Lattice QCD for Nuclear Physics

Wick Fest

Looking for ν physics on Earth and in the Cosmos

Berkeley, CA

André Walker-Loud

CalLat

$LECs$

δ^{LQCD}

A Controlled Nonrelativistic ET applicable to nuclei

↔

↔

Cold Lattice QCD focused on NN scattering observables

experimental observables

connect to fundamental theory

California Lattice Collaboration

W. Haxton, T. Luu, P. Vranas

Lattice QCD for Nuclear Physics

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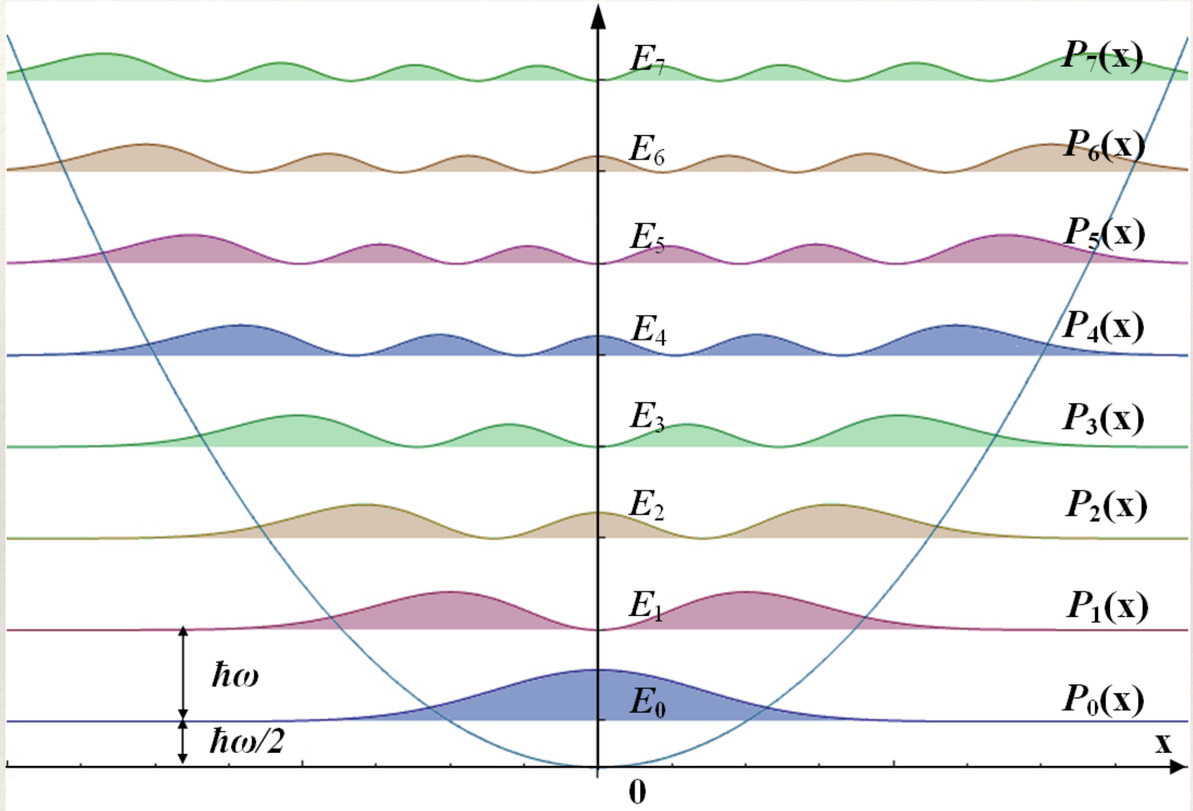
Current view of nuclear physics from QCD

BERKELEY LAB

How has Wick impacted lattice QCD?

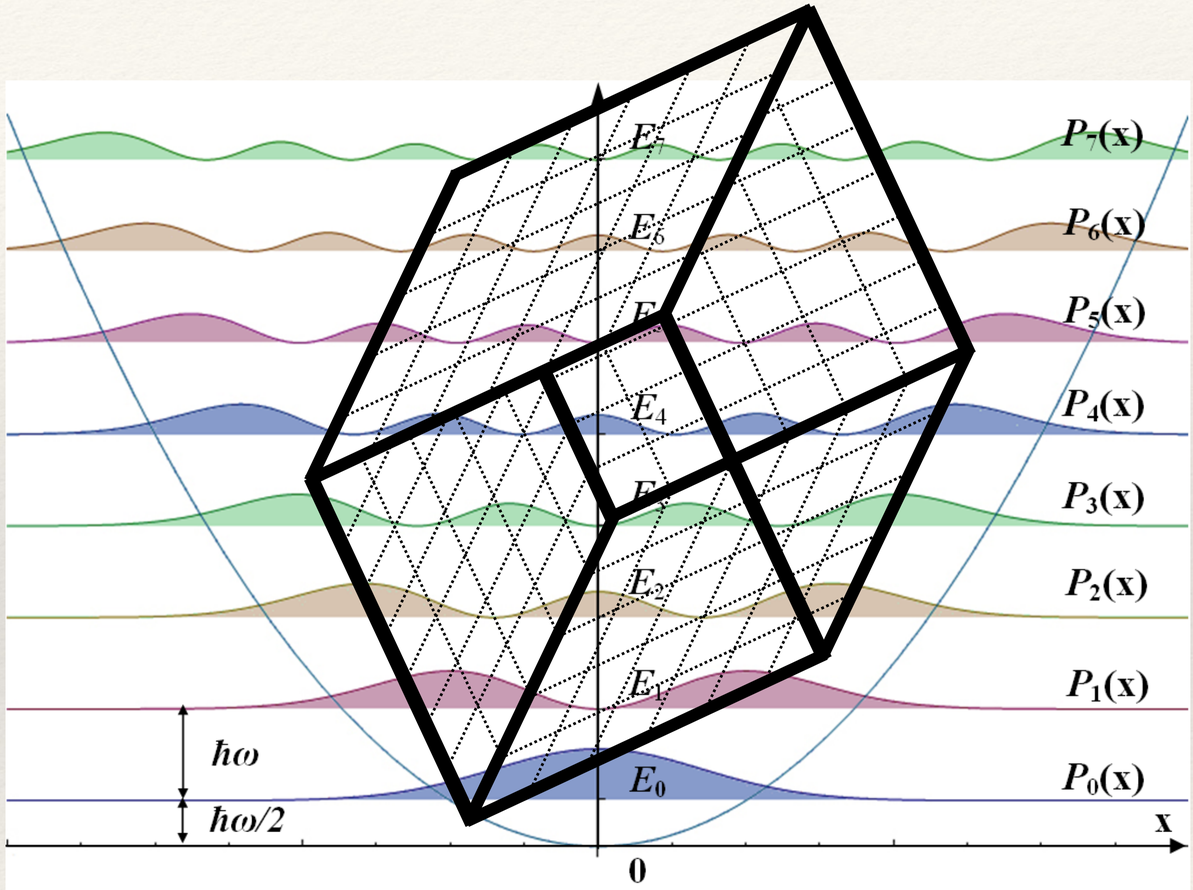
- As some of you may know, Wick does not work on the lattice, but rather lives in a harmonic oscillator



How has Wick impacted lattice QCD?

- As some of you may know, Wick does not work on the lattice, but rather lives in a harmonic oscillator

- But he is very welcoming and is encouraging us to fit the lattice in a harmonic oscillator as well



How has Wick impacted lattice QCD?

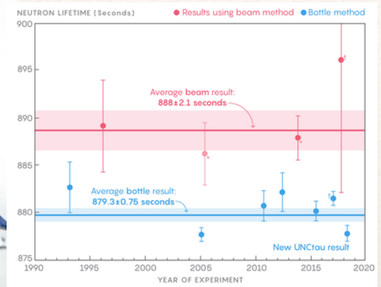
- In 2010 - Wick spent more or less all of his LBNL start up funds to hire two lattice QCD postdocs - Sergey Syritsyn and myself
  - my "unbiassed" opinion is this is fantastic!
  - The goal was(is) to build a quantitative bridge between QCD and our understanding of low-energy nuclear physics of nucleons and nuclei
- I never asked, but I am certain my opportunity to come to LBNL then was at the strong recommendation of Tom Luu (my first physics TA) and Martin Savage (my PhD advisor) [I spent 11 years @ UW as a student, u-grad then grad - during which, I never interacted with Wick]
  - I also would bet none of them (Martin, Tom, Wick) anticipated exactly how exciting the times would become from this move

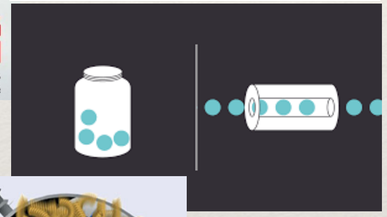
How has Wick impacted lattice QCD?

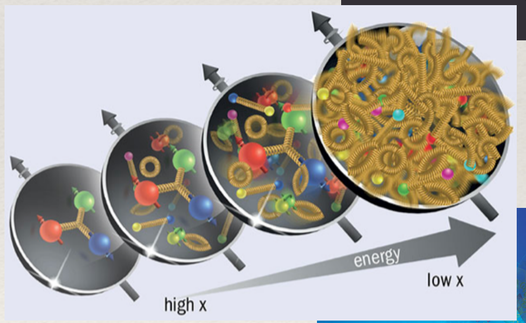
- What I learned from Wick from 2010-2013
  Building on the experience I had in effective field theory and lattice QCD
- Over cups of coffee, discussions of harmonic oscillators and the fractional quantum hall effect, I developed a keen vision of applying lattice QCD and EFT for problems in
  - "fundamental symmetry tests" of the Standard Model in low-energy nuclear environments (which I was mostly ignorant of)
  - connections to nuclear astrophysics (for which I had a somewhat vague vision previously)
- Not to say that others did not already have this vision, just that it finally became my own vision (up to this point, I was very focussed on NN and YN interactions from LQCD and XPT and I was missing this bigger picture)

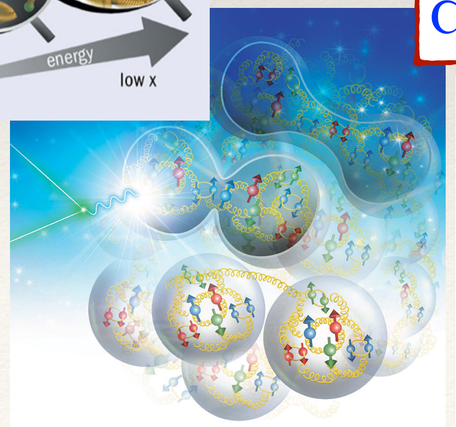
LQCD and Forefront Questions in Nuclear Physics

nucleon structure

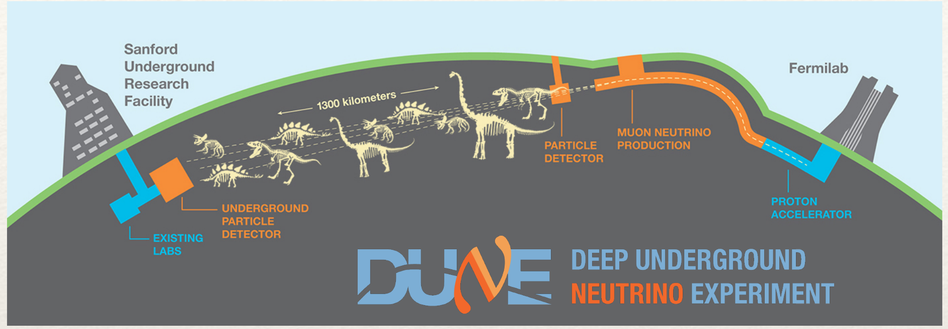


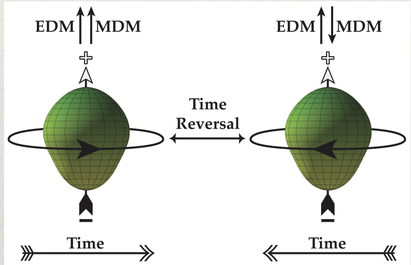


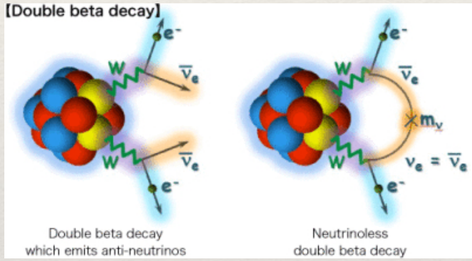




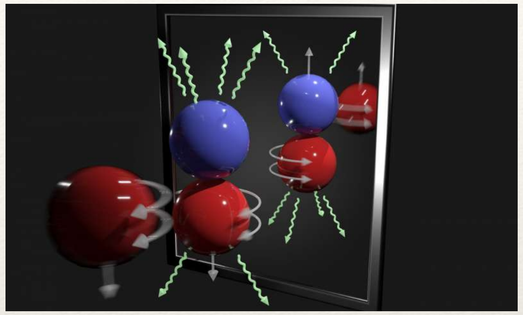
origin of matter



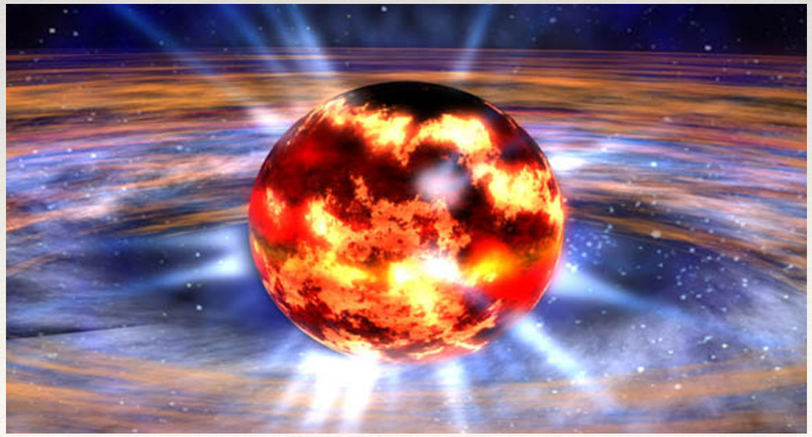




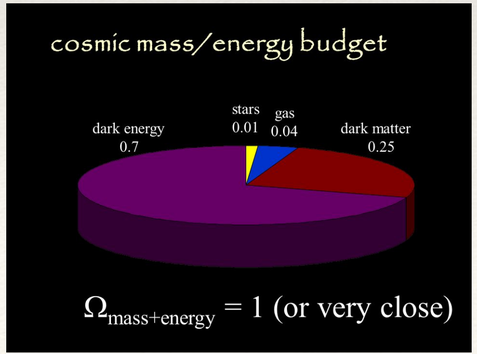
hadronic parity violation

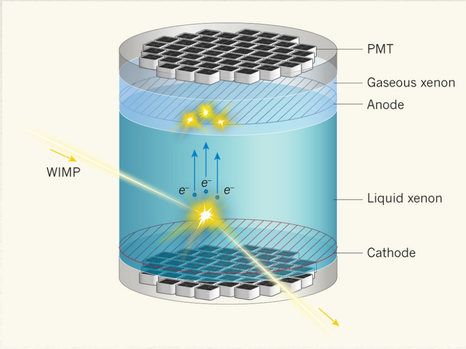


properties of dense nuclear matter



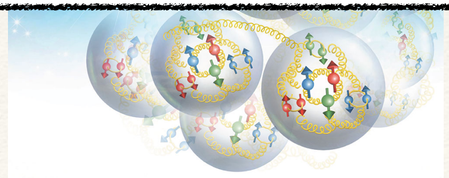
dark matter/matter interactions

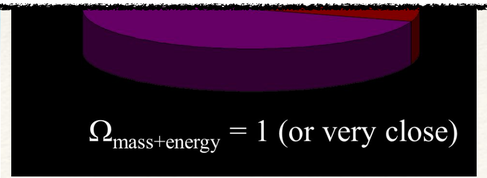


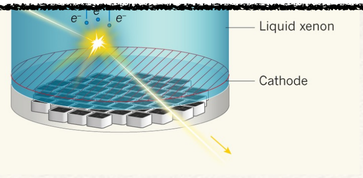


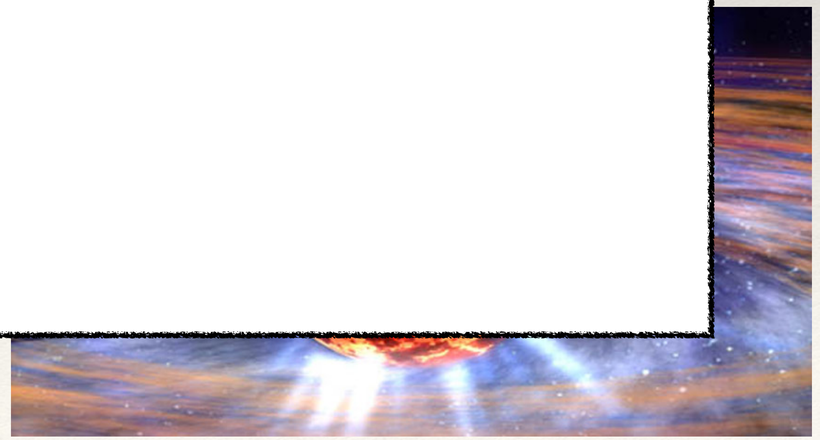
LQCD and Forefront Questions in Nuclear Physics

