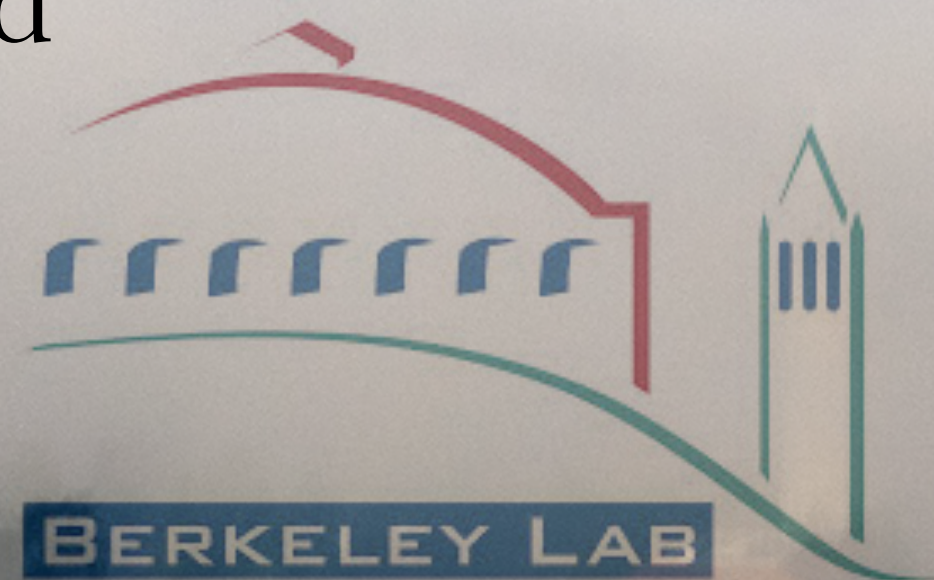


What is Lattice QCD? (and why do we need it?)

UC Berkeley 290e
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What is Lattice QCD (LQCD) and Why do we Need it?

- ❑ Quantum Chromodynamics (QCD) is one of the three gauge theories that make up the Standard Model (SM) of Particle Physics
- ❑ QCD is the fundamental theory of nuclear strong interactions (to the best of our knowledge). It is interesting to understand how to compute properties of strongly interacting (nuclear) matter both
 - ❑ To understand how nuclear physics emerges from QCD and to predict properties of strongly interacting matter
 - ❑ Nuclear Equation of State (neutron stars)
 - ❑ Properties of the Quark Gluon Plasma
 - ❑ ...
 - ❑ To understand how new, beyond the Standard Model (BSM) physics might effect precision, low-energy tests of the SM
 - ❑ Why is the universe composed of matter and not anti-matter? (are there permanent EDMs in nucleons and nuclei?)
 - ❑ Are neutrinos Majorana in nature, thus allowing for neutrinoless double beta-decay of nuclei?
 - ❑ Are there corrections to the SM V-A beta-decay processes (as can be measured with ultra-cold neutron decays?)
 - ❑ ...

What is Lattice QCD (LQCD) and Why do we Need it?

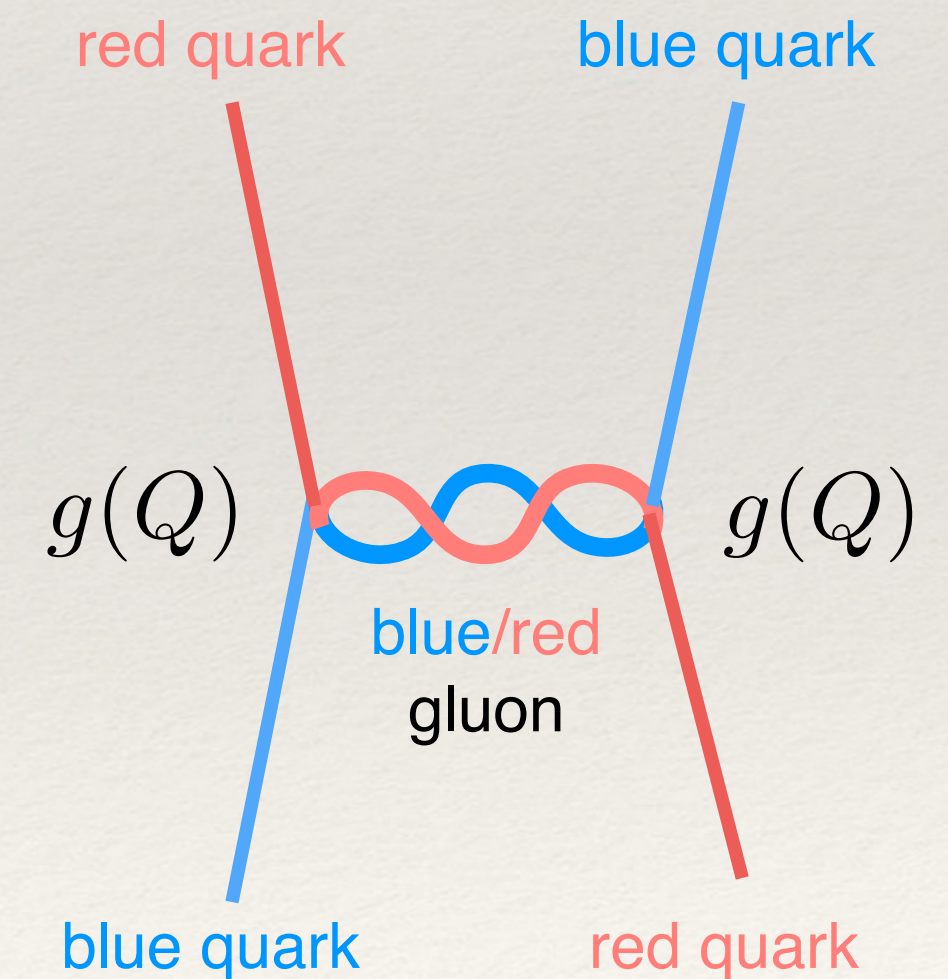
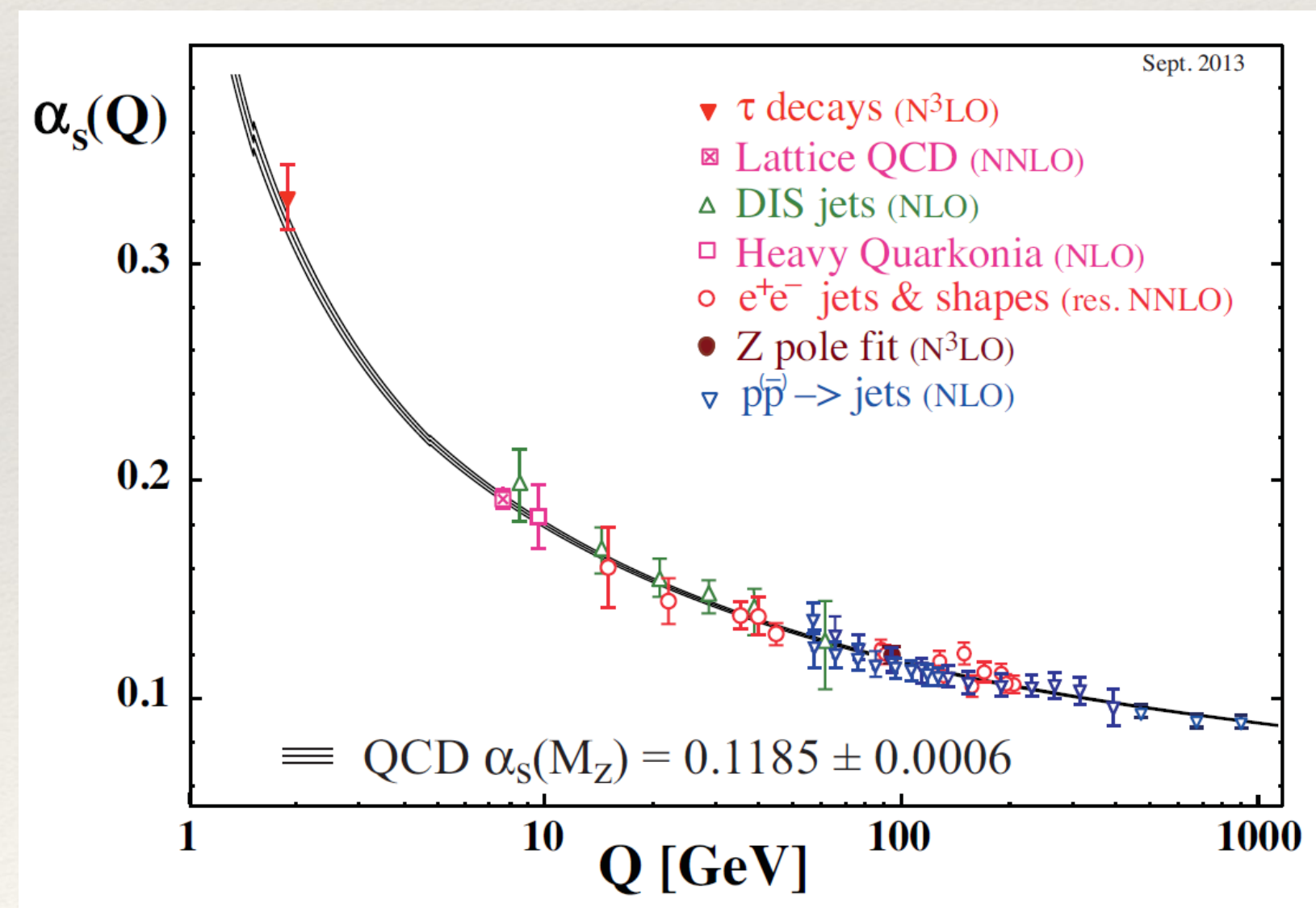
- QCD is a very “predictive” theory (it only has a few parameters)

