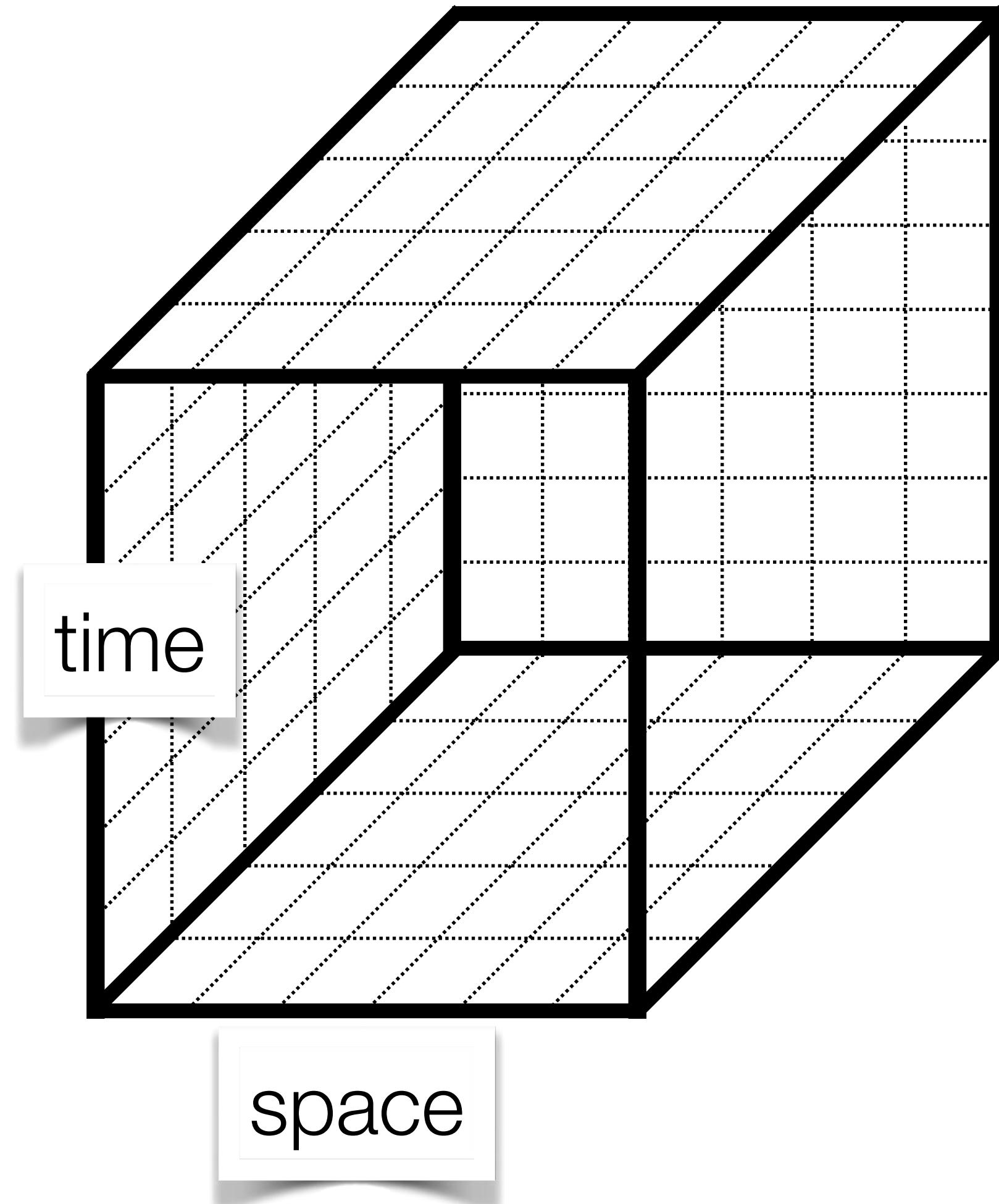
# Introduction to LQCD

$$\begin{aligned} C(t) = \langle \mathcal{O}(t)\mathcal{O}^\dagger(0) \rangle &= \frac{1}{\mathcal{Z}} \int D\psi D\bar{\psi} DU \mathcal{O}(t)\mathcal{O}(0) e^{iS_M[\bar{\psi},\psi,U]} \\ &= \frac{1}{\mathcal{Z}} \int DU \det(iD - M) \mathcal{O}(t)\mathcal{O}(0) e^{iS_M[\bar{\psi},\psi,U]} \end{aligned}$$

# Introduction to LQCD

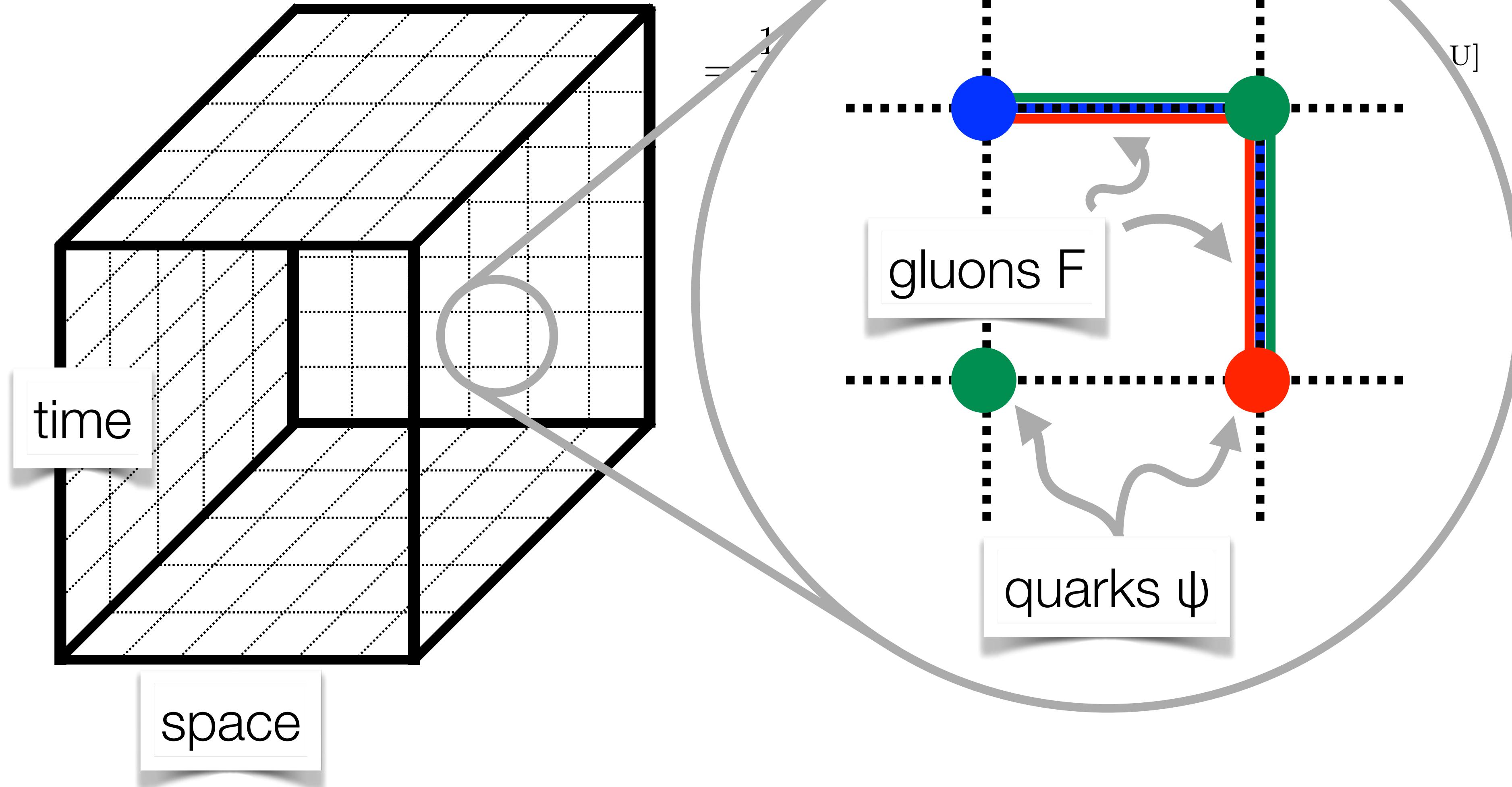
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lattice  
finite volume



# Introduction to LQCD

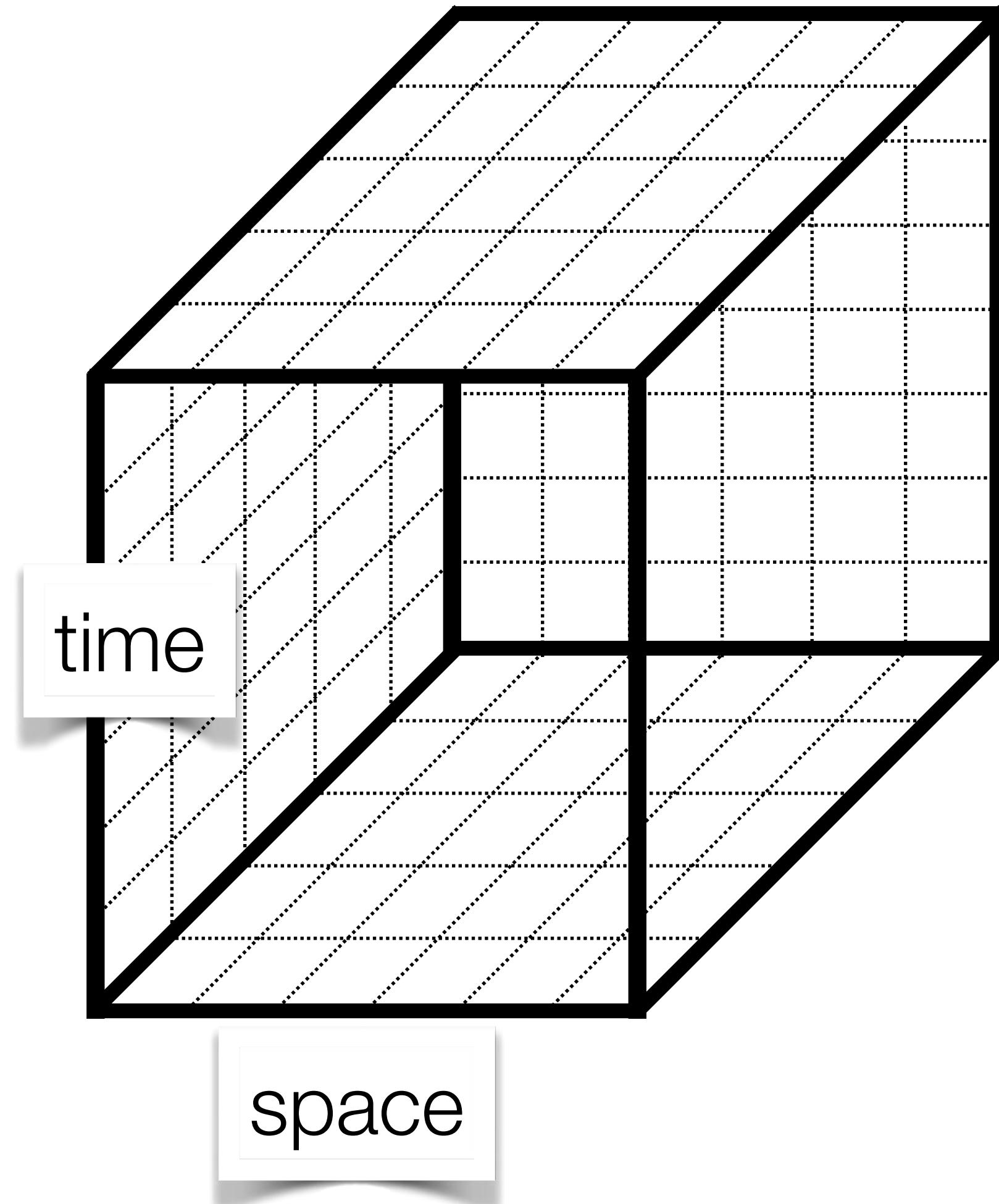
$$C(t) = \langle \mathcal{O}(t)\mathcal{O}^\dagger(0) \rangle = \frac{1}{\mathcal{Z}} \int D\psi \bar{\psi} \psi U^\dagger(t) \psi U(0)$$



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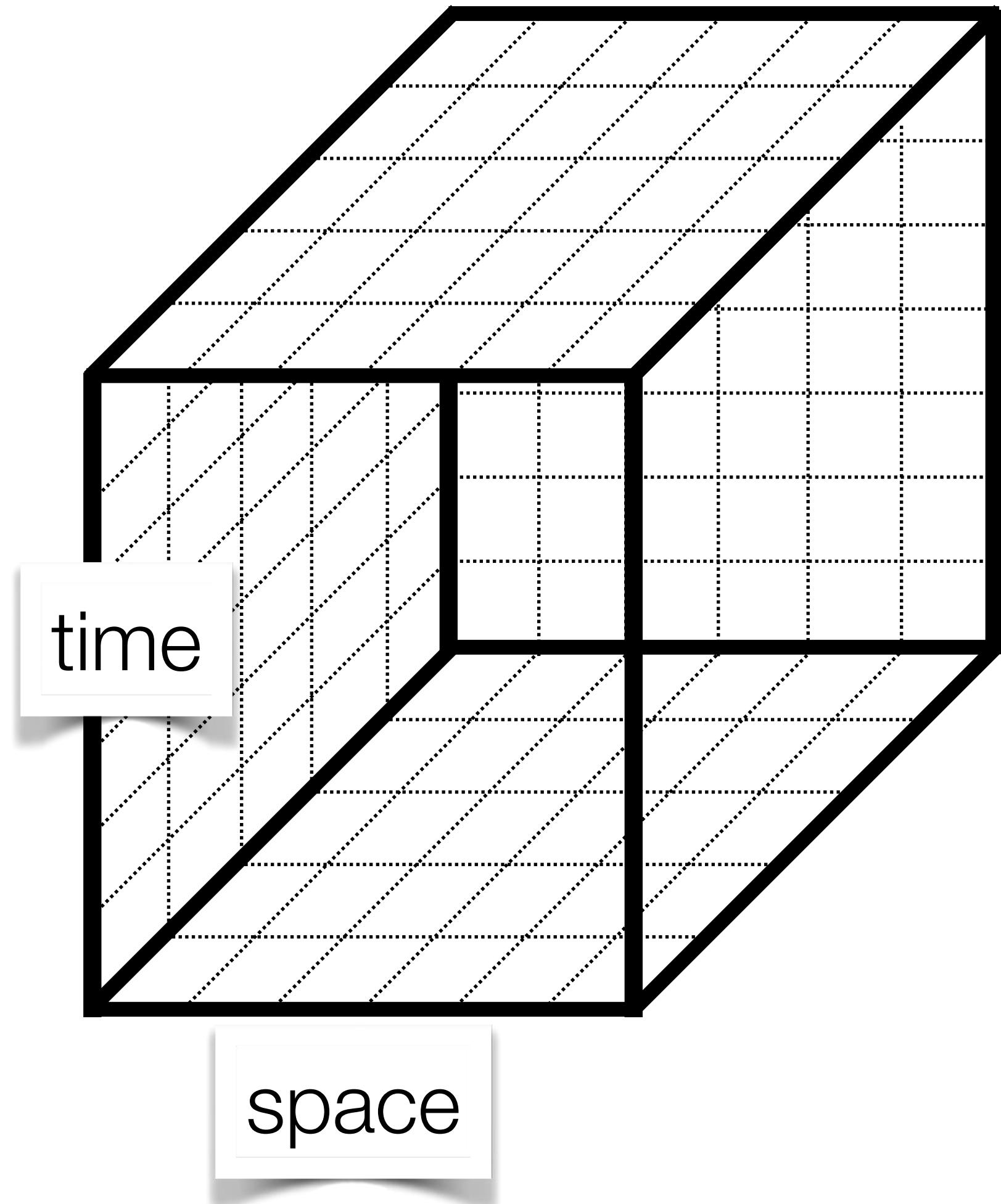
lattice  
finite volume



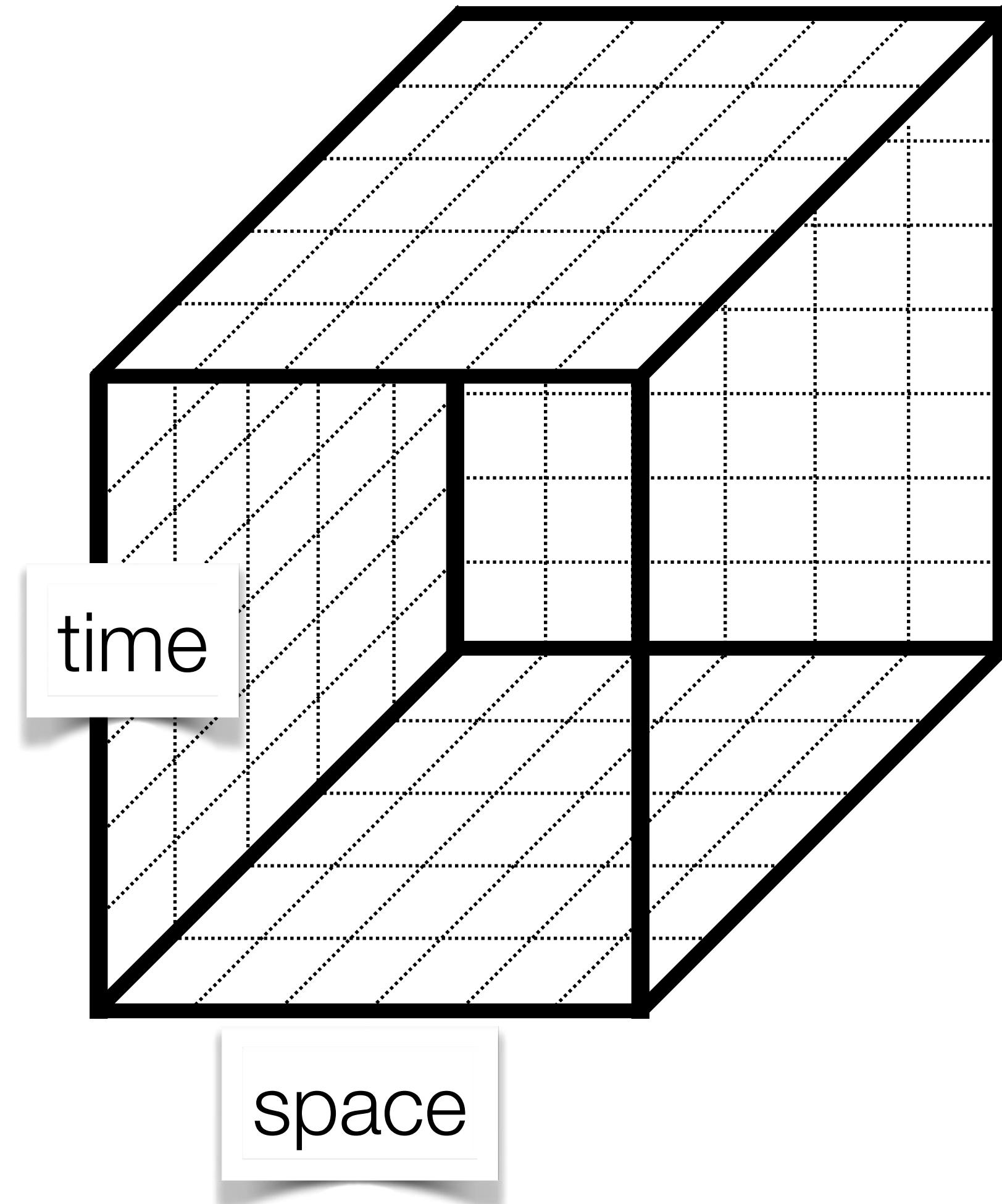
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$$= \frac{1}{\mathcal{Z}} \int \mathcal{D}U \det(\not{D} + M) e^{-S[U]} \mathcal{O}(t)\mathcal{O}^\dagger(0)$$

lattice  
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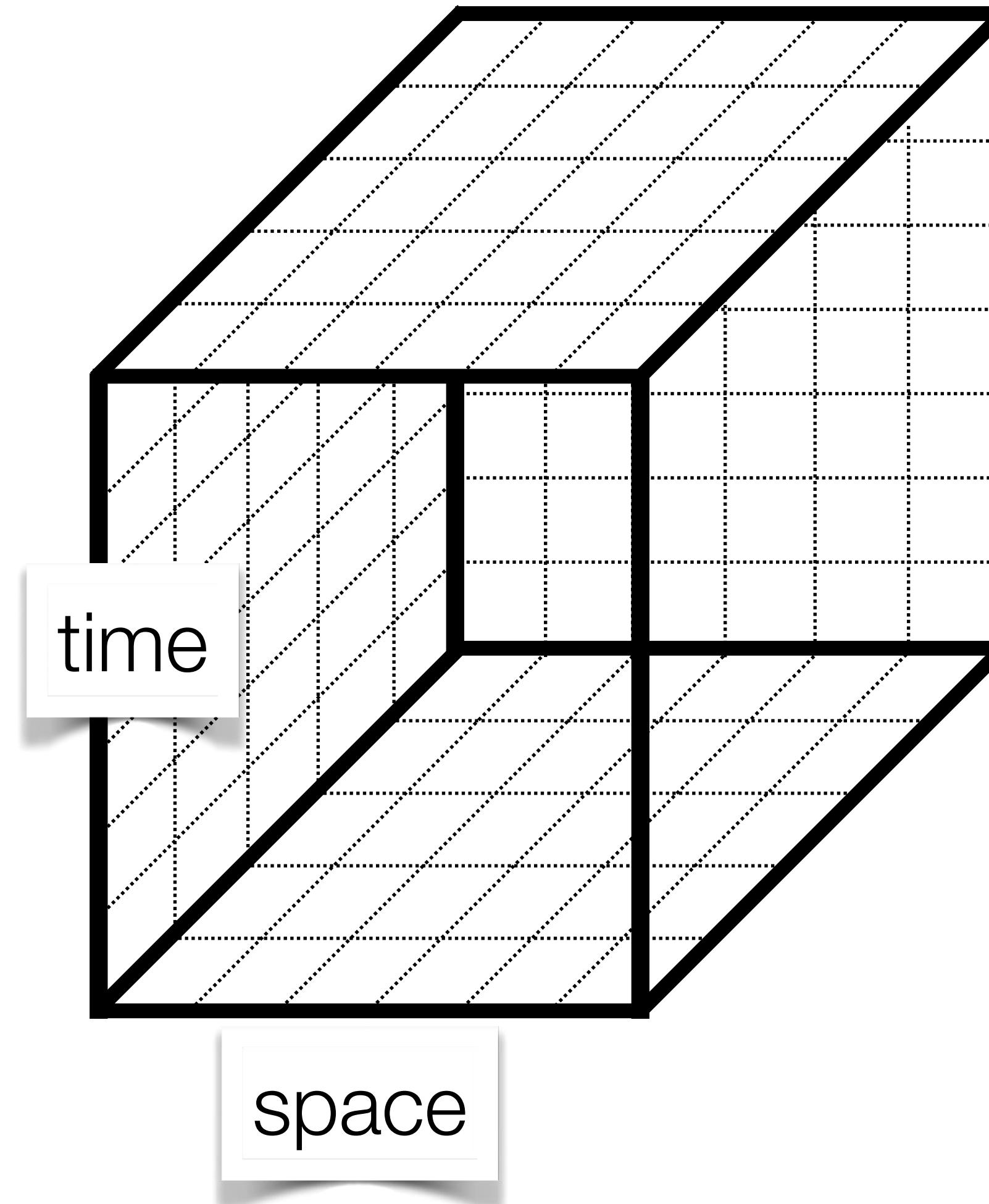
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Probability

# Introduction to LQCD



$$C(t) = \langle \mathcal{O}(t)\mathcal{O}^\dagger(0) \rangle = \frac{1}{\mathcal{Z}} \int \mathcal{D}\psi \mathcal{D}\bar{\psi} \mathcal{D}U \mathcal{O}(t)\mathcal{O}^\dagger(0)e^{-S[\bar{\psi},\psi,U]}$$

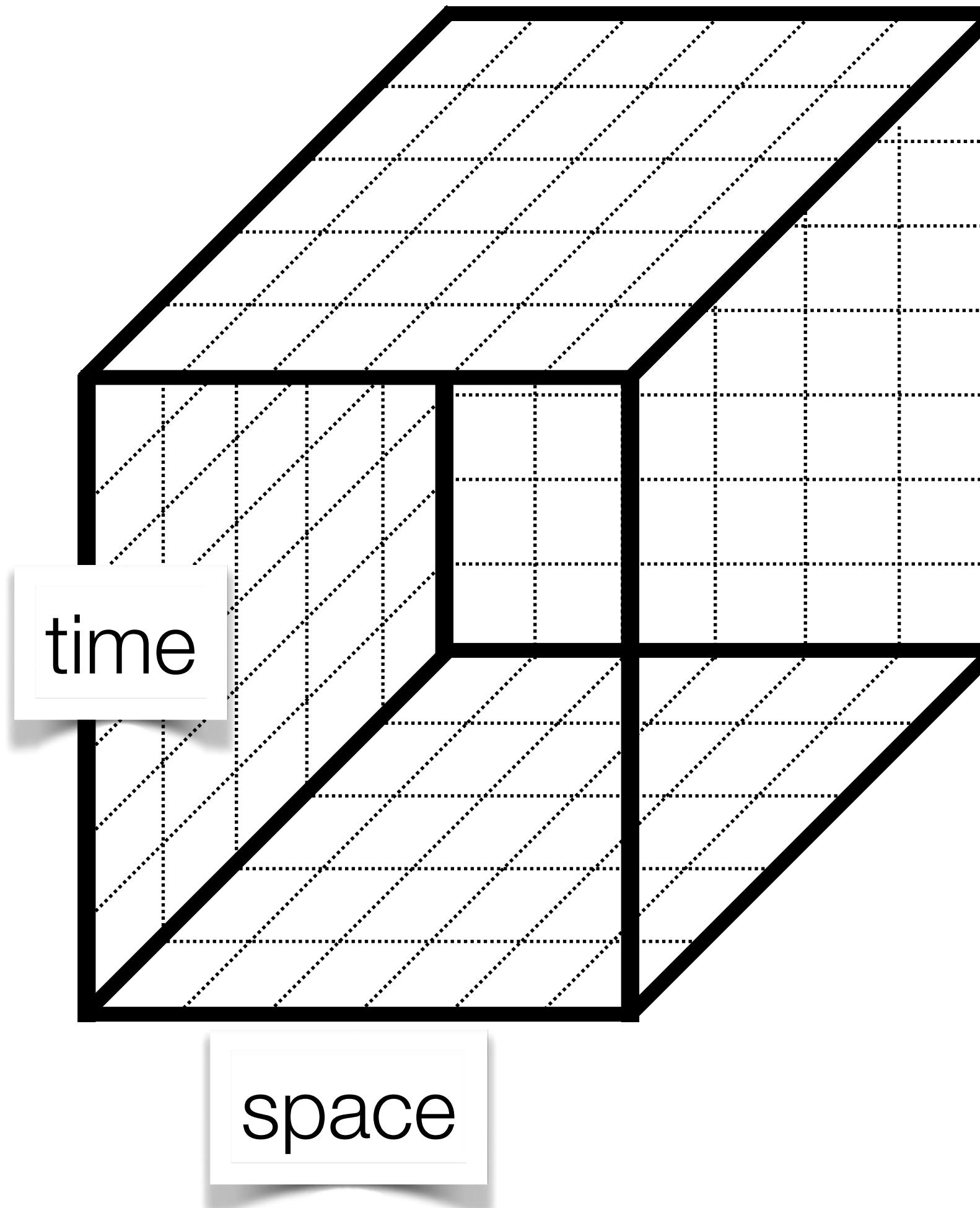
$$= \frac{1}{\mathcal{Z}} \int \mathcal{D}U \det(\not{D} + M) e^{-S[U]} \mathcal{O}(t)\mathcal{O}^\dagger(0)$$