- 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 will require a coordinated effort between LQCD, Effective Field Theory (EFT) and 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









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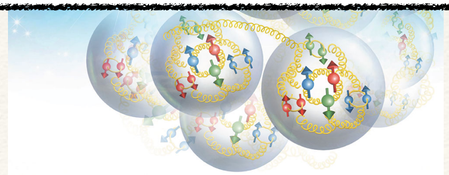
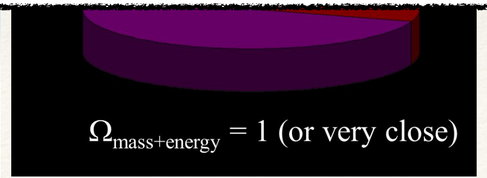
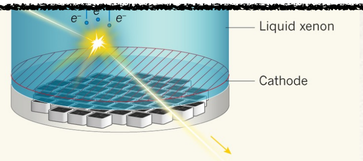
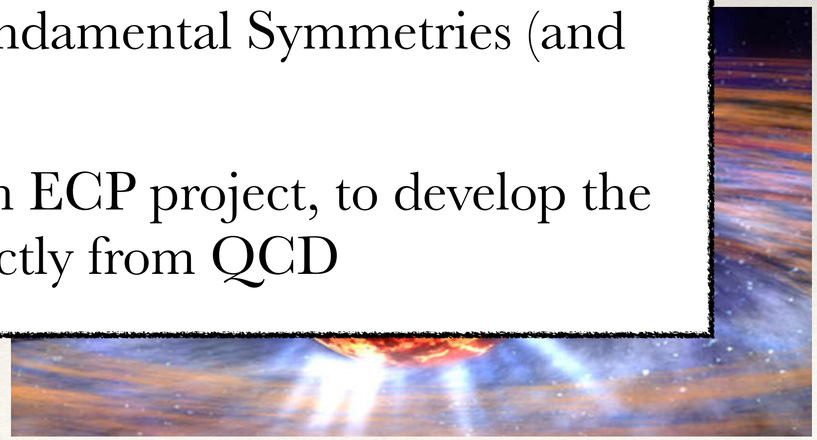
- In fact - we have two new efforts precisely to develop and strengthen this coupling between LQCD and theories of nuclear physics:
  - DOE Nuclear Physics Topical Collaboration for ββ-decay and Fundamental Symmetries (and friends) https://a51.lbl.gov/~0nubb/webhome
  - We are now working with ExaStar (D. Kasen and many others), an ECP project, to develop the software necessary to constrain the nuclear Equation of State directly from QCD









LQCD and Forefront Questions in Nuclear Physics

Cornell University

Our grandiose vision

We gratefully acknowledge support from the Simons Foundation and Lawrence Berkeley National Laboratory (LBL).

arXiv.org > nucl-th > arXiv:1910.07961

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Nuclear Theory

Towards grounding nuclear physics in QCD

Christian Drischler, Wick Haxton, Kenneth McElvain, Emanuele Mereghetti, Amy Nicholson, Pavlos Vranas, André Walker-Loud

(Submitted on 17 Oct 2019)

Exascale computing could soon enable a predictive theory of nuclear structure and reactions rooted in the standard model of particle physics, with quantifiable and systematically improvable uncertainties. Such a predictive theory will help us more fully exploit experiments that use nucleons and nuclei as laboratories for testing the standard model and its limitations. Examples include direct dark matter detection, neutrinoless double beta decay, and searches for permanent electric dipole moments

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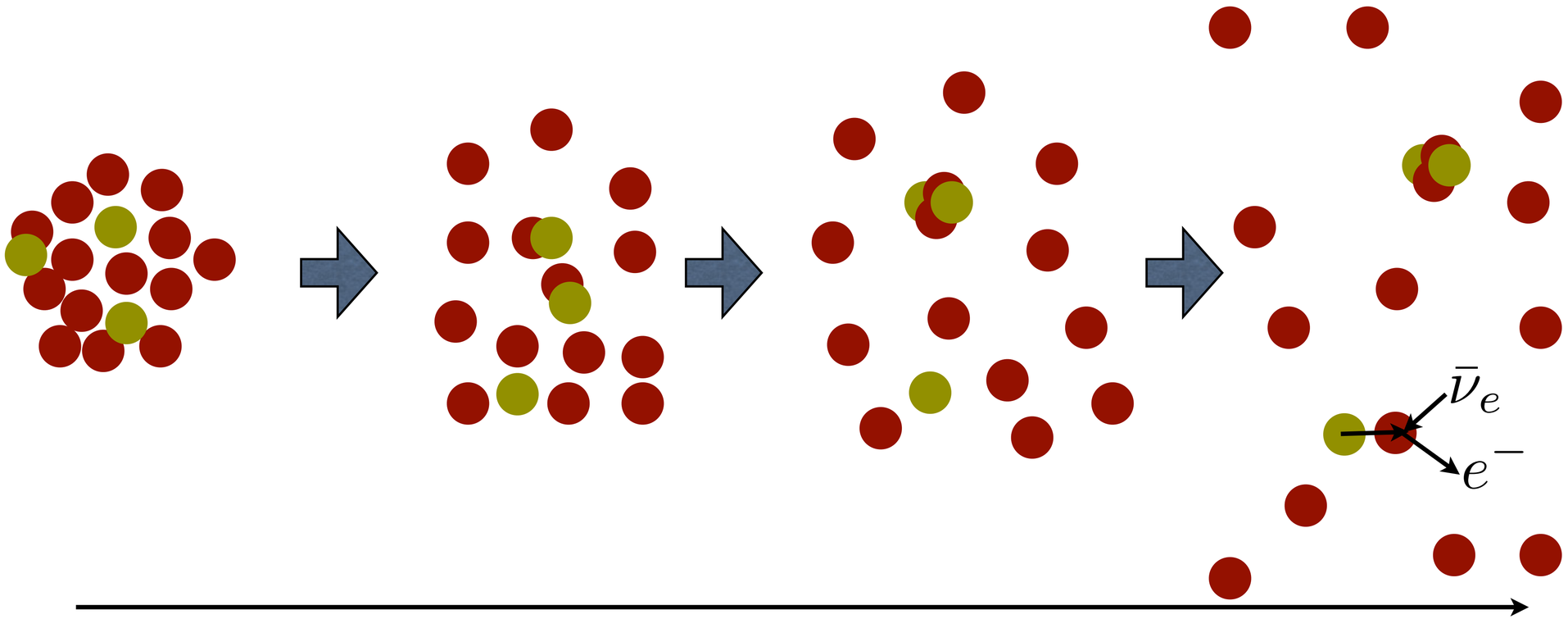
Big Bang Nucleosynthesis and $m_n - m_p$

Heffernan, Banerjee and AWL - arXiv:1706.04991



$t \sim 1$ sec	$t \sim 3$ min	$t \sim 3^+$ min	$t \sim 15$min
$T \sim 1$ MeV	$T \sim 0.1$ MeV	$T \sim 0.1^-$ MeV	$T \sim 0.01$ MeV

$$\frac{X_n}{X_p} = e^{-(m_n - m_p)/T}$$

Initial conditions

B_d deuterium binding energy

What is the sensitivity of BBN to isospin breaking?

τ_n

neutron lifetime

Big Bang Nucleosynthesis and $m_n - m_p$

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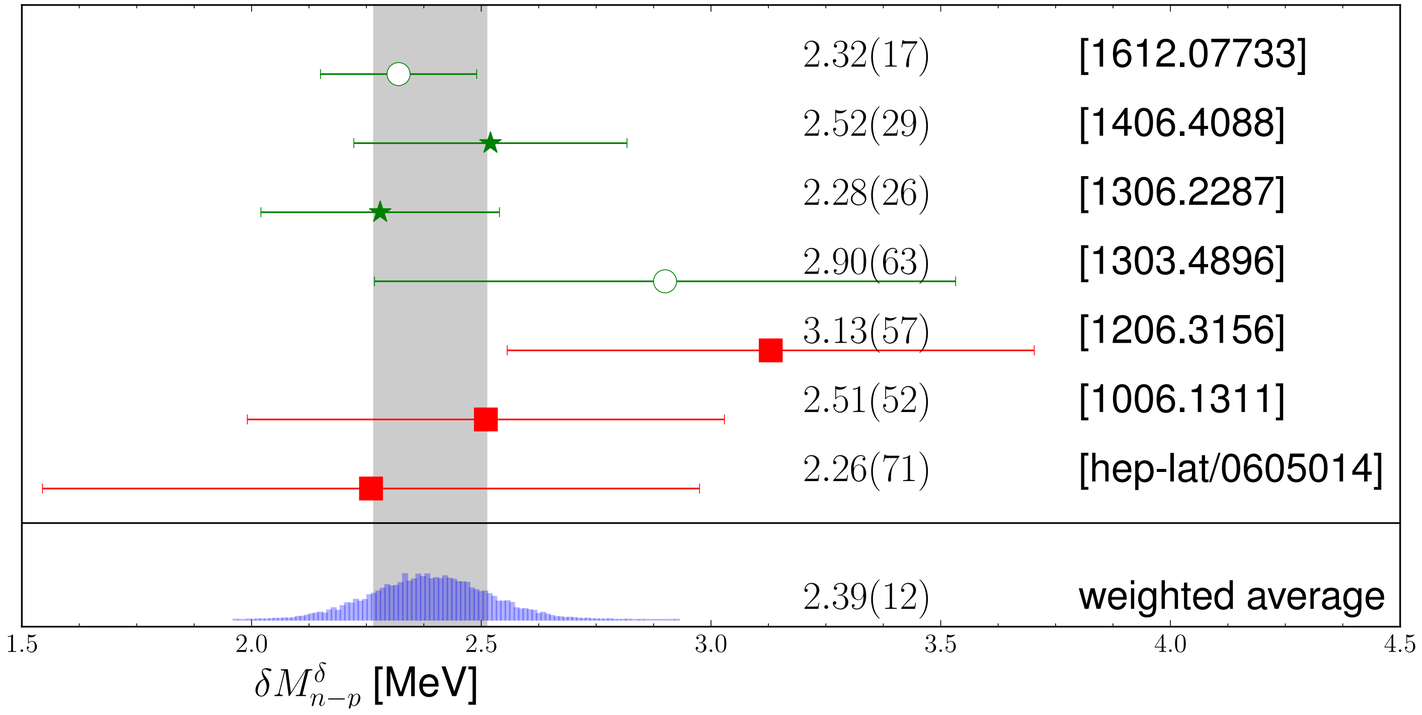


we now have a precise determination of the QCD contribution to the nucleon mass splitting

$$\delta M_{n-p}^{m_d - m_u} = 2.39(.12) \text{ MeV}$$

we can use this to determine the electromagnetic contribution

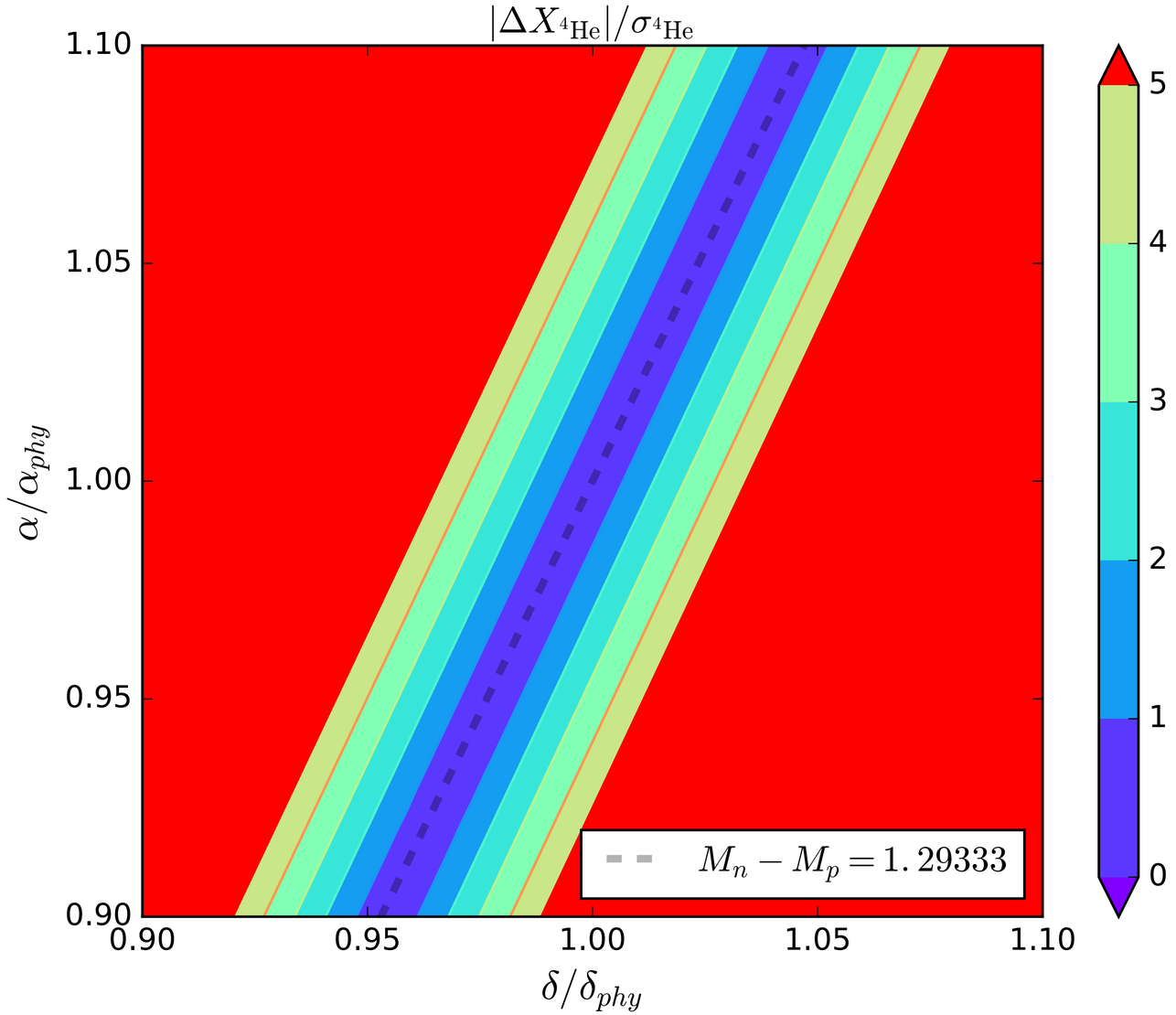
$$\delta M_{n-p}^{\gamma} = \delta M_{n-p}^{PDG} - \delta M_{n-p}^{m_d - m_u}$$
$$= -1.10(.12) \text{ MeV}$$