$$\mathcal{L}_{\text{QCD}} = \sum_{q=u,d,s,c,b,t} \bar{\psi}_q [i(\partial_\mu + igA_\mu)\gamma^\mu - m_q] \psi_q - \frac{1}{4} G_{\mu\nu} G^{\mu\nu}$$

↑ quarks ↑ gluons

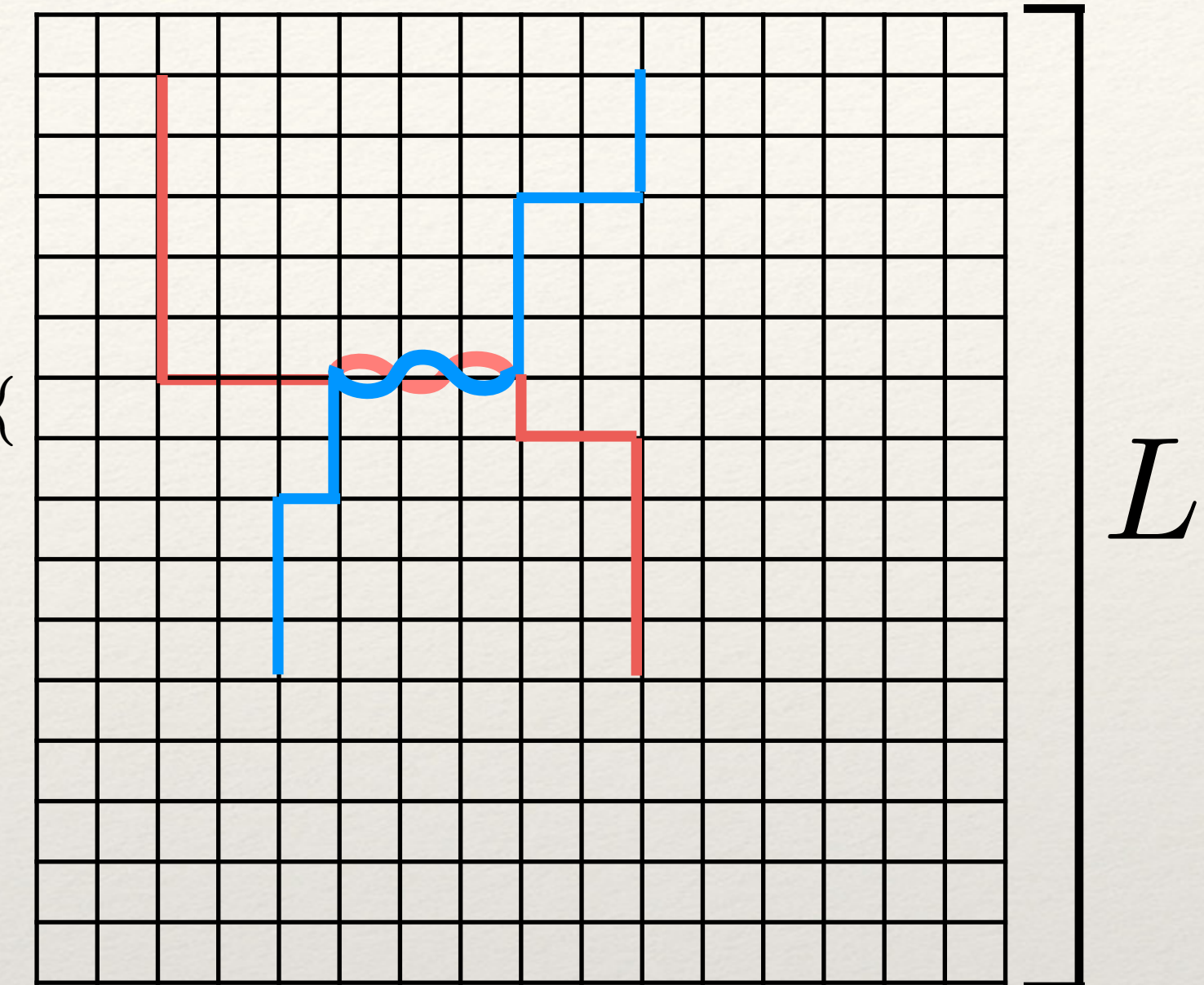
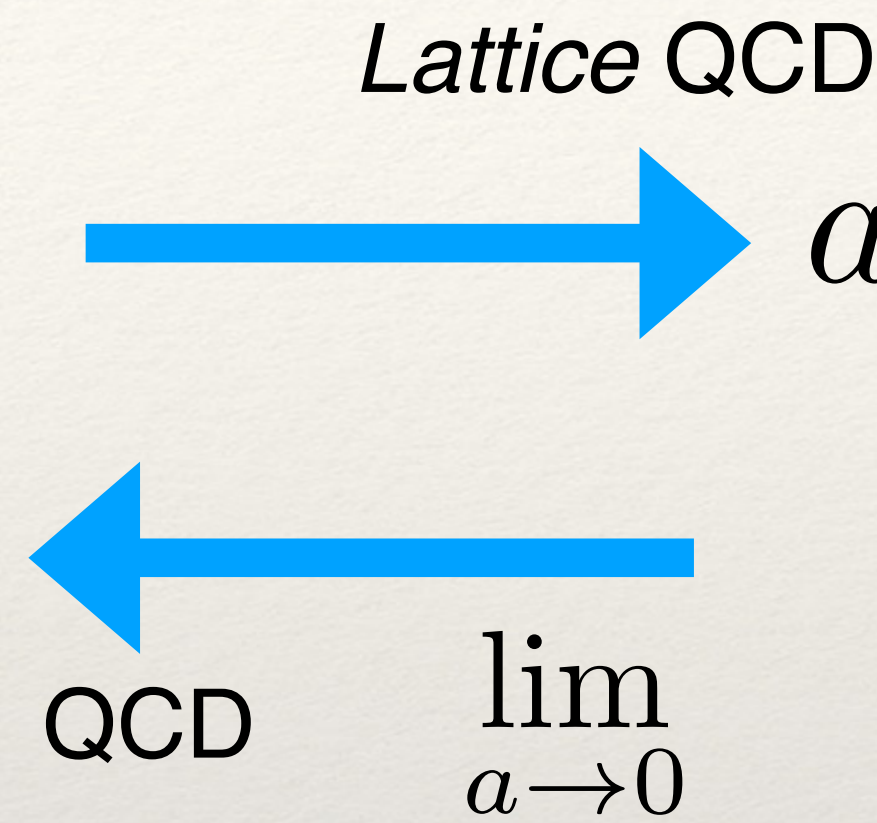
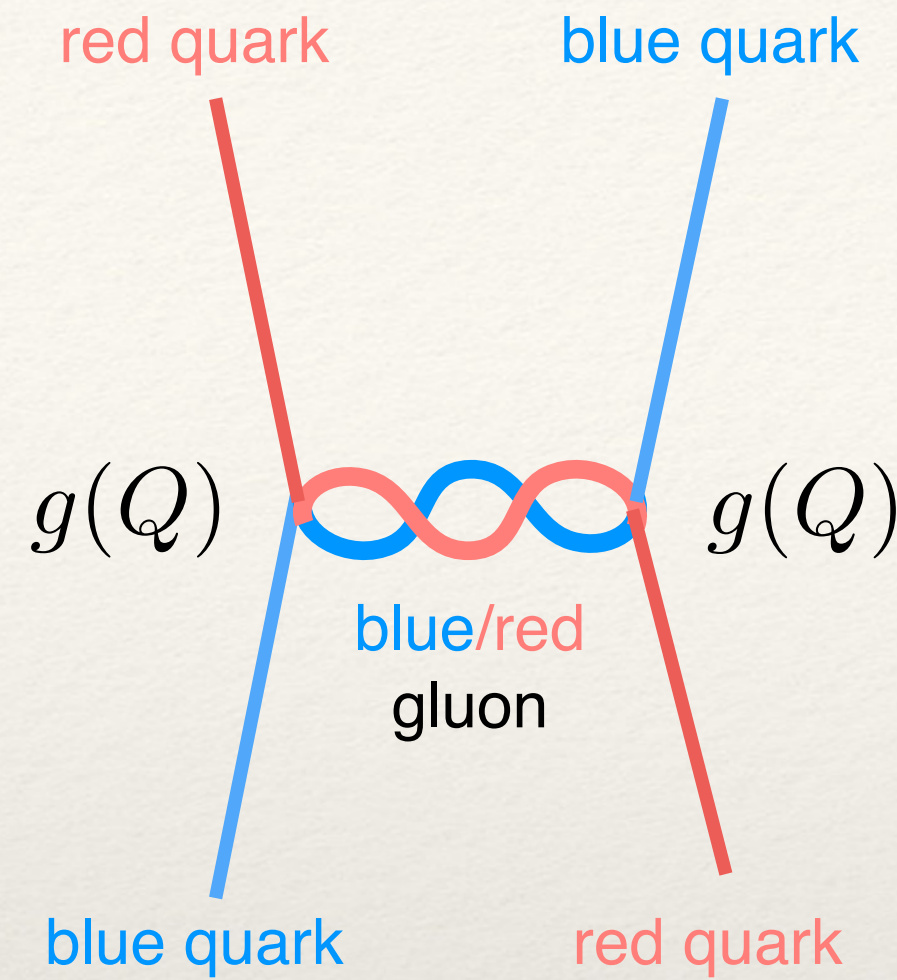
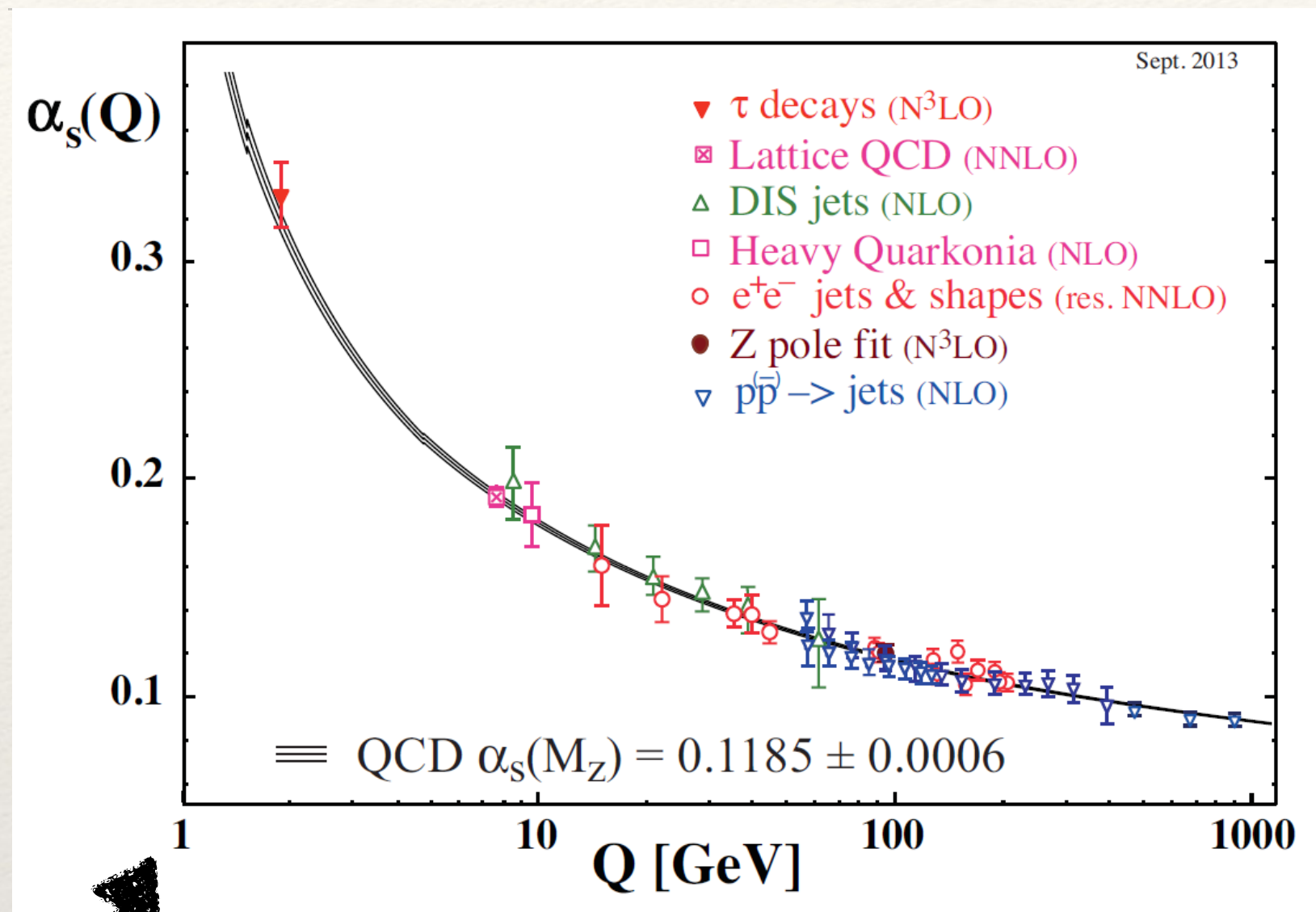
- At “nuclear” energies, 3 parameters: g , m_u , m_d
- Once these 3 parameters are determined with experimental input, everything else is a prediction
Nuclear physics “emerges” from QCD

- But - at low energy, QCD is strongly coupled
- Very challenging to compute processes and quantities directly from QCD



$$\alpha_s(Q) = \frac{g^2(Q)}{4\pi}$$

QCD is a “most perfect” theory: perturbative at short distance



Proton mass
 $M_p = 0.938 \text{ GeV}$

$$\alpha_s(Q) = \frac{g^2(Q)}{4\pi}$$

The gluon self-interactions (the gluons carry the “color” charge) leads to a very different theory from QED.