Probability

$$\{U_1, U_2, U_3, \dots, U_N\}$$

Markov Chain Monte Carlo

# Introduction to LQCD



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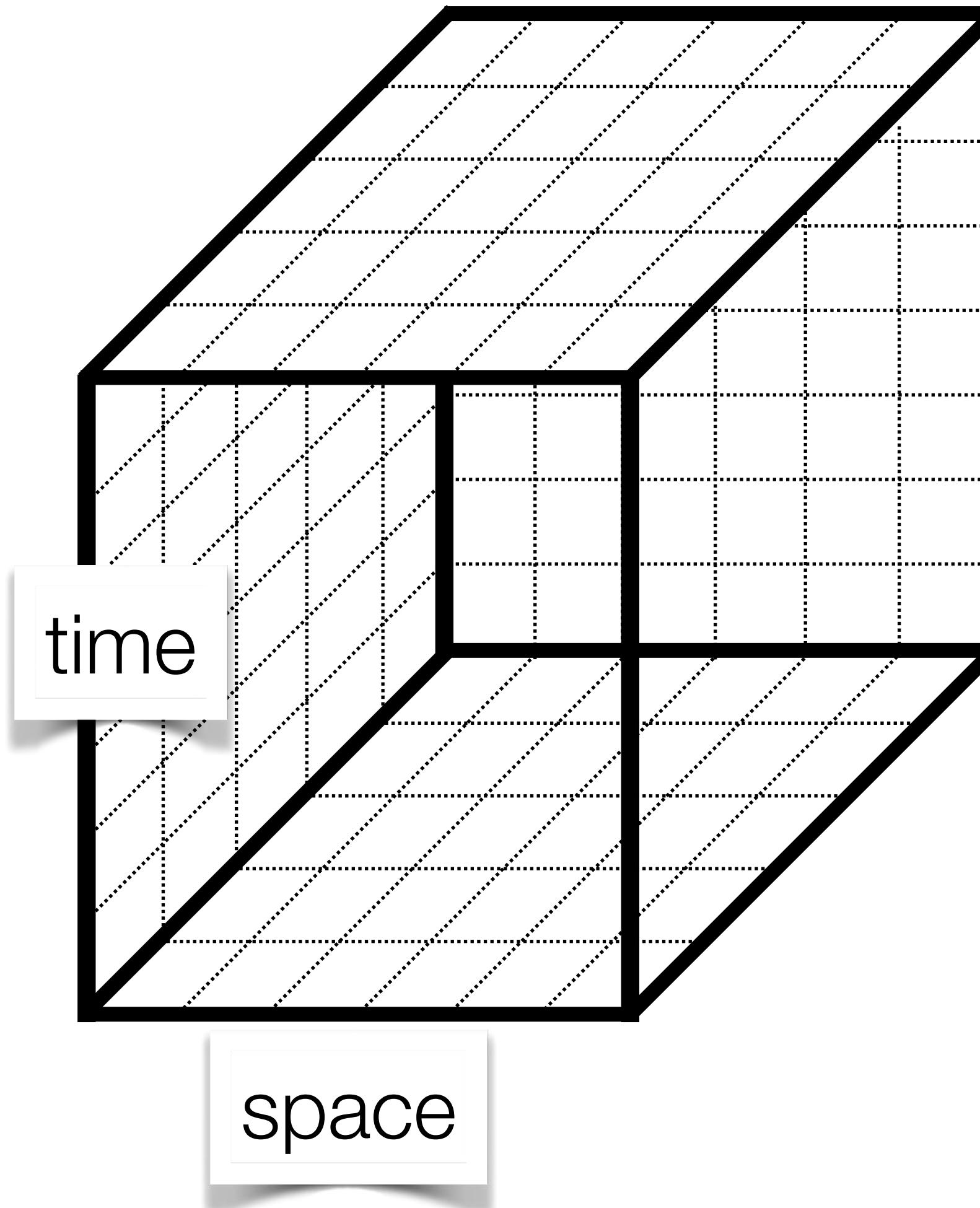
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Markov Chain Monte Carlo

$$\approx \frac{1}{N} \sum_{i=1}^N \mathcal{O}(t)\mathcal{O}^\dagger(0)[U_i]$$

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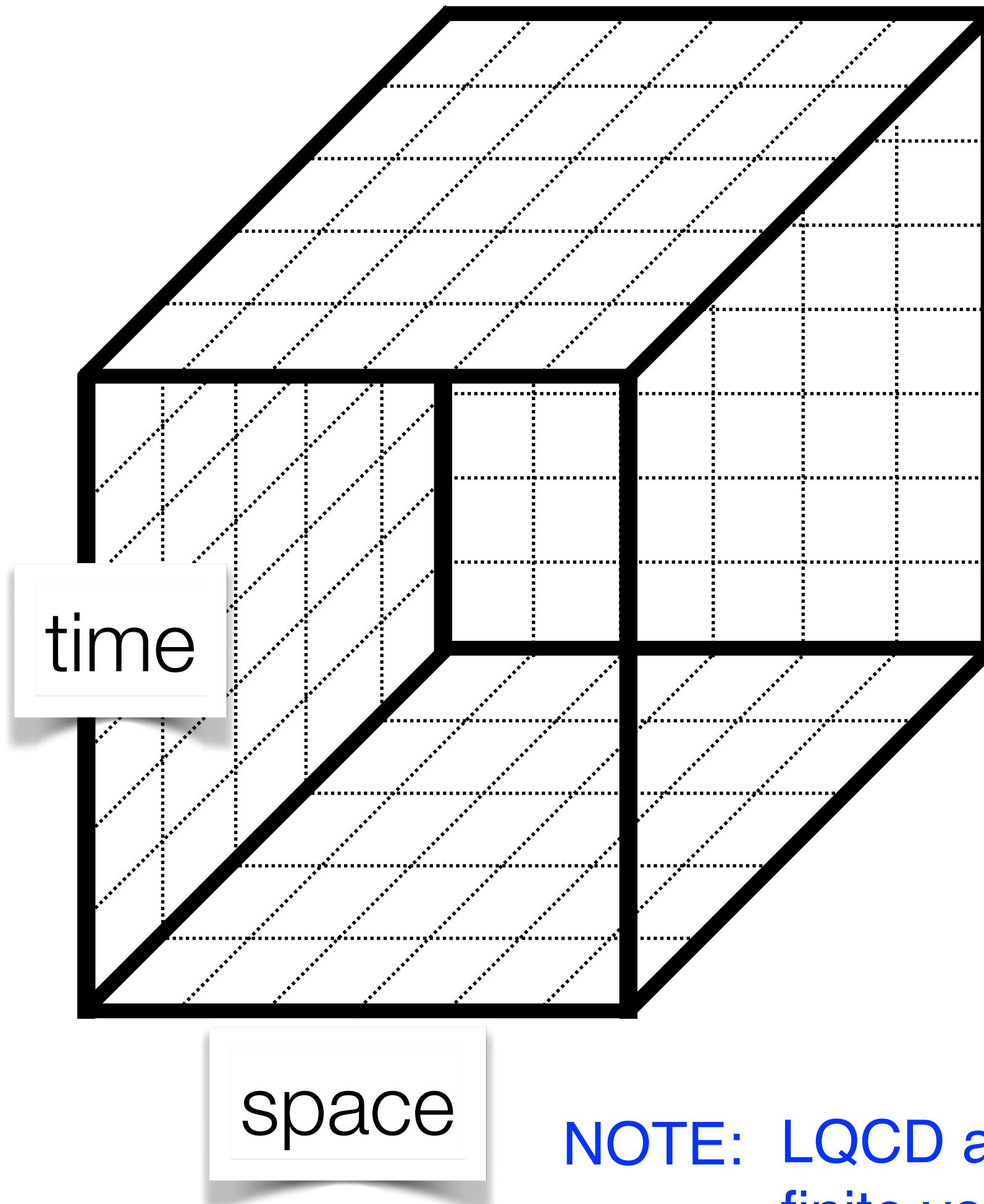
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Markov Chain Monte Carlo

$$\approx \frac{1}{N} \sum_{i=1}^N \mathcal{O}(t)\mathcal{O}^\dagger(0)[U_i] + O\left(\frac{1}{\sqrt{N}}\right)$$

# Introduction to LQCD



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Probability

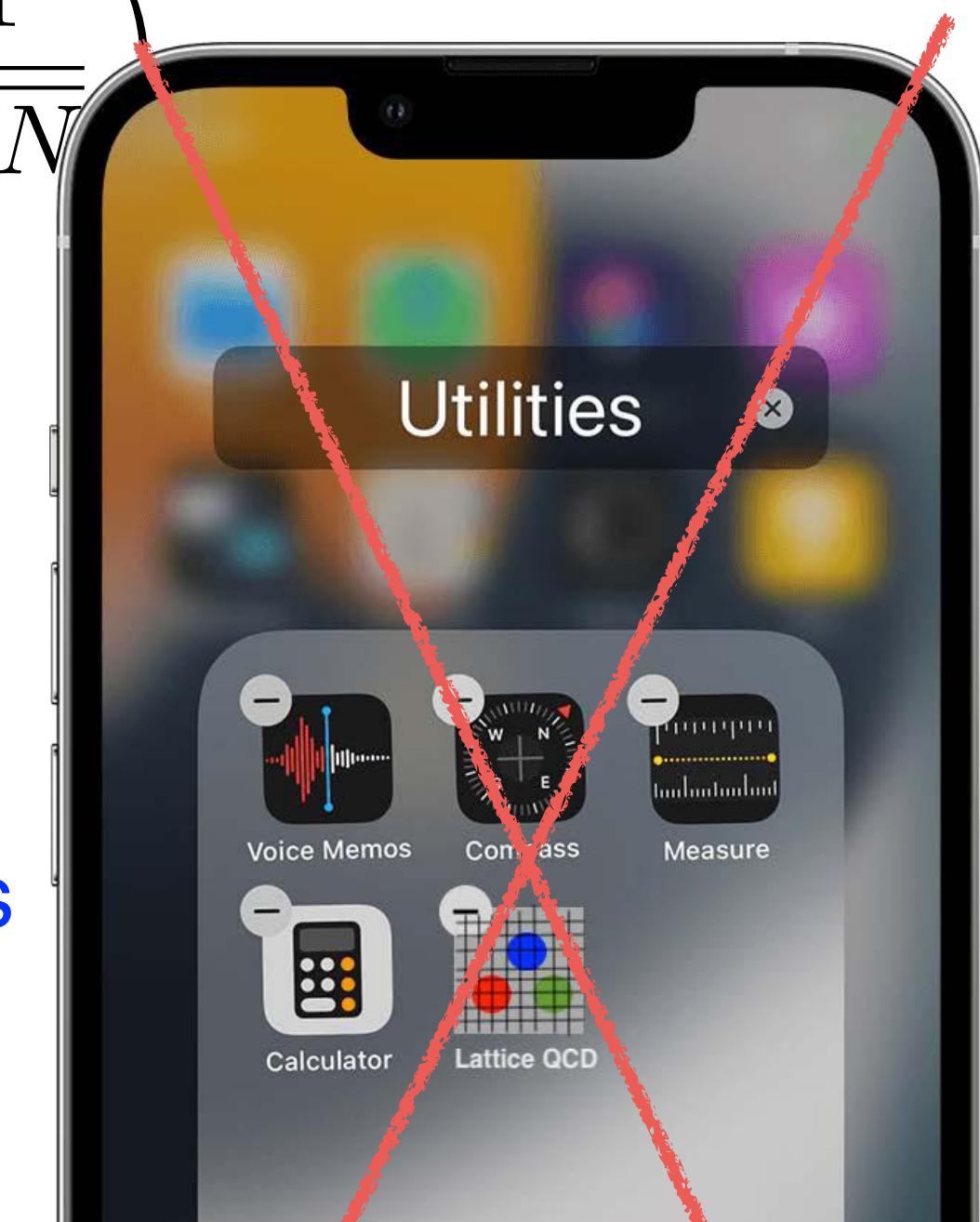
$$\{U_1, U_2, U_3, \dots, U_N\}$$

Markov Chain Monte Carlo

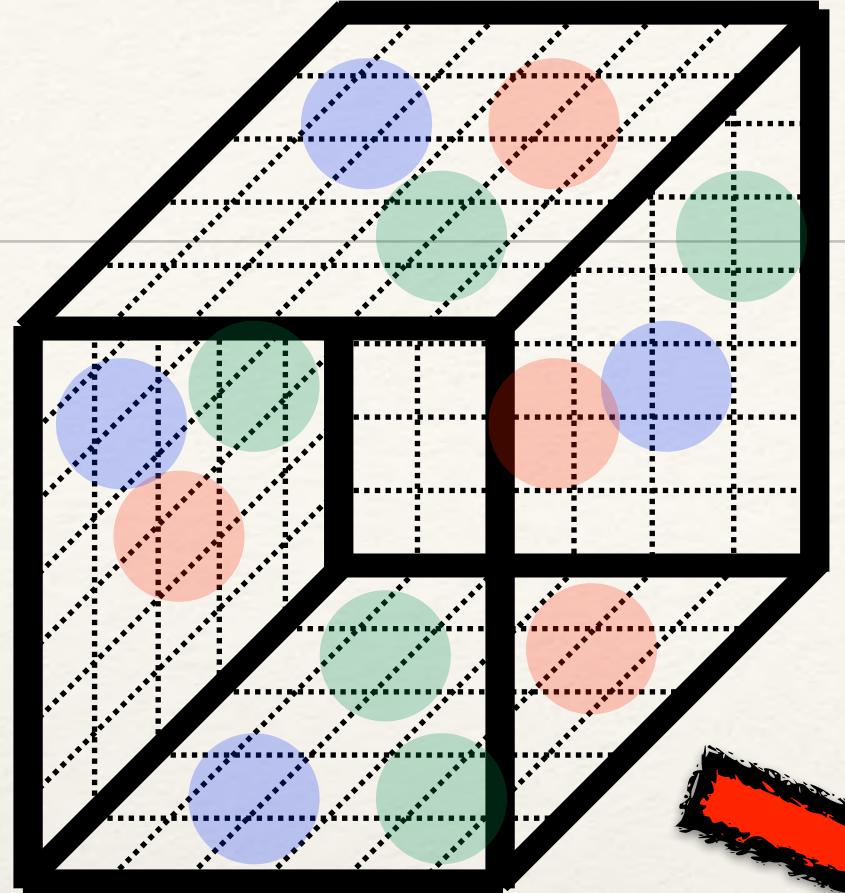
$$\approx \frac{1}{N} \sum_{i=1}^N \mathcal{O}(t)\mathcal{O}^\dagger(0)[U_i] + O\left(\frac{1}{\sqrt{N}}\right)$$

NOTE: LQCD allows us to compute Euclidean space, finite volume, correlation functions

Non-trivial numerical analysis (and sometimes formalism) to extract spectrum, matrix elements, form factors, ...



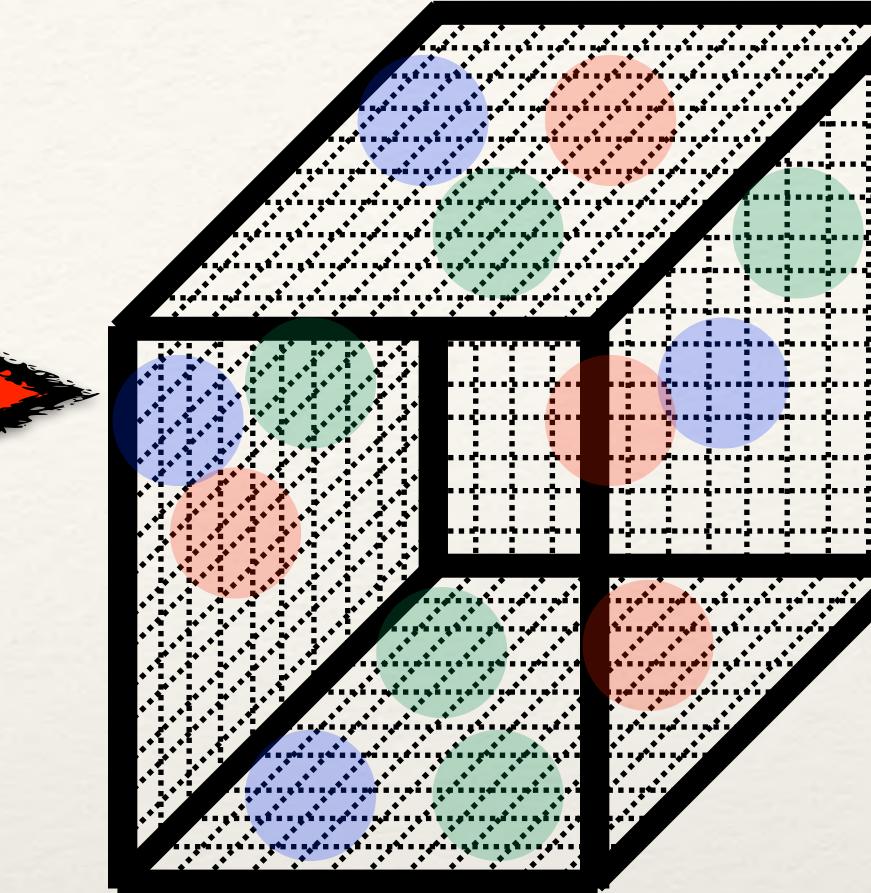
# What does it mean to have a LQCD result?



**continuum limit**

need 3 or more  
lattice spacings

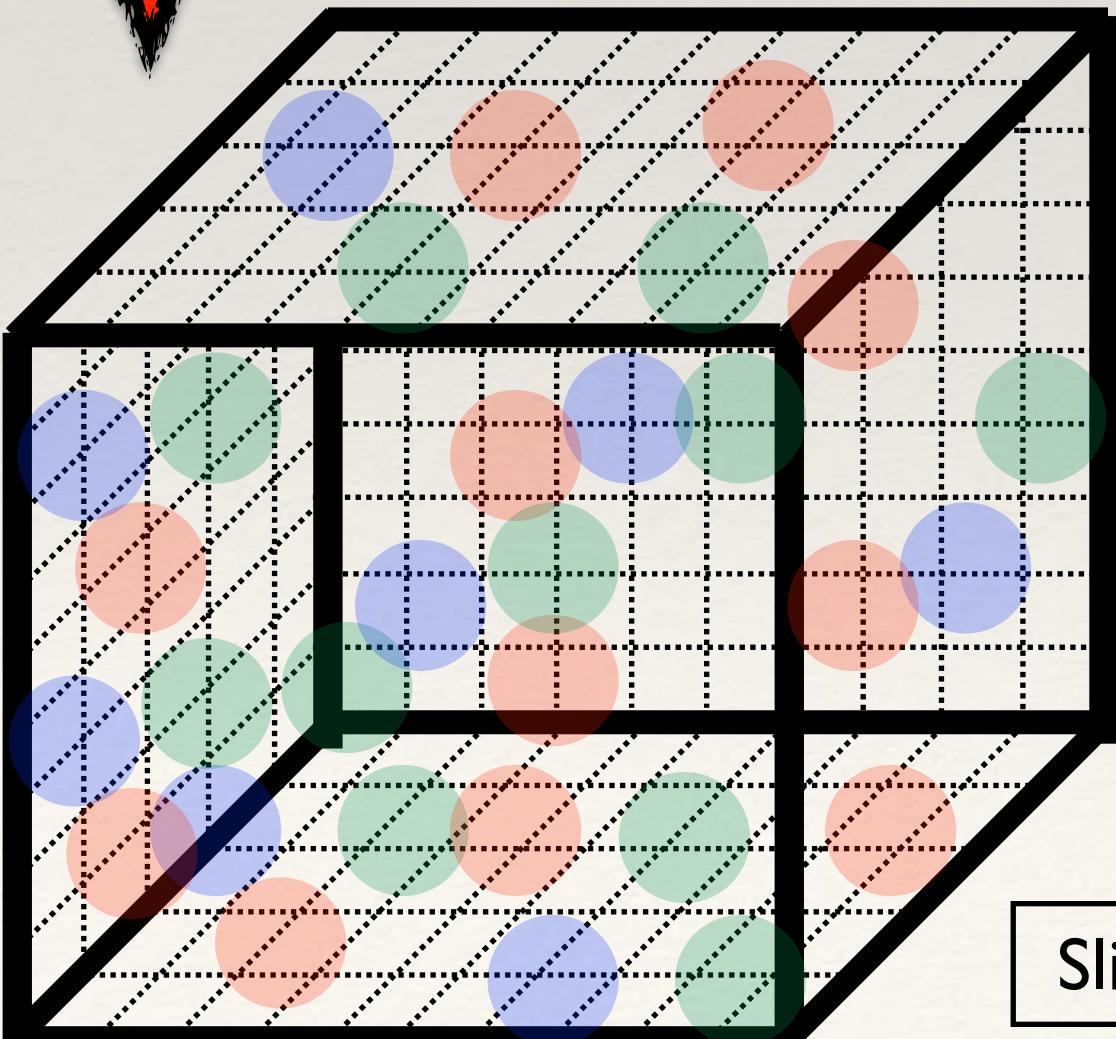
$$t_{comp} \propto \frac{1}{a^6}$$



**infinite volume limit**

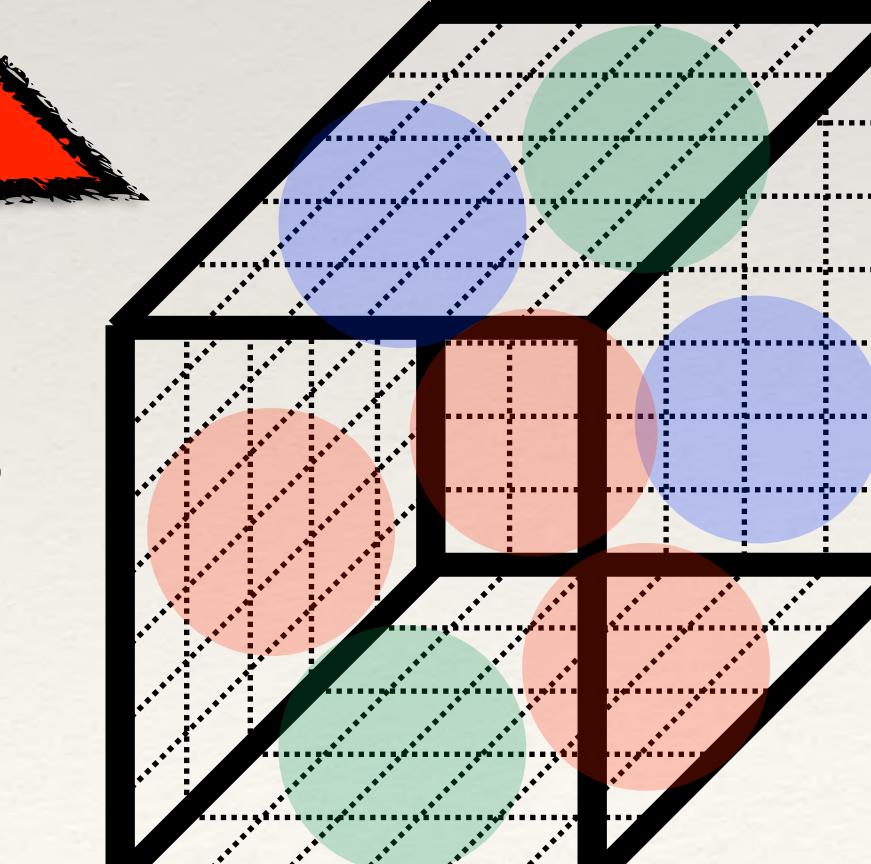
$$t_{comp} \propto V^{5/4}$$

$$V = N_L^3 \times N_T$$



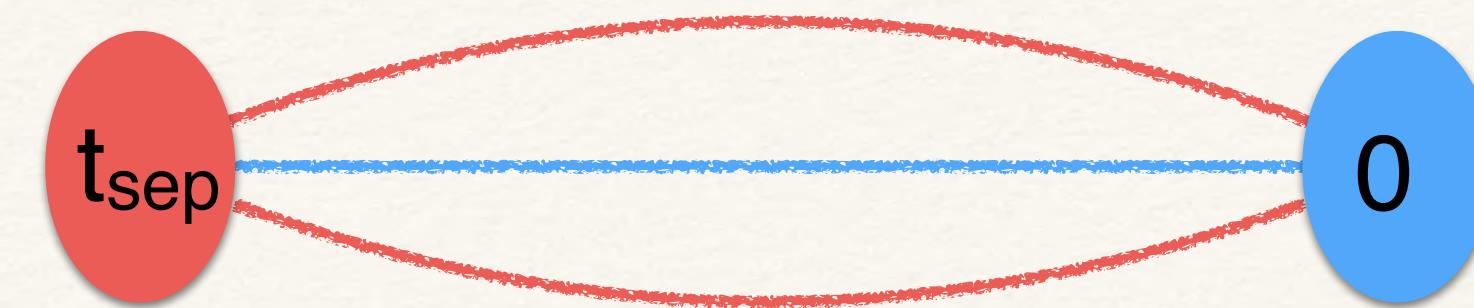
**physical pion masses**

exponentially bad  
signal-to-noise problem



# LQCD: 2 point functions

$$C(t, \mathbf{p}) = \sum_{\mathbf{x}} e^{-i\mathbf{p} \cdot \mathbf{x}} \langle \Omega | O(t, \mathbf{x}) O^\dagger(0, \mathbf{0}) | \Omega \rangle$$



$$\begin{aligned} C(t) &= \sum_{\mathbf{x}} \langle \Omega | O(t, \mathbf{x}) O^\dagger(0, \mathbf{0}) | \Omega \rangle \\ &= \sum_{\mathbf{x}} \langle \Omega | e^{\hat{H}t} O(0, \mathbf{x}) e^{-\hat{H}t} O^\dagger(0, \mathbf{0}) | \Omega \rangle \\ &= \sum_n \sum_{\mathbf{x}} \langle \Omega | e^{\hat{H}t} O(0, \mathbf{x}) e^{-\hat{H}t} | n \rangle \langle n | O^\dagger(0, \mathbf{0}) | \Omega \rangle \\ &= \sum_n e^{-E_n t} \sum_{\mathbf{x}} \langle \Omega | O(0, \mathbf{x}) | n \rangle \langle n | O^\dagger(0, \mathbf{0}) | \Omega \rangle \\ &= \sum_n e^{-E_n(\mathbf{p}=0)t} \langle \Omega | O(0) | n, \mathbf{p} = 0 \rangle \langle n, \mathbf{p} = 0 | O^\dagger(0) | \Omega \rangle \\ &= \sum_n e^{-E_n t} z_n z_n^\dagger \end{aligned}$$

focus on 0-momentum

time-evolve operator

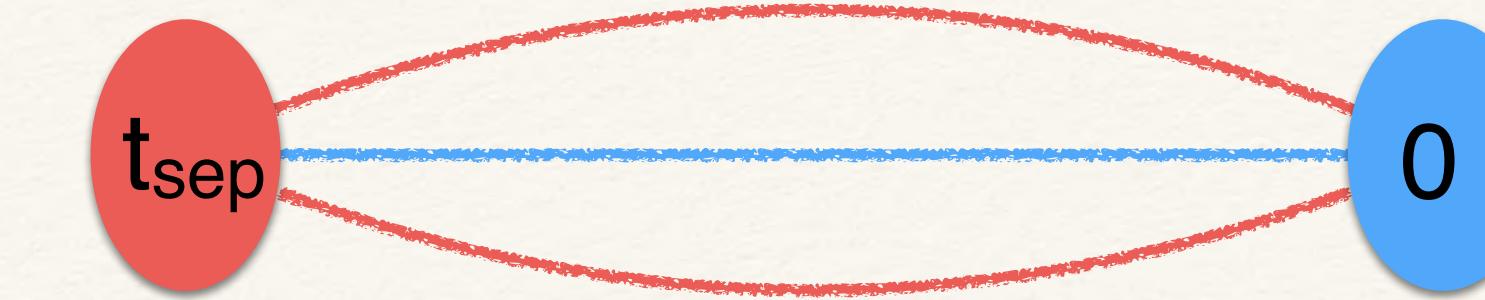
multiply by 1,  $1 = \sum_n |n\rangle \langle n|$

define vacuum to have 0-energy

sum of exponentials

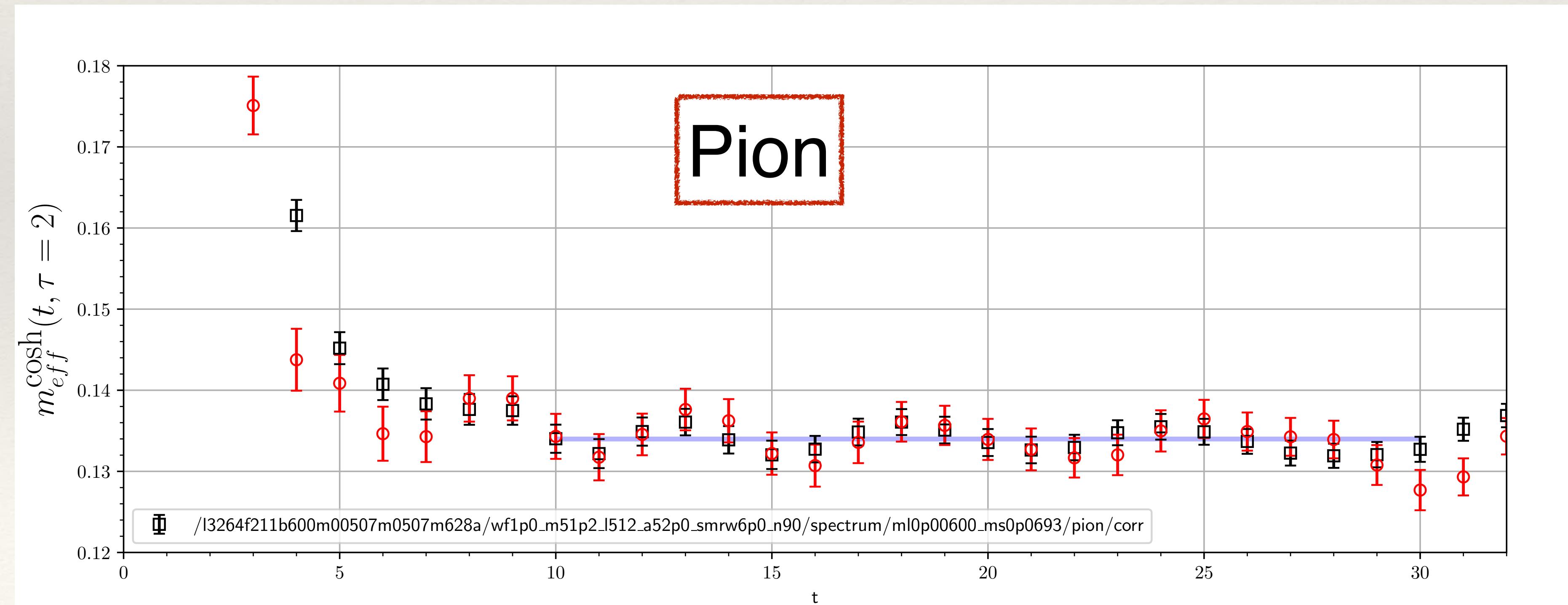
# LQCD: 2 point functions

$$\begin{aligned} C(t, \mathbf{p} = 0) &= \sum_{\mathbf{x}} \langle \Omega | N(t, \mathbf{x}) N^\dagger(0, \mathbf{0}) | \Omega \rangle \\ &= A_0 e^{-E_0 t} \left( 1 + \sum_{n>0} r_n e^{-\Delta_{n0} t} \right) \\ \Delta_{n0} &= E_n - E_0 \end{aligned}$$