Big Bang Nucleosynthesis and $m_n - m_p$

Heffernan, Banerjee and AWL - arXiv:1706.04991

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

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



Big Bang Nucleosynthesis and $m_n - m_p$

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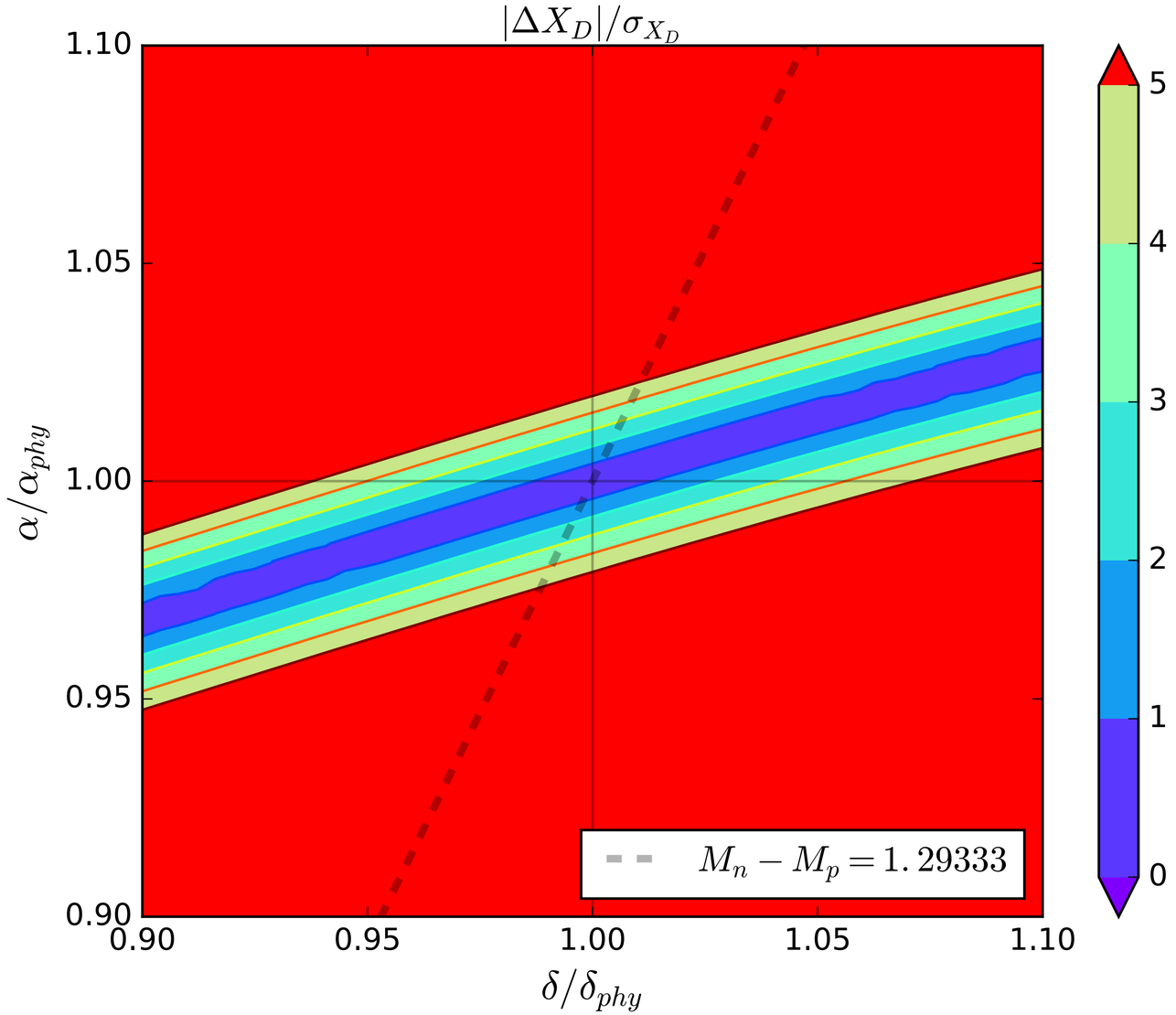
- Comparing the variation of Deuterium to the observed abundance
- electromagnetic effects in fusion cross sections are important, such that lines on constant D do not line up with M_n-M_p



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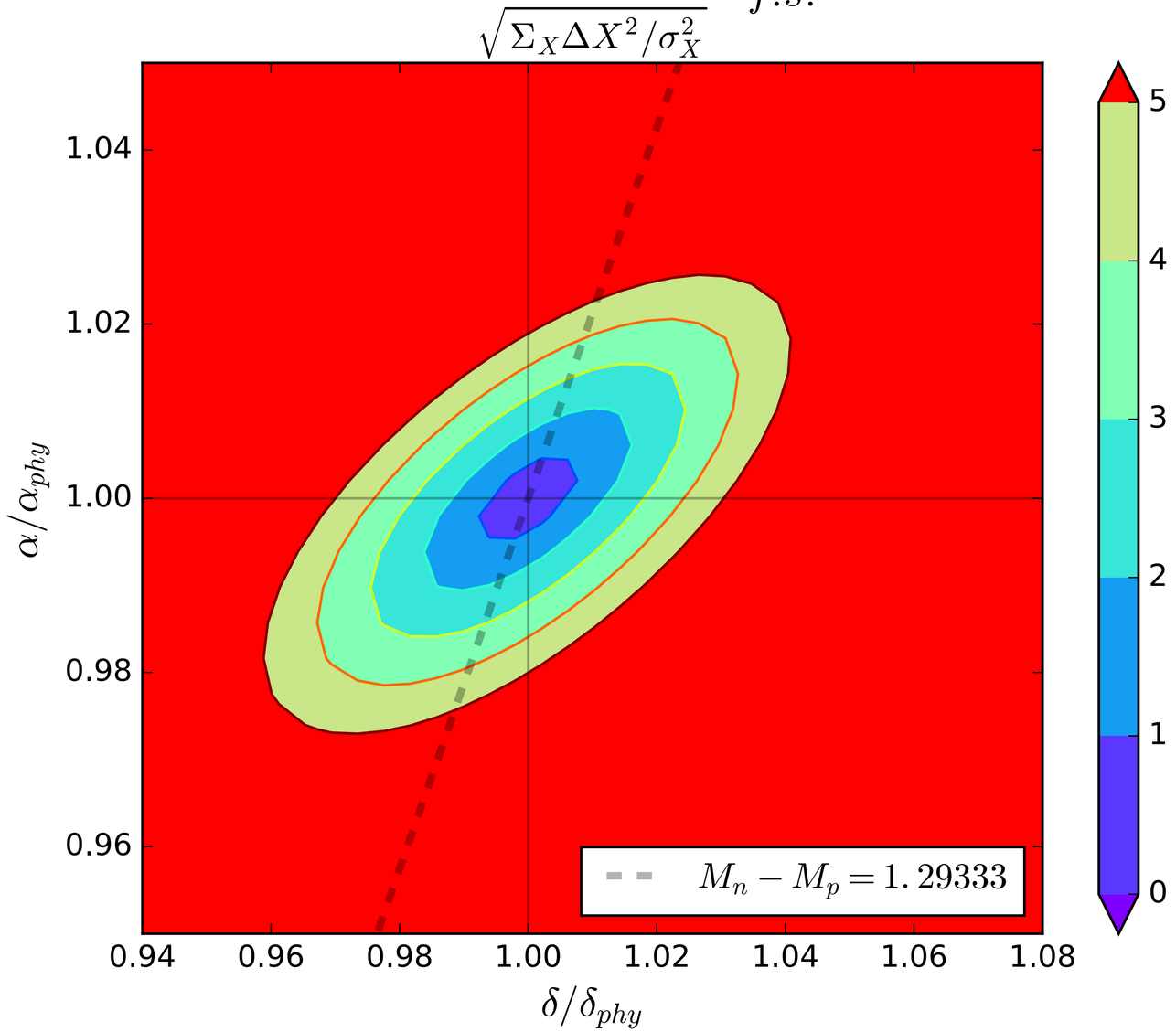
- The combined variation of D, ^{3}He and ^{4}He restrict possible primordial variations of isospin breaking to less than 2% at the 95% confidence level
- This places tight constraints on possible extensions of the Standard Model



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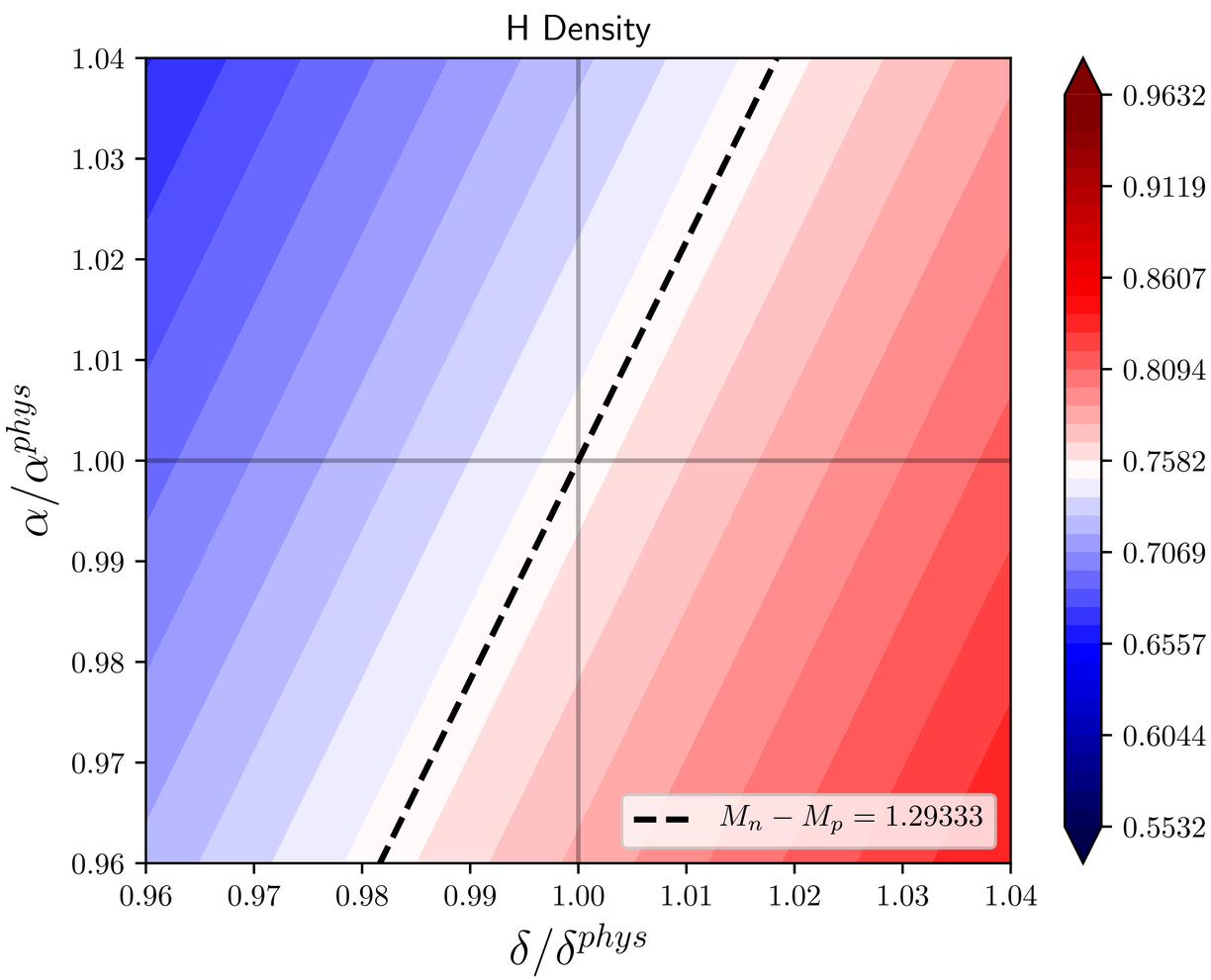
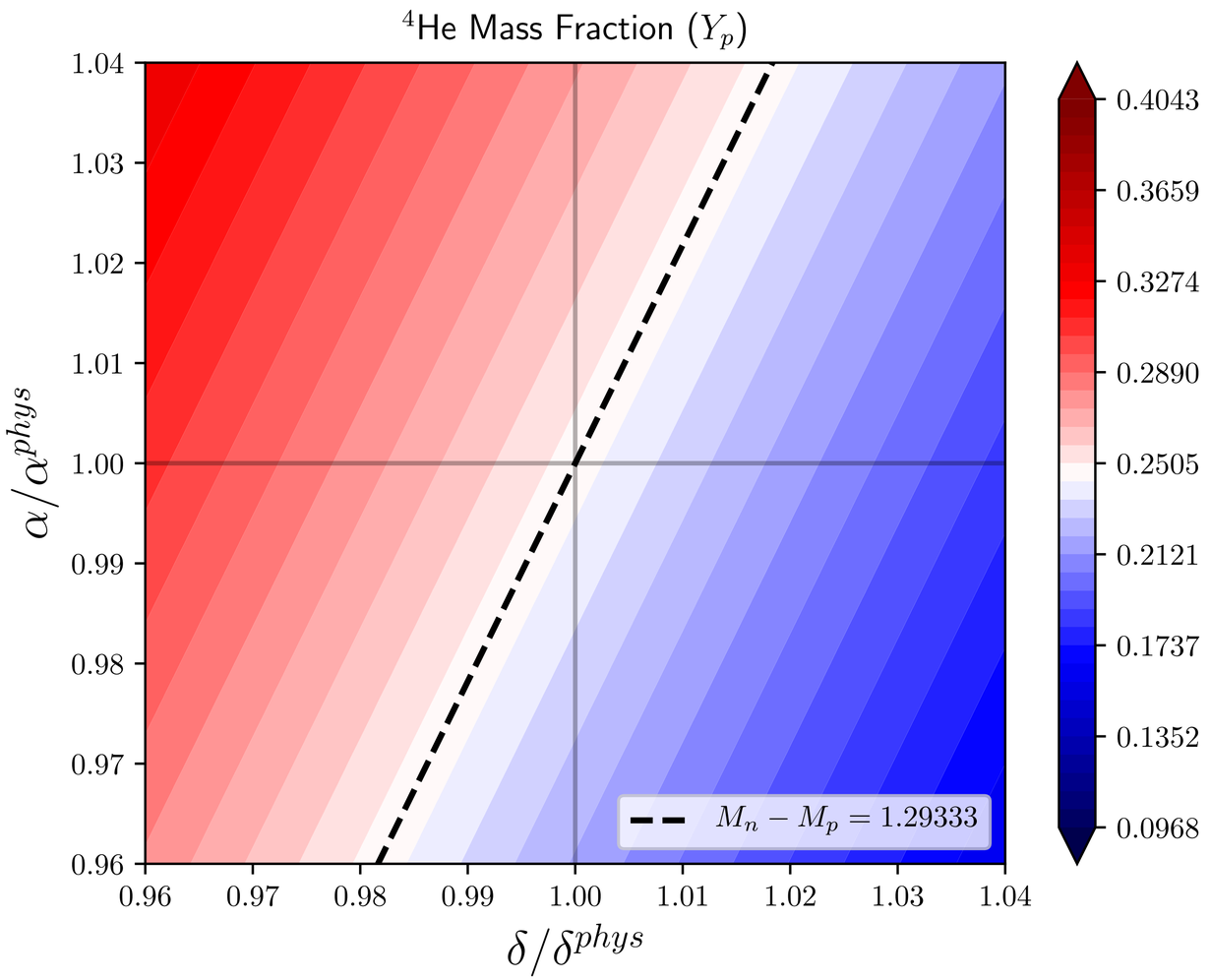
- For fun - we can see what the ^{4}He density would be for larger variations