Solving QCD at low (nuclear) energy scales ($\approx 1 \text{ GeV}$) is currently impossible with pen/paper techniques (no small parameter to control a perturbation series).

At high energy scales, the interaction coupling becomes small, $\alpha_s(Q)$ allowing for perturbation theory to work.

We can discretize QCD on a space-time *lattice*, conveniently coined lattice QCD

The quantum uncertainty principle means as we reduce the lattice spacing, $a \rightarrow 0$, this is equivalent to probing the theory at high energies ($a \sim \Delta x$)

$$\Delta x \Delta Q \geq \frac{\hbar}{2}$$

We know the exact theory to discretize without uncertainty quantification and the computer can handle the non-perturbative long-range QCD interactions

QCD is a “most perfect” theory: perturbative at short distance

- There are 2 important symmetries of QCD which are important for understanding the dynamics of the theory
 - Exact gauge-invariance (invariance of theory under local $SU(3)$ -color rotations), which gives rise to massless gluons
 - Approximate symmetry under global $SU(2)$ chiral rotations of up and down quarks

QCD: symmetry and low-energy

□ Approximate global chiral symmetry of QCD

- In the limit that the up and down quark masses are 0, QCD has an exact $SU(2)_L \times SU(2)_R$ chiral symmetry

$$\mathcal{L}_{\text{QCD}} = \bar{\psi}_L i\gamma^\mu D_\mu \psi_L + \bar{\psi}_R i\gamma^\mu D_\mu \psi_R - m (\bar{\psi}_L \psi_R + \bar{\psi}_R \psi_L)$$

$$\psi = \begin{pmatrix} \psi_u \\ \psi_d \end{pmatrix}$$

$$m = \begin{pmatrix} m_u & 0 \\ 0 & m_d \end{pmatrix}$$

- Global $SU(2)$ rotation $\psi_{L,R} \rightarrow e^{i\theta_{L,R}^a \tau_{L,R}^a / 2} \psi$

$$\mathcal{L}_{\text{QCD}}^D \rightarrow \mathcal{L}_{\text{QCD}}^D$$

$$\psi_R = \frac{1 + \gamma_5}{2} \psi \quad \psi_L = \frac{1 - \gamma_5}{2} \psi$$

- While the mass operator is only invariant if $\theta_L = \theta_R$, **the vector subgroup**
The quark mass **explicitly breaks** the full $SU(2)_L \times SU(2)_R$ symmetry

- We also know (now) that $m_{u,d} \ll \Lambda_{\text{QCD}} \approx 1 \text{ GeV}$ so we expect that this global symmetry should be realized in nature

QCD: symmetry and low-energy

- Approximate global $SU(2)_L \times SU(2)_R$ chiral symmetry of QCD

$$\mathcal{L}_{\text{QCD}} = \bar{\psi}_L i\gamma^\mu D_\mu \psi_L + \bar{\psi}_R i\gamma^\mu D_\mu \psi_R - m (\bar{\psi}_L \psi_R + \bar{\psi}_R \psi_L)$$

- If this approximate symmetry were a symmetry of the QCD vacuum, we would observe that the negative parity nucleon has the same mass as the nucleon

$$m_N \approx 940 \text{ MeV} \quad m_{N^*} \approx 1535 \text{ MeV}$$

- We also observe — all hadrons made of u,d quarks have masses $\geq 770 \text{ MeV}$ except for the pions:

$$m_{\pi_0} \approx 135 \text{ MeV} \quad m_{\pi_\pm} \approx 139 \text{ MeV}$$

- Why are there three relatively light hadrons in the spectrum?
And why do we not observe a near degeneracy between the parity partner states?

QCD: symmetry and low-energy

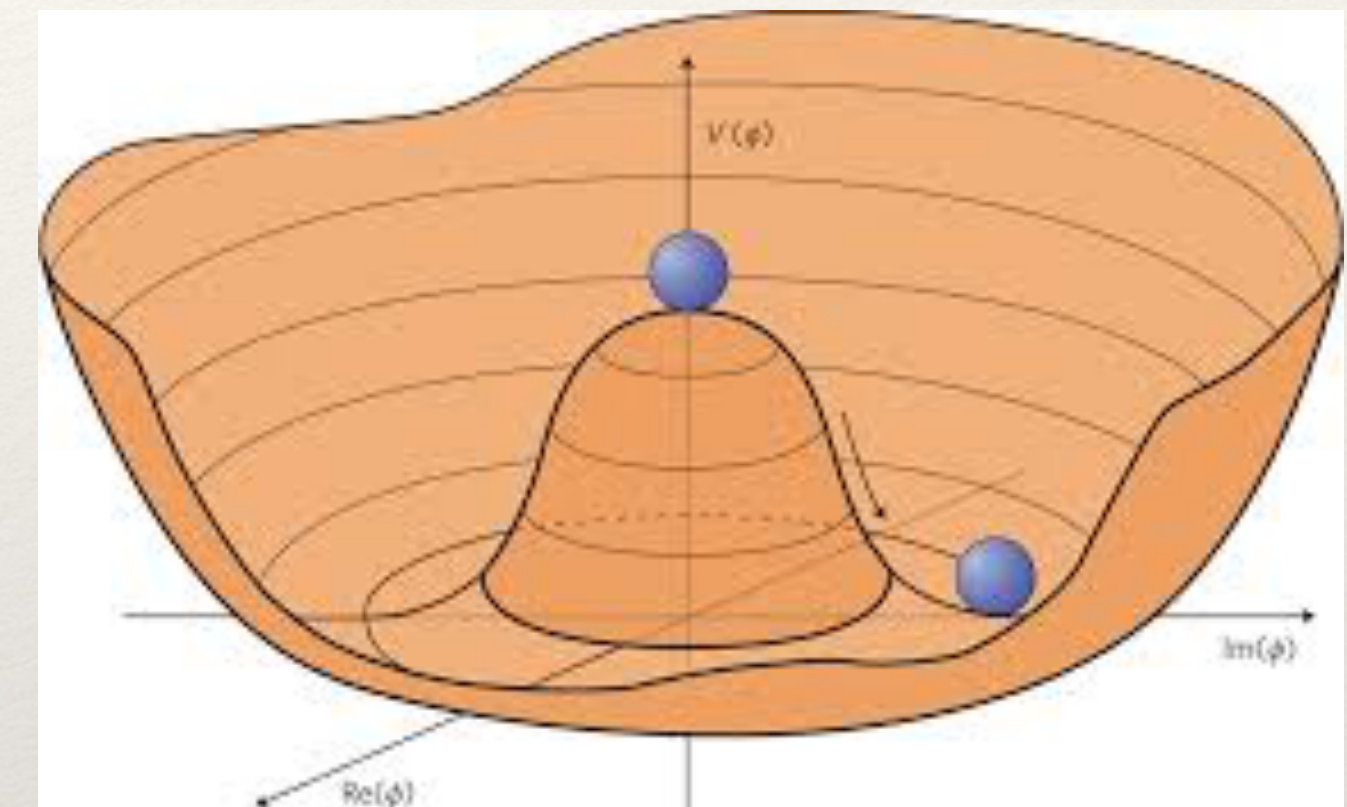
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- The situation reminded us of spontaneous symmetry breaking. If a global symmetry is spontaneously broken, there must emerge Nambu-Goldstone modes which are massless excitations (along the vacuum)
- In our case, we have an approximate symmetry. We postulate that the QCD vacuum spontaneously breaks this approximate symmetry down to the vector subgroup

$$SU(2)_L \times SU(2)_R \rightarrow SU(2)_V \quad \text{— the remaining } SU(2) \text{ symmetry is Isospin symmetry}$$