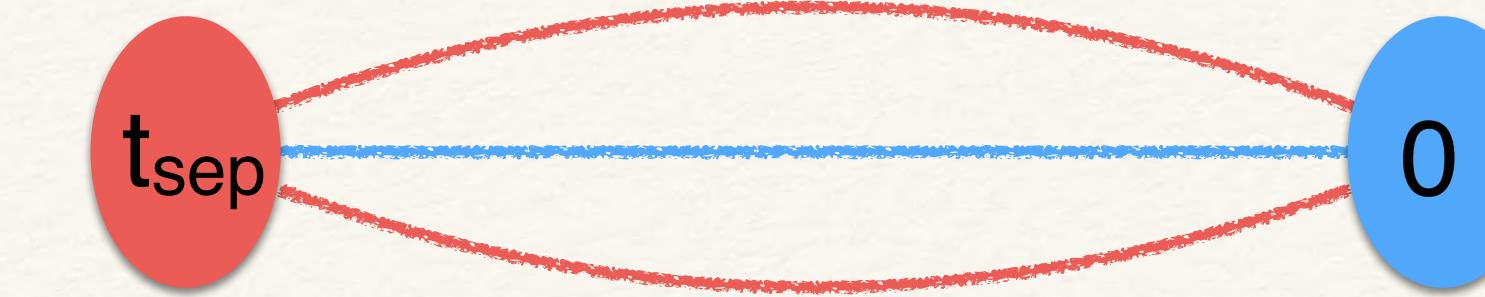
$$m_{\text{eff}}(t) = \ln \left( \frac{C(t)}{C(t+1)} \right) \xrightarrow[\text{large } t]{} E_0 + \sum_{n>0} r_n (e^{-\Delta_{n0} t} - e^{-\Delta_{n0} (t+1)})$$

**NOTE:** if the creation operator is conjugate to the annihilation operator  
 $r_n \geq 0$



# LQCD: 2 point functions

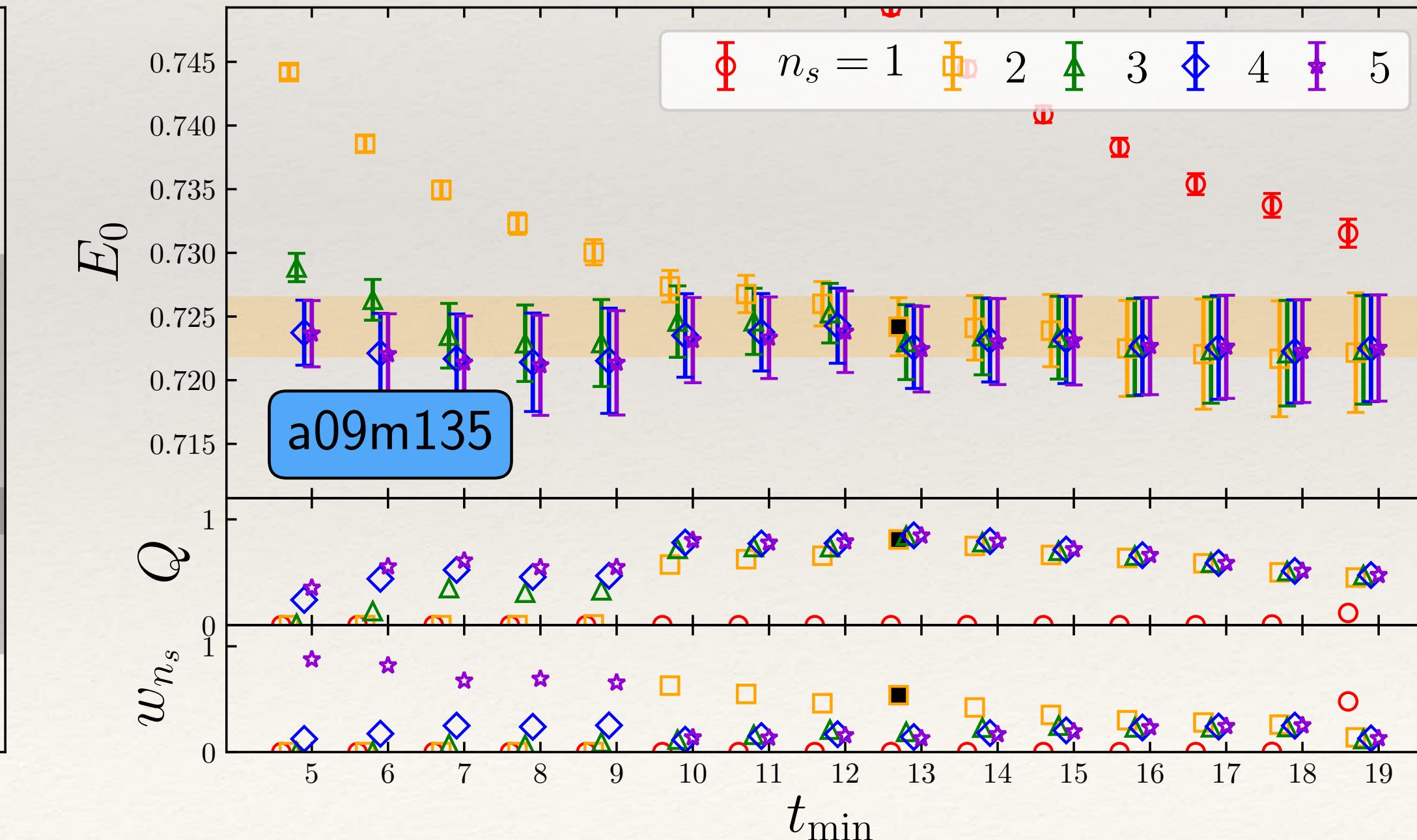
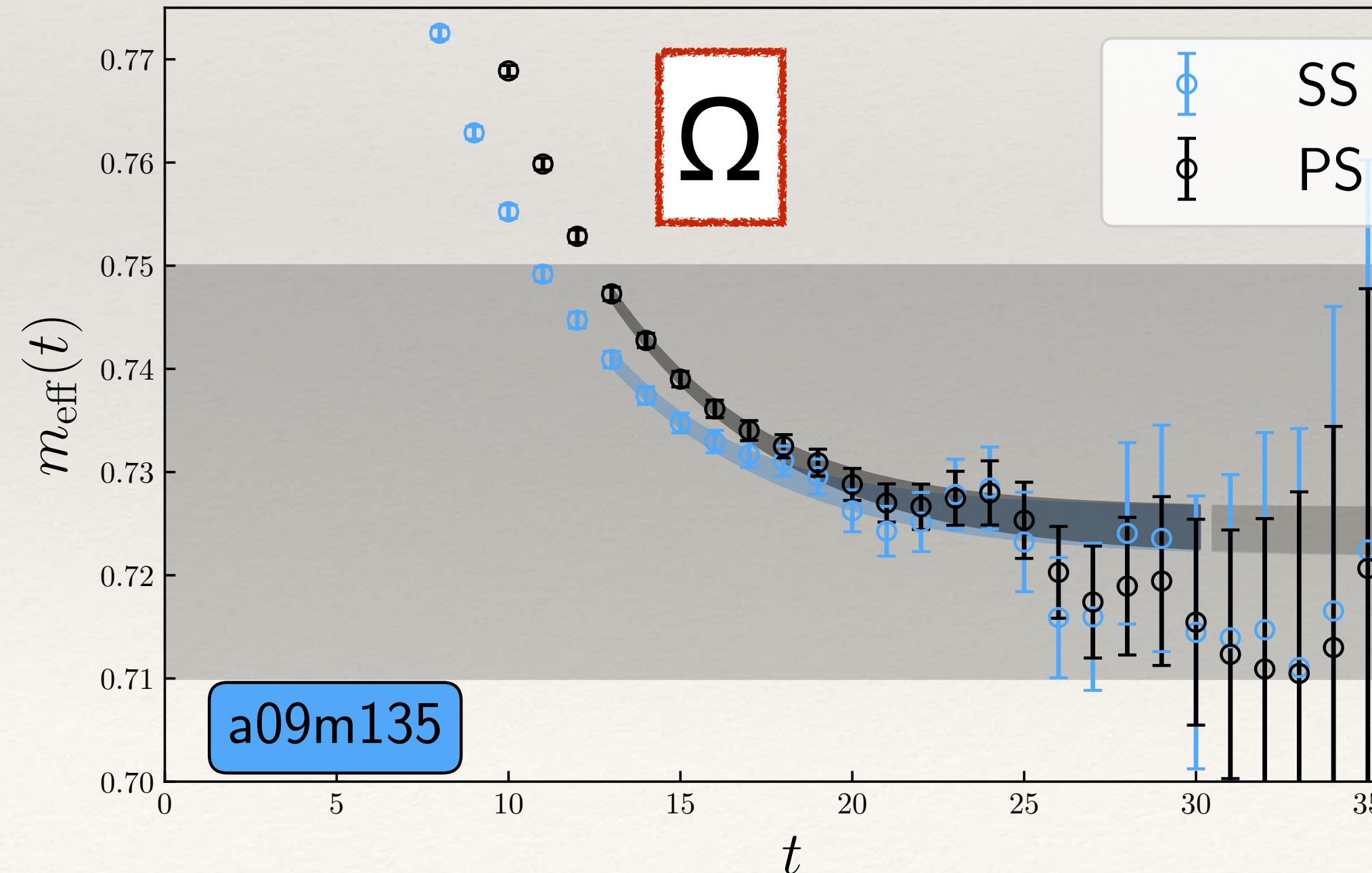
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**NOTE:** if the creation operator is conjugate to the annihilation operator  
 $r_n \geq 0$

but... signal-to-noise - can not simply “wait till long time” to get ground state (g.s.)

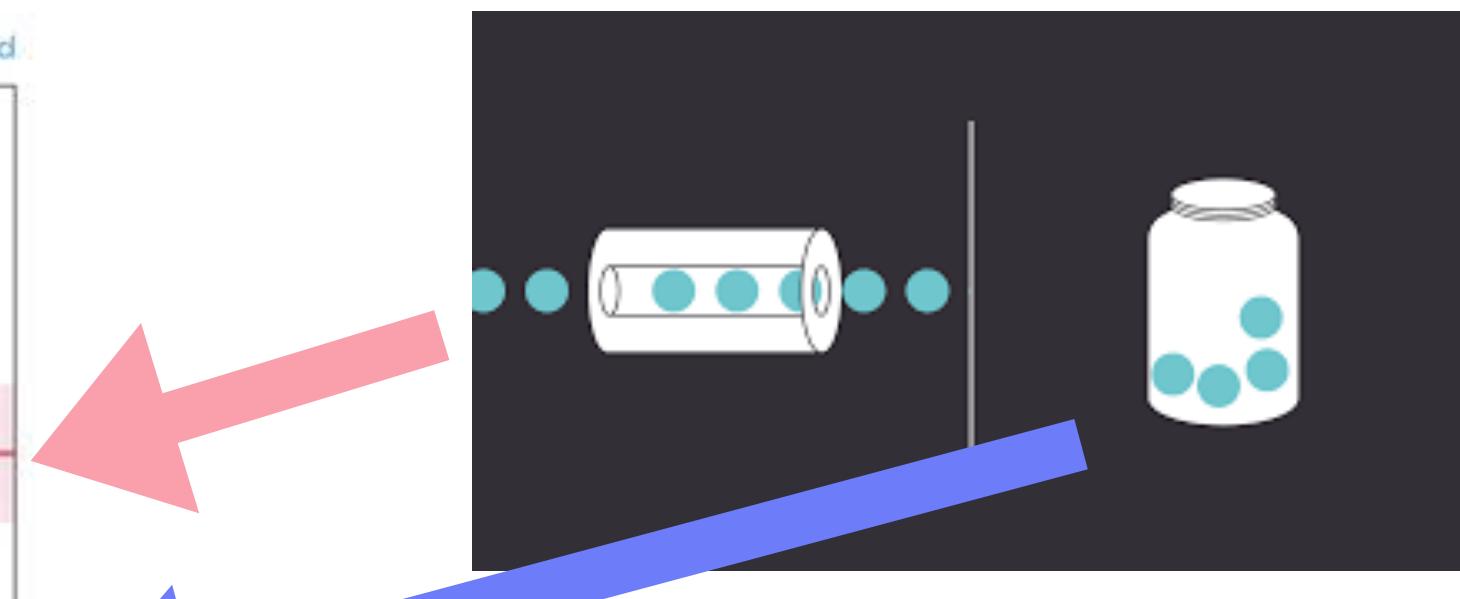
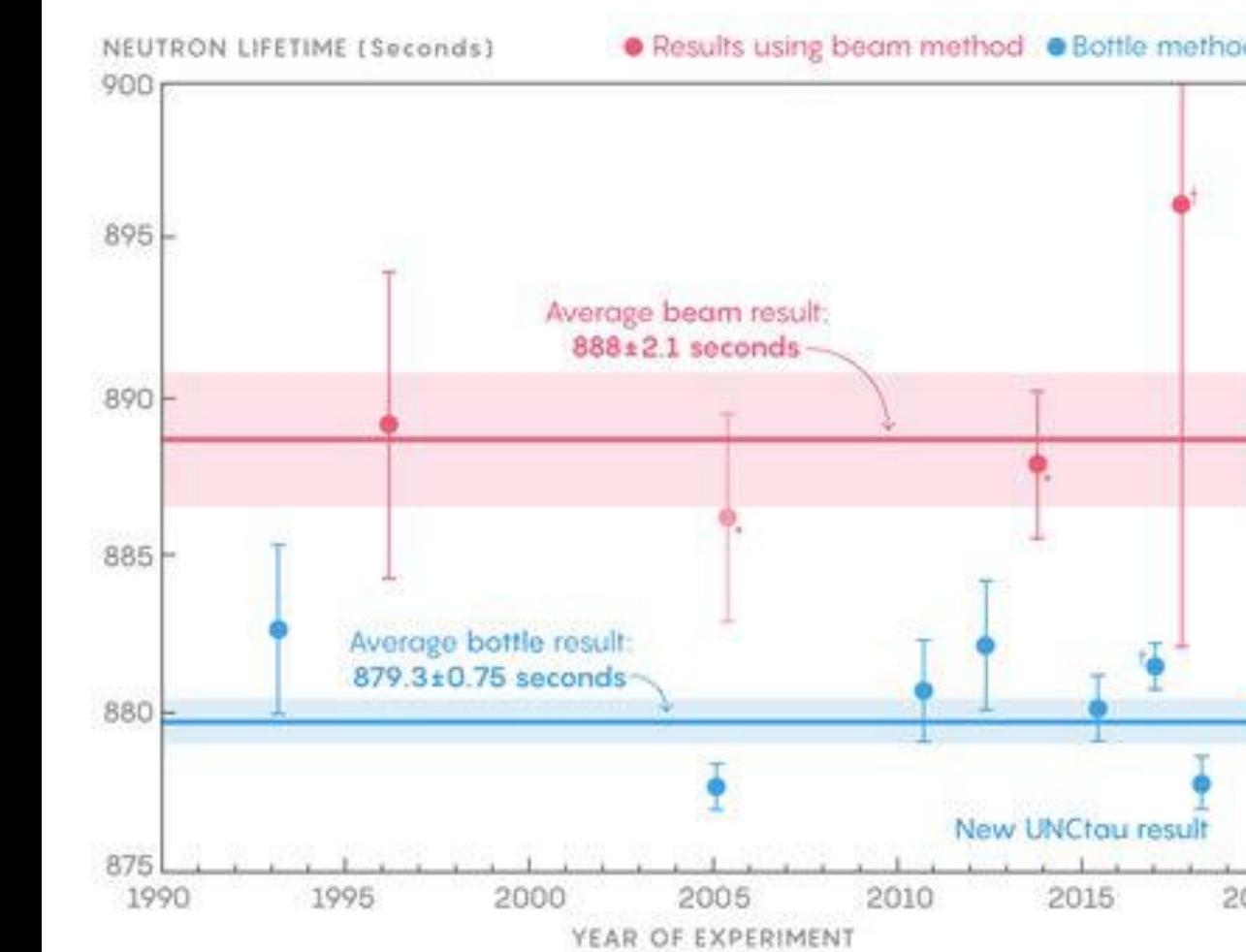
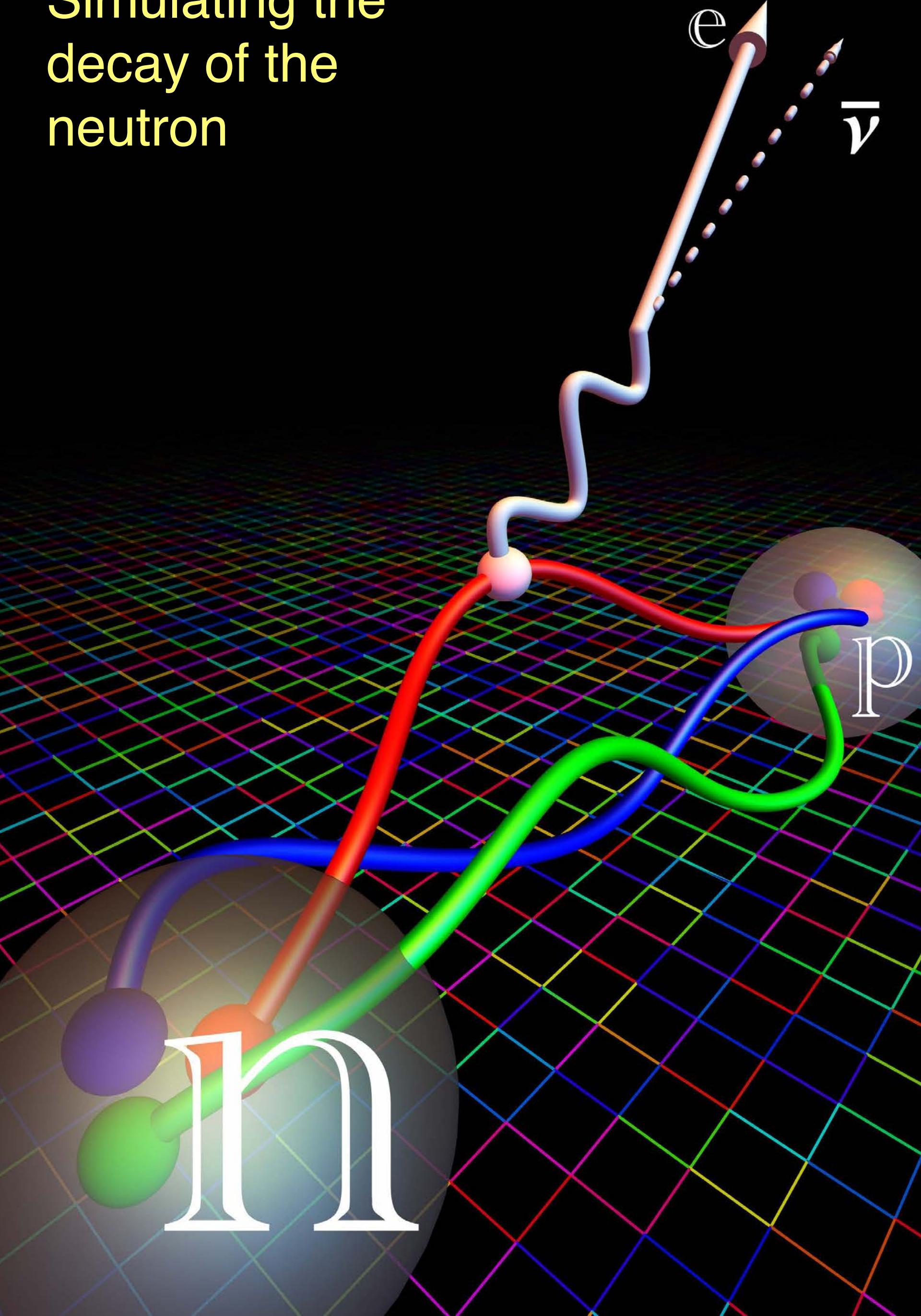


# Selective Highlights

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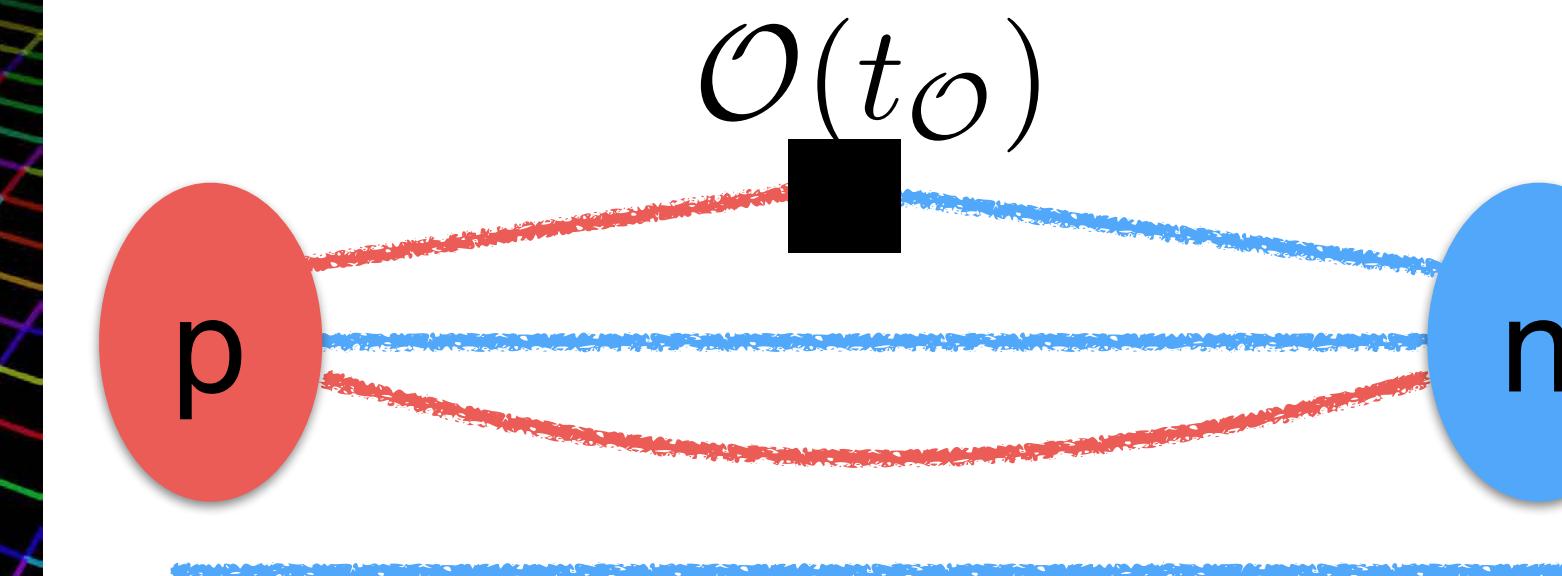
- The nucleon axial coupling  $g_A$
- The nucleon axial form factor
- $\pi \rightarrow \pi$  from short-distance 4-quark/2-electron operators:  $0\nu\beta\beta$
- BBN vs Isospin breaking

# Simulating the decay of the neutron



Neutron lifetime puzzle:  
There is currently a 4-sigma discrepancy  
between the **beam** and **bottle**  
measurements of the neutron lifetime

$$\frac{1}{\tau_n} = \frac{G_\mu^2 |V_{ud}|^2}{2\pi^3} m_e^5 (1 + 3g_A^2)(1 + RC)f$$



$S_Q(t,0) = \text{Quark Propagator}$

$$[D + M]_{y,z} S_{z,x} = \delta_{y,x}$$

Solve the Quark Propagators with  
Conjugate Gradient Matrix Multiplication

Known Matrix, Sparse, Large :  
 $\sim 400,000,000$

**GPUs are what allow us to do the calculations very efficiently**

# LETTER

<https://doi.org/10.1038/s41586-018-0161-8>

# Lattice QCD Team

(postdoc, grad student)

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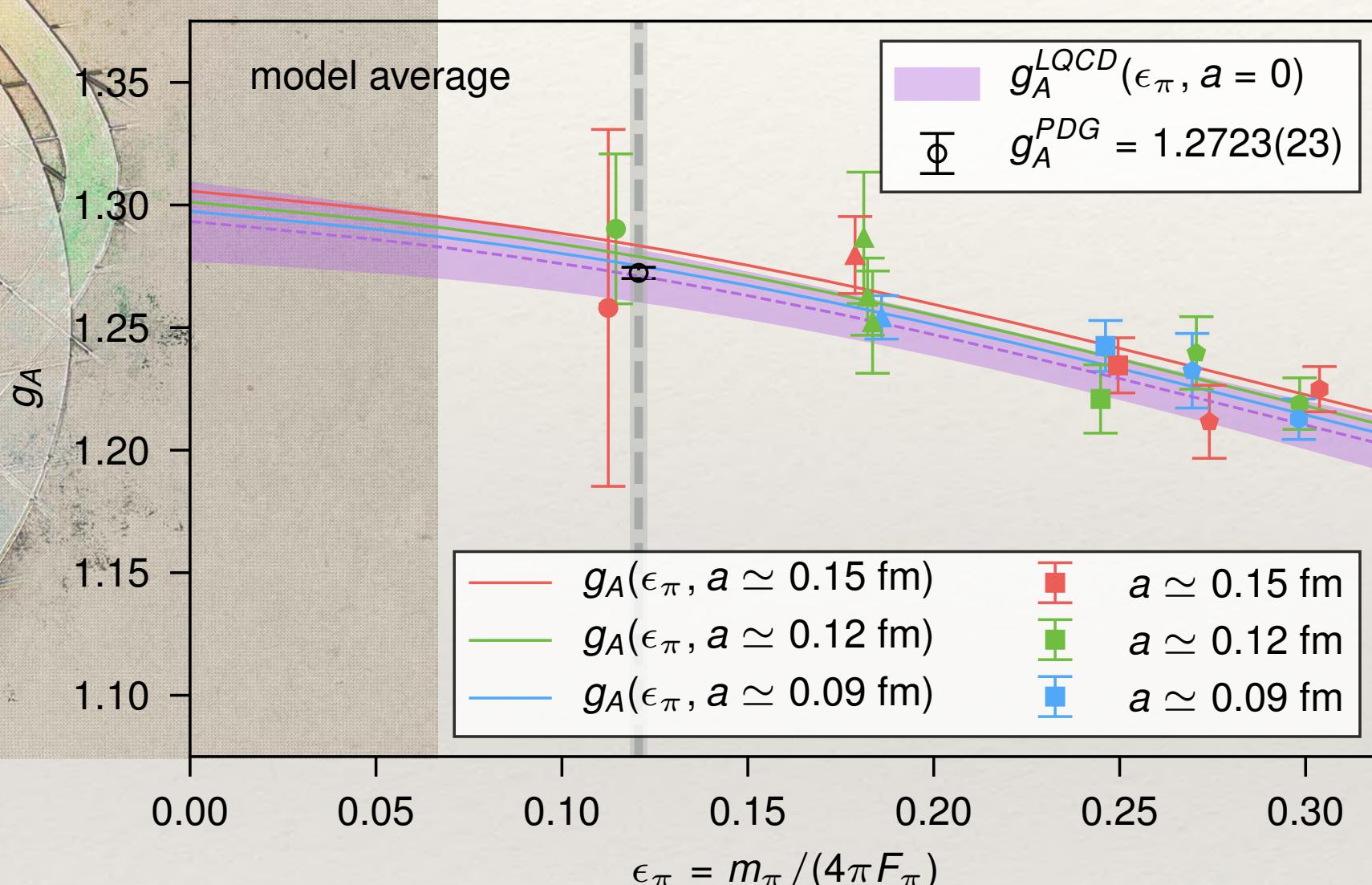
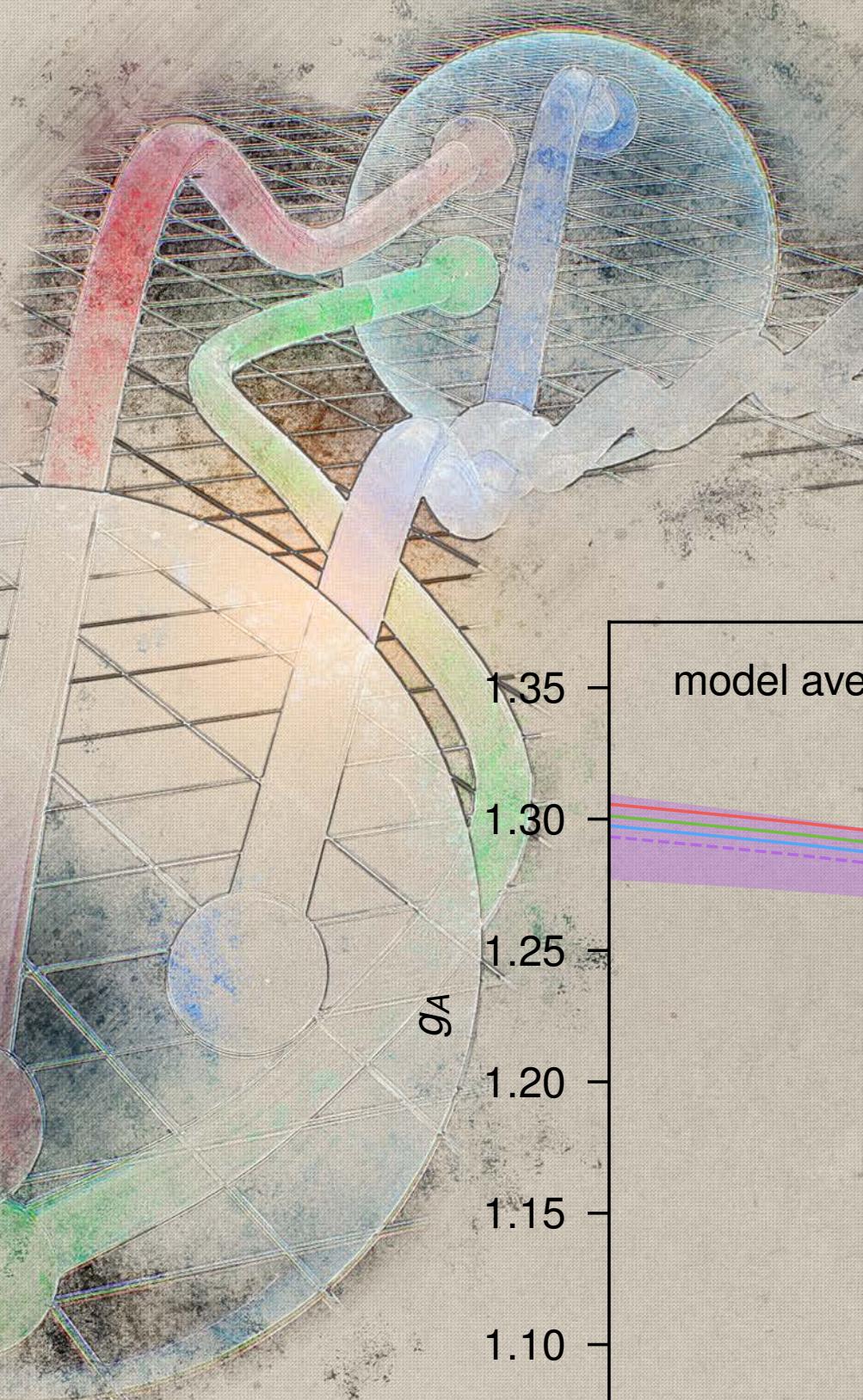
Pavlos Vranas