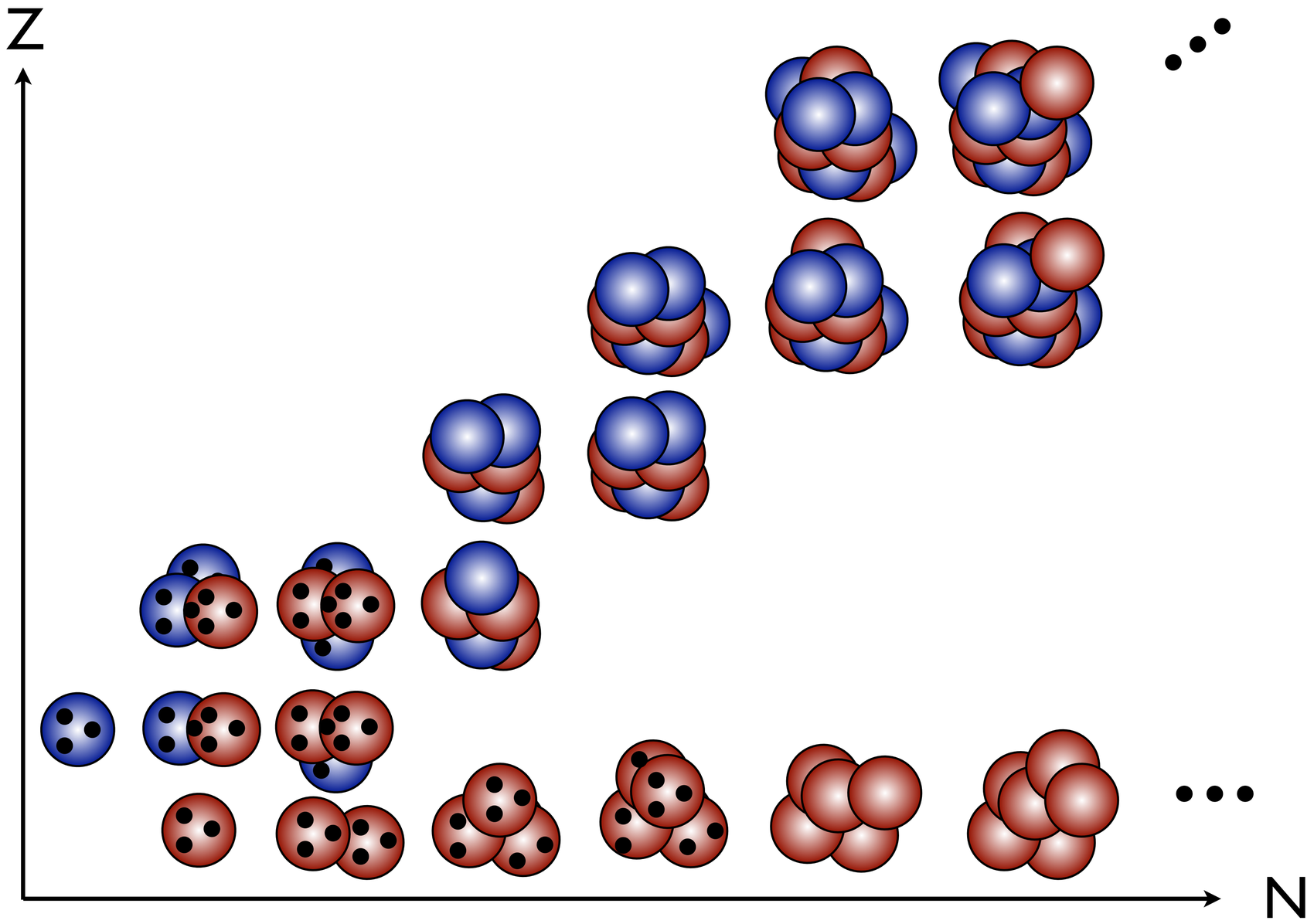
How has Wick impacted lattice QCD?

- Wick's guidance, this new vision, and a growing independence
  - pushed me over the edge to getting a faculty job
  - wrote a successful Early Career Proposal

- With Wick's support and encouragement
  - I ultimately ended up back at LBNL to help cement a new lattice QCD effort here
  - It is no longer true that all US LQCD people are members of USQCD
    - Increased competition leads to improved science!
    - All of the exciting results we have been generating (g_A, $0\nu BB$, …) would not have been possible had I and others remained in USQCD
      - access to INCITE resources were essential for the results
      - USQCD prohibits its members from writing independent INCITE proposals
    - BUT - we still maintain a close working relationship with members of USQCD - the partnership is also very valuable!

Lattice QCD for Nuclear Physics

- Lattice QCD offers us the promise of quantitatively connecting our understanding of nuclear physics to QCD
  - not just academically interesting - but essential for quantities difficult/impossible to measure
    - hadronic parity violation!
    - hyperon-nucleon interactions
    - three-nucleon (YNN) interactions
    - matrix elements of BSM currents ($0\nu\beta\beta$)
    - …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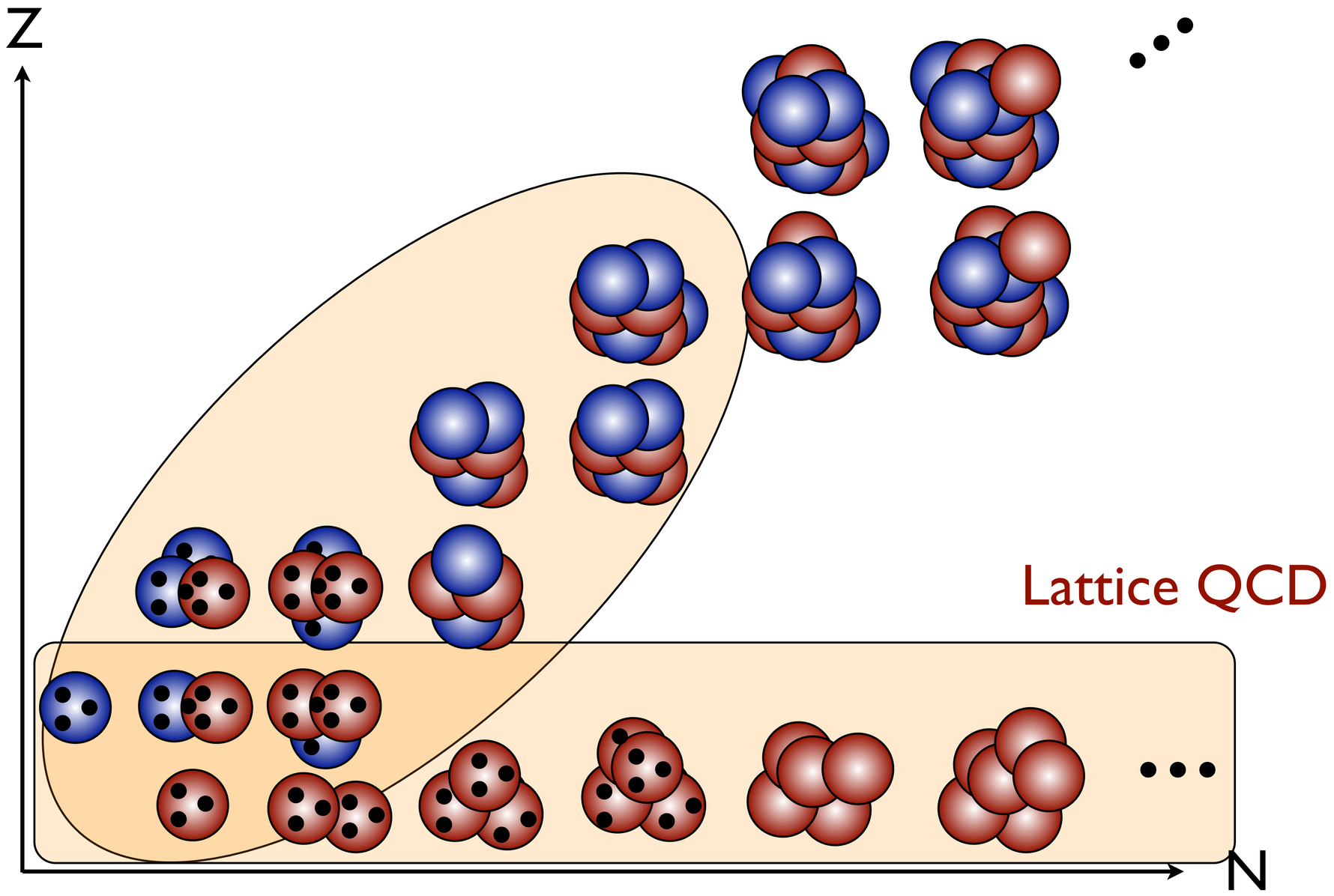
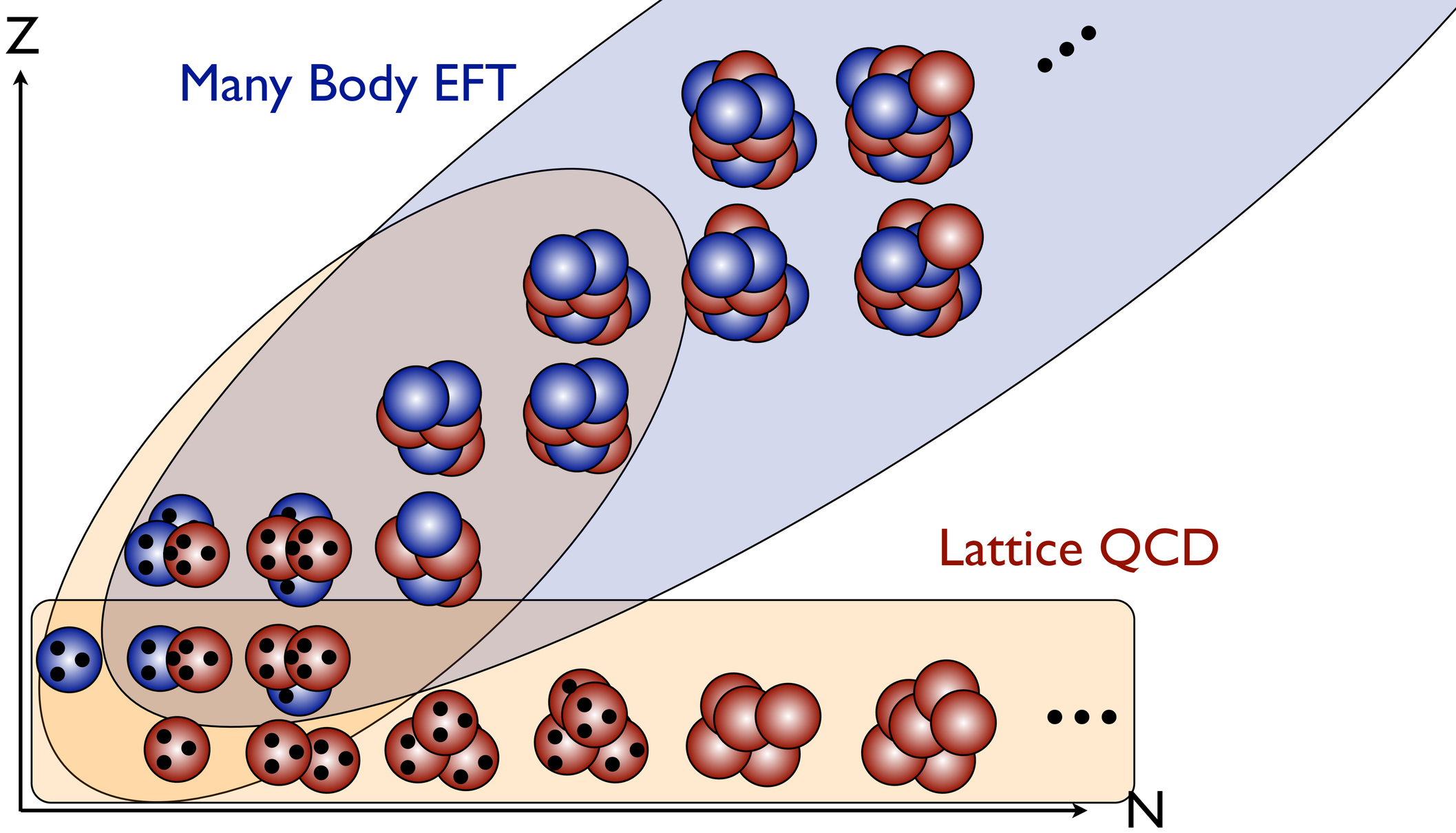
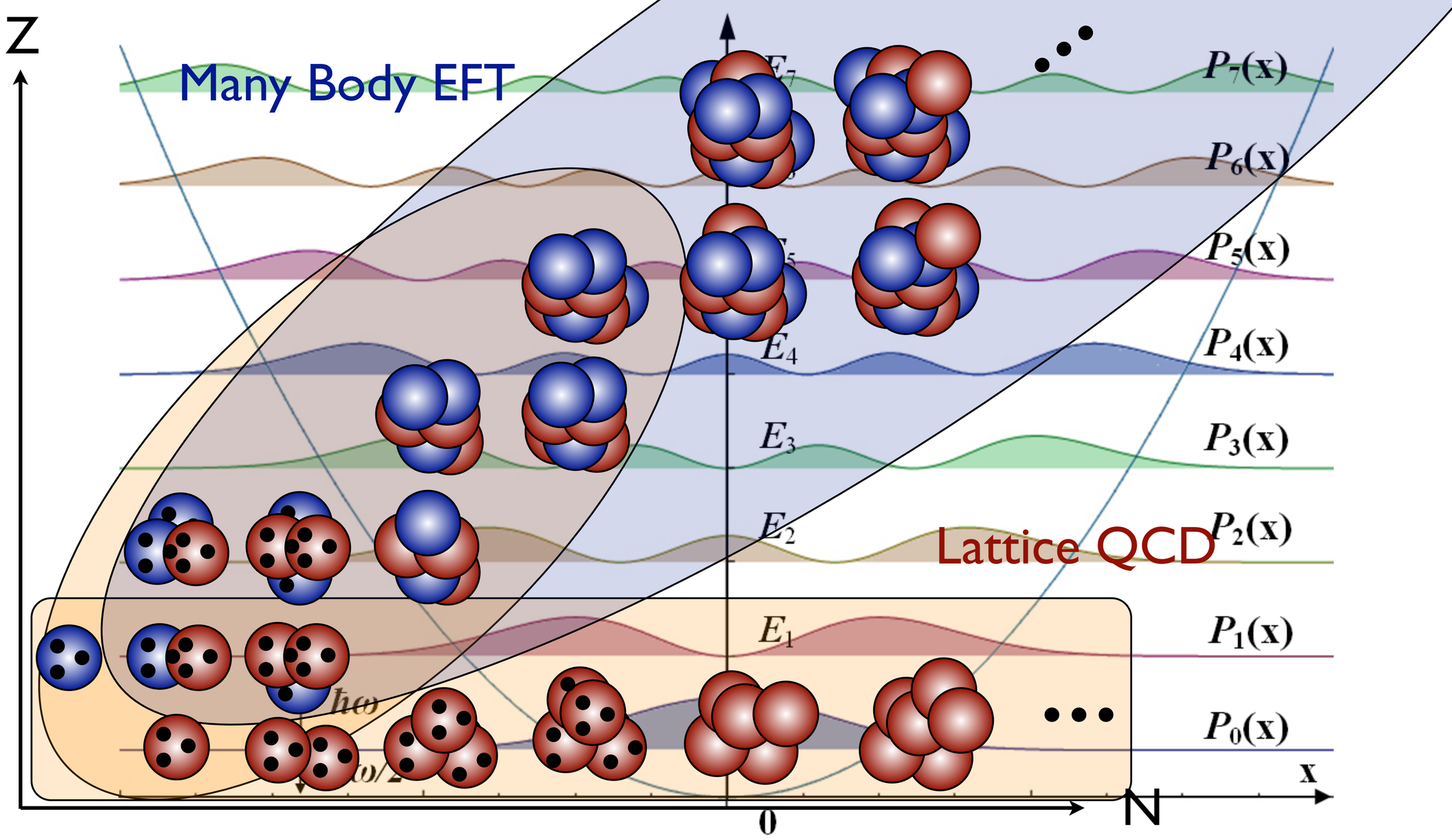