- Because we start with an approximate, not exact, symmetry, the Nambu-Goldstone modes will have a small mass arising from the explicit breaking of the symmetry



QCD: symmetry and low-energy

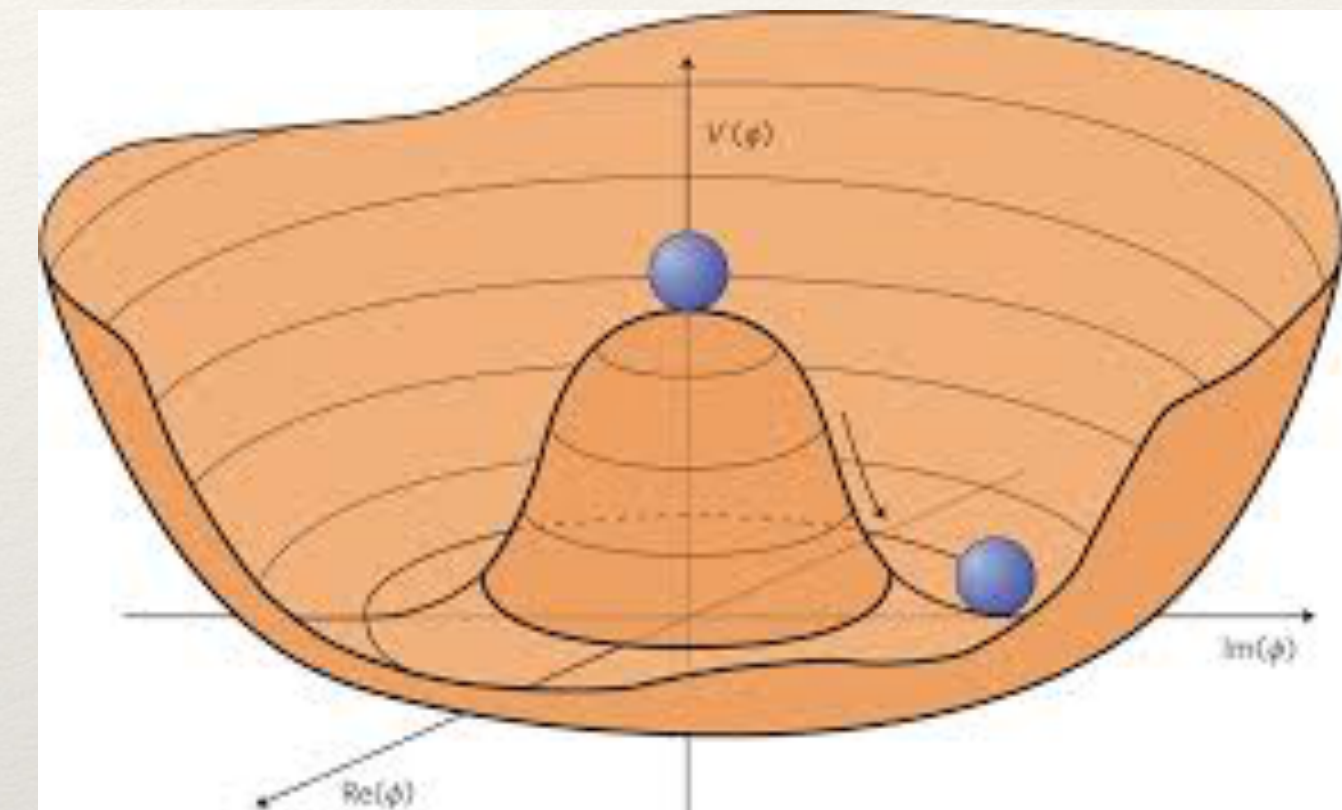
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- The global chiral symmetry has 3+3 generators (from each $SU(2)$)
- We end with 3 symmetry generators of $SU(2)_V$
- The Nambu-Goldstone Theorem tells us we should end up with 3 nearly massless particles associated with each broken generator
- There is a theorem that this spontaneous symmetry breaking can not break into a parity broken phase
Vafa, Witten, Phys.Rev.Lett. 53 (1984)

suggesting that the Nambu-Goldstone modes should be parity-odd (as they are associated with the breaking of axial symmetries), and indeed, we observe the pions have intrinsic odd parity

- Our understanding of low-energy QCD is heavily based upon the realization of this approximate global chiral symmetry and its spontaneous breaking by the QCD vacuum



QCD: gauge “symmetry”

- A key feature of QCD is the exact gauge invariance — the theory remains the same under local SU(3) transformations

$$\mathcal{L}_{\text{QCD}} = \bar{\psi}^a(x) [i\partial_\mu \gamma^\mu \delta_{ab} - \gamma_\mu A_{ab}^\mu - m\delta_{ab}] \psi_b(x) - \frac{1}{4} G_{\mu\nu}^a G_a^{\mu\nu}$$

a,b are “color” indices

- The gauge fields also carry “color charge”, which leads to the gluon self-interactions