André Walker-Loud



(CallLat)

\*not all in California

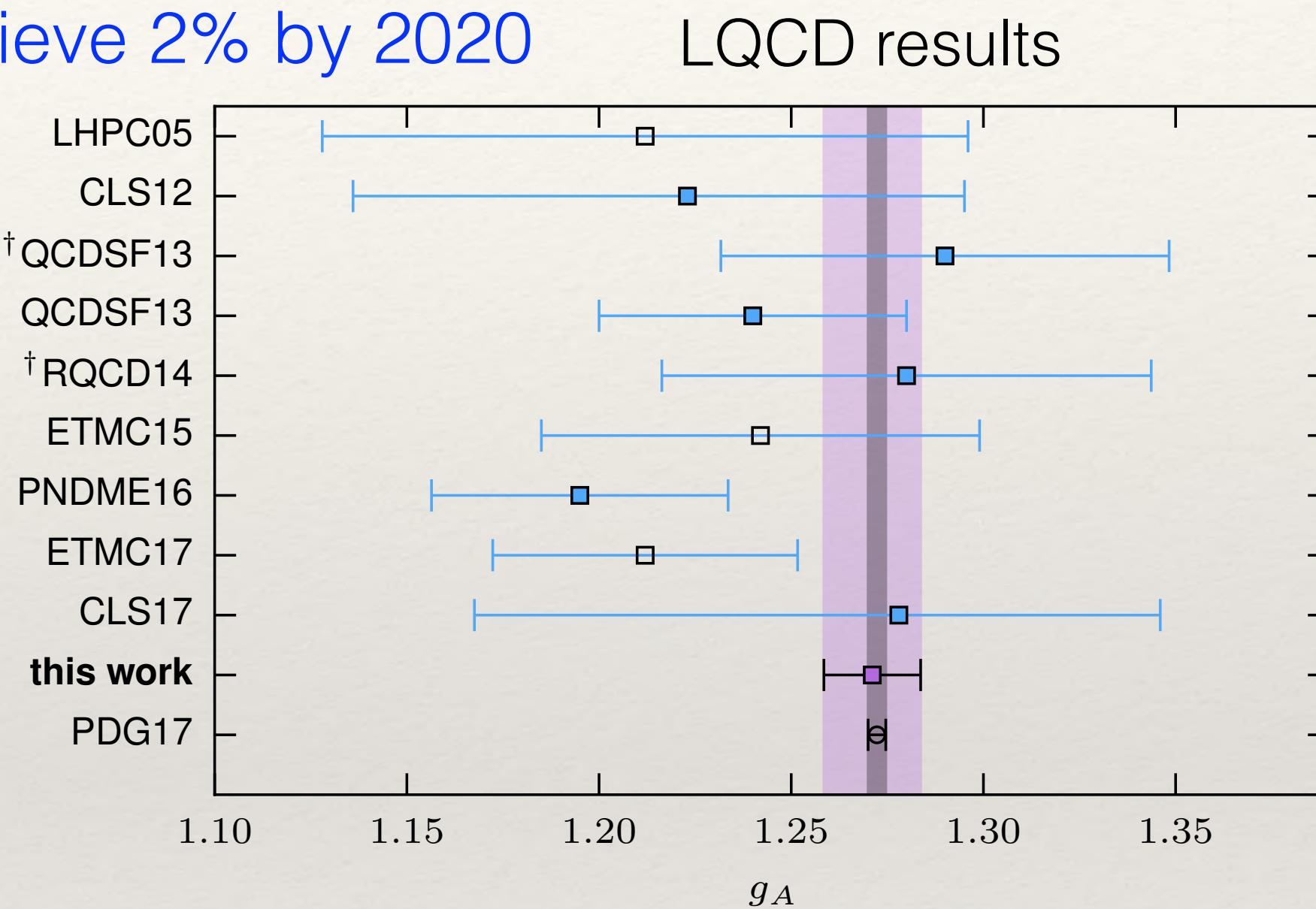


$$g_A^{\text{QCD}} = 1.2711(103)^s(39)^x(15)^a(19)^V(04)^I(55)^M$$

$$= 1.2711(126)$$

$$g_A^{\text{UCNA}} = 1.2772(020)$$

experiment factor of 6 more precise



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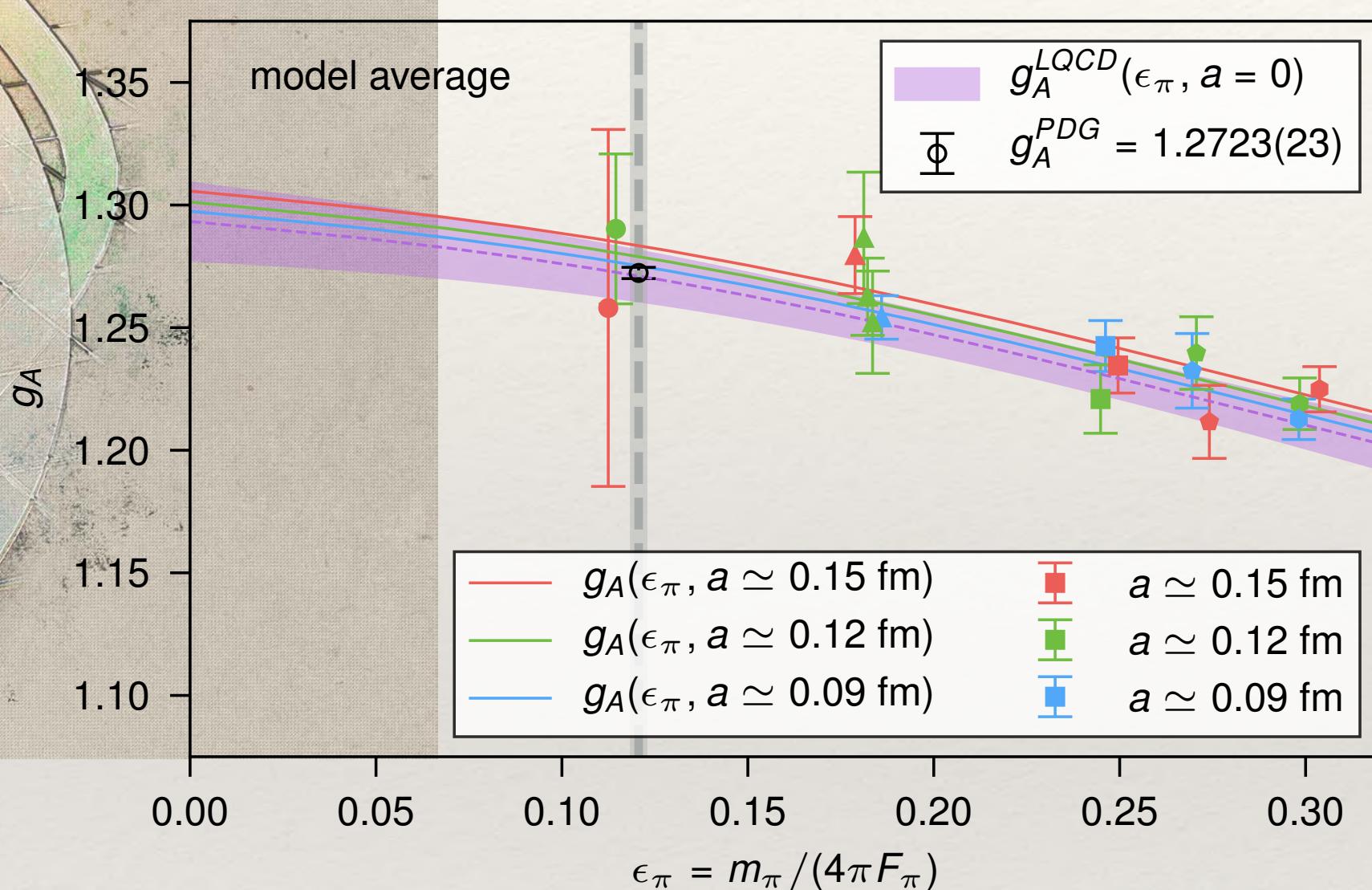
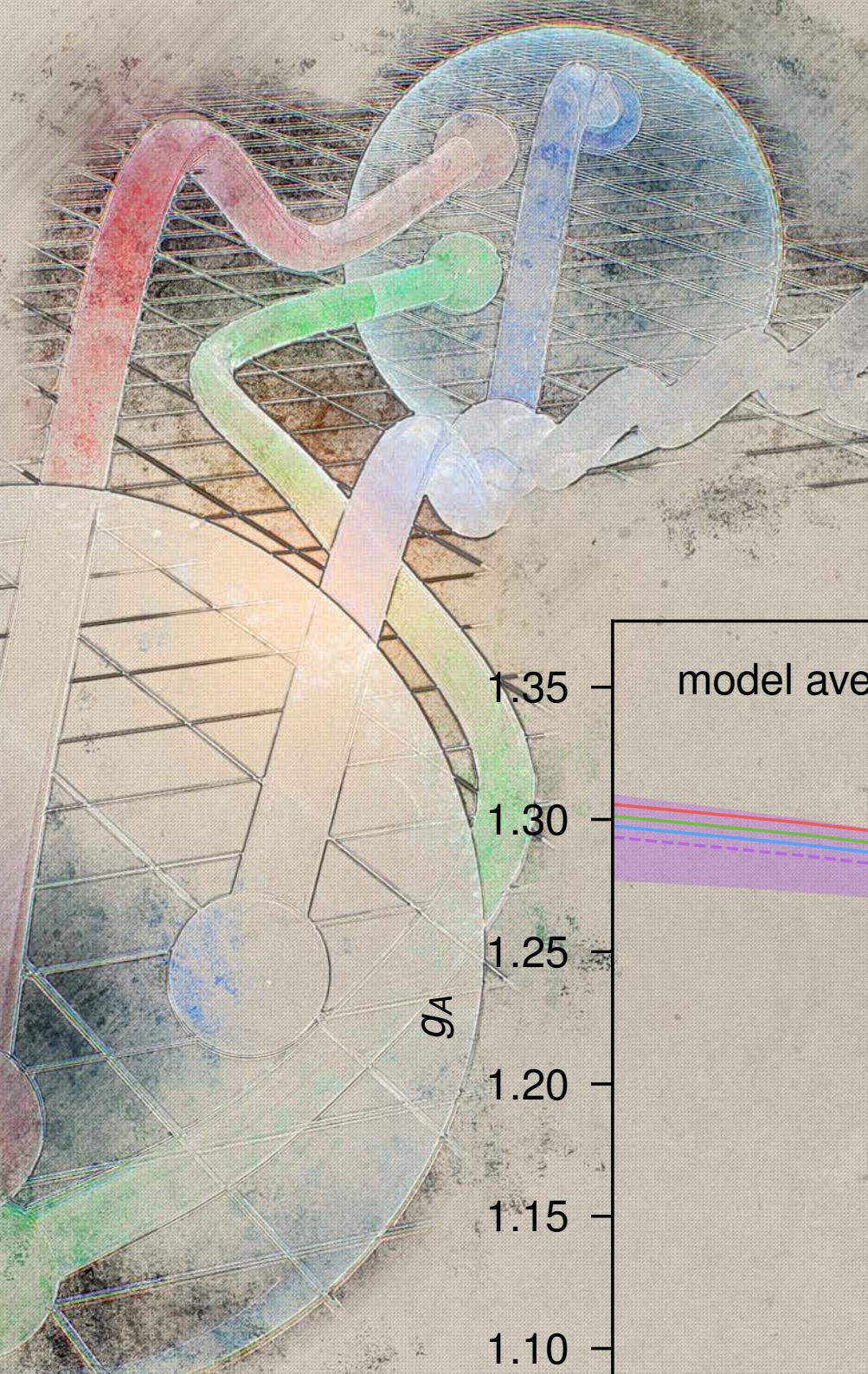
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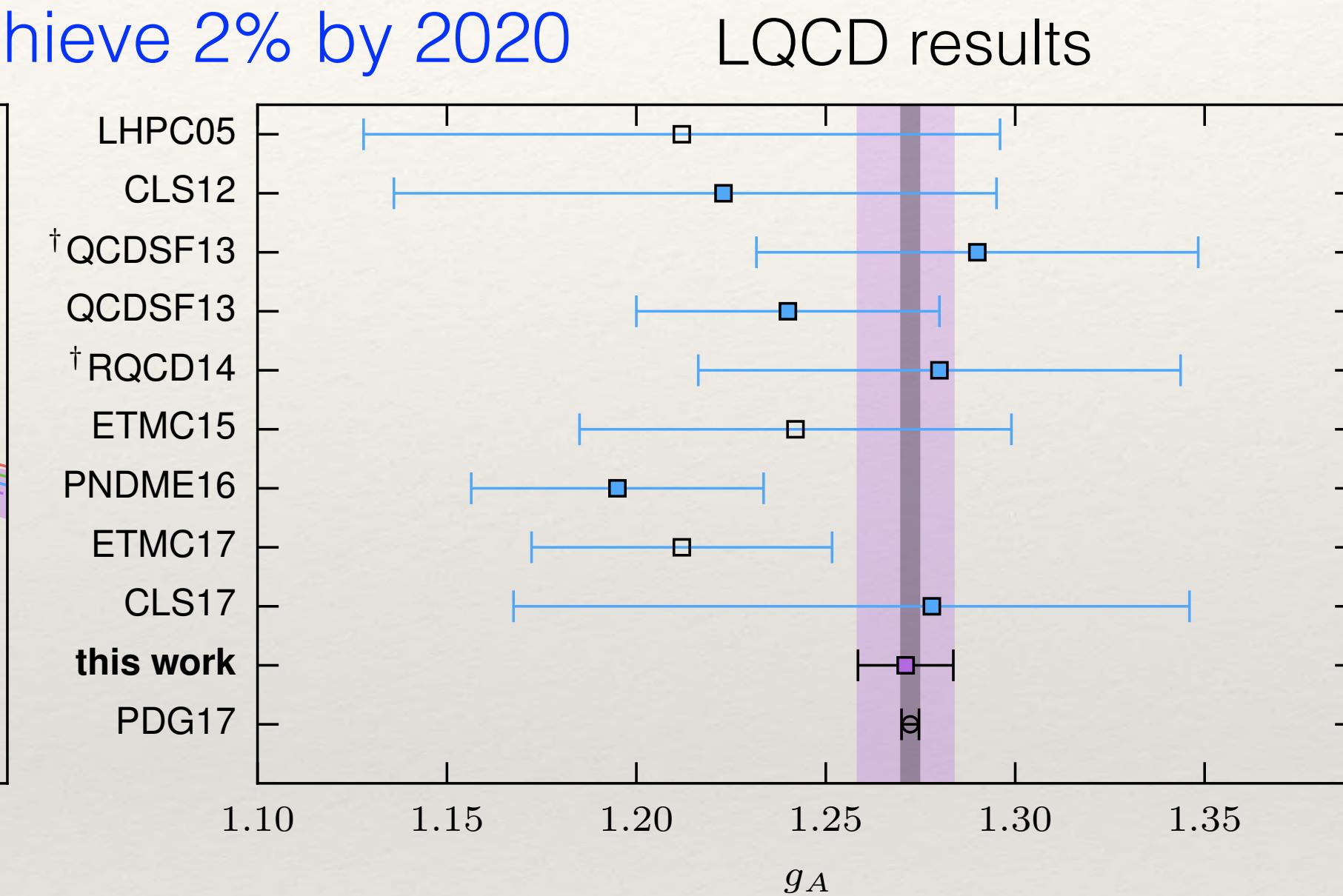
(CallLat)

\*not all in California



previously estimated to achieve 2% by 2020

[https://github.com/callat-qcd/project\\_gA](https://github.com/callat-qcd/project_gA)



$$\begin{aligned} g_A^{\text{QCD}} &= 1.2711(103)^s(39)^x(15)^a(19)^V(04)^I(55)^M \\ &= 1.2711(126) \end{aligned}$$

$$g_A^{\text{UCNA}} = 1.2772(020) \quad \text{experiment factor of 6 more precise}$$

$$g_A^{\text{PERKEO III}} = 1.27641(0055) \quad \text{experiment factor of 22 more precise}$$

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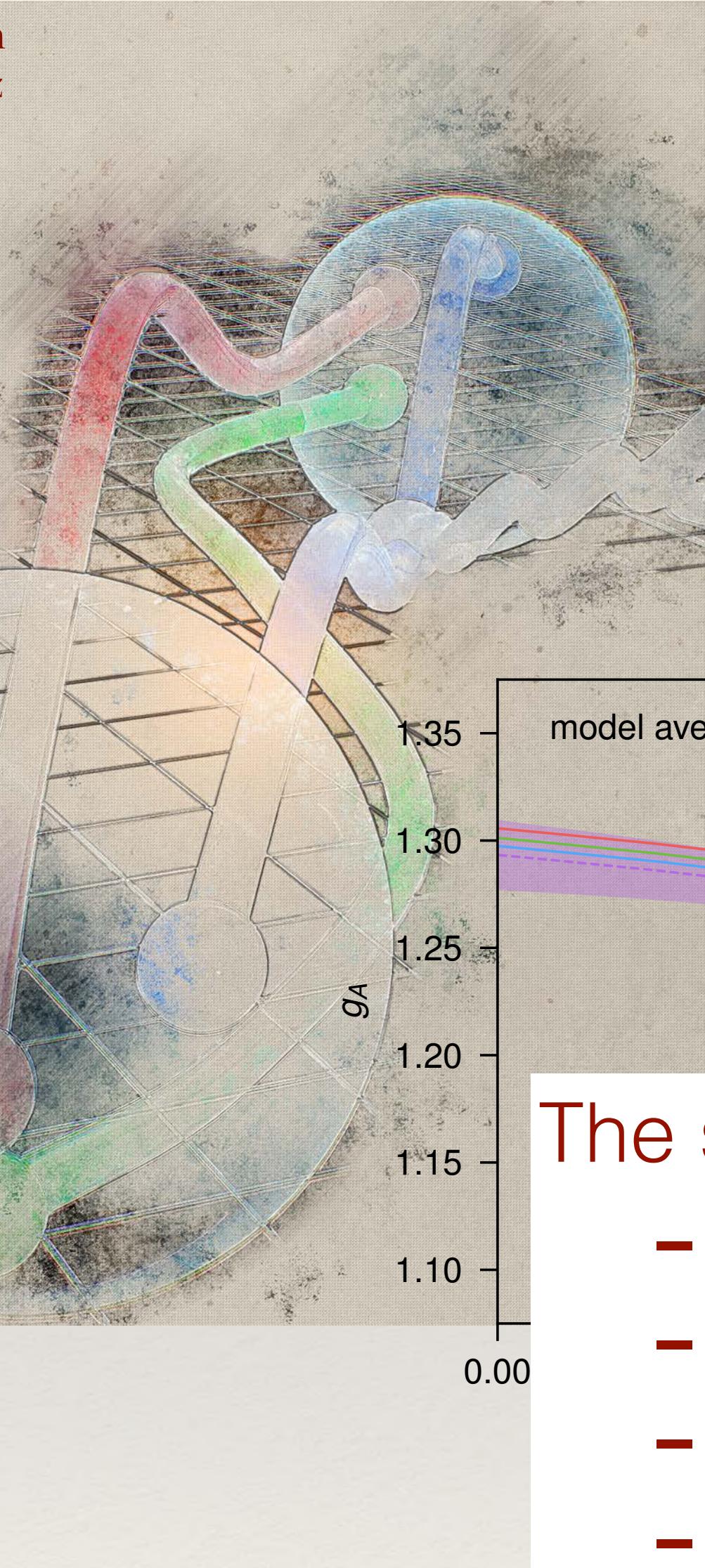
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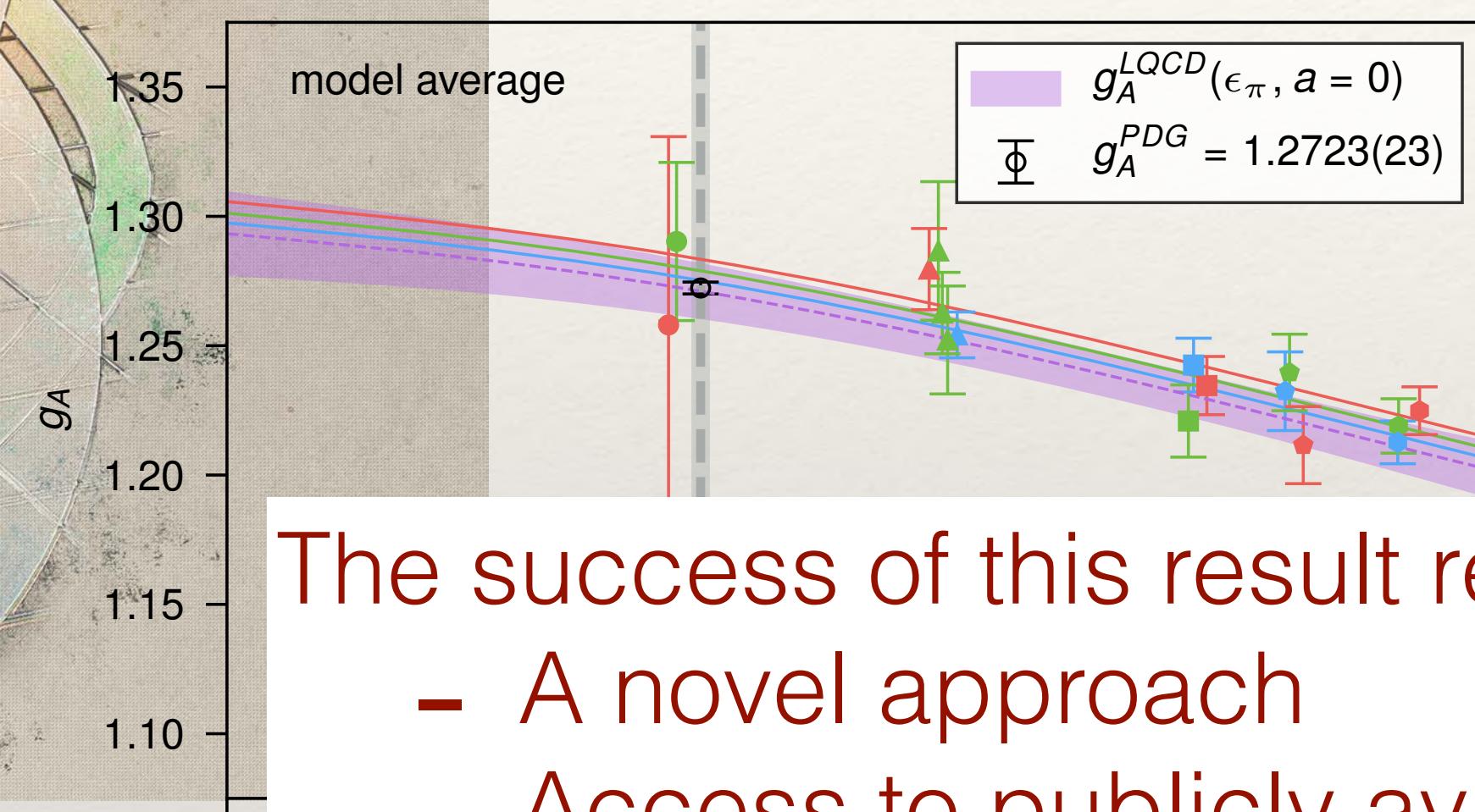


Nature 558 (2018) no.7708, 91-94 [arXiv:1805.12130]

## A per-cent-level determination of the nucleon axial coupling from quantum chromodynamics

[https://github.com/callat-qcd/project\\_gA](https://github.com/callat-qcd/project_gA)

previously estimated to achieve 2% by 2020



The success of this result required:

- A novel approach
- Access to publicly available configurations (MILC)
- Ludicrously fast GPU code (Kate Clark of NVIDIA)
- Access to Leadership Class Computing (INCITE)

$$= 1.2711(126)$$

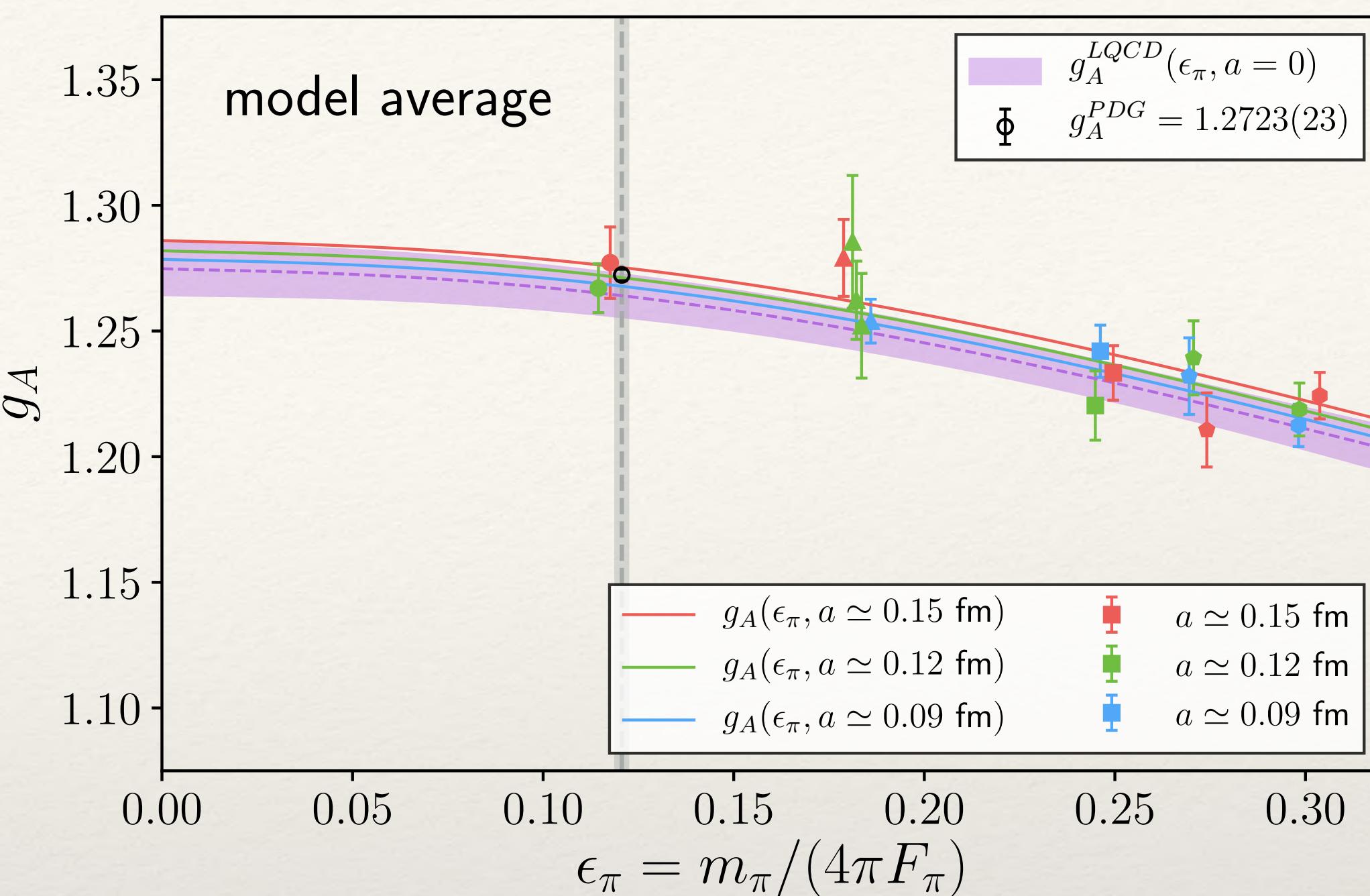
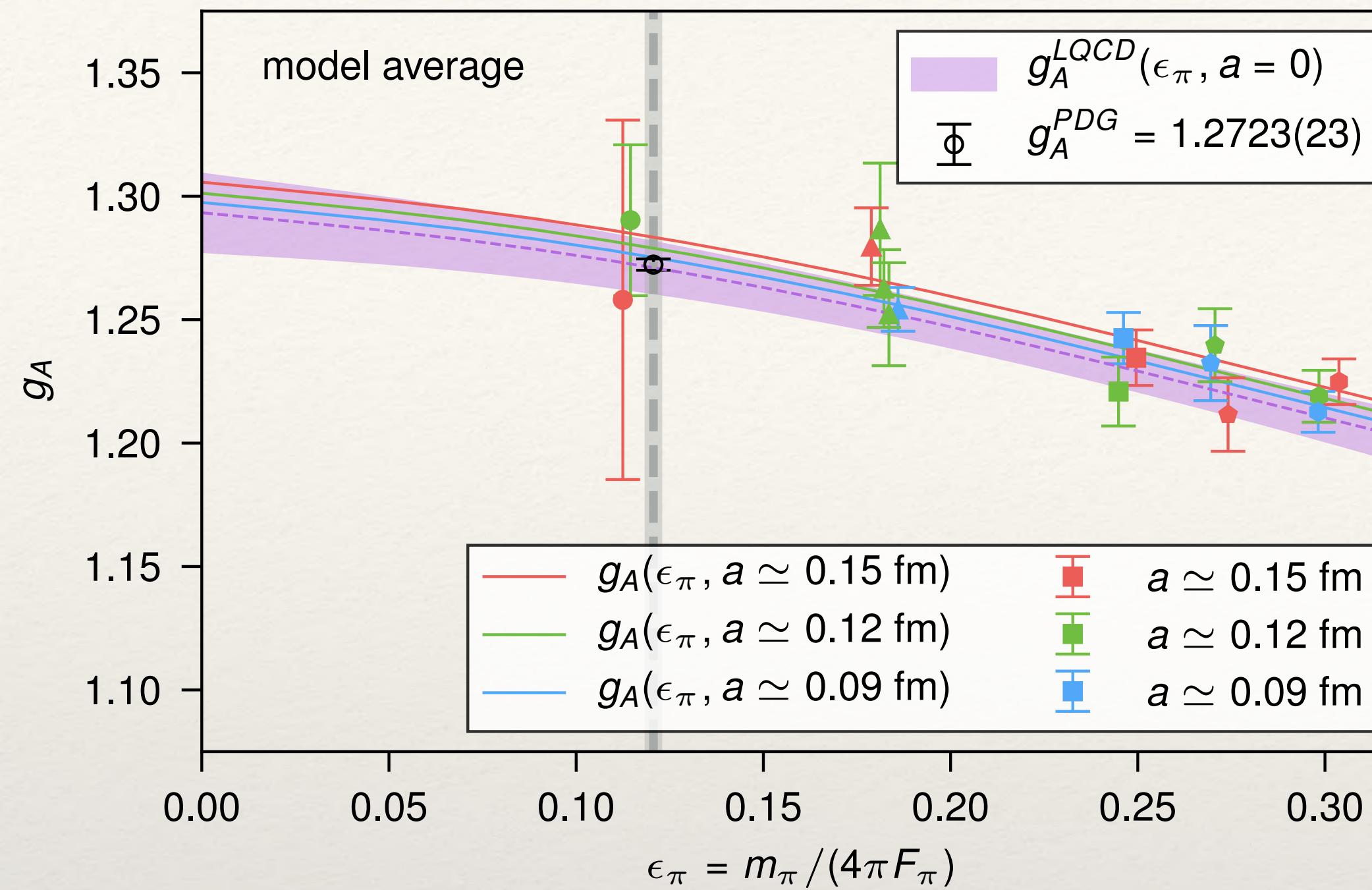
$$g_A^{\text{UCNA}} = 1.2772(020) \quad \text{experiment factor of 6 more precise}$$

$$g_A^{\text{PERKEO III}} = 1.27641(0055) \quad \text{experiment factor of 22 more precise}$$



DOE Topical Collaboration  
Double Beta Decay

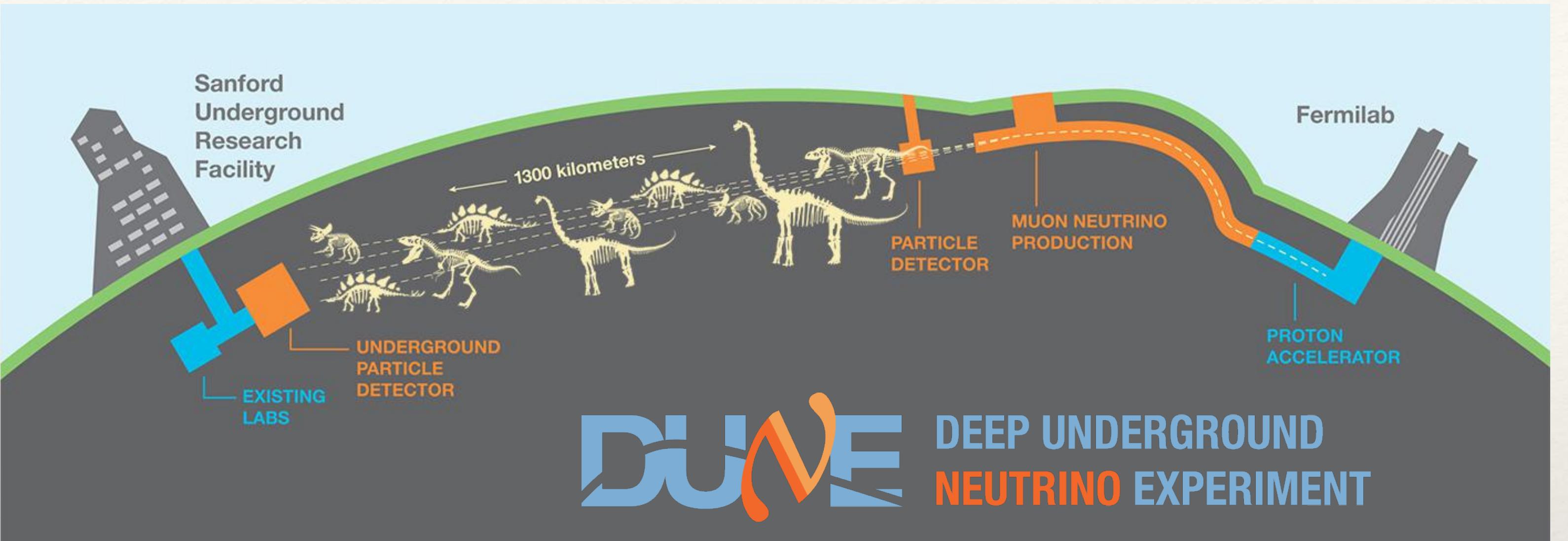




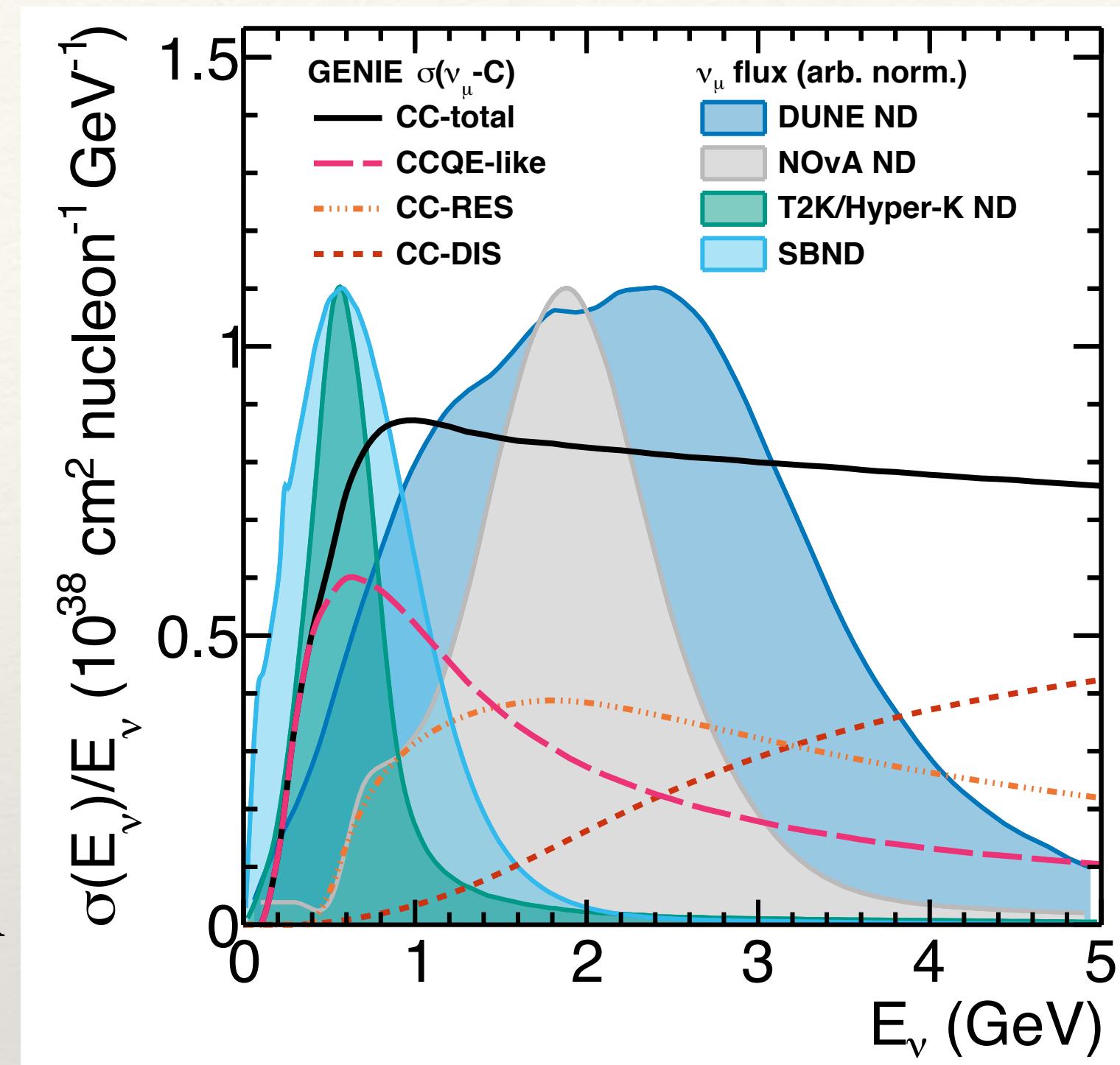
- The **a12m130** ( $48^3 \times 64 \times 20$ ) with 3 sources cost as much as all other ensembles combined
  - 2.5 weekends on Sierra → 16 srcs
  - Now, 32 srcs (un-constrained, 3-state fit)
- We generated a new **a15m135XL** ( $48^3 \times 64$ ) ensemble (old **a15m130** is  $32^3 \times 48$ )
  - $M\pi L = 4.93$  (old  $M\pi L = 3.2$ )
  - $L_5 = 24$ ,  $N_{src} = 16$
- We are running  $g_A(Q^2)$  on Summit this year (DOE INCITE)
- We anticipate improving  $g_A$  to ~0.5%

$g_A = 1.2711(125) \rightarrow 1.2641(93) [0.74\%]$

# Nucleon Axial Form Factor



- DUNE and Hyper-K science goals reliant upon accurate and precise modeling of  $\nu$ -A cross sections
- The 50-year old pion-production model that is currently used in event generators was described by its authors as *naive and obviously wrong in its simplicity* [FKR]
- No experimental path forward to improve these basic  $\nu$ N reactions
- With Lattice QCD, we can pin down certain contributions to the cross section to minimize the modeling uncertainty
- $\nu n \rightarrow \ell p$ ,  $\nu N \rightarrow \ell \Delta$ ,  $\nu N \rightarrow \ell N \pi$ ,  $\nu NN \rightarrow \nu NN$ , ...

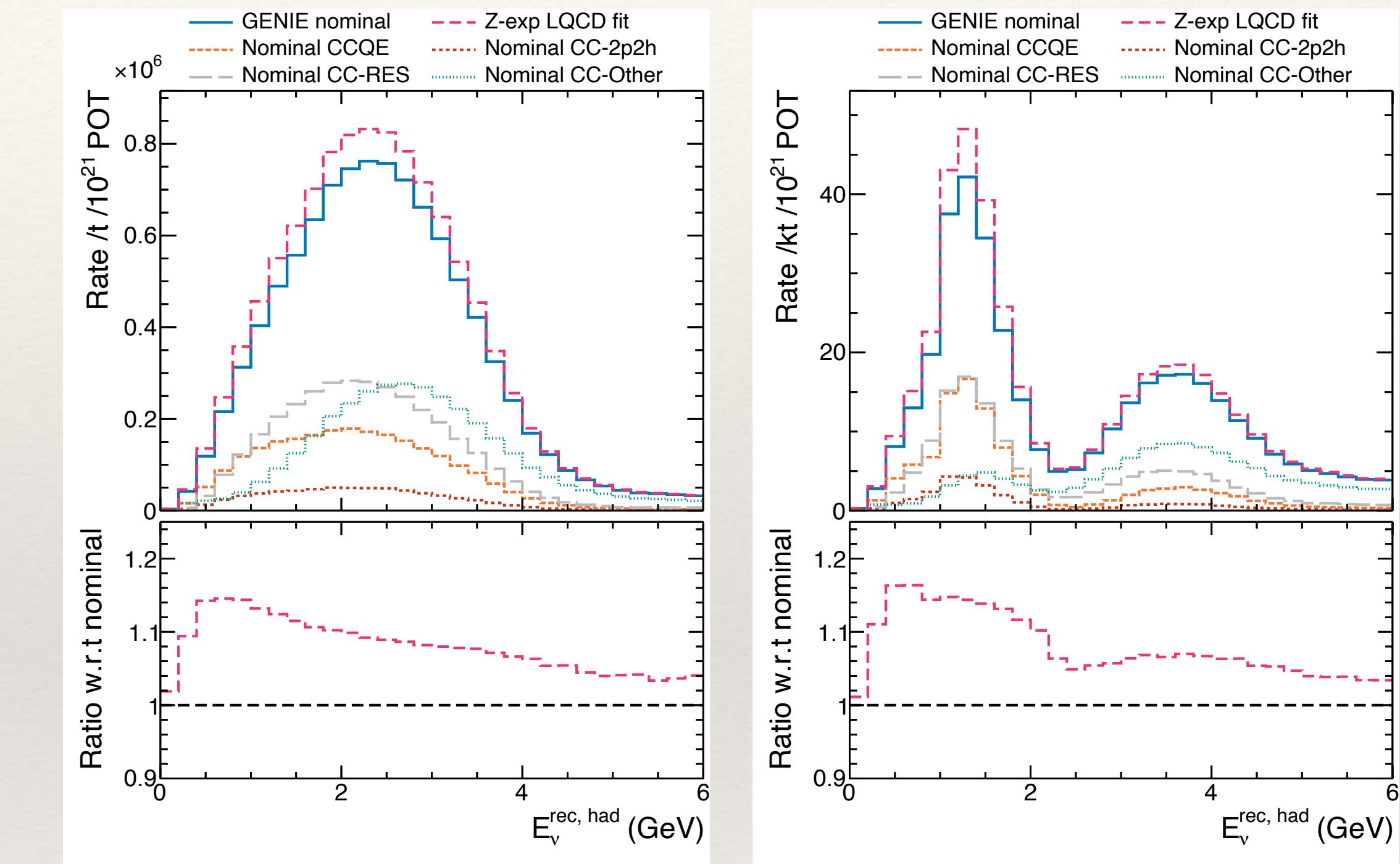
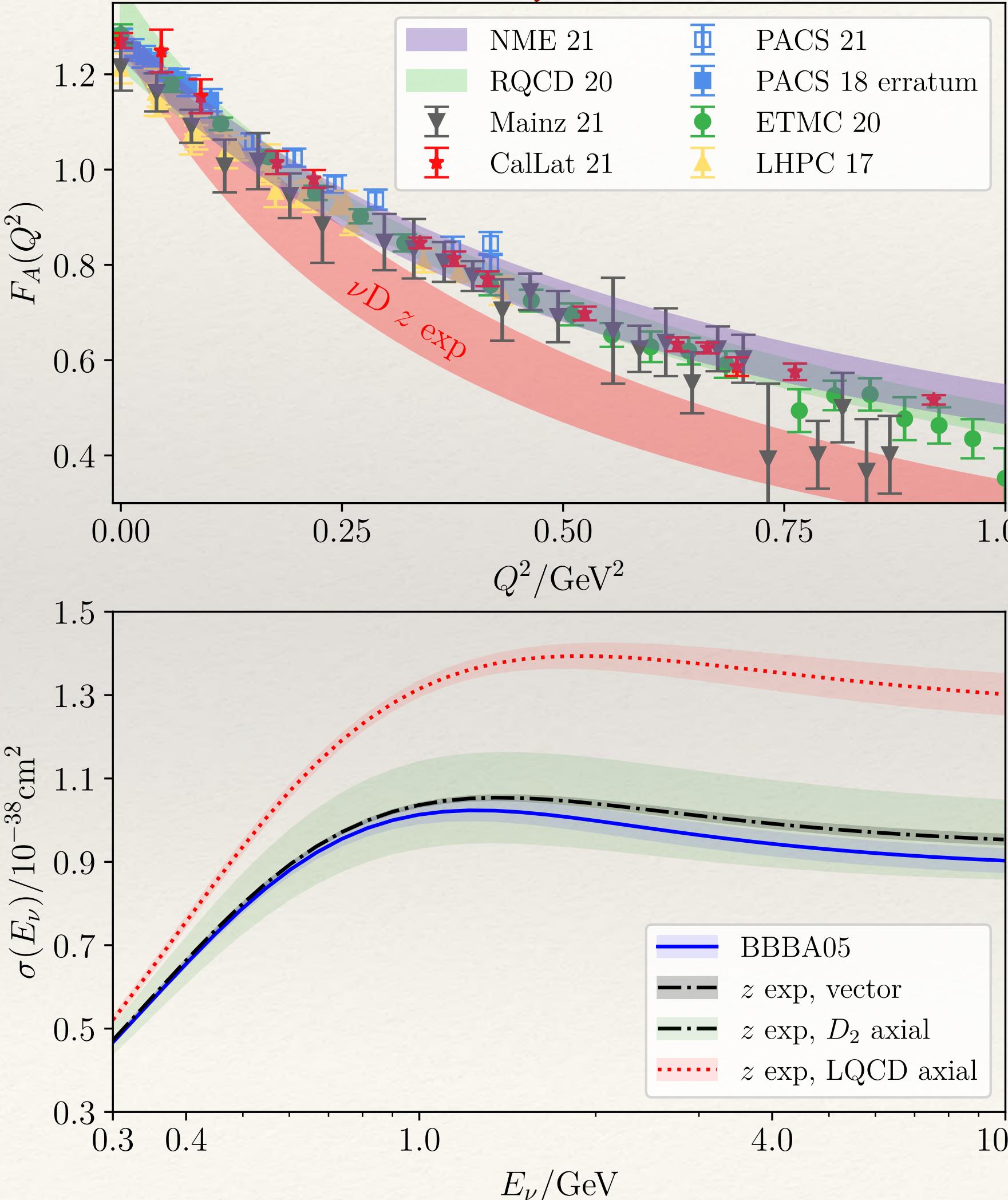


Unoscillated flux from different  $\nu$ -A mechanisms

[FKR] Feynman, Kislinger, Ravndal  
PRD 3 (1971)

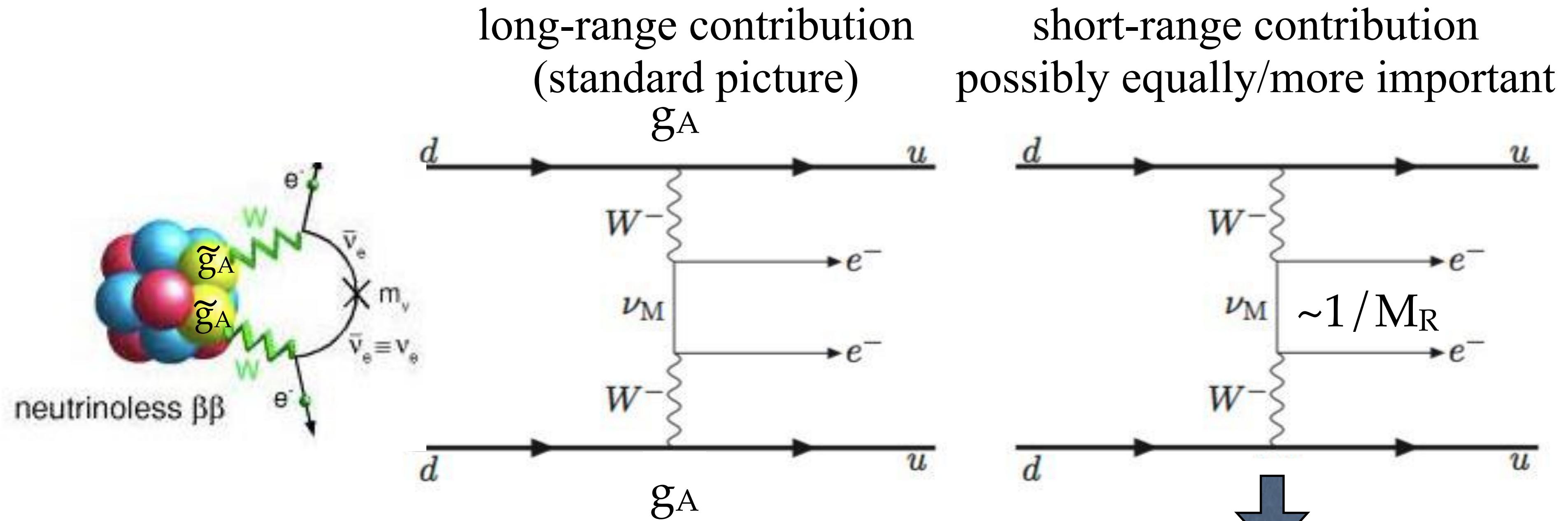
# Nucleon Axial Form Factor

- Current lattice QCD results show significant tension for even the simplest quasi-elastic form factor - [A. Meyer, A. Walker-Loud, C. Wilkinson, Ann. Rev. Nucl. Part. Sci. 72 \(2022\)](#)



- Within a couple years, lattice QCD will deliver “final” FA results
- We are not expecting any surprise systematics that will change this picture
- Frontier is the delta-resonance and pion-production amplitudes

# Neutrinoless Double Beta-Decay

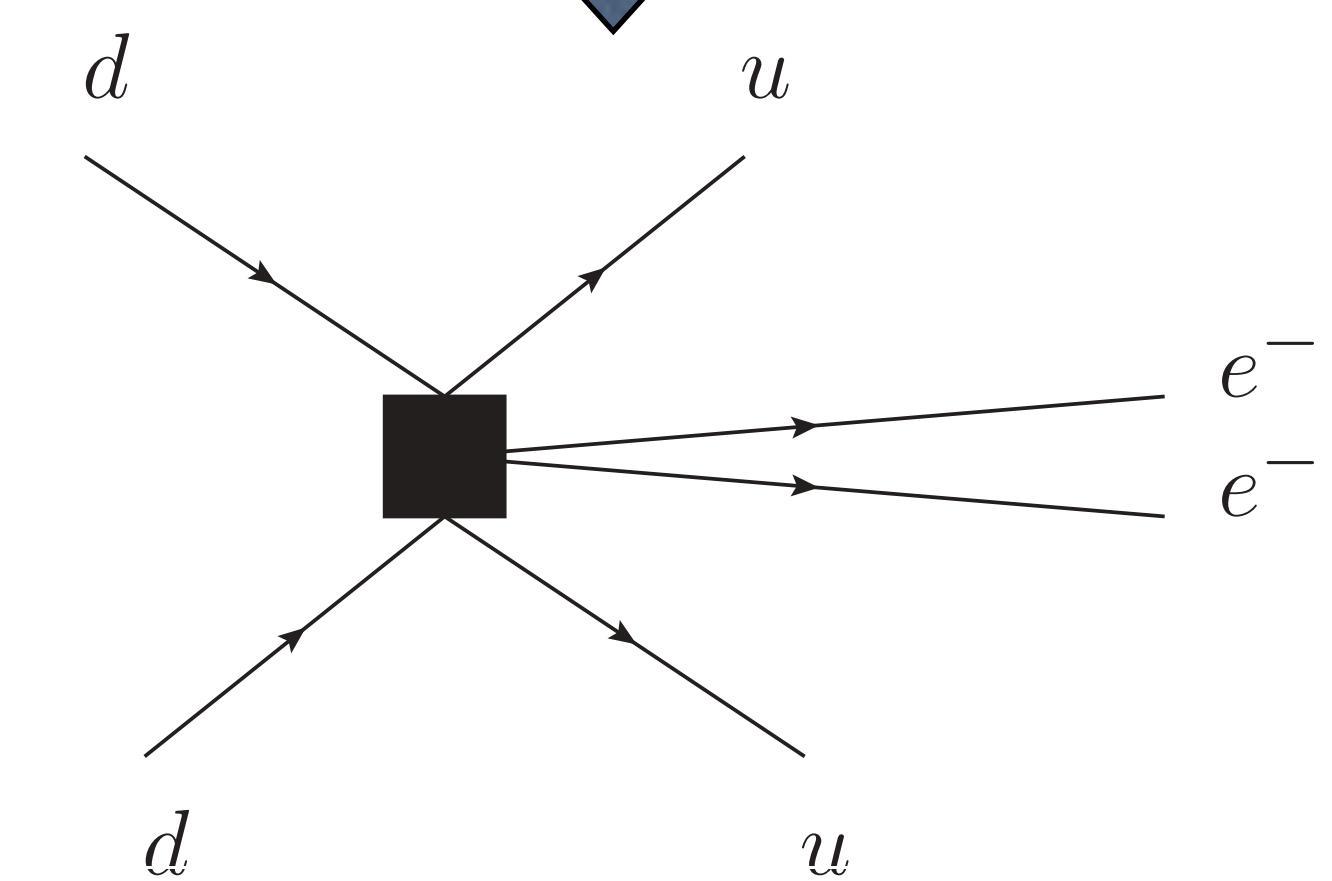


Long Range: lattice QCD can help understand “quenching” of  $g_A$  in a nucleus -  
although - see Gysbers et al. Nature Phys (2019) [1903.00047]