Determine 2, 3, 4 body forces directly from QCD



Determine 2, 3, 4 body forces directly from QCD

match onto many body effective field theory



Determine 2, 3, 4 body forces directly from QCD

match onto many body effective field theory

Lattice QCD for Nuclear Physics

- Lattice QCD offers us the promise of quantitatively connecting our understanding of nuclear physics to QCD
  - The first dynamical LQCD calculation of NN interactions was performed in 2006
    Beane, Bedaque, Orginos, Savage, PRL 97 (2006) [hep-lat/0602010] (NPLQCD)
    Mpi ~ {350, 450, 580} MeV
  - Shortly after - the first approach to a new method for computing the NN potential
    Ishii, Aoki, Hatsuda PRL 99 (2007) [nucl-th/0611096] (HAL QCD)
    quenched-QCD: Mpi ~ {360, 530} MeV

  - These papers set off many years of *fiery* debate (still going) about the validity of the second method and systematic control in the first method culminating in the present situation
    - In many important ways, we still have no reliable calculation of NN interactions from LQCD near the physical pion mass (near = Mpi ≲ 200 MeV) or even lighter than the original work (Mpi~350 MeV)
    - It is not even clear/certain whether two nucleons are bound at Mpi~800 MeV where the numerical challenges are exponentially easier

Lattice QCD for Nuclear Physics

- You have probably been hearing since 2006, that "in 5 years, we'll have NN results at the physical pion mass…"
- Here we are, 14 years later, pretty much in the same position
  - Why is this problem so challenging?
  - What did the gurus miss for their estimates to be so off?

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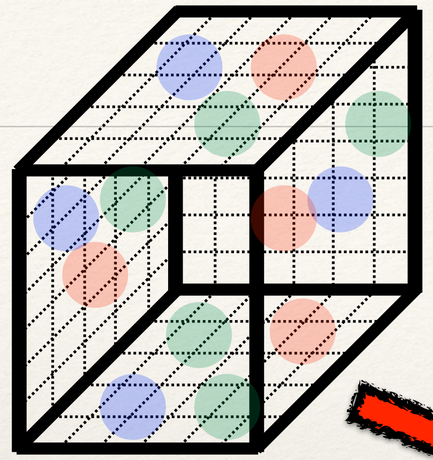
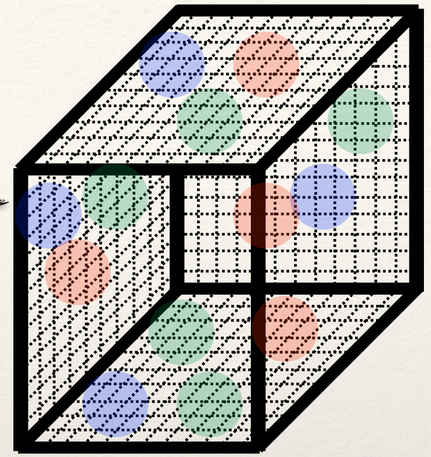
- Here we are, 14 years later, pretty much in the same position
  - Why is this problem so challenging?
  - What did the gurus miss for their estimates to be so off?
  - Why should you believe me when I tell you "Within 5 years, we'll have reliable NN results at the physical pion mass"?

What does it mean to have a LQCD result?



continuum limit
need 3 or more
lattice spacings

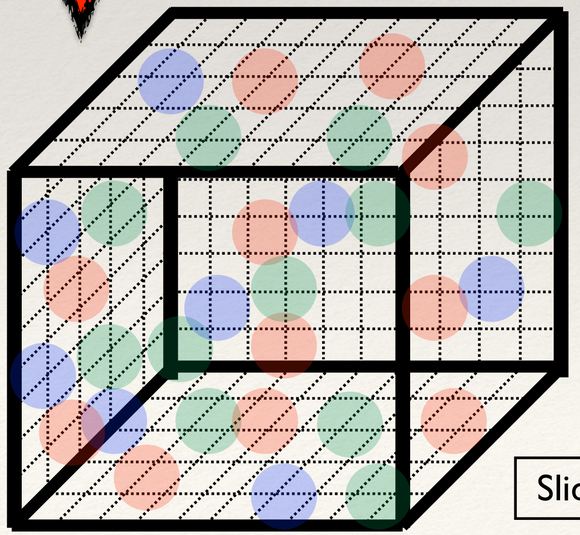
$$t_{comp} \propto \frac{1}{a^6}$$



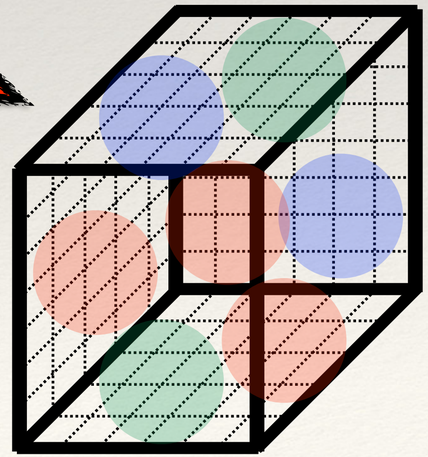
infinite volume limit

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

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



physical pion masses
exponentially bad
signal-to-noise problem



Slide adapted from E. Berkowitz

LQCD challenges for NP

2-point correlation function

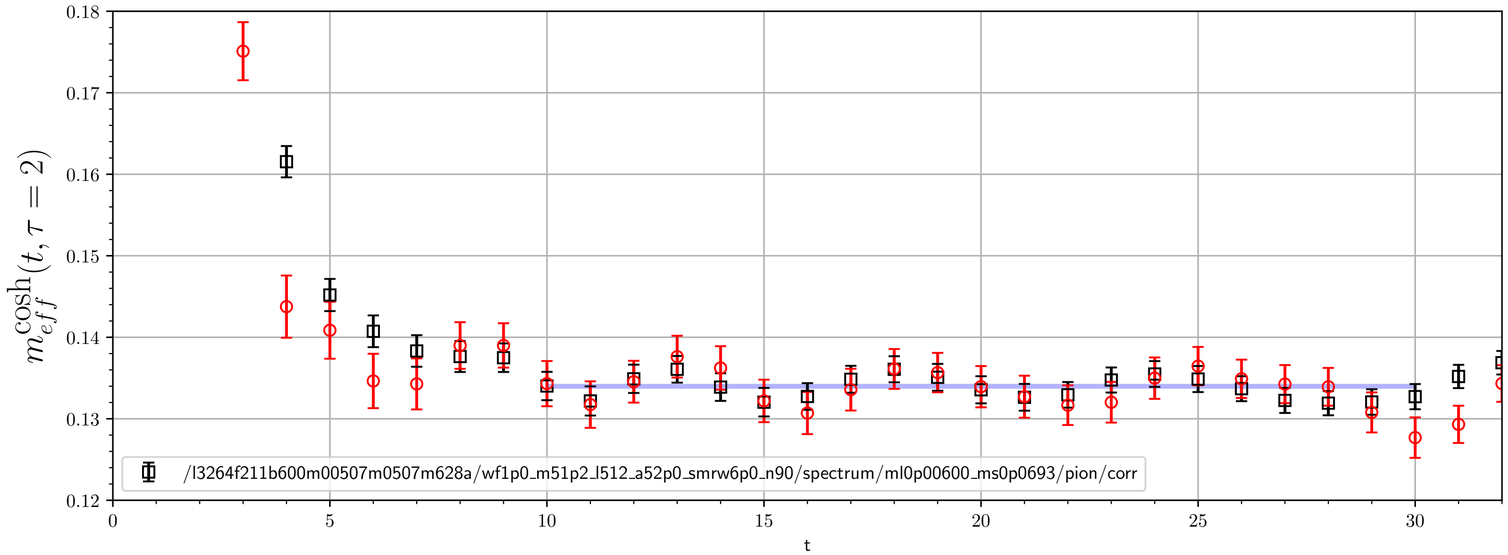
$$C(t) = \sum_n z_n z_n^\dagger e^{-E_n t}$$

$$m_{eff}(t) = \frac{1}{\tau} \ln \left(\frac{C(t)}{C(t+\tau)} \right)$$

For pions, need to consider leading finite temperature effects

$$C(t) = \sum_n z_n z_n^\dagger \left(e^{-E_n t} + e^{-E_n (T-t)} \right)$$

$$m_{eff}^{\cosh}(t,\tau) = \frac{1}{\tau} \cosh^{-1} \left(\frac{C(t+\tau) + C(t-\tau)}{2C(t)} \right)$$



Effective mass of Pion 2-point correlation function
red and black "data" are from different choices of *interpolating* operators

Noise is constant in time - can determine very clean ground state (blue band)

Challenges in applying LQCD to NN

- There are a few substantial challenges which make this problem particularly difficult
  - The signal of interest decays exponentially faster than the noise

$$\frac{\text{Signal}}{\text{Noise}} \propto \sqrt{N_{\text{samples}}} e^{A(m_N - \frac{3}{2} m_\pi)t}$$

  - There is a much higher density of low-lying excitations (need to filter out e.s. to get isolated state)

$$E_0 = 2m_N + \Delta_0 \qquad E_n = 2\left(m_N + \frac{1}{2}\frac{|\vec{n}|(2\pi/L)^2}{m_N} + \cdots\right) + \Delta_n \qquad \vec{n} = (1,0,0) \text{ for example}$$

  - The physics of interest lies in the interactions, which are relatively very small

$$\Delta_{0,n} \ll 2m_N \qquad \Delta_0^{\text{deuteron}} = B_d = 2.2 \text{ MeV} \simeq 0.001 \times 2m_N$$

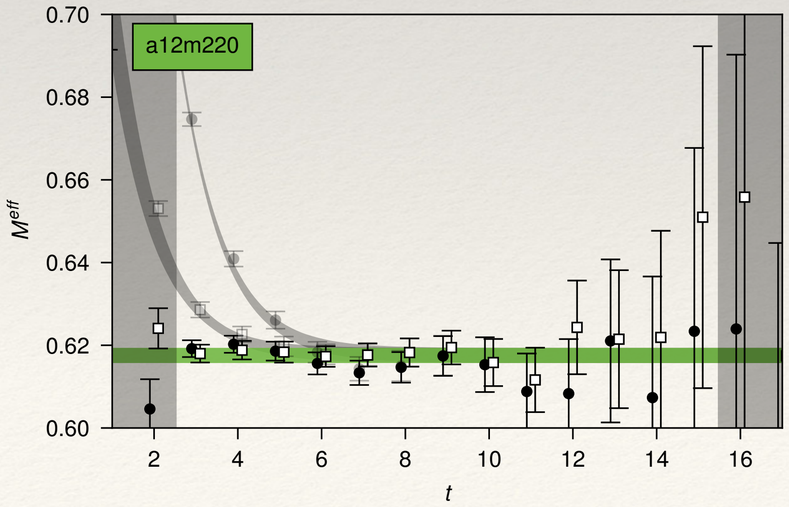
  - The numerical expense to Wick contract all the quarks is exponentially high (the nice tricks you've likely heard of to exploit symmetry to reduce this cost only work for unrealistically simple "wave functions")

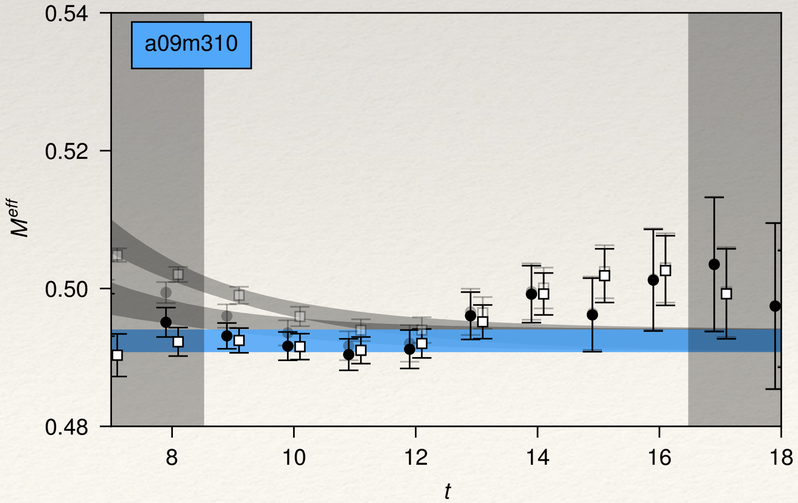
$$\text{cost} \propto N_u! \times N_d! \qquad \text{deut: } 36, \ \text{nn: } 48, \ \text{npp: } 2880, \ \text{nnpp: } 518400$$

Challenges in applying LQCD to NN

- We have to
  - Precisely determine a quantity which is at the per-mill level $\Delta_{0,n} \ll 2m_N$
  - of a signal that is decaying exponentially $\frac{\text{Signal}}{\text{Noise}} \propto \sqrt{N_{\text{samples}}} e^{A(m_N - \frac{3}{2}m_\pi)t}$
  - in a system with a pile up of low-lying excited states (requiring either long time to resolve $t \propto 1/(E_1 - E_0)$ $E_n = 2\left(m_N + \frac{1}{2}\frac{|\vec{n}|(2\pi/L)^2}{m_N} + \cdots\right) + \Delta_n$
  - and the numerical cost of Wick contractions exceeds the rest of the computation $\text{cost} \propto N_u! \times N_d!$

deut: 36, nn: 48, npp: 2880, nnpp: 518400





single nucleon

$A = 1$

NN LQCD Controversy

- NPLQCD
  Yamazaki+Ishikawa+Kuramashi+Ukawa
  CalLat

  observe that for $300 \lesssim m_\pi \lesssim 800$ MeV
  - $B_d > B_d^{\rm phys}$ $\quad B_{nn} > 0$