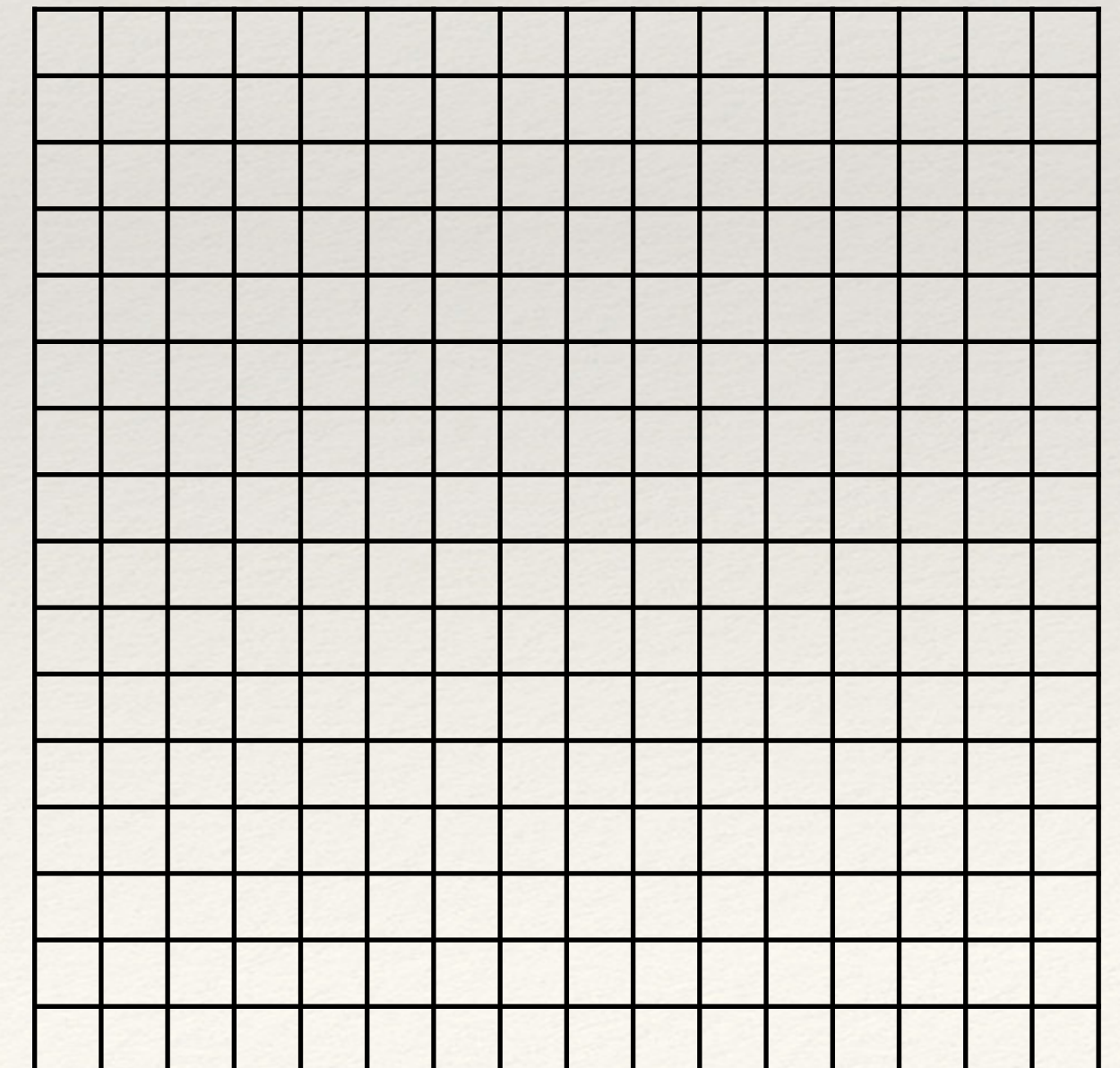
- We demand the theory is invariant under $\psi_a(x) \rightarrow e^{i\frac{1}{2}\theta_i(x)\lambda_{ab}^i} \psi_b(x)$ where λ^i are the Gell-Mann matrices

- A key question when discretizing a theory - how do you preserve the invariance of these local transformations?

$$\bar{\psi}(x) i\gamma^\mu \partial_\mu \psi(x) \longrightarrow \bar{\psi}(x) i\gamma^\mu \frac{1}{2a} [\psi(x + a\mu) - \psi(x - a\mu)]$$

$a =$ lattice spacing

- A local transformation at \mathbf{x} and $\mathbf{x}+a\mu$ will not longer exactly cancel



QCD: gauge “symmetry”

- A key feature of QCD is the exact gauge invariance

$$\bar{\psi}(x)i\gamma^\mu\partial_\mu\psi(x) \longrightarrow \bar{\psi}(x)i\gamma^\mu\frac{1}{2a}[\psi(x+a\mu) - \psi(x-a\mu)]$$

- Gauge links $U_\mu(x) = \exp\left\{ia\int_0^1 dt A_\mu(x+(1-t)a\hat{\mu})\right\} \approx \exp\{ia\bar{A}_\mu(x)\}$

enable for a gauge-invariant construction of a finite-difference operator

$$\bar{\psi}(x)i\gamma^\mu D_\mu\psi(x) \longrightarrow \frac{i}{2a}[\bar{\psi}(x)\gamma^\mu U_\mu(x)\psi(x+a\mu) - \bar{\psi}(x)\gamma^\mu U_\mu^\dagger(x)\psi(x-a\mu)]$$