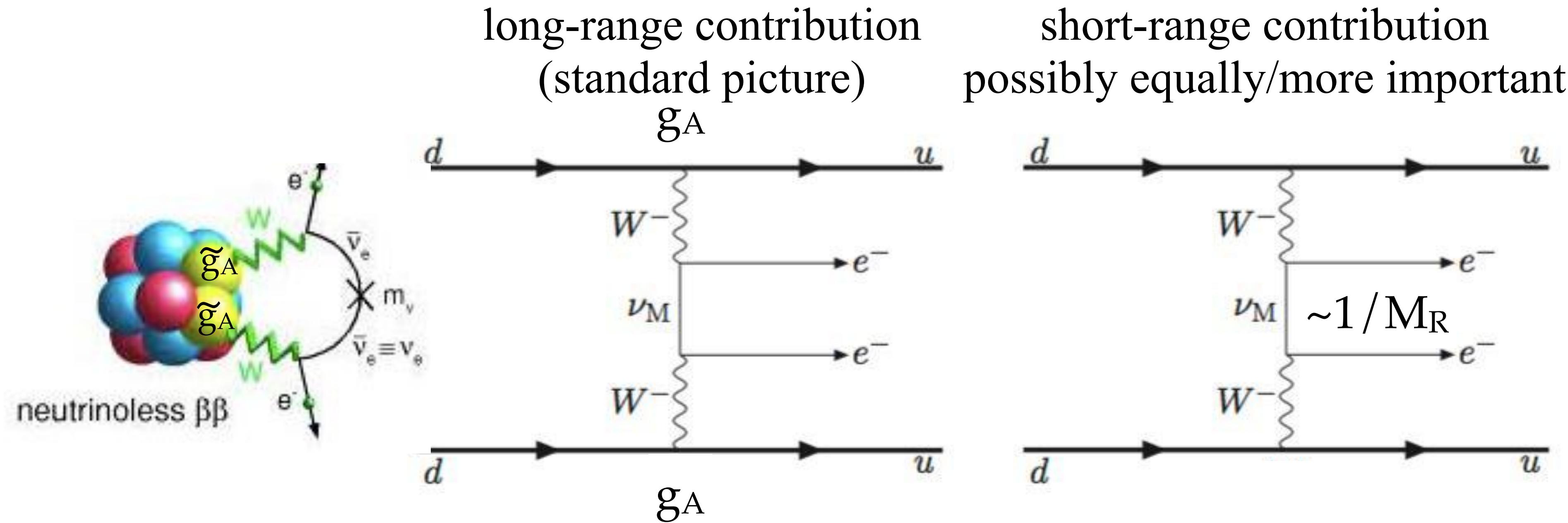
Short Range: lattice QCD is the ONLY theoretical tool we have to understand  
these contributions with quantified uncertainties

Lattice QCD: compute 2-nucleon matrix elements to determine unknown  
couplings/transition rates

Many Body Nuclear Effective Theory: take lattice QCD results as input and  
compute transition rate in nucleus (Haxton, others)



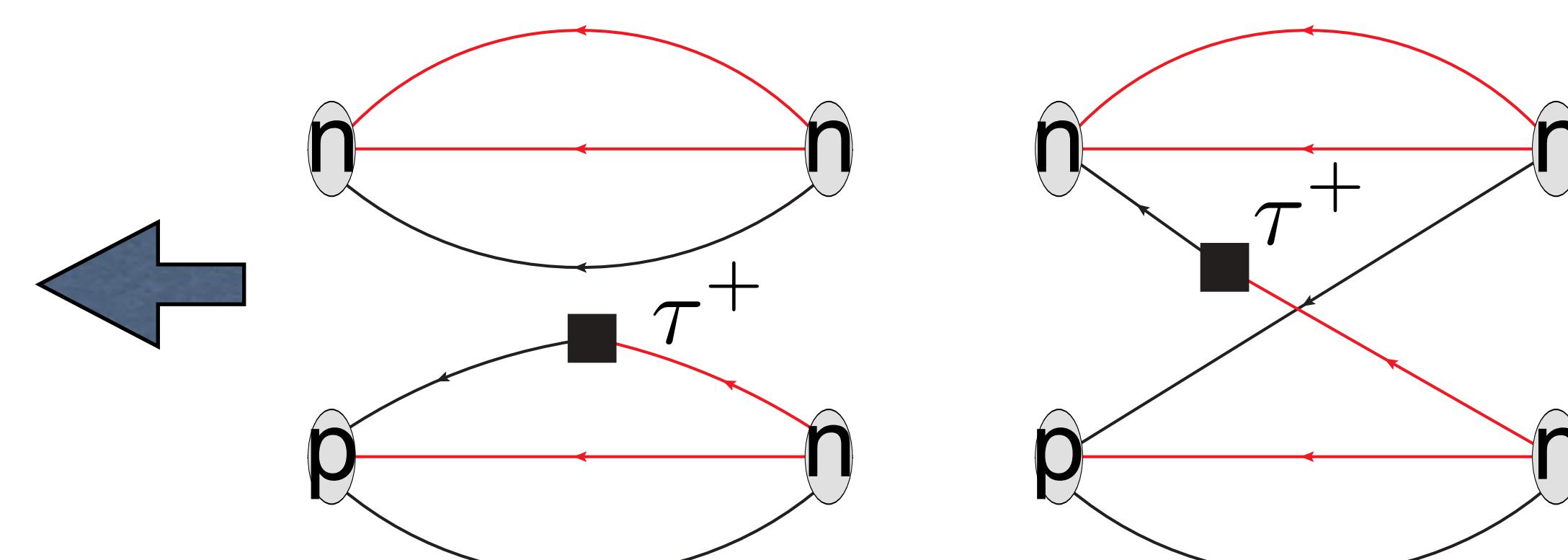
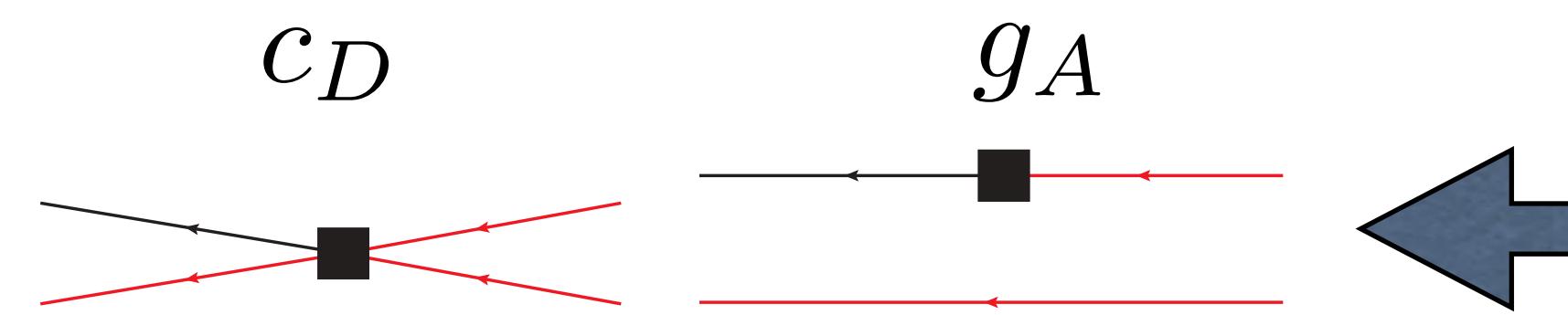
# Neutrinoless Double Beta-Decay



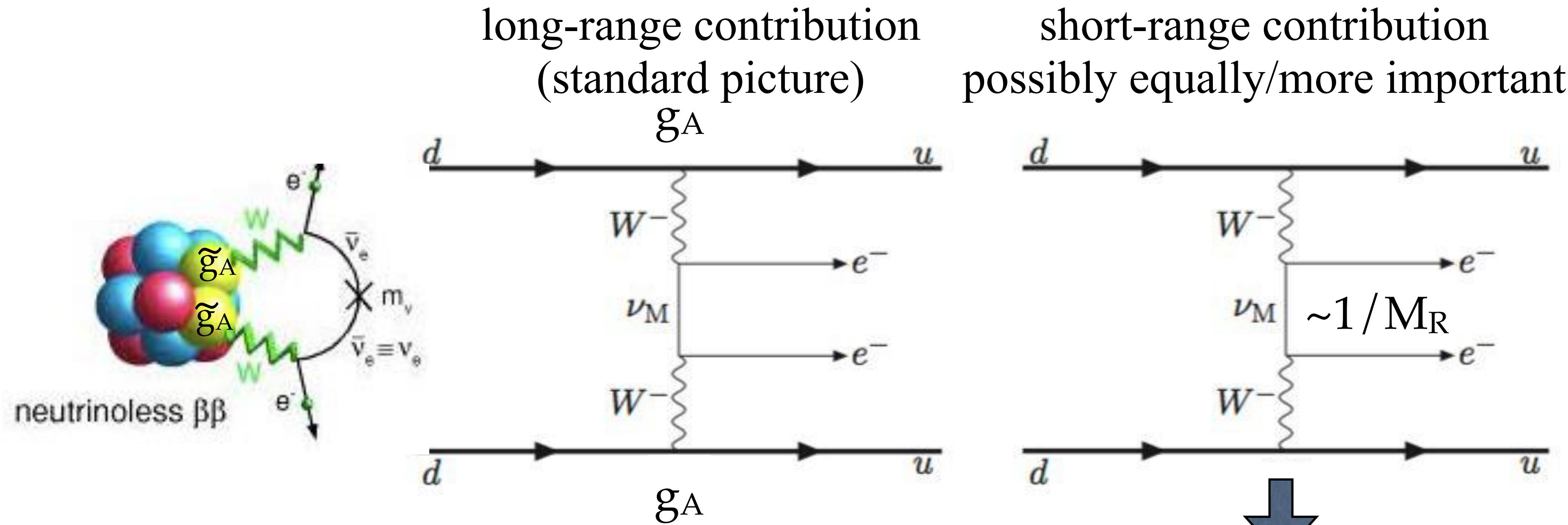
*Long Range Contribution*

Lattice QCD

EFT Level

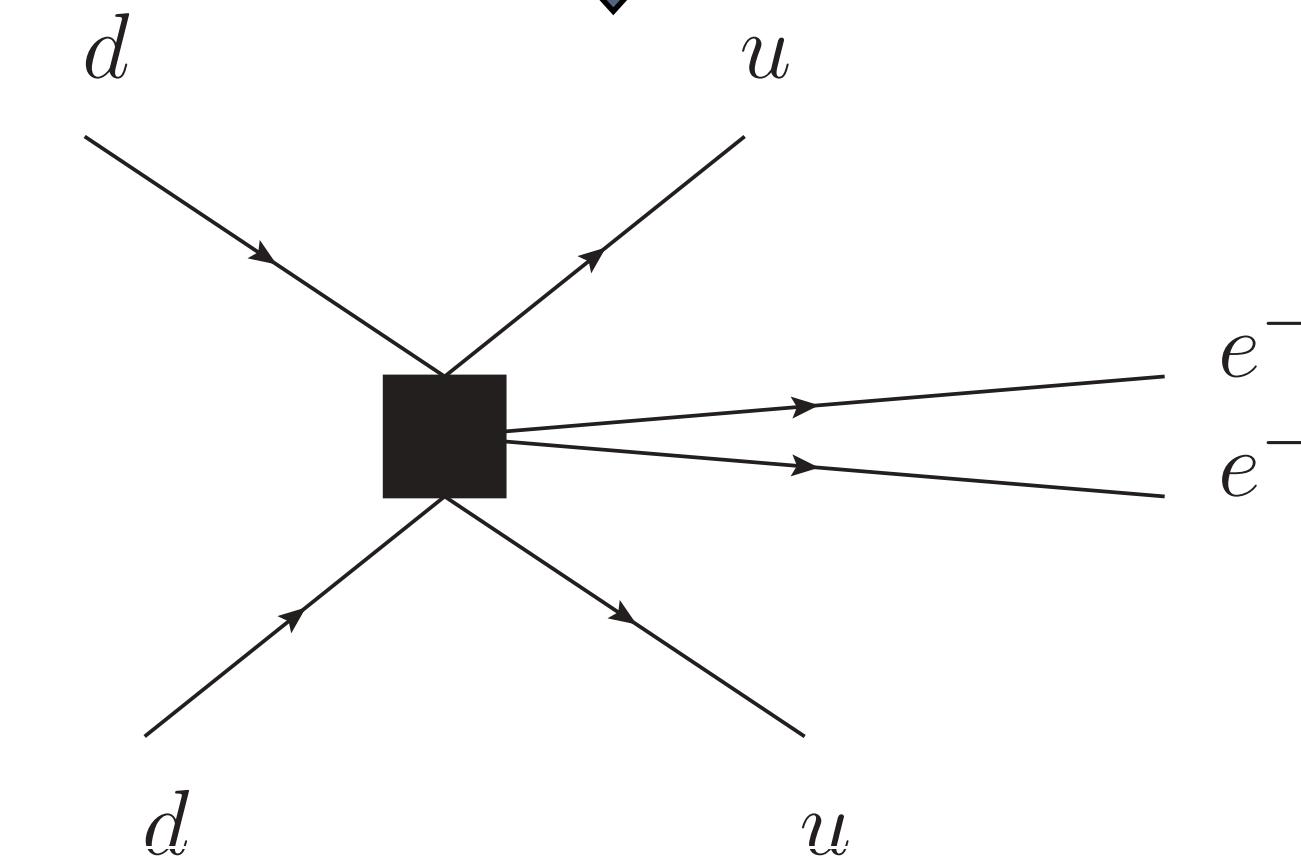


# Neutrinoless Double Beta-Decay



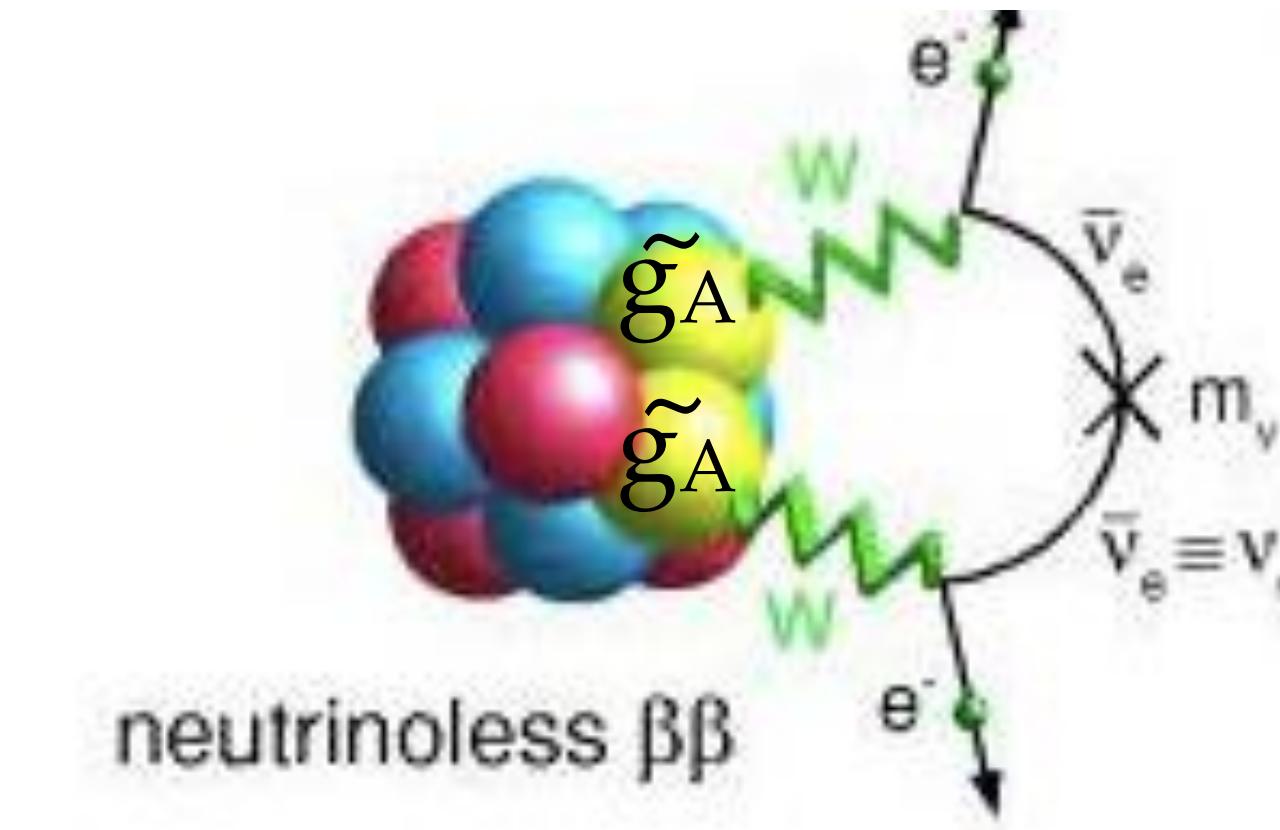
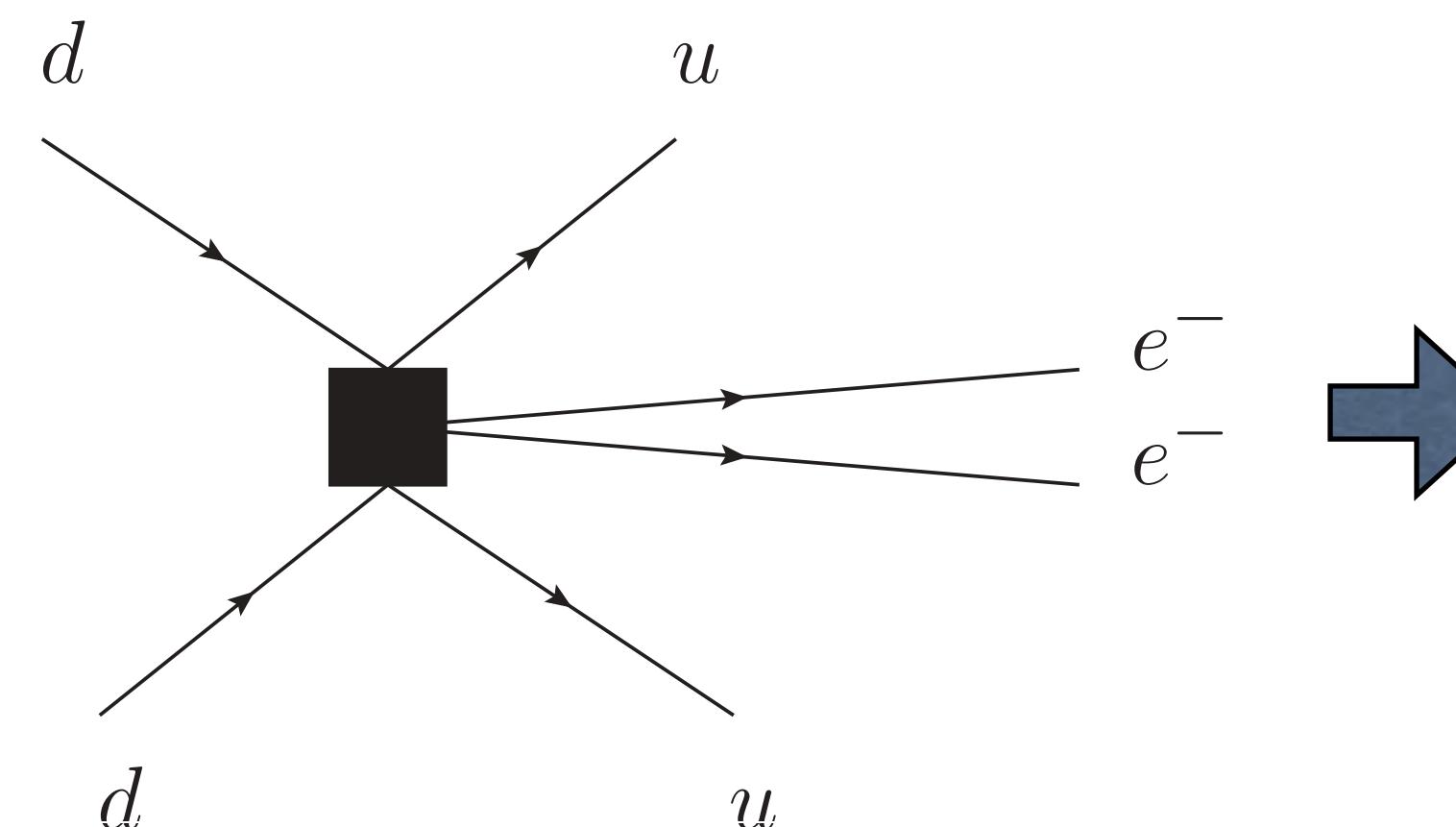
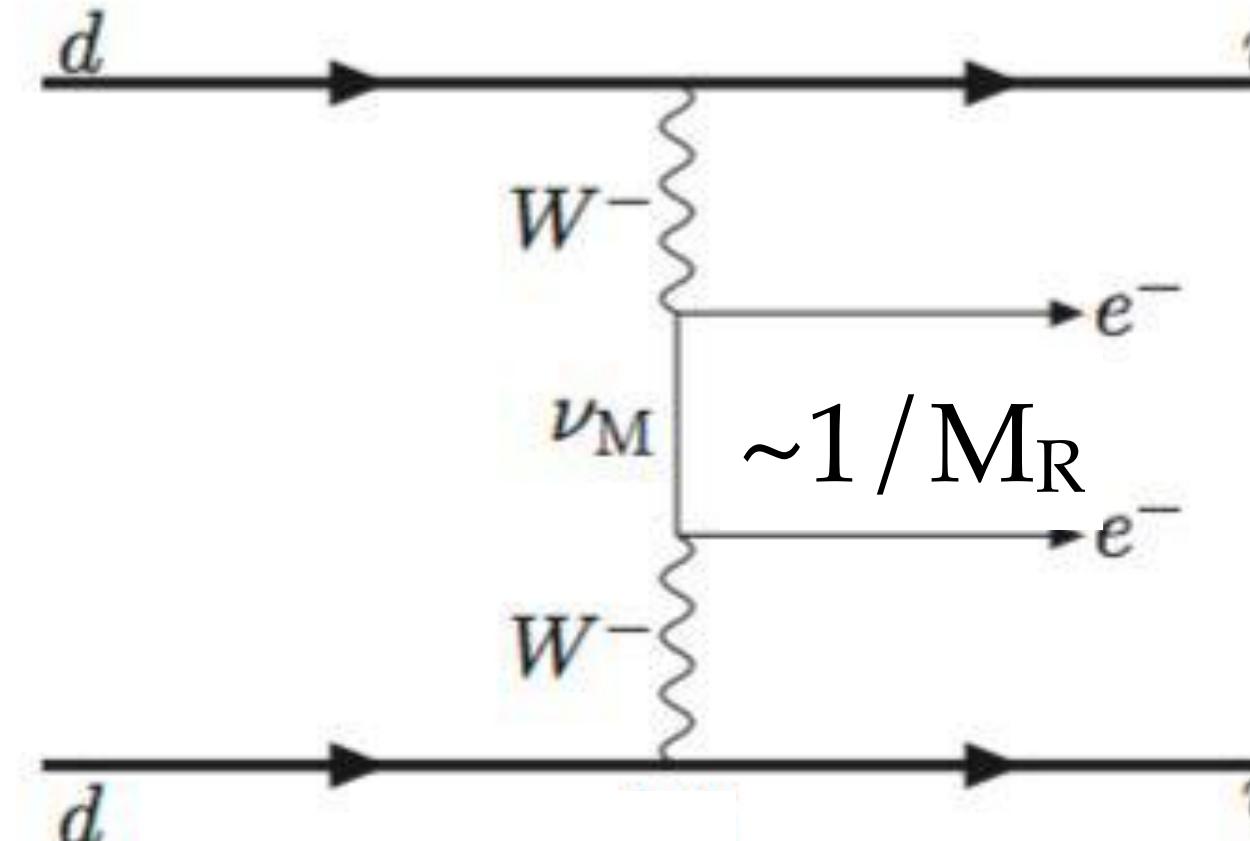
## *Short Range Contribution*

Need to know value of 4-quark matrix element in two-nucleon systems: LQCD is the only tool we have as we are not able to measure  $0\nu\beta\beta$  in few-nucleon systems - so need fundamental theory calculation

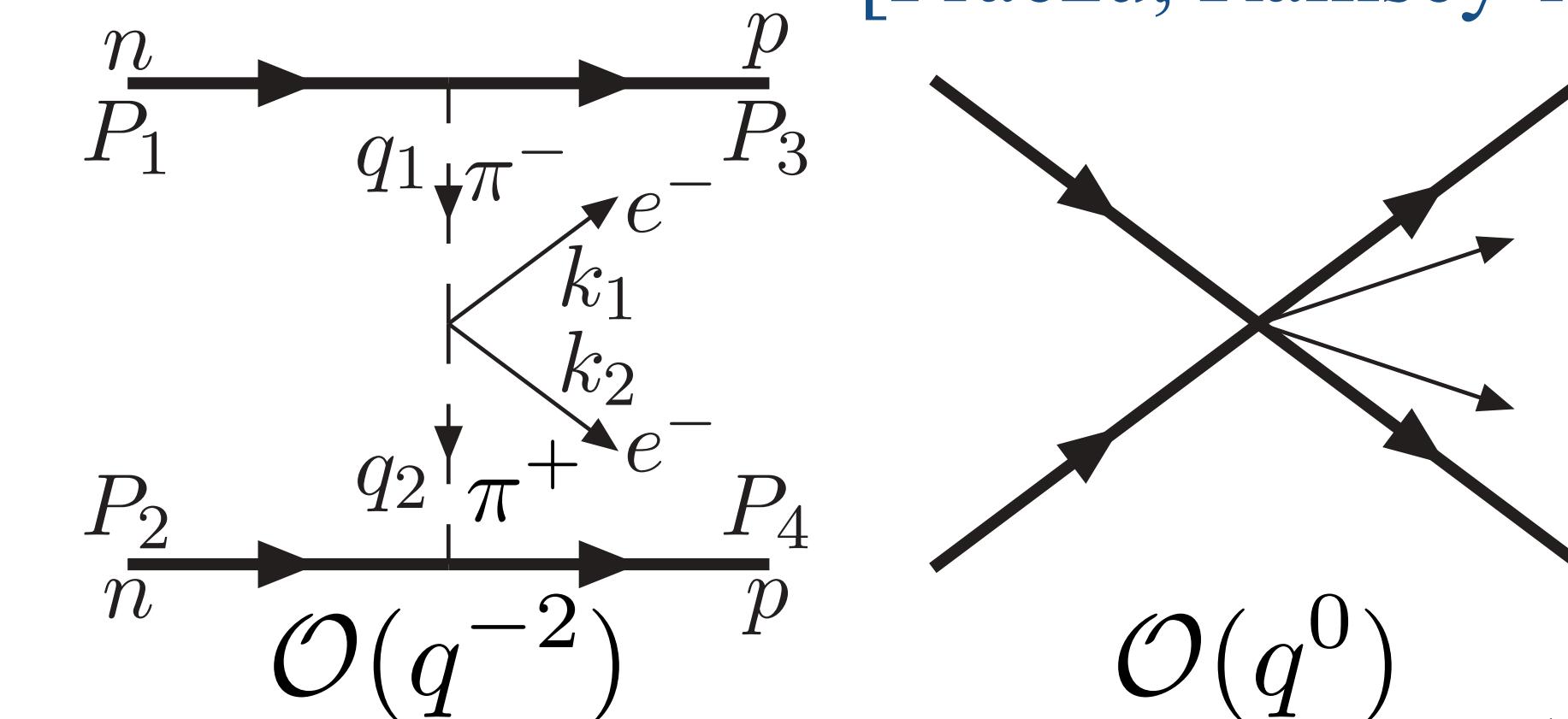


# Neutrinoless Double Beta-Decay

Short-range contribution: probe for heavy physics

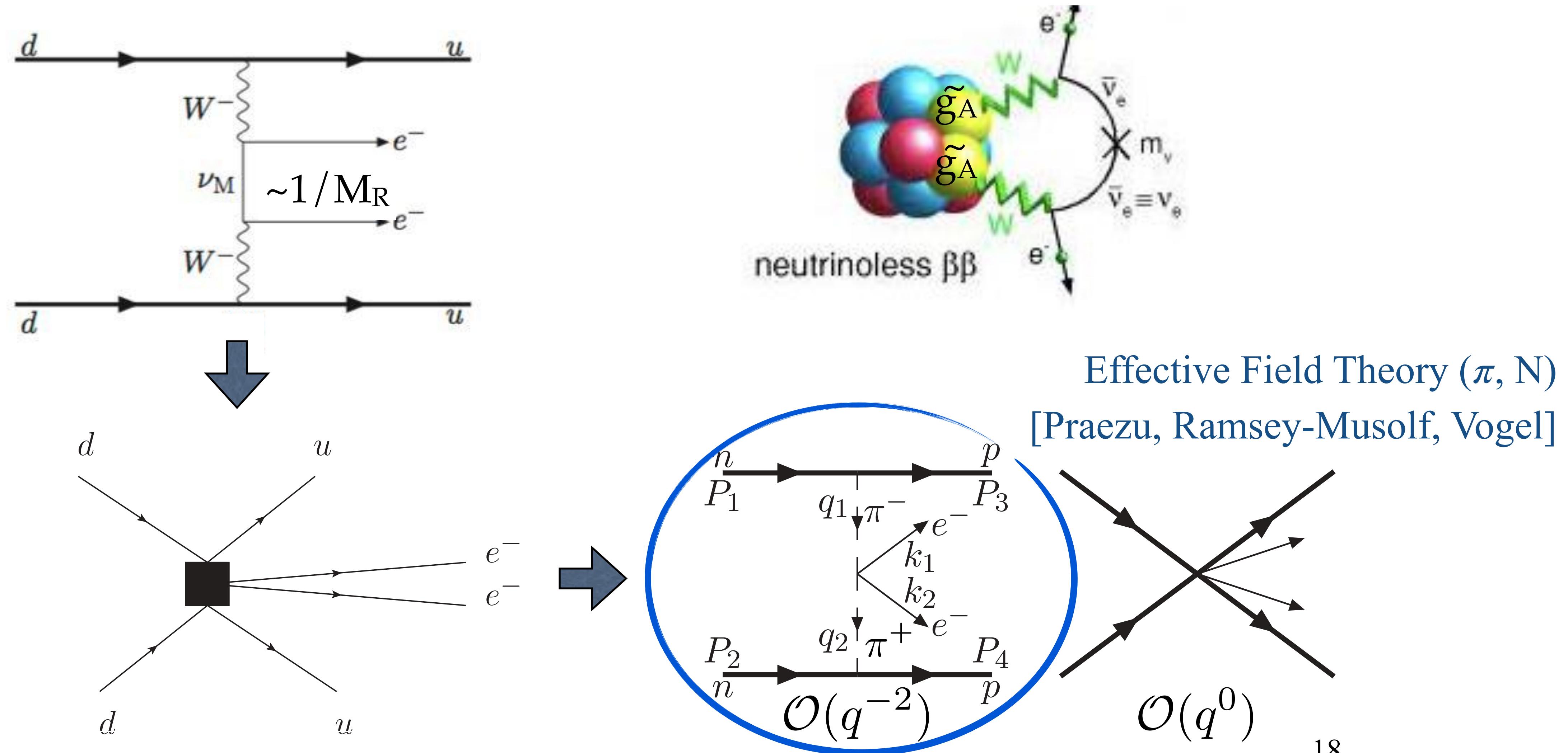


Effective Field Theory ( $\pi, N$ )  
[Praezu, Ramsey-Musolf, Vogel]