- HAL QCD
  using a different method based on a
  Nambu-Bethe-Salpeter Kernel (potential)

  observe that for similar pion masses
  no bound deuteron or di-neutron

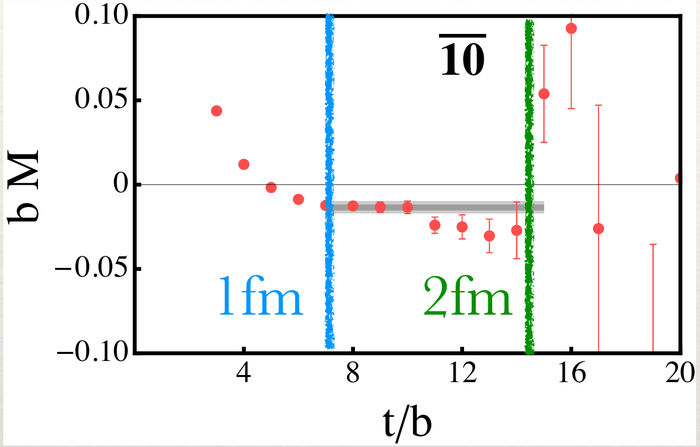
- At first, most of us dismissed this controversy as the HAL QCD method requires additional assumptions that are more difficult to quantify

- However, HAL QCD has more thoroughly studied the systematics in their method, as well as the standard method, than any other group, and they have presented criticism of all of our results that at present, are not definitively refuted

- (Tetsuo Hatsuda originally thought he could be here, and I guess might have discussed some of their results)

NN LQCD Controversy

- The heart of the issues lies in the Signal-to-Noise and density of states problem
  - Signal-to-Noise → need early time
  - Density of states → need late time (or sophisticated "wave functions" to couple to single states much better)



suppress elastic excited states: $e^{t\Delta_E} \ll 1$

$$t\Delta_E \simeq 1 \qquad t \simeq \frac{1}{\Delta_E} \qquad \Delta_E \sim \frac{p^2}{m_N}$$

$$\rightarrow \quad t \simeq 10 \text{ fm}$$

- These arguments are only qualitative - we need quantitative information
- Further evidence: all results with deep binding come from "wave functions" in which all 6 quarks originate from the same space-time point
- If we pull the nucleons apart - the binding energy reduces or vanishes
  - Deep binding is fake? (HAL QCD suggestion)
  - overlap of deep binding state on diffuse operator is too small to detect state? (CalLat hypothesis)
- The resolution requires the use of sophisticated "wave functions" that do a much better job of coupling to single states → can extract the signal early in time before the noise swamps the signal

NN LQCD Controversy

- I returned to LBNL to work on building this bridge between QCD and nuclear physics

NN LQCD Controversy

- I returned to LBNL to work on building this bridge between QCD and nuclear physics and promptly focussed on properties of the single nucleon… (it is relatively so much easier!)

- Our results are evidence that you should be excited about the prospect of understanding nuclear physics (two or more nucleons) from QCD
  - They show that precision properties involving nucleons with the full continuum, infinite volume, physical pion mass limits are possible
  - The new supercomputers are disruptively fast (and the exascale machine is already commissioned)
  - These results were made possible through new ideas in both physics and algorithms
    - Ben Hörz (a postdoc I am working with) re-organized the Wick contraction code for two-nucleons (the sophisticated way) and achieved a 400 (500) x speed up for deuteron (nn)!

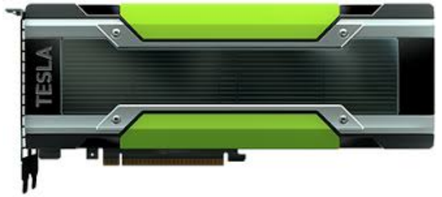
  - Combining the 400x algorithmic speed up for contractions, with the computing speed up (15x for Summit vs Titan), we can now afford to implement sophisticated "wave functions" (physics optimization) and prepare the two-nucleon states at the source and sink to strongly overlap onto the states of interest and extract the physics early in time where the signal is exponentially more precise

Peta scale computing era

Vulcan (BG/Q)
5 PetaFlops

Lawrence Livermore National Laboratory

Surface



RZHasGPU

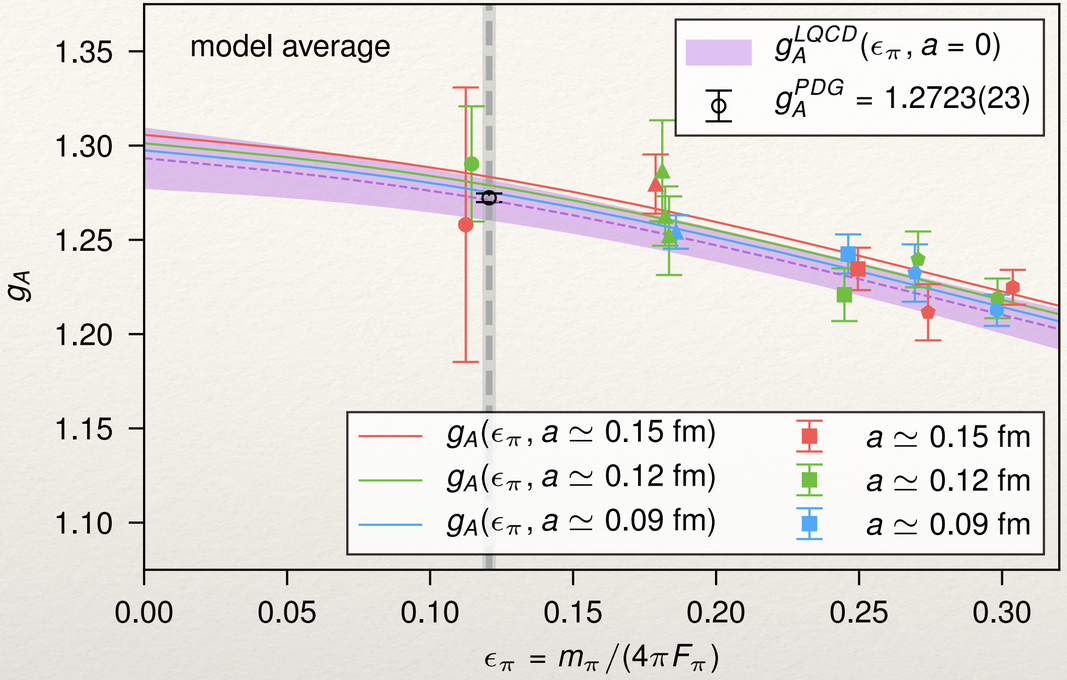
OAK RIDGE National Laboratory | LEADERSHIP COMPUTING FACILITY

O(100 PFlops)

O(ExaFlops)

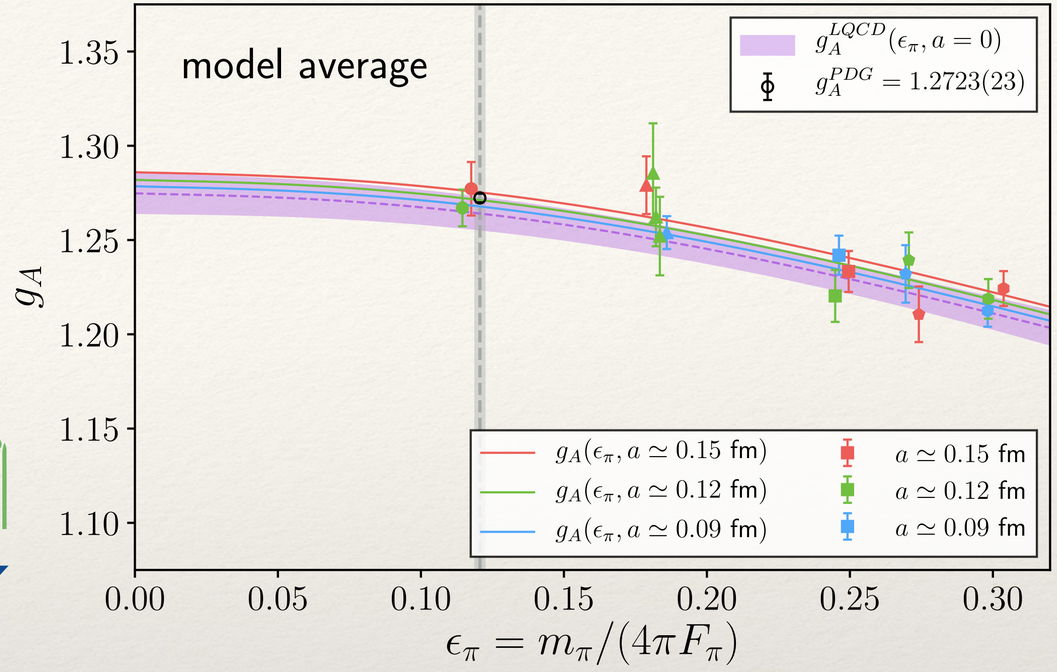
Nature 558 (2018) no. 7708, 91-94
Chang et al. [arXiv:1805.12130]

1 year on Titan (ORNL) + 2 years on GPU machines at LLNL



Sierra Early Science

PRELIMINARY

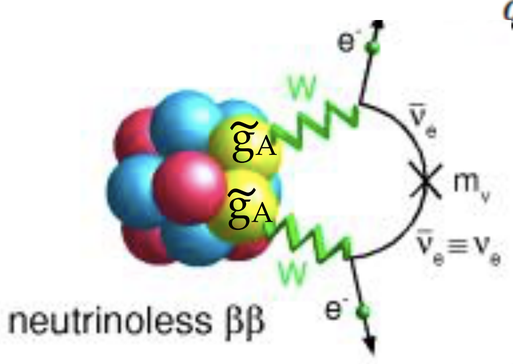


California Lattice Collaboration

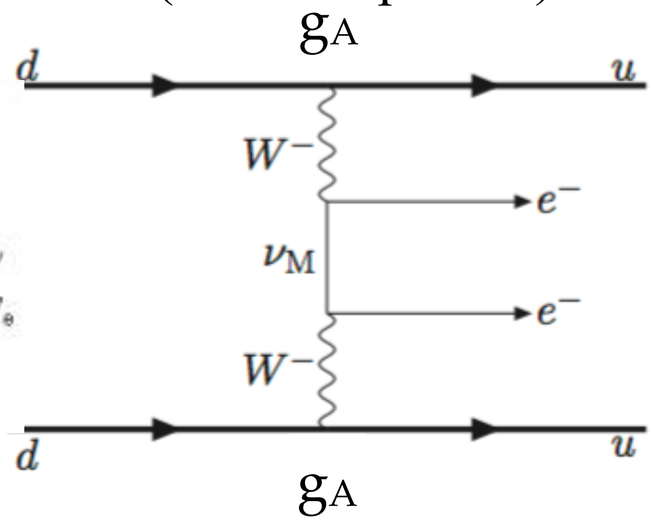
- The a12m130 (48^3 x 64 x 20) with 3 sources cost as much as all other ensembles combined
  - 2.5 weekends on Sierra → 16 srcs
  - Now, 32 srcs (un-constrained, 3-state fit)
- We generated a new a15m135XL (48^3 x 64) ensemble (old a15m130 is 32^3 x 48)
  - $M\pi L = 4.93$ (old $M\pi L = 3.2$)
  - $L_5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

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

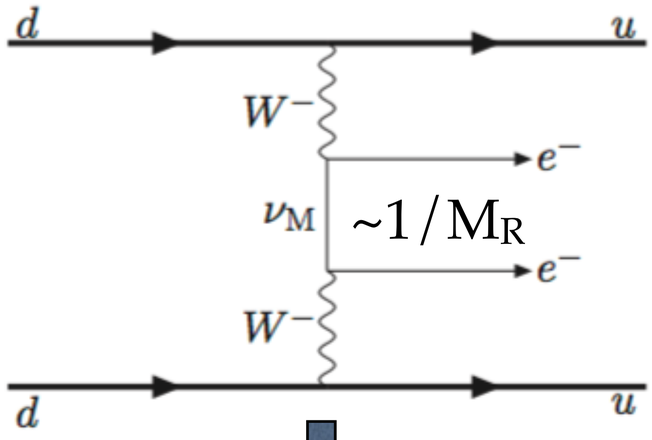
Neutrinoless Double Beta-Decay

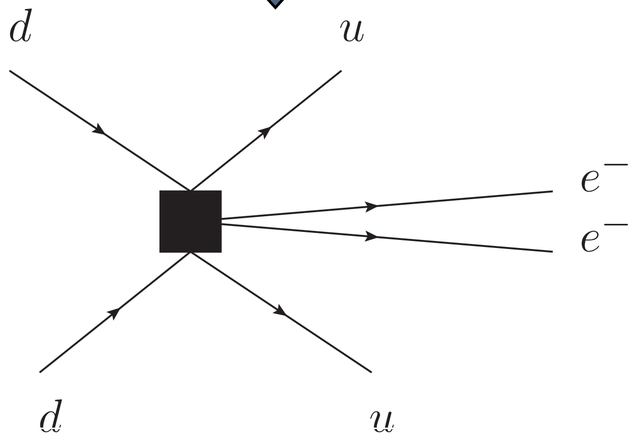


long-range contribution
(standard picture)



short-range contribution
possibly equally/more important





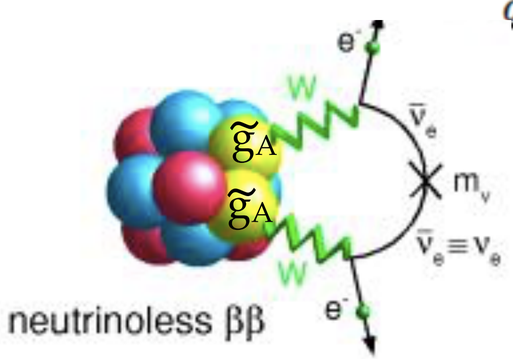
Long Range: lattice QCD can help understand "quenching" of g_A in a nucleus - although - see Gysbers et al. Nature Phys (2019) [1903.00047]

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

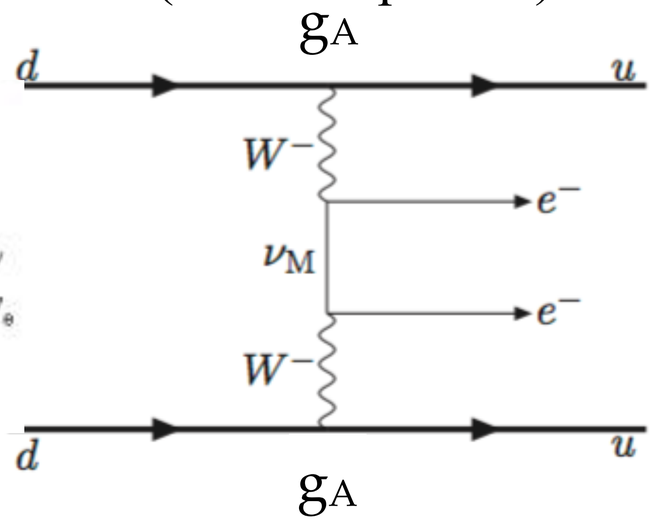
Lattice QCD: compute 2-nucleon matrix elements to determine unknown couplings/transition rates

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
(standard picture)