Introduction to LQCD

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

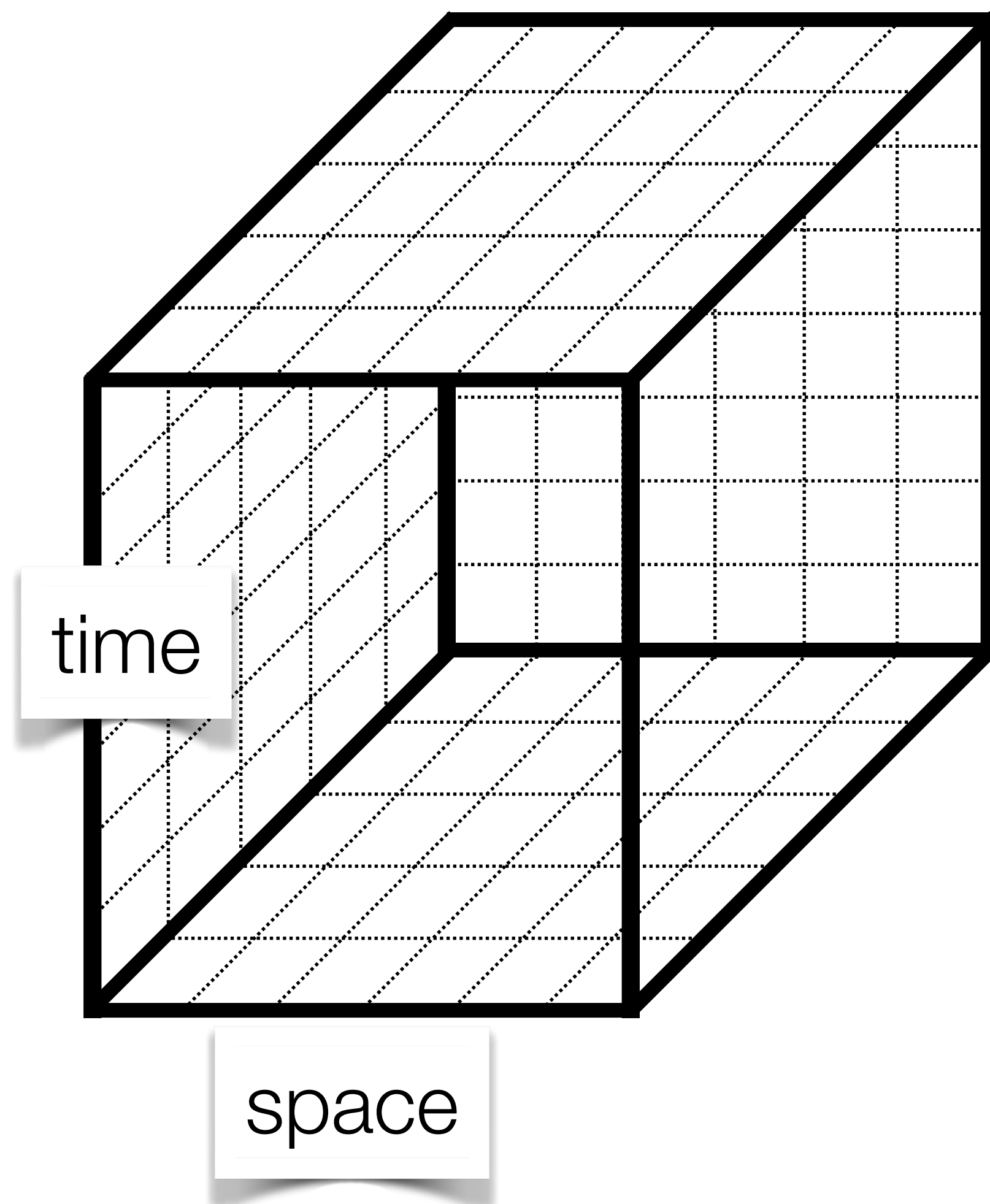
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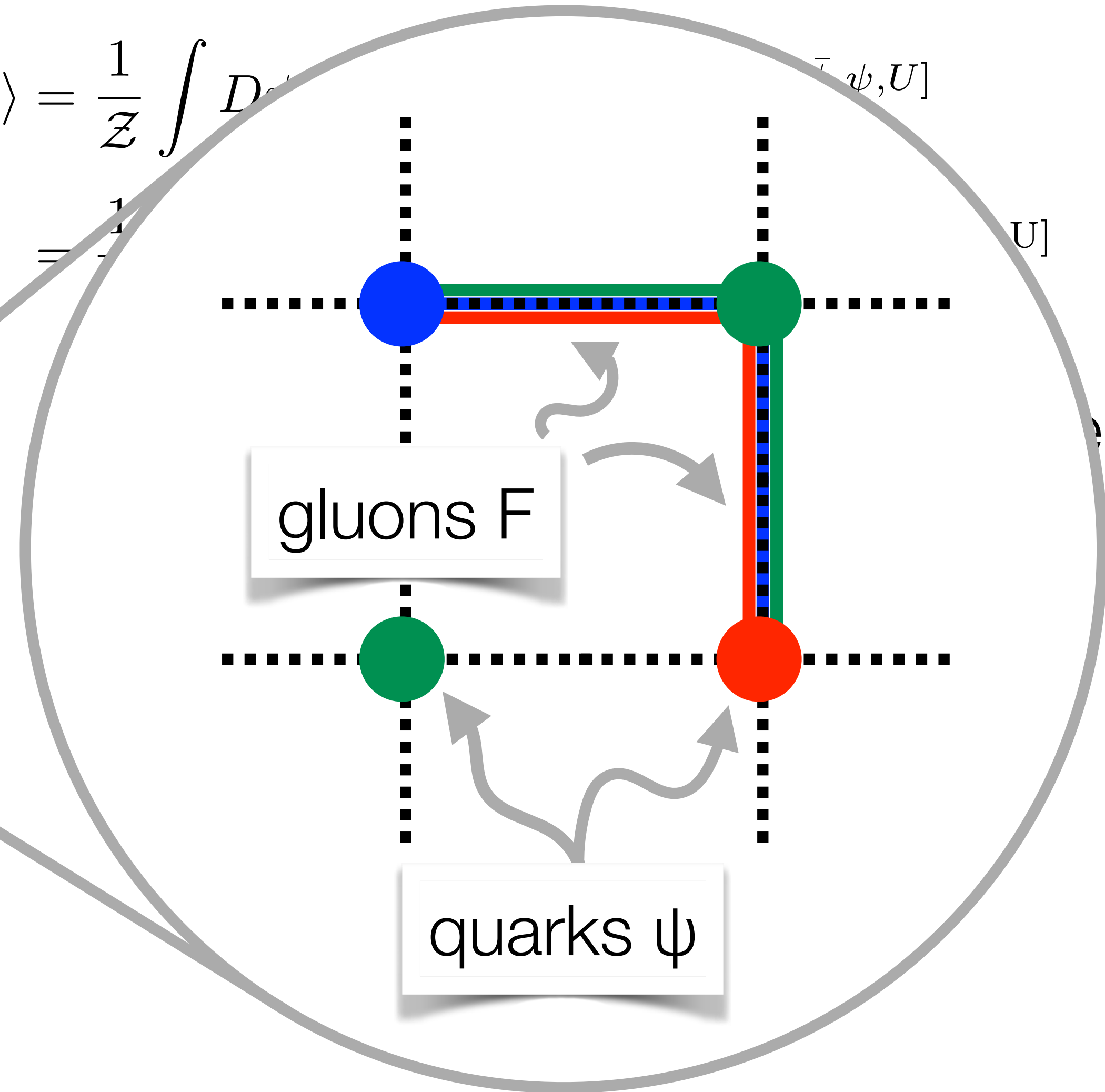
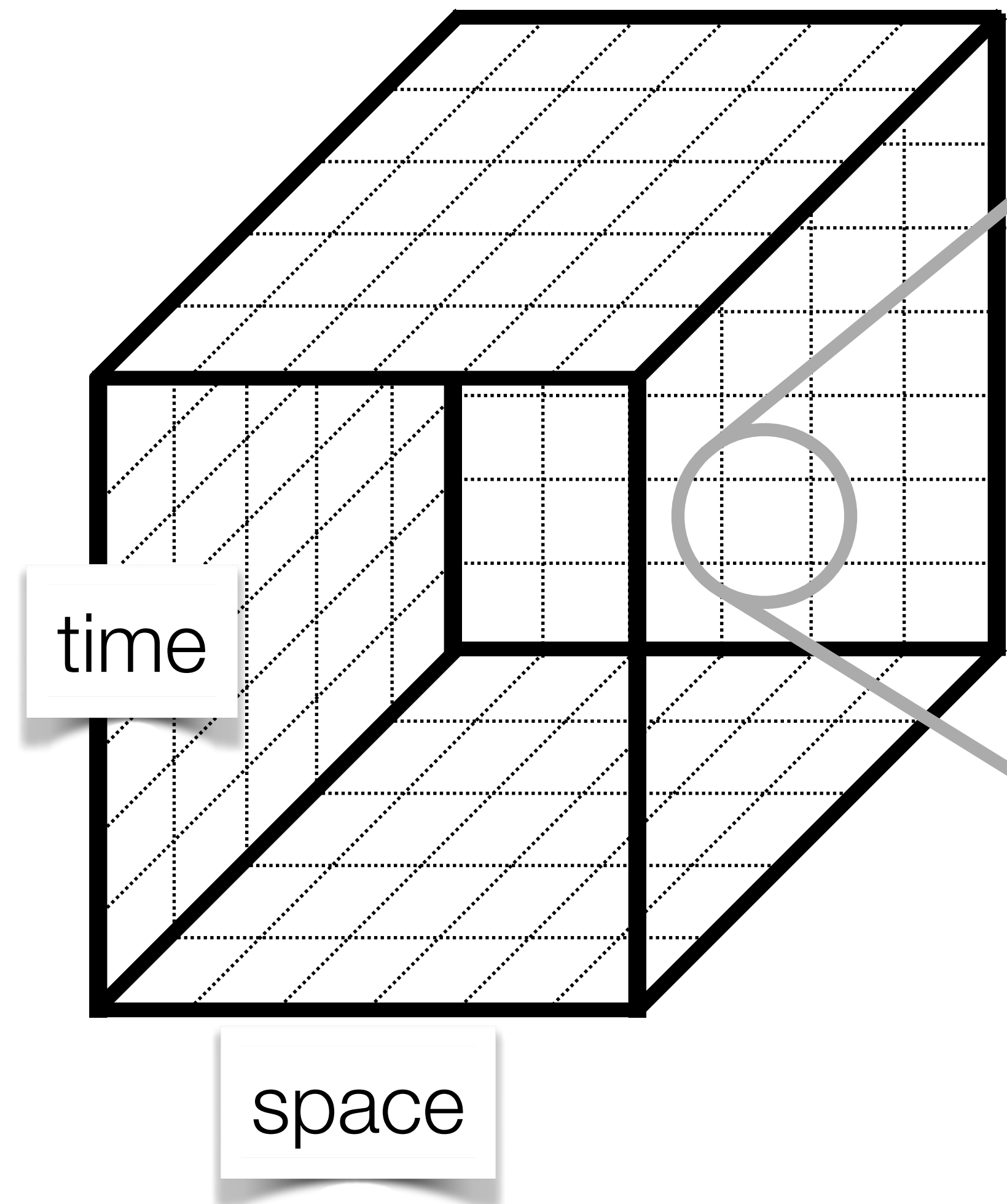
lattice