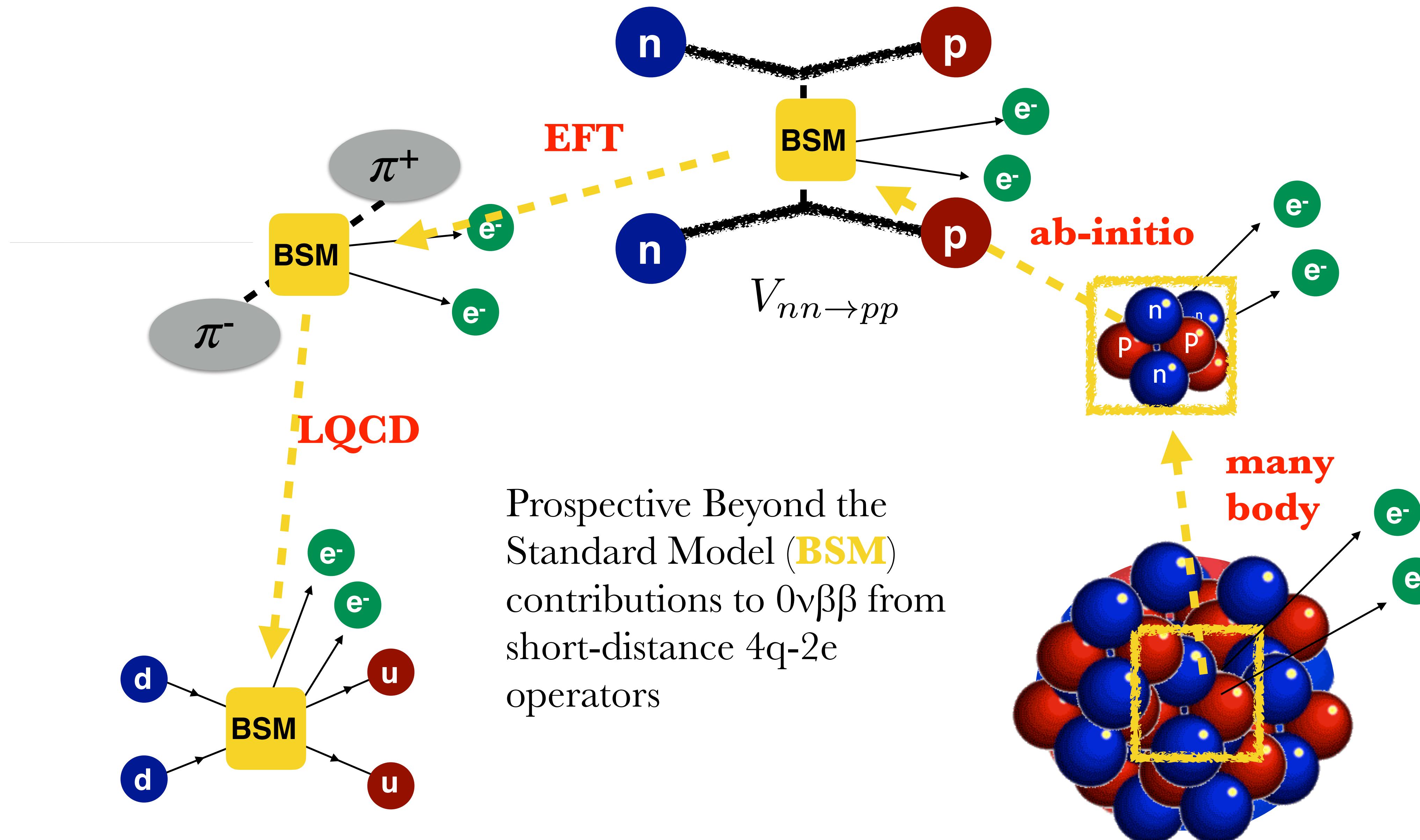


# Neutrinoless Double Beta-Decay

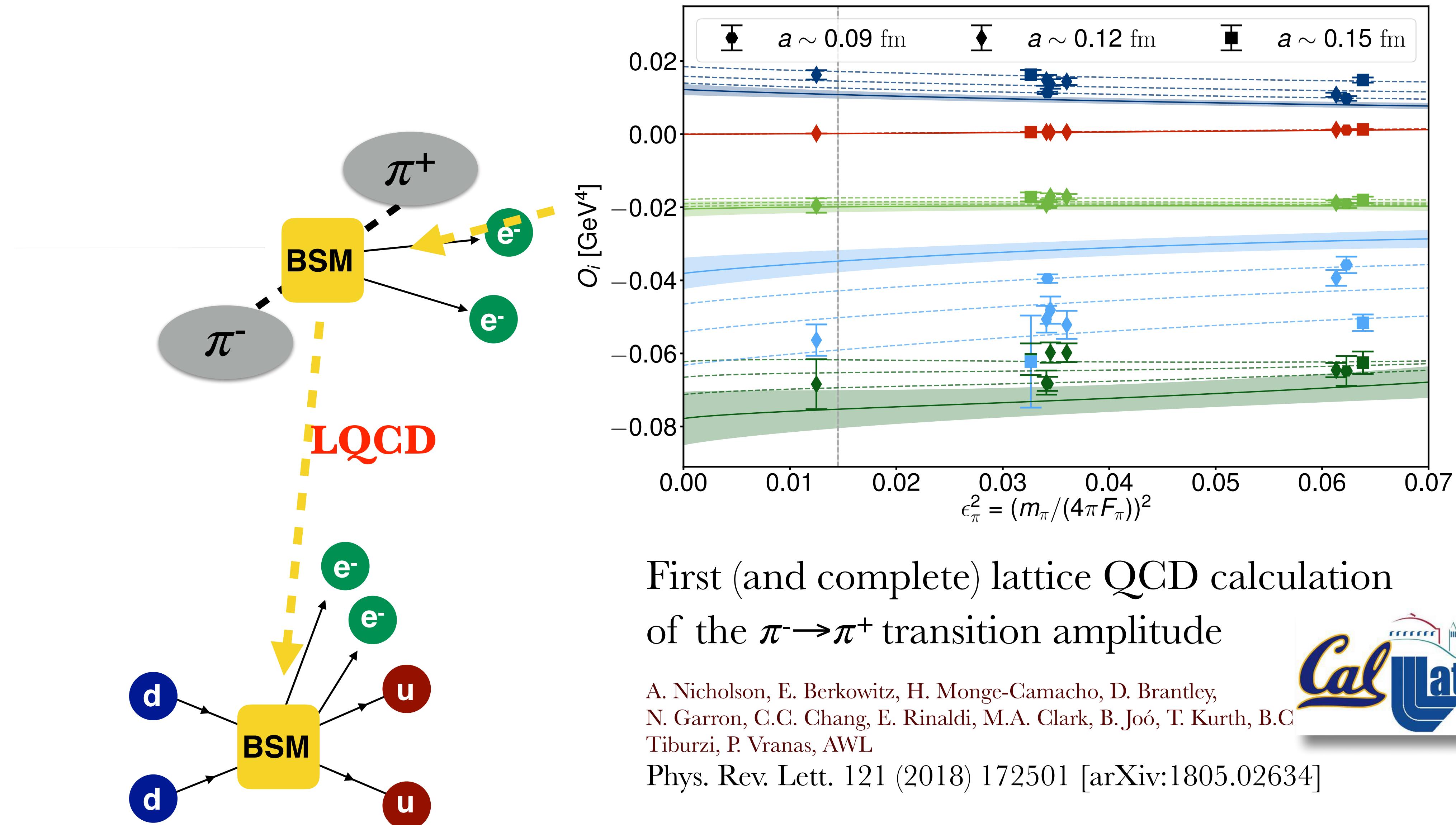
Short-range contribution: probe for heavy physics



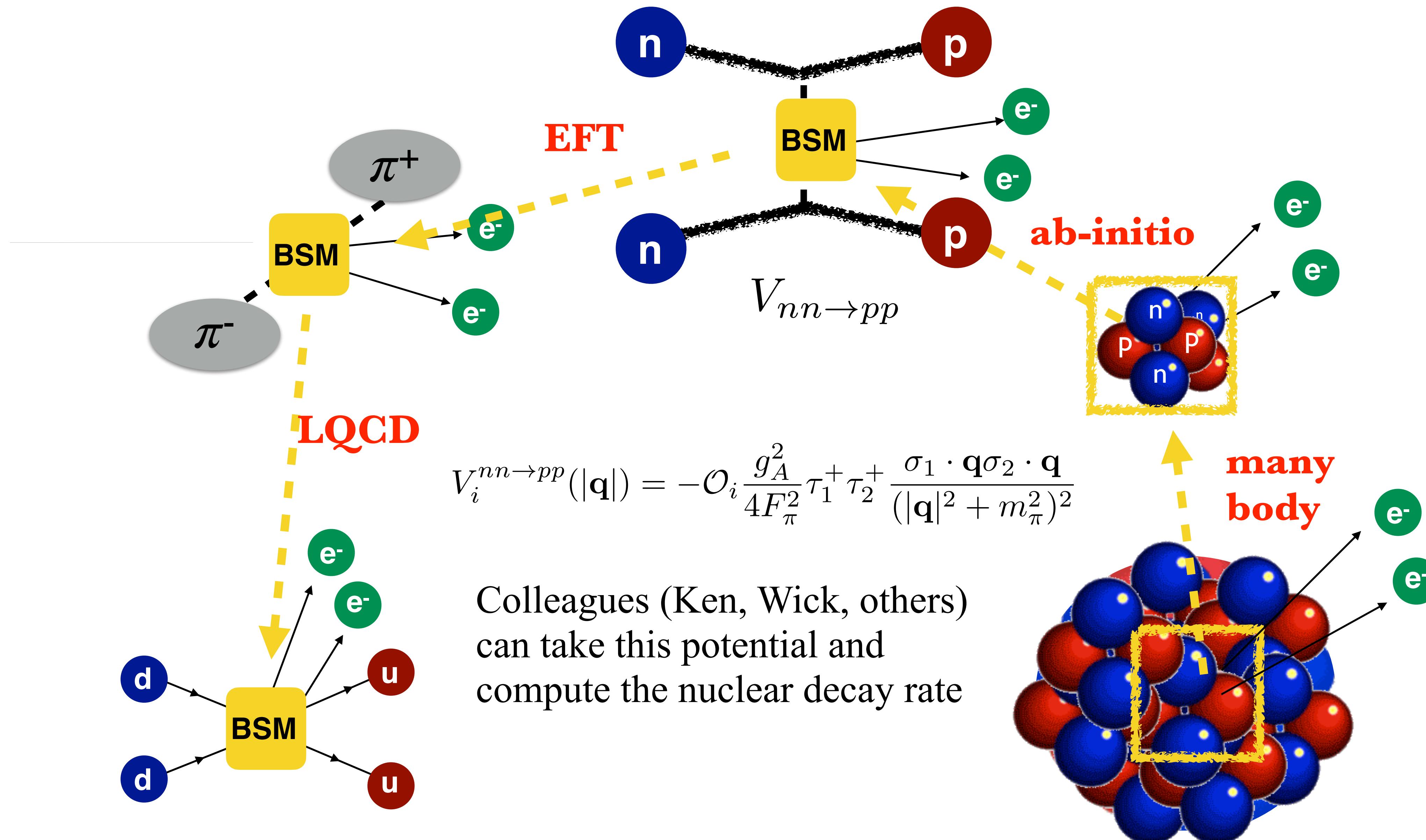
# Lattice QCD for Neutrinoless Double Beta-Decay



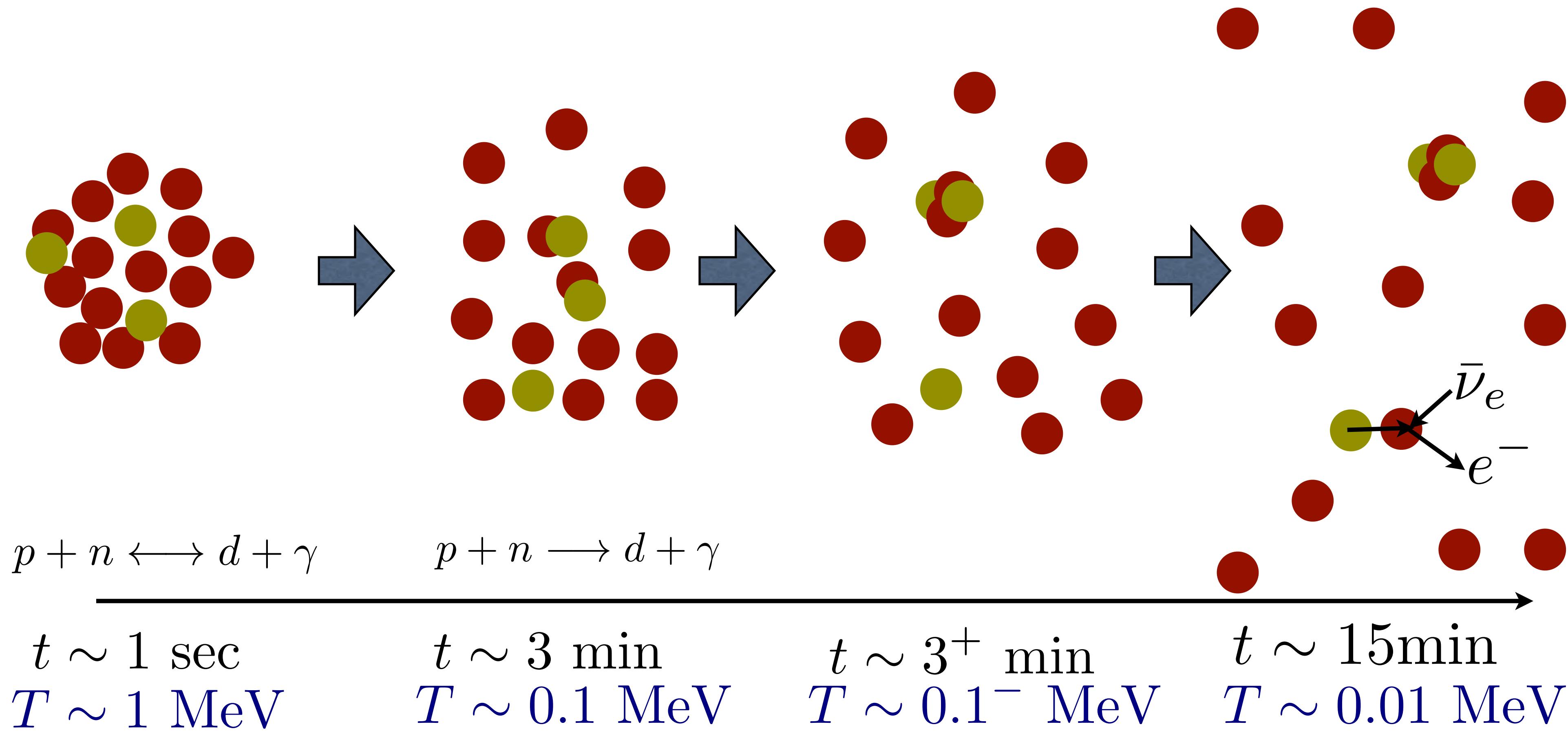
# Lattice QCD for Neutrinoless Double Beta-Decay



# Lattice QCD for Neutrinoless Double Beta-Decay



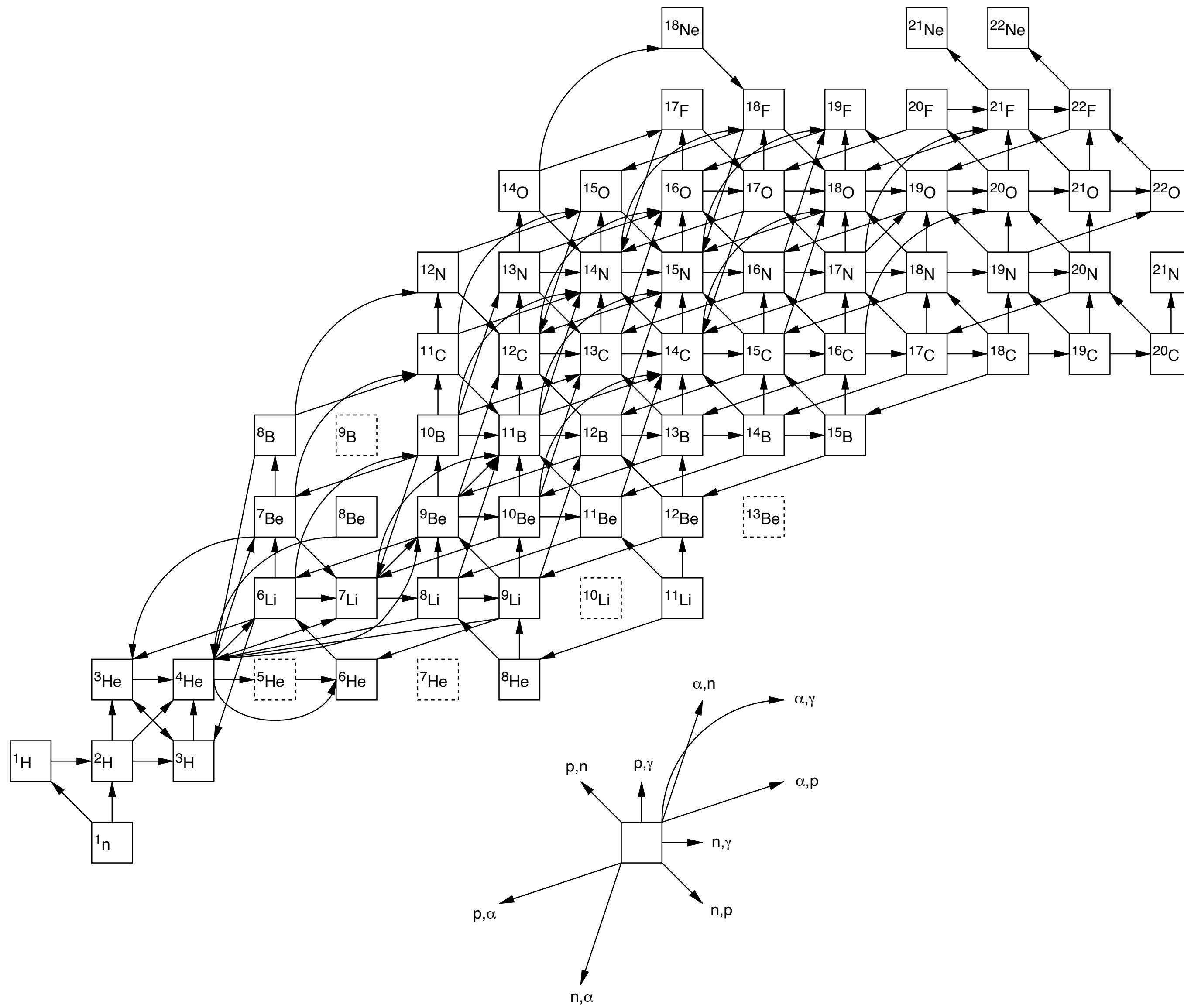
# Primordial Abundance of Light Nuclei & Fine Tunings



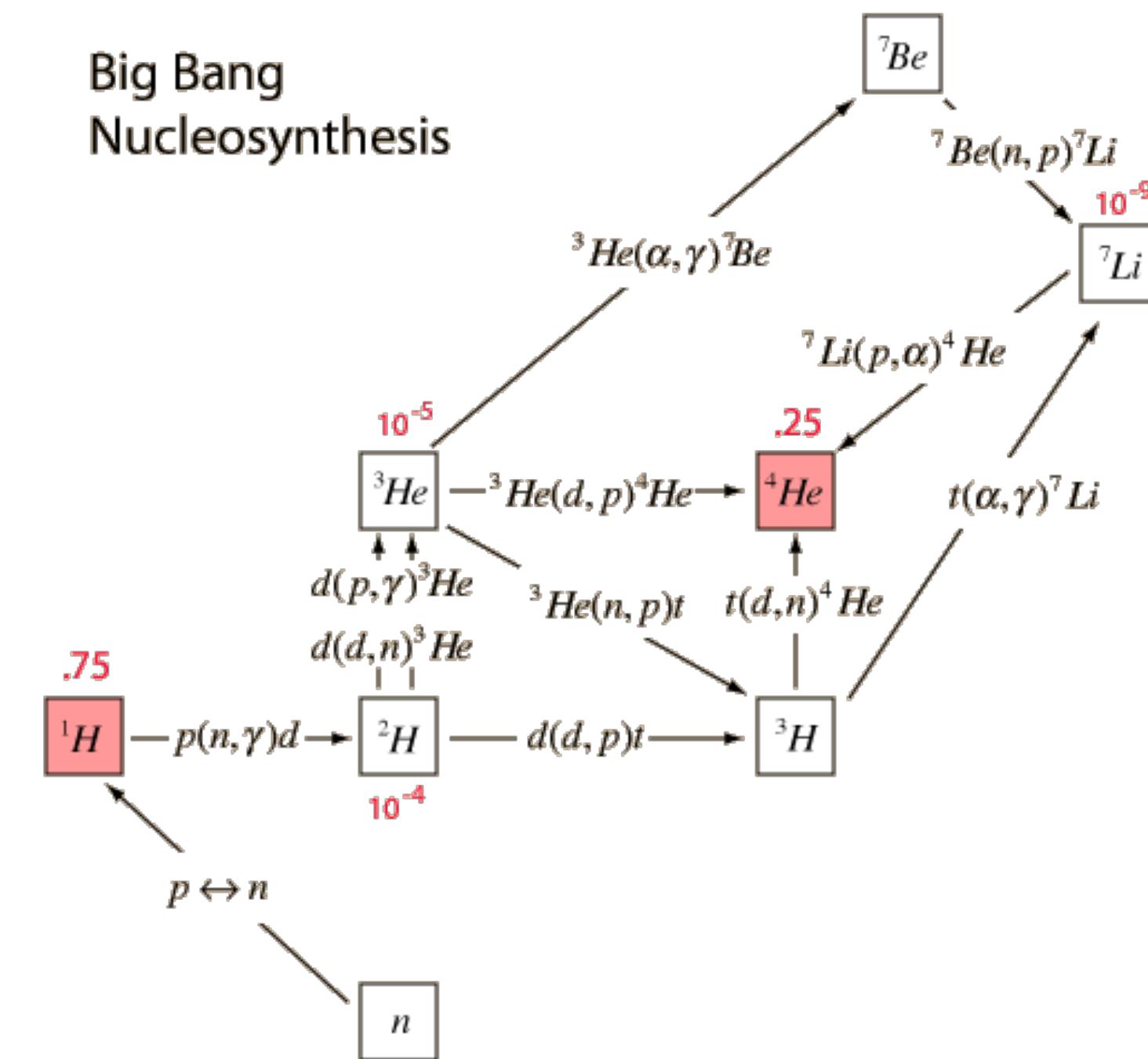
Light Ion reactions in early universe produce primordial abundances of light nuclei  
reactions dominated by radiation  
absence of bound  $A=5,8$  nuclei limit synthesis (no  $^{12}\text{C}$ )

Alpher, Gamow; Fermi, Turkevich; Hayashi; Alpher; Peebles; Hoyle, Tayler; Wagoner, Fowler, Hoyle;  
Kawano; Olive; ...