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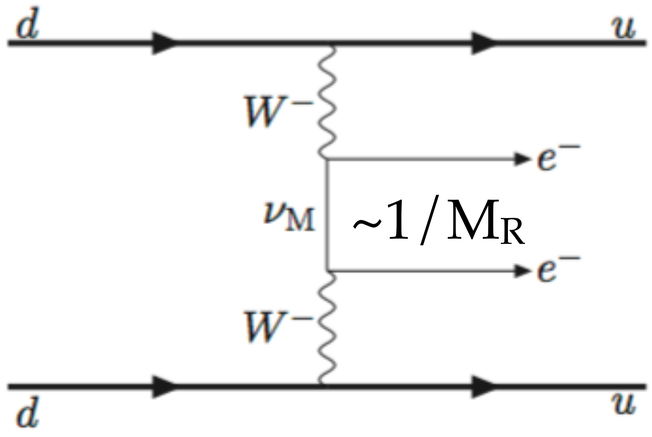
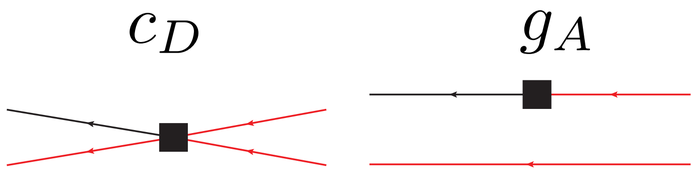
possibly equally/more important

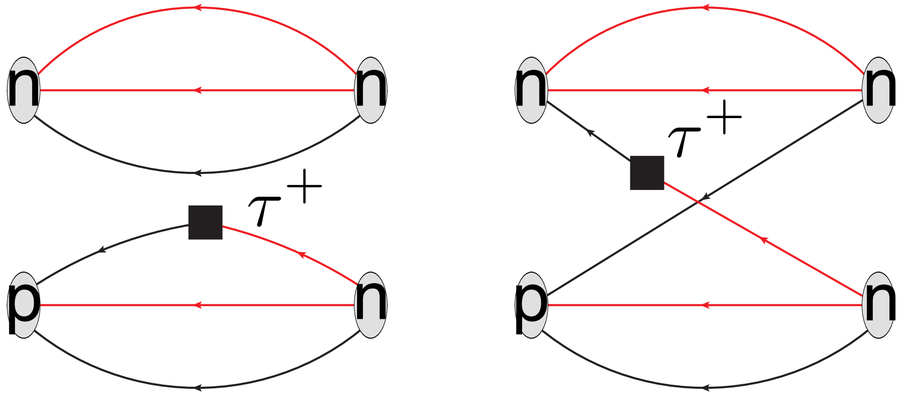


Long Range Contribution

EFT Level



Lattice QCD



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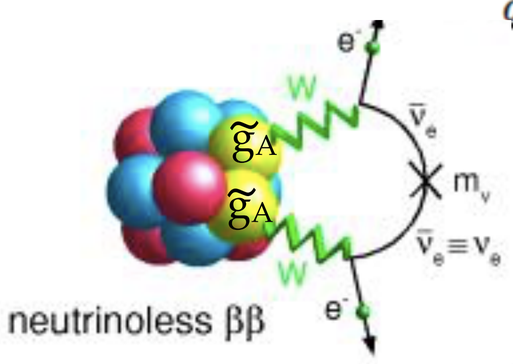
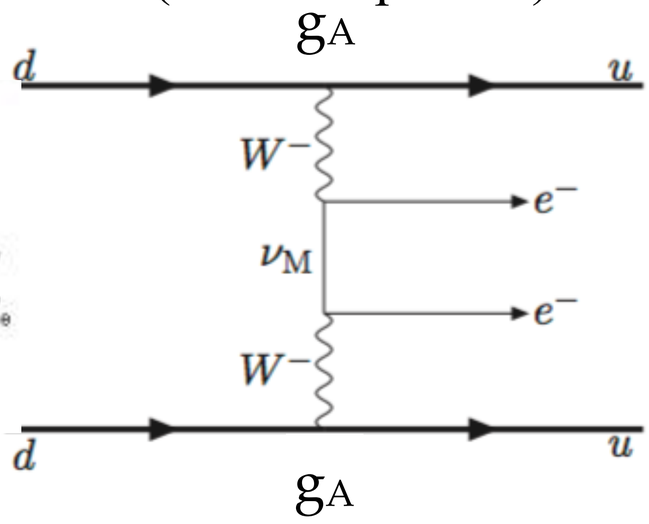
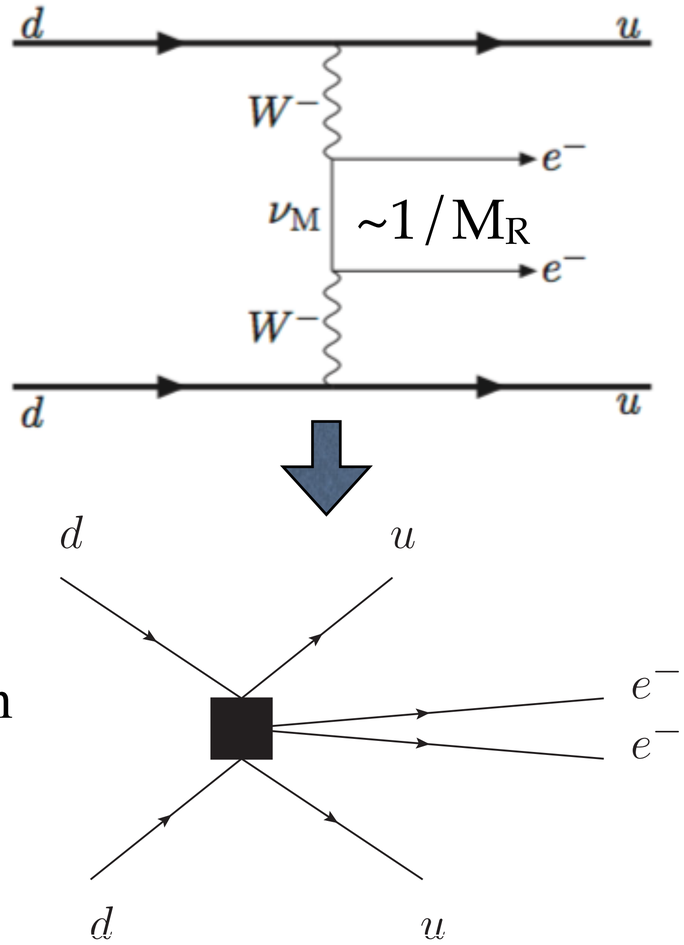


long-range contribution
(standard picture)



short-range contribution
possibly equally/more important

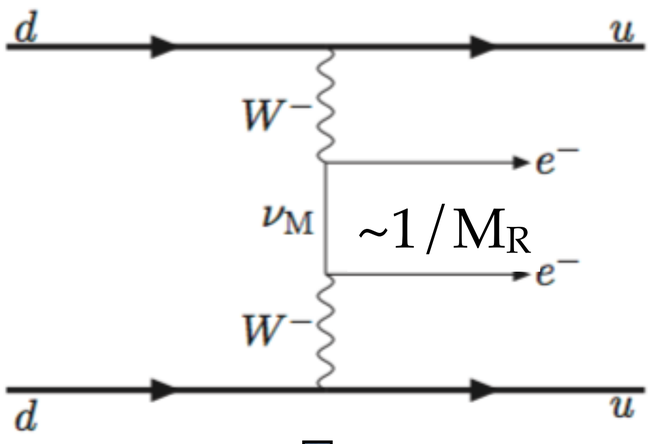


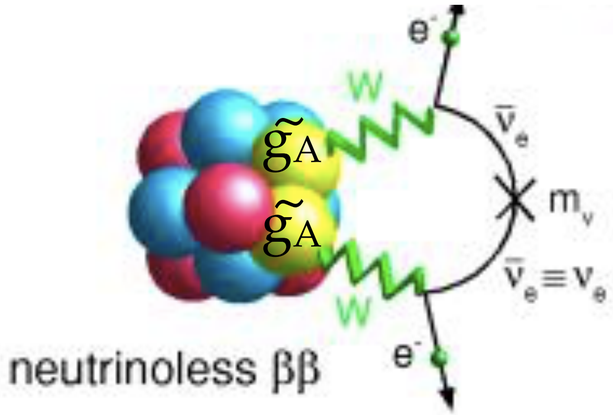
Short Range Contribution

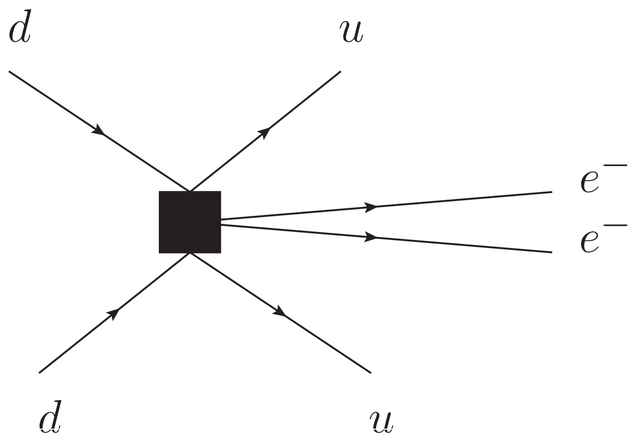
Need to know value of 4-quark matrix element in two-nucleon systems: LQCD is the only tool we have as we are not able to measure 0νββ in few-nucleon systems - so need fundamental theory calculation

Neutrinoless Double Beta-Decay

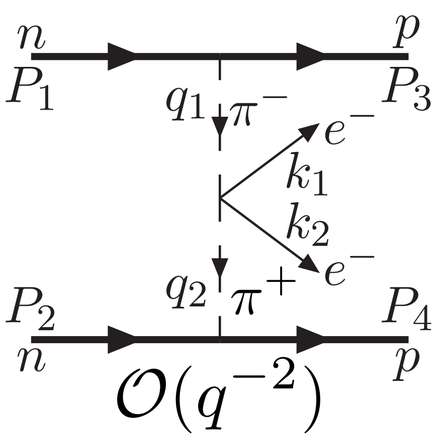
Short-range contribution: probe for heavy physics

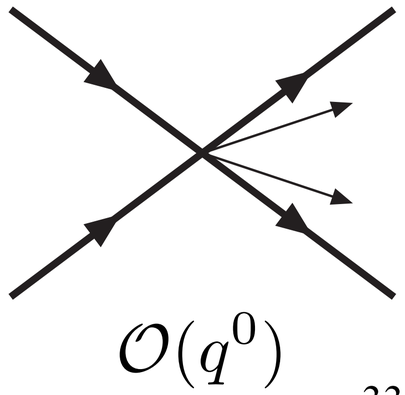






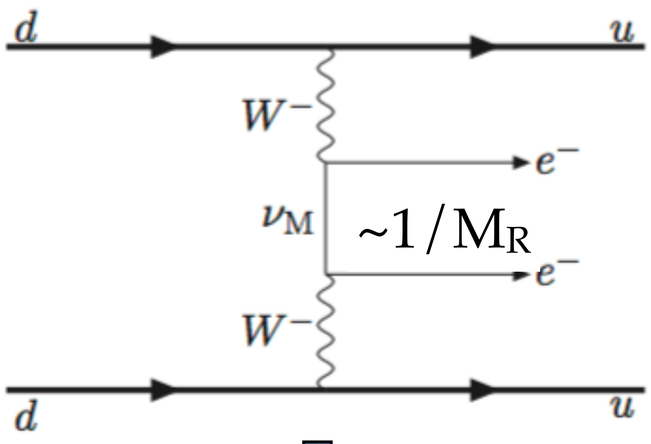
Effective Field Theory (π, N)
[Praezu, Ramsey-Musolf, Vogel]

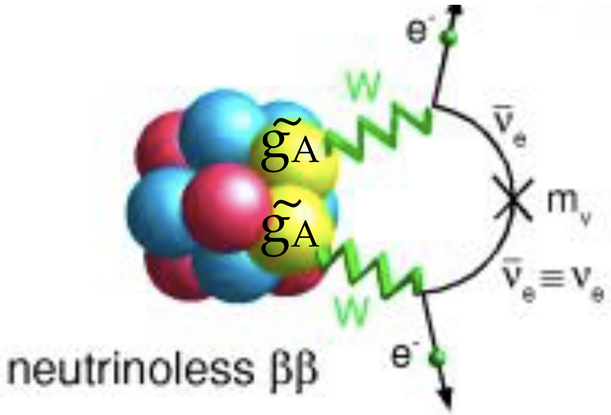


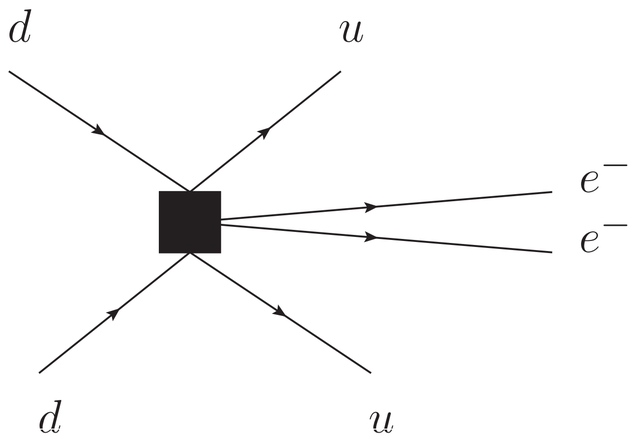


Neutrinoless Double Beta-Decay

Short-range contribution: probe for heavy physics







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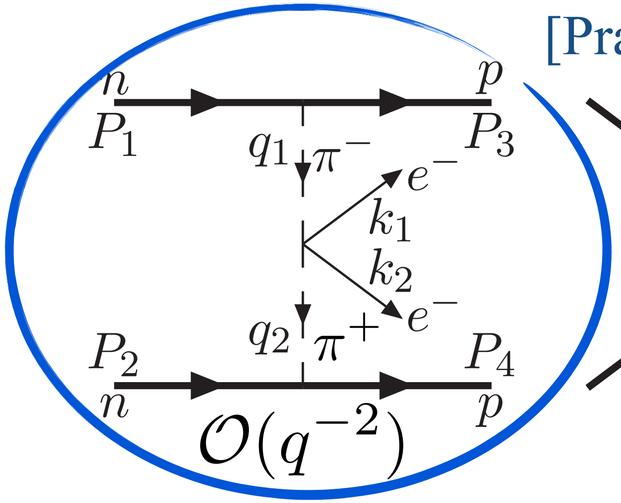
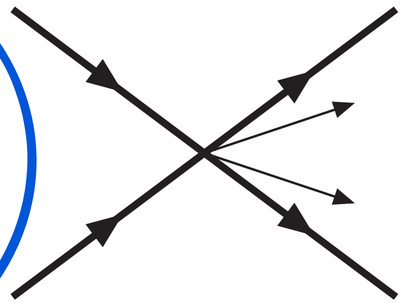
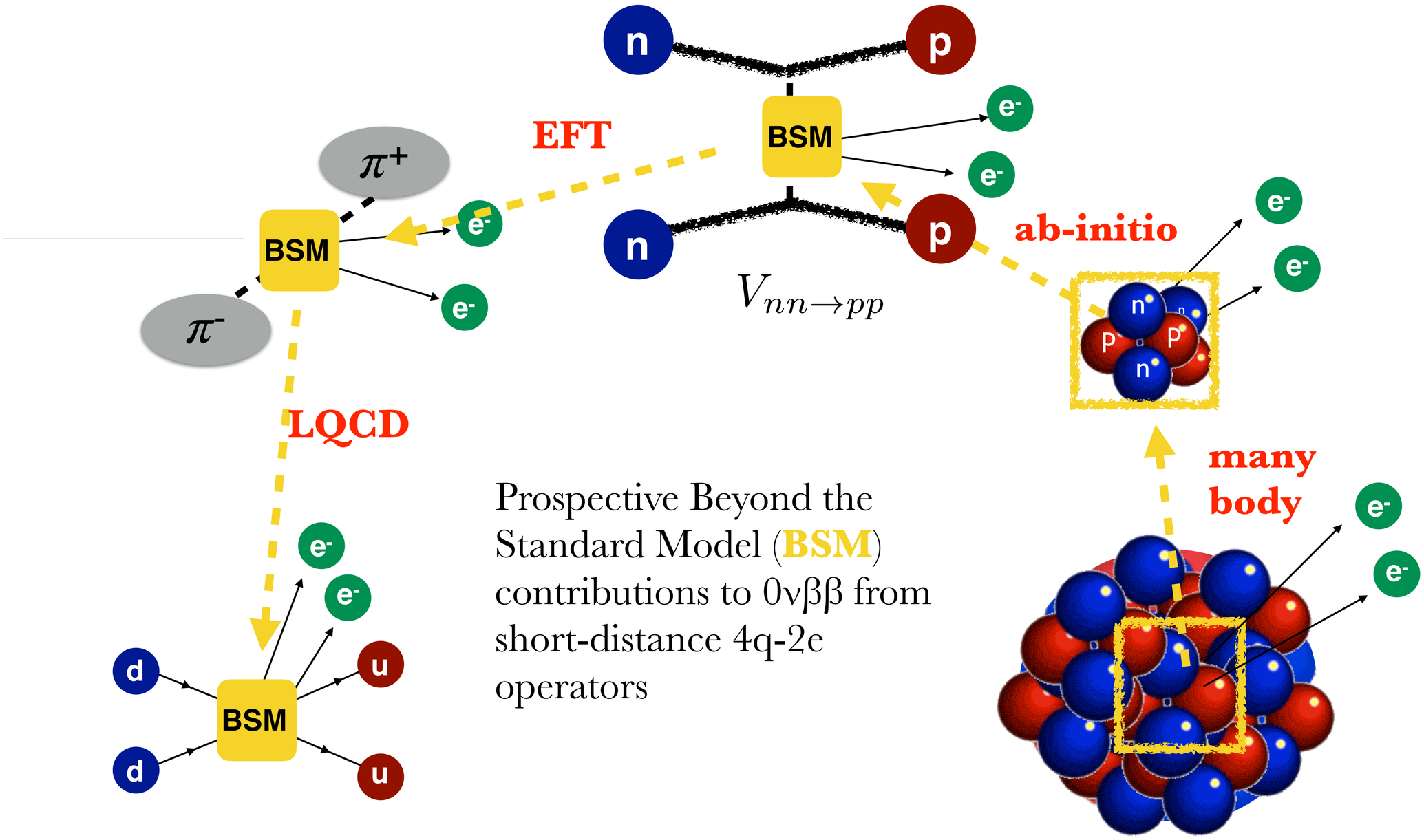




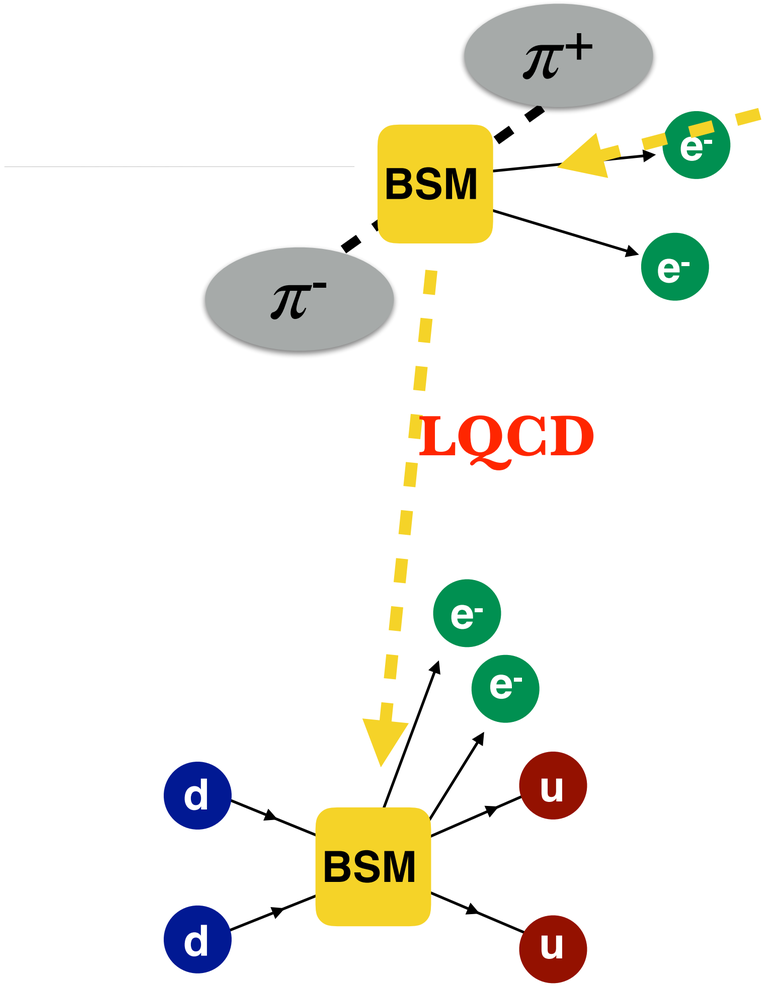
$\mathcal{O}(q^0)$

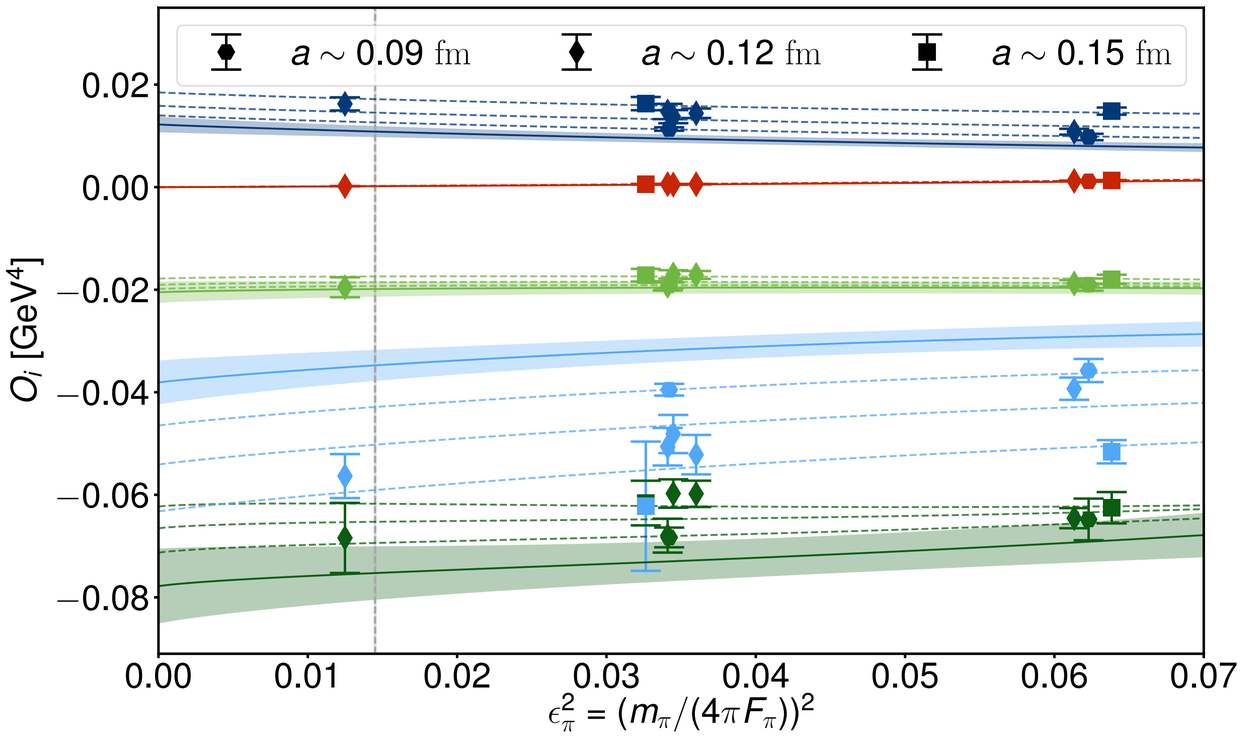
Lattice QCD for Neutrinoless Double Beta-Decay



Prospective Beyond the Standard Model (**BSM**) contributions to 0νββ from short-distance 4q-2e operators

Lattice QCD for Neutrinoless Double Beta-Decay



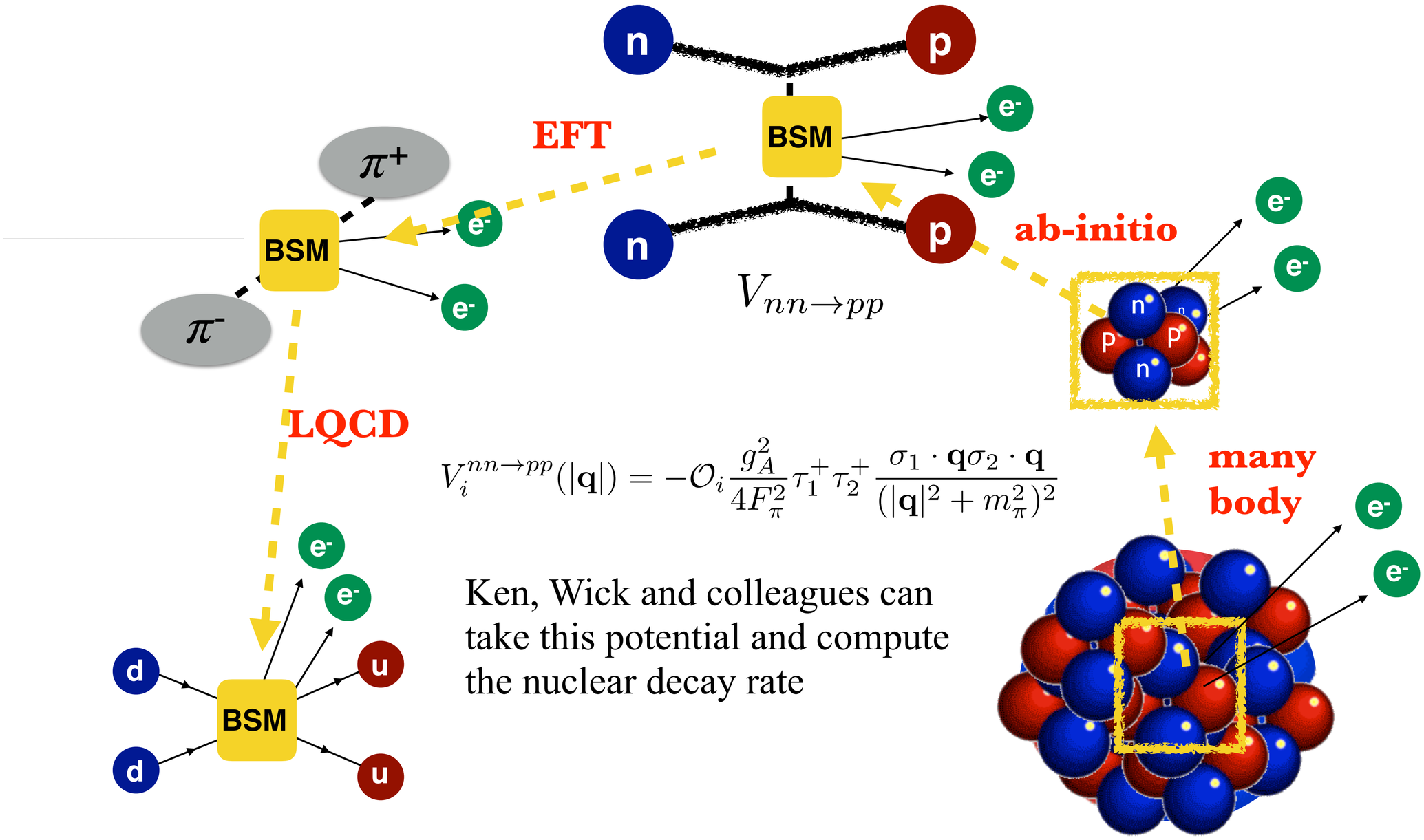


First (and complete) lattice QCD calculation of the $\pi^- \rightarrow \pi^+$ transition amplitude

A. Nicholson, E. Berkowitz, H. Monge-Camacho, D. Brantley, N. Garron, C.C. Chang, E. Rinaldi, M.A. Clark, B. Joó, T. Kurth, B.C Tiburzi, P. Vranas, AWL

Phys. Rev. Lett. 121 (2018) 172501 [arXiv:1805.02634]

Lattice QCD for Neutrinoless Double Beta-Decay



$$V_i^{nn\to pp}(|\mathbf{q}|) = -\mathcal{O}_i \frac{g_A^2}{4F_\pi^2}\tau_1^+\tau_2^+ \frac{\sigma_1\cdot\mathbf{q}\sigma_2\cdot\mathbf{q}}{(|\mathbf{q}|^2+m_\pi^2)^2}$$

Ken, Wick and colleagues can take this potential and compute the nuclear decay rate

Yesterday, Today and Tomorrow

- Yesterday
  - Neutron Lifetime
    g_A with 1% uncertainty
  - $0\nu\beta\beta$
    $\pi^- \rightarrow \pi^+$

- Today (≤5years)
  - g_A to <0.5%
    proton charge radius
    Deuteron
    Hyperon-Nucleon interactions
  - $g_A(Q^2)$
    two-nucleon axial response
    short distance NN matrix elements (4quark operators)

- Tomorrow
  three-neutron force
  hyperon-nucleon-nucleon forces

Yesterday, Today and Tomorrow

- Yesterday
  - Neutron Lifetime
    g_A with 1% uncertainty
  - $0\nu\beta\beta$
    $\pi^- \rightarrow \pi^+$

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  - $g_A(Q^2)$
    two-nucleon axial response
    short distance NN matrix elements (4quark operators)

- Tomorrow
  three-neutron force
  hyperon-nucleon-nucleon forces
  - figure out how to formulate lattice QCD in a harmonic oscillator!

Collaborators

New Collaborators
John Bulava
Christian Drischler
Drew Hanlon
Wick Haxton
Ben Horz
Chris Körber
Colin Morningstar

Nucleon Axial Coupling
Nature 558 (2018) no. 7708
Chia Cheng (Jason) Chang
Amy Nicholson
Enrico Rinaldi
Evan Berkowitz
Nicolas Garron
David Brantley
Henry Monge-Camacho
Chris Monahan
Chris Bouchard
Kate Clark
Balint Joó
Thorsten Kurth
Kostas Orginos
Pavlos Vranas
André Walker-Loud

0νββ
Phys.Rev.Lett. 121 (2018)
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Enrico Rinaldi
Kate Clark
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Happy Birthday Wick!

- I have not worked with harmonic oscillators
- Wick has not worked with lattice QCD
- Despite this lack of obvious overlap, Wick has been very generous with his time, advice and resources
- I am very grateful for your mentorship and support as I have developed my research vision and career
  - especially since I seem to have chosen to butt heads with more traditional sources of support for young lattice/nuclear theorists