finite volume



Introduction to LQCD

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

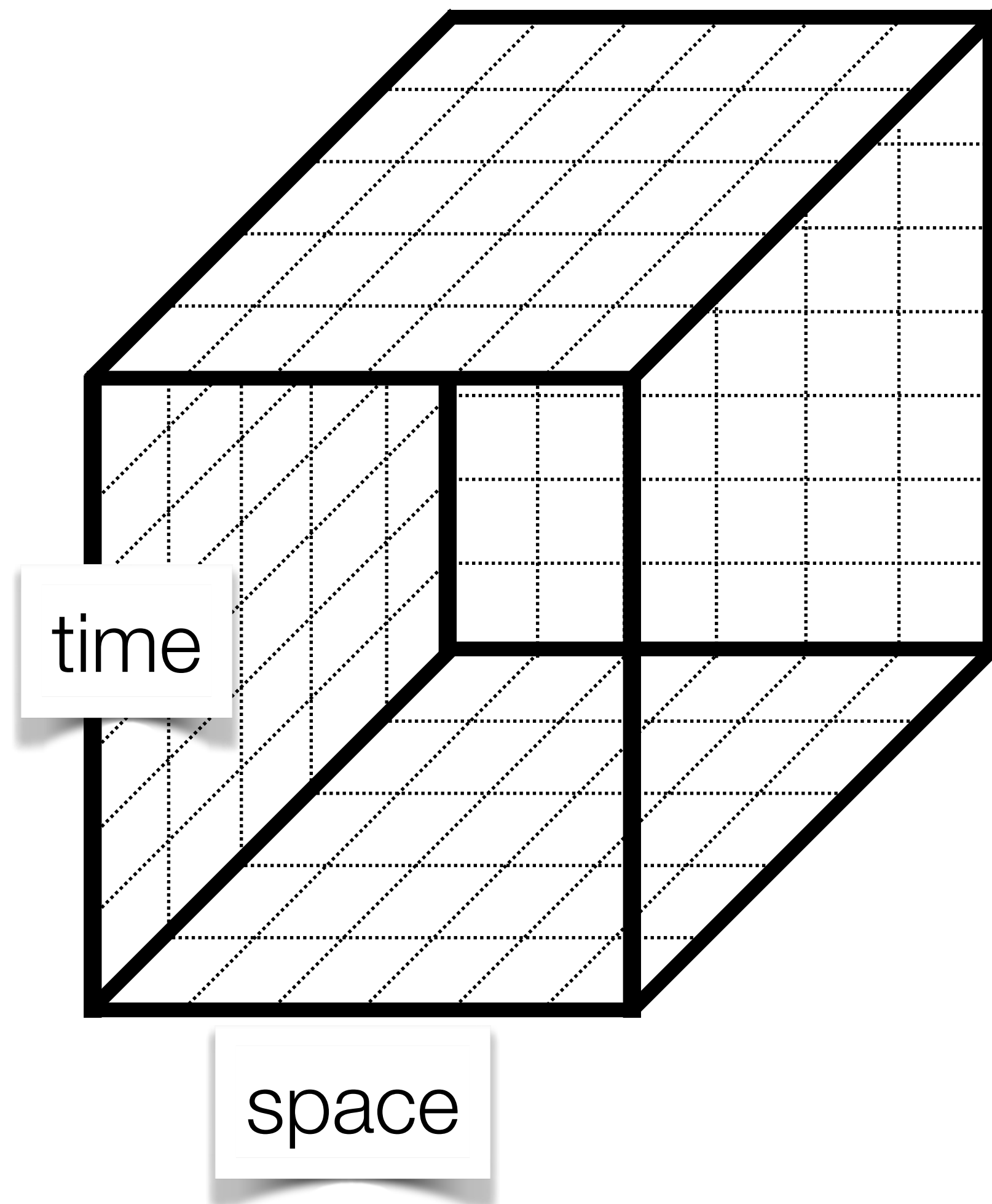


Introduction to LQCD

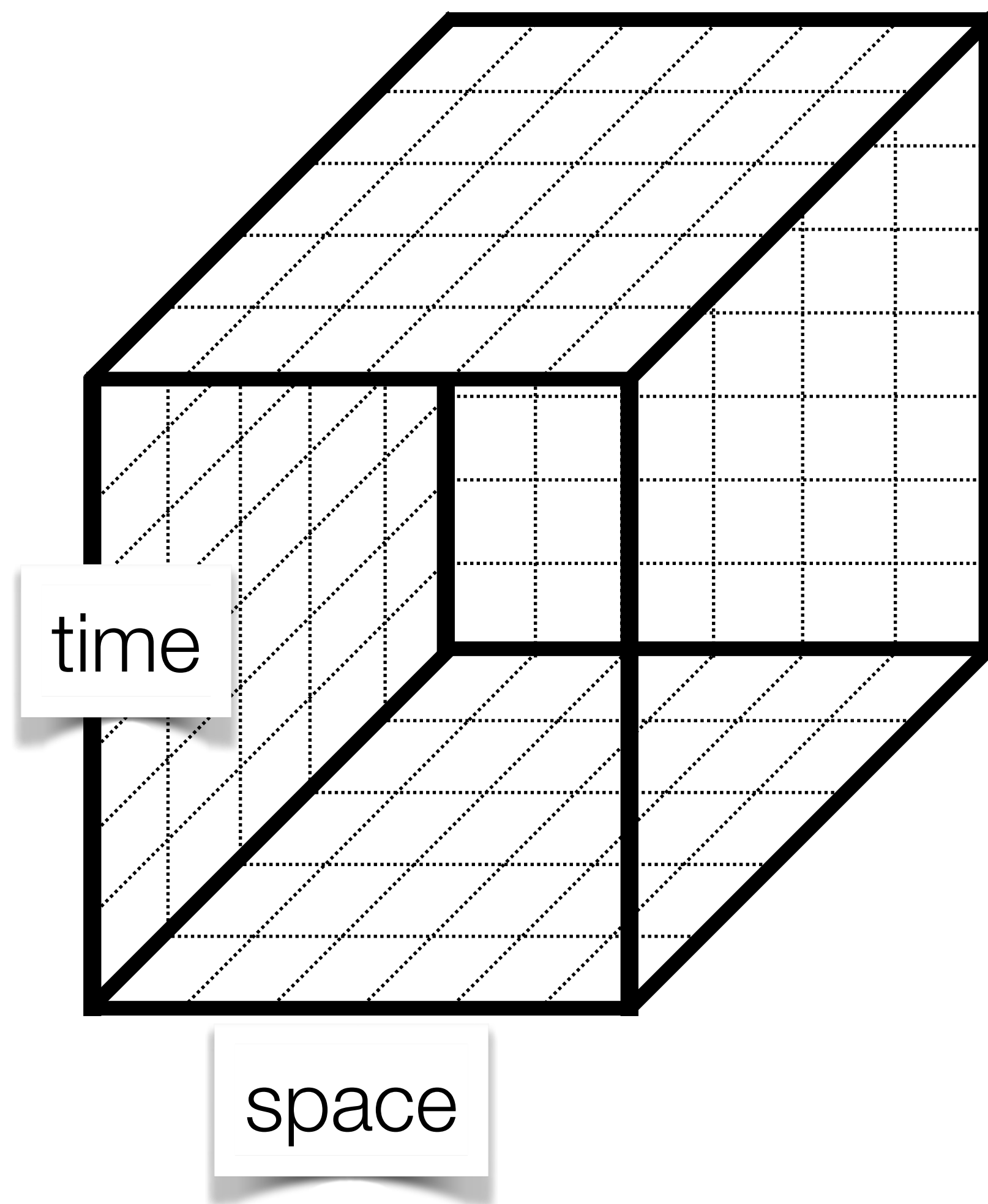
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lattice
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Introduction to LQCD