# Primordial Abundance of Light Nuclei & Fine Tunings



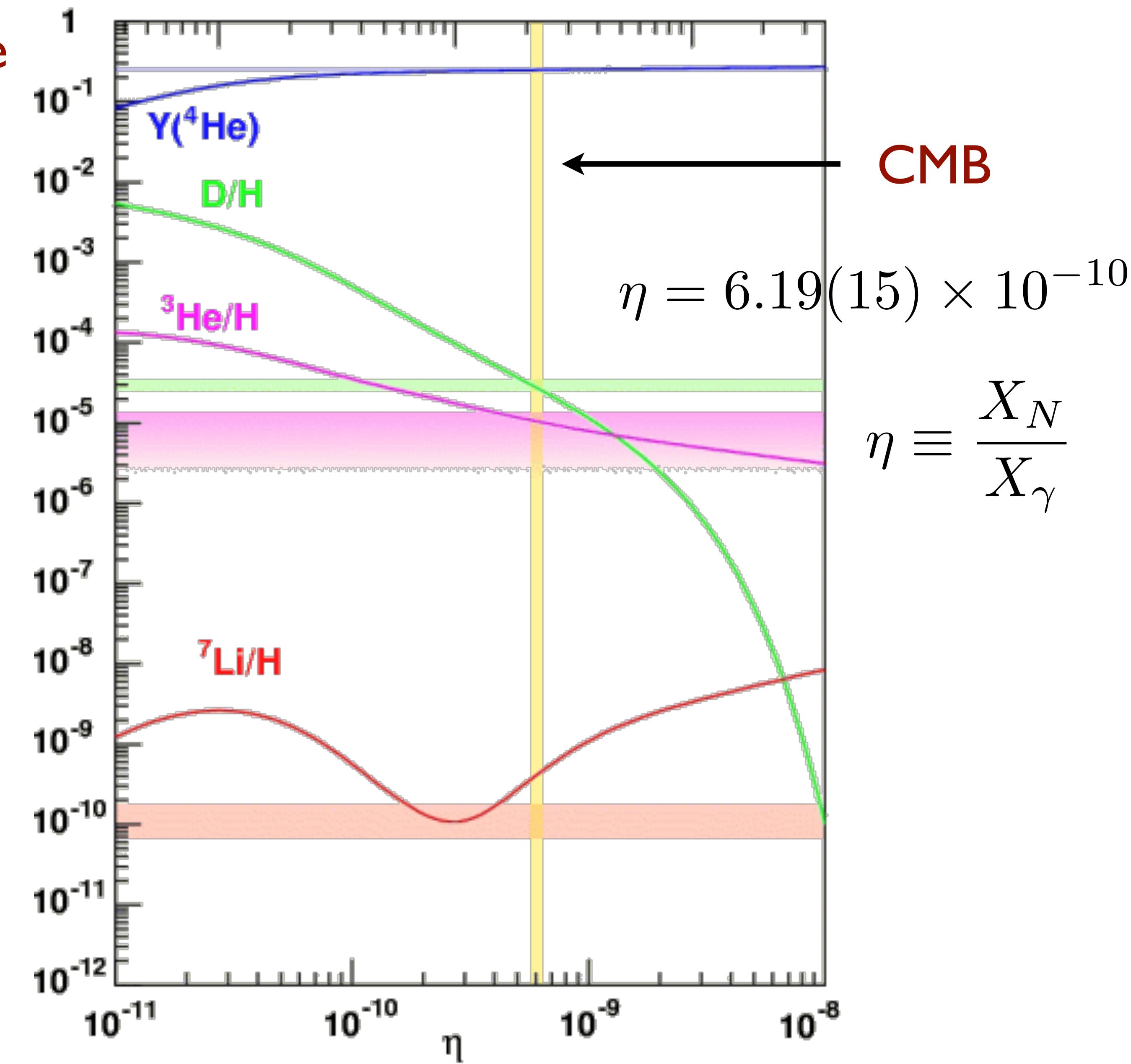
# Big Bang Nucleosynthesis



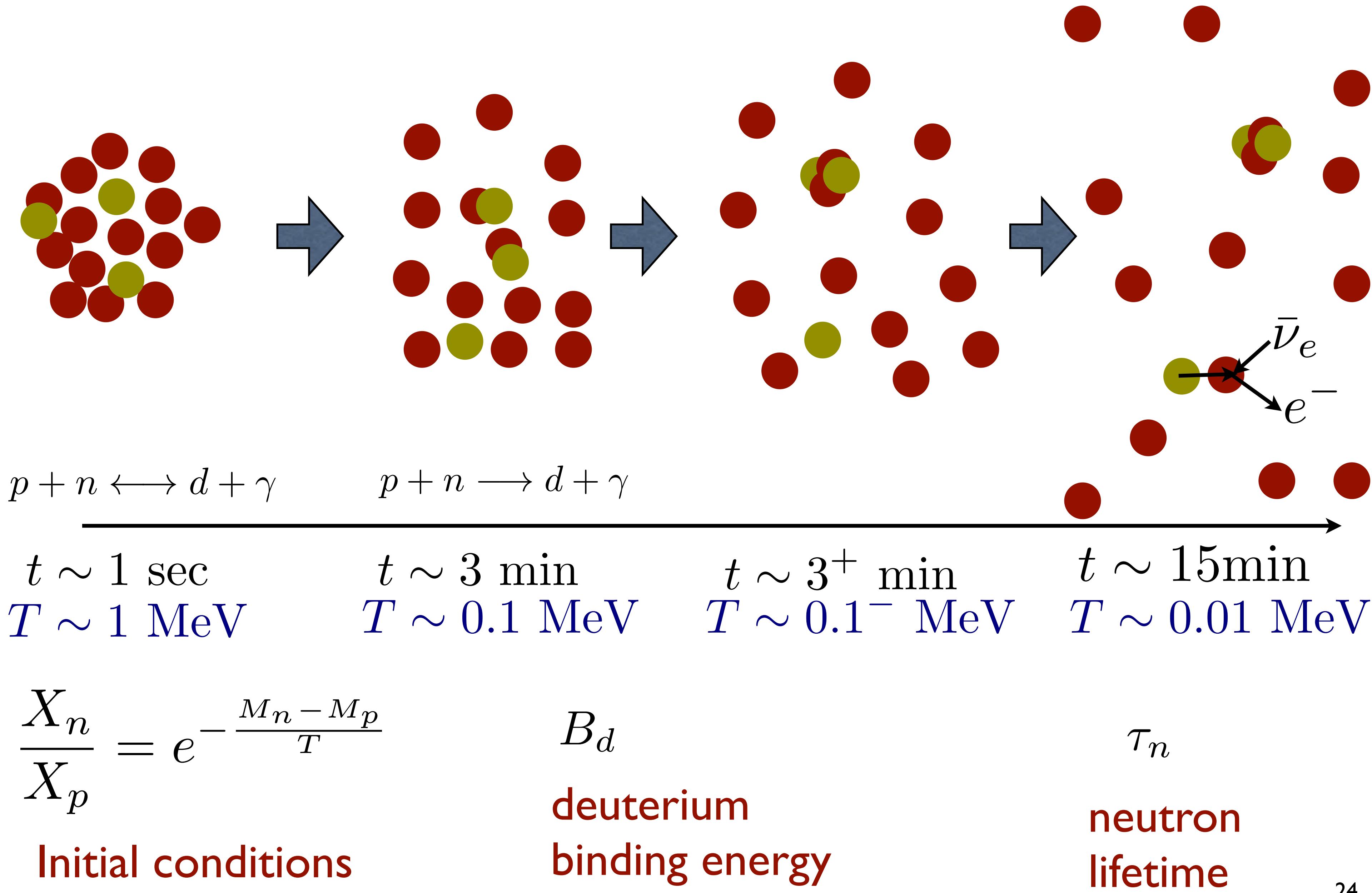
# Primordial Abundance of Light Nuclei & Fine Tunings

Primordial Universe  
(Mass Fraction)

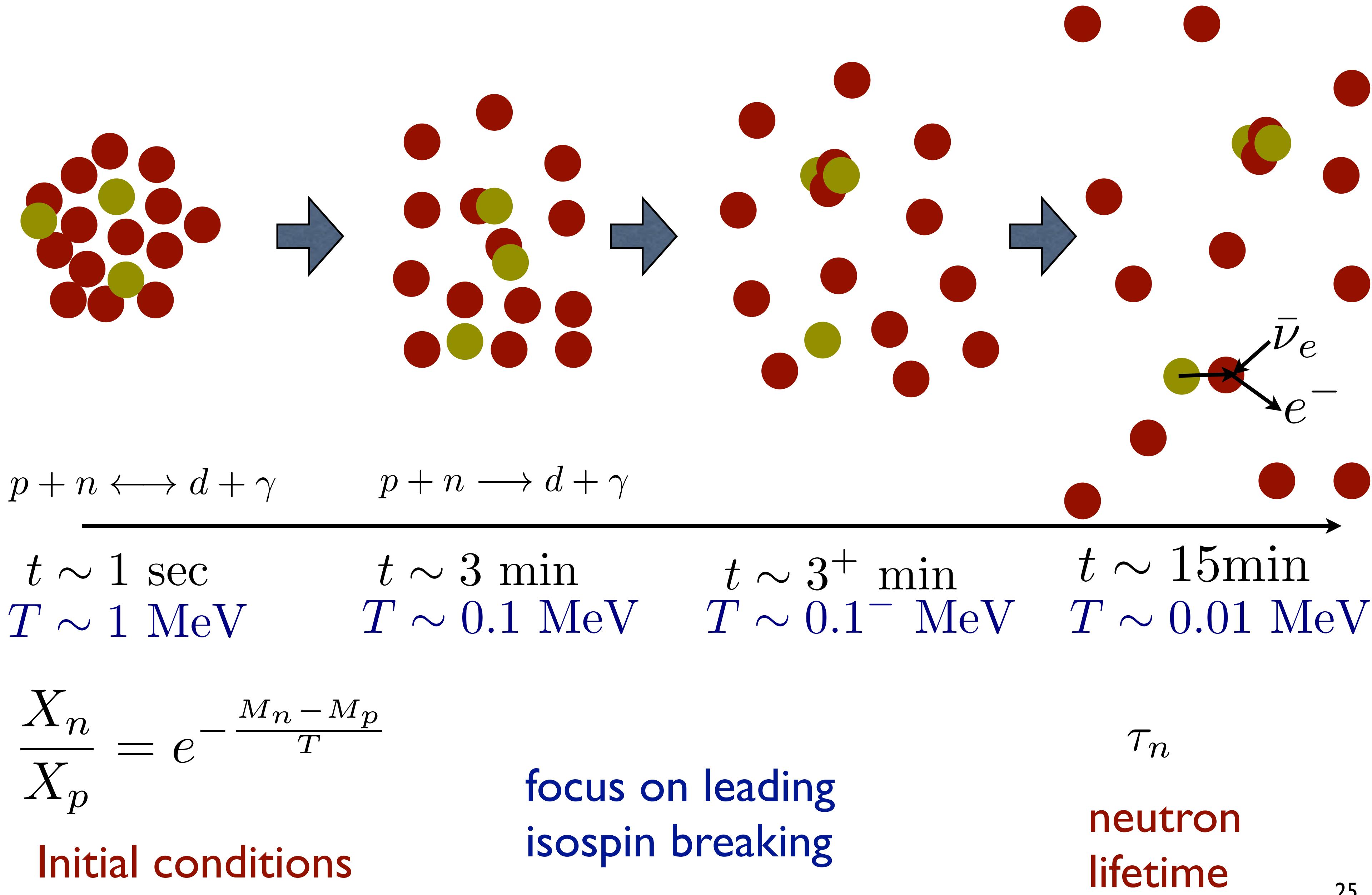
~75% H  
~25%  ${}^4\text{He}$



# Primordial Abundance of Light Nuclei & Fine Tunings



# Primordial Abundance of Light Nuclei & Fine Tunings



# Big Bang Nucleosynthesis and $M_n - M_p$

---

initial conditions for ratio of neutron to protons exponentially sensitive to mass splitting

$$\frac{X_n}{X_p} = e^{-\frac{M_n - M_p}{T}}$$

neutron lifetime very sensitive to mass splitting

$$\frac{1}{\tau_n} = \frac{(G_F \cos \theta_C)^2}{2\pi^3} m_e^5 (1 + 3g_A^2) f \left( \frac{M_n - M_p}{m_e} \right)$$
$$f(a) \simeq \frac{1}{15} (2a^4 - 9a^2 - 8) \sqrt{a^2 - 1} + a \ln \left( a + \sqrt{a^2 - 1} \right)$$

Griffiths “Introduction to Elementary Particles”

10% change in  $M_n - M_p$  corresponds to  $\sim$ 100% change  
neutron lifetime

# Big Bang Nucleosynthesis and $M_n - M_p$

---

$$M_n - M_p = 1.29333217(42) \text{ MeV}$$

two sources of isospin breaking in the Standard Model

quark mass

$$m_q = \hat{m} \mathbf{1} - \delta \tau_3$$

quark electric charge

$$Q = \frac{1}{6} \mathbf{1} + \frac{1}{2} \tau_3$$

at leading order in isospin breaking

$$M_n - M_p = \delta M_{n-p}^\gamma + \delta M_{n-p}^{m_d - m_u}$$

$$< 0 \qquad > 0$$

# Big Bang Nucleosynthesis and $M_n - M_p$

---

## PRELIMINARY

$$\begin{aligned} M_n - M_p &= \delta M_{n-p}^\gamma + \delta M_{n-p}^{m_d - m_u} \\ &= -178(04)(64) \text{ MeV} \times \alpha_{f.s.} + 1.08(6)(9) \times (m_d - m_u) \\ &\quad (\text{lattice average}) \end{aligned}$$

**Big Bang Nucleosynthesis (BBN) highly constrains variation of  $M_n - M_p$  and hence variation of fundamental constants**

- Observe gas clouds with low metalicity (very few heavy elements).
- Assume these are representative of nuclear abundances shortly after the Big Bang (for some quantities, extrapolations are required)
- Run BBN code, changing input parameters connected to QCD, and compare predicted abundances to observed

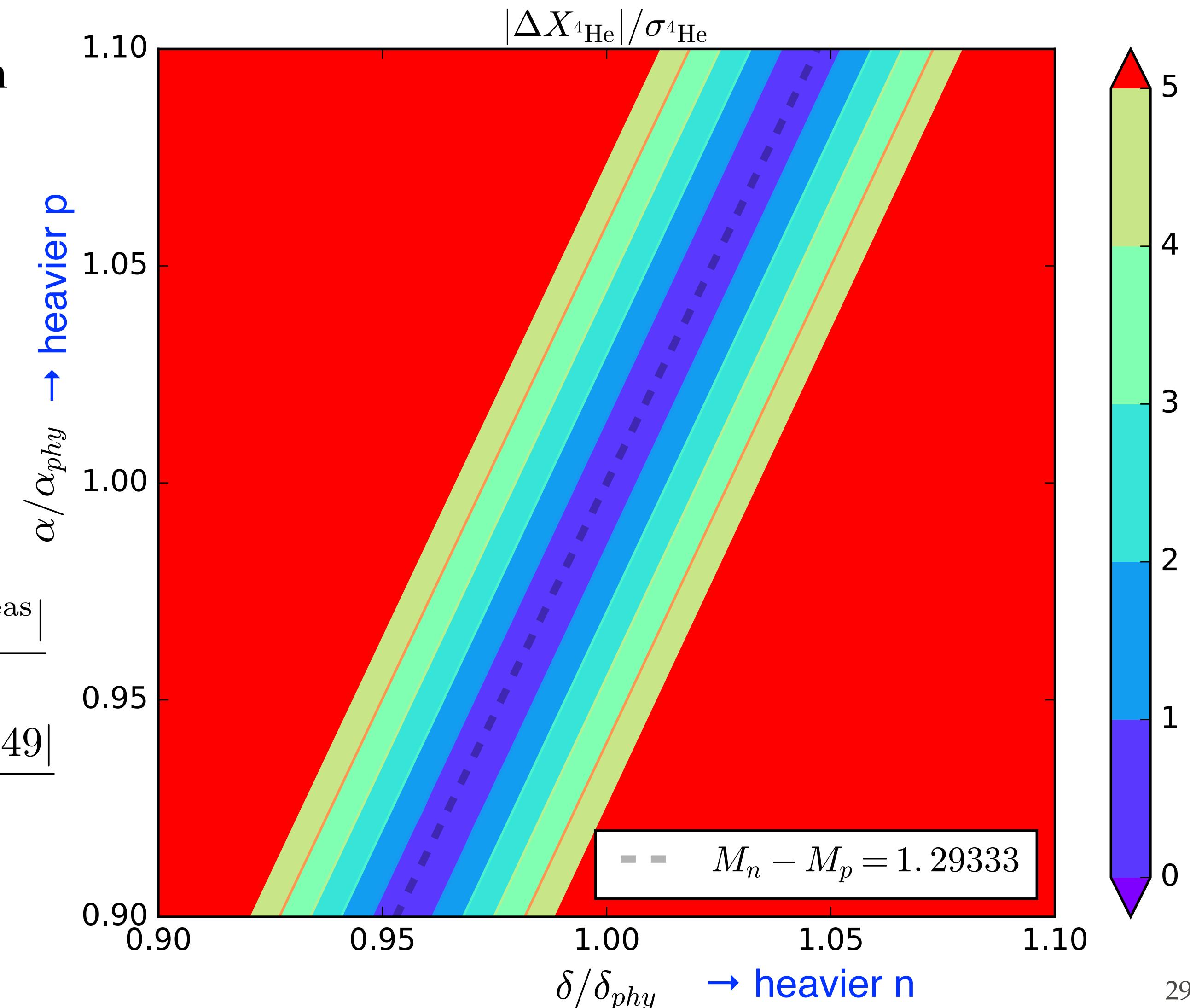
$${}^4\text{He} : Y_p = 0.2449 \pm 0.0040$$

$$\left(\frac{\text{D}}{\text{H}}\right)_p = (2.53 \pm 0.04) \times 10^{-5}$$

$$\delta M_{n-p} = \delta M_{n-p}^\delta + \delta M_{n-p}^\gamma = 2.39 \frac{\delta}{\delta_{\text{phys}}} - 1.10 \frac{\alpha_{f.s.}}{\alpha_{\text{phys}}^{\text{phys}}} \text{ MeV}$$

- Comparing the variation of  ${}^4\text{He}$  to the observed abundance
- ${}^4\text{He}$  tracks almost perfectly the nucleon mass splitting

$$\begin{aligned} \frac{|\Delta X_{{}^4\text{He}}|}{\sigma_{{}^4\text{He}}} &= \frac{|Y_p(\delta, \alpha_{f.s.}) - Y_p^{\text{meas}}|}{\sigma_{Y_p}} \\ &= \frac{|Y_p(\delta, \alpha_{f.s.}) - 0.2449|}{0.0040} \end{aligned}$$



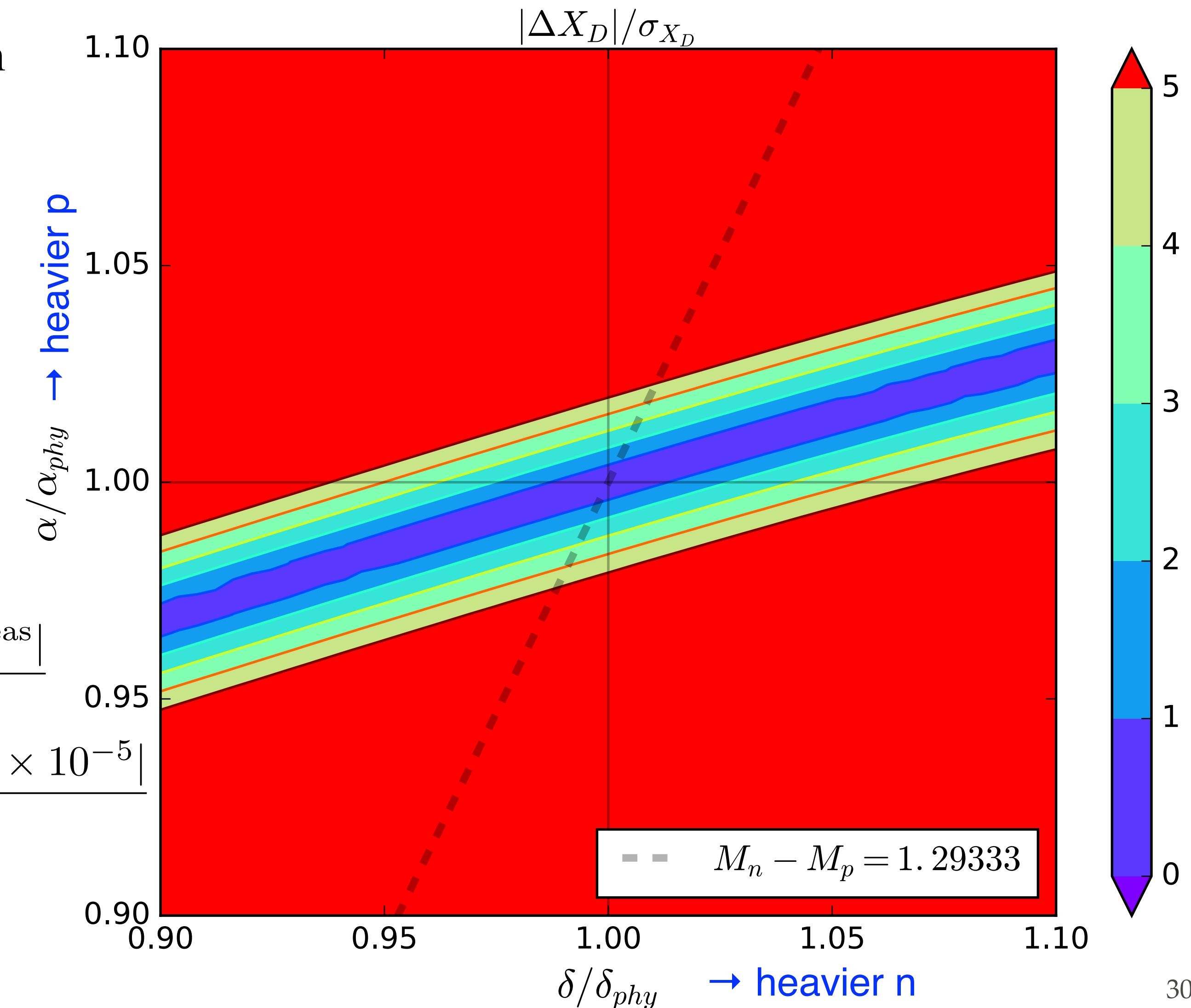
# Big Bang Nucleosynthesis and $m_n - m_p$

Heffernan, Banerjee and  
AWL - 1706.04991

$$\delta M_{n-p} = \delta M_{n-p}^\delta + \delta M_{n-p}^\gamma = 2.39 \frac{\delta}{\delta_{\text{phys}}} - 1.10 \frac{\alpha_{f.s.}}{\alpha_{\text{phys}}^{\text{phys}}} \text{ MeV}$$

- Comparing the variation of Deuterium to the observed abundance
- electromagnetic effects in fusion cross sections are important, such that lines on constant D do not line up with  $M_n - M_p$

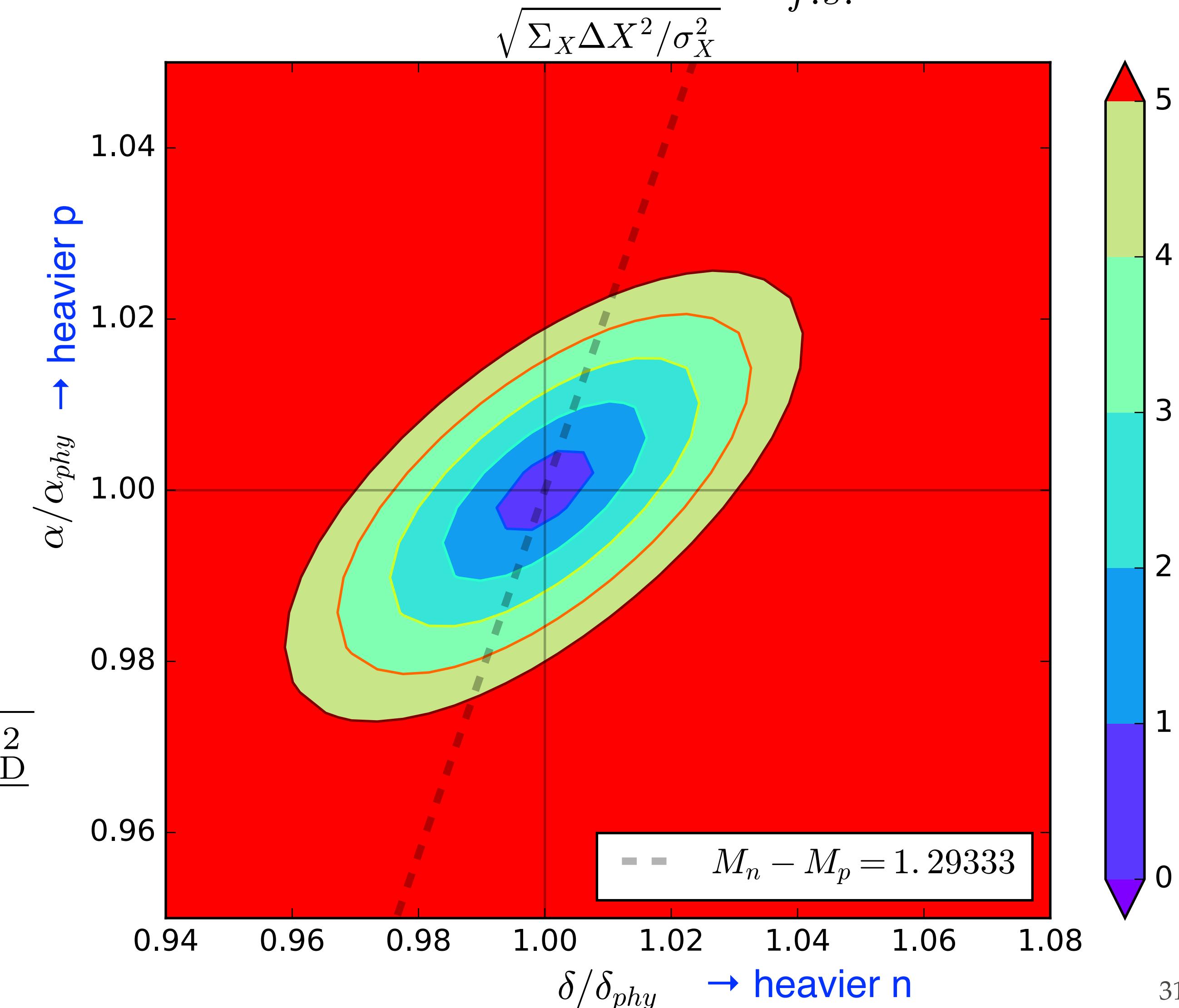
$$\begin{aligned} \frac{|\Delta X_D|}{\sigma_D} &= \frac{|X_D(\delta, \alpha_{f.s.}) - X_D^{\text{meas}}|}{\sigma_{X_D}} \\ &= \frac{|X_D(\delta, \alpha_{f.s.}) - 2.53 \times 10^{-5}|}{0.04 \times 10^{-5}} \end{aligned}$$



$$\delta M_{n-p} = \delta M_{n-p}^\delta + \delta M_{n-p}^\gamma = 2.39 \frac{\delta}{\delta_{\text{phys}}} - 1.10 \frac{\alpha_{f.s.}}{\alpha_{\text{phys}}^{\text{phys}}} \text{ MeV}$$

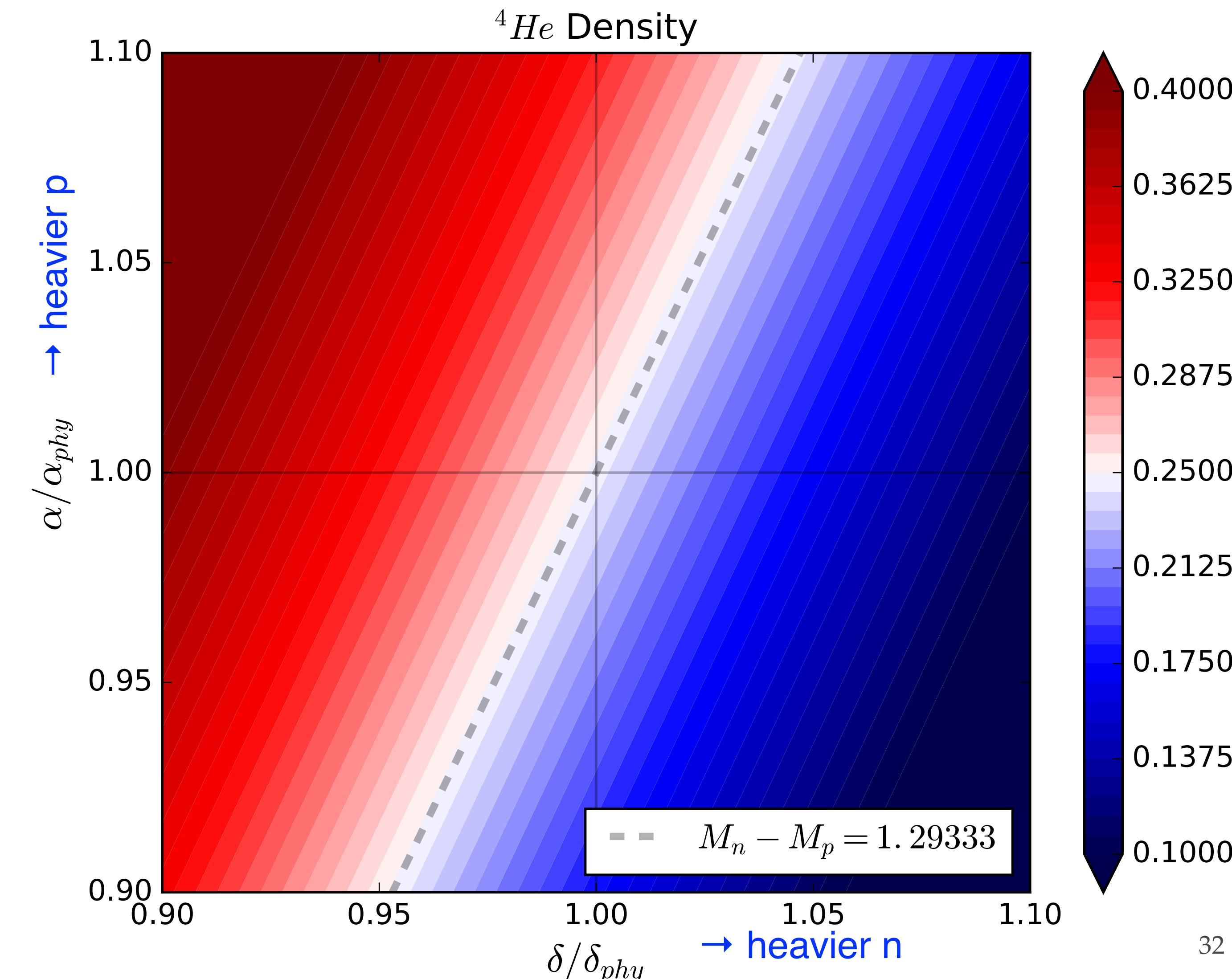
- The combined variation of D,  ${}^3\text{He}$  and  ${}^4\text{He}$  restrict possible primordial variations of isospin breaking to less than 2% at the 95% confidence level
- This places tight constraints on possible extensions of the Standard Model

$$\frac{\Delta X}{\sigma_X} = \sqrt{\frac{\Delta X_{{}^4\text{He}}^2}{\sigma_{{}^4\text{He}}^2} + \frac{\Delta X_{\text{D}}^2}{\sigma_{\text{D}}^2}}$$



$$\delta M_{n-p} = \delta M_{n-p}^\delta + \delta M_{n-p}^\gamma = 2.39 \frac{\delta}{\delta_{\text{phys}}} - 1.10 \frac{\alpha_{f.s.}}{\alpha_{f.s.}^{\text{phys}}} \text{ MeV}$$

- For fun - we can see what the  ${}^4\text{He}$  density would be for larger variations



# Outlook

- We are now in the era in which lattice QCD is delivering precise single-nucleon quantities relevant to the nuclear physics program
  - nucleon charges (axial, scalar, tensor)
- In the next few years, we will see more dynamic quantities pinned down
  - form factors
  - radiative QED corrections to beta-decay
- The frontier for lattice QCD is moving towards the two-hadron processes
  - $\pi$ -N scattering,  $N \rightarrow N\pi$  transition matrix elements, NN matrix elements, YN, (NNN) interactions, ...
  - These two-hadron quantities (and notoriously two-nucleon) suffer from more extreme systematic challenges
    - The last couple years have seen the application of more sophisticated methods known to work for  $\pi\pi$ -scattering, to the NN problem: most likely, nearly all previous NN calculations (and their matrix elements) are unquantifiable wrong

*Thank You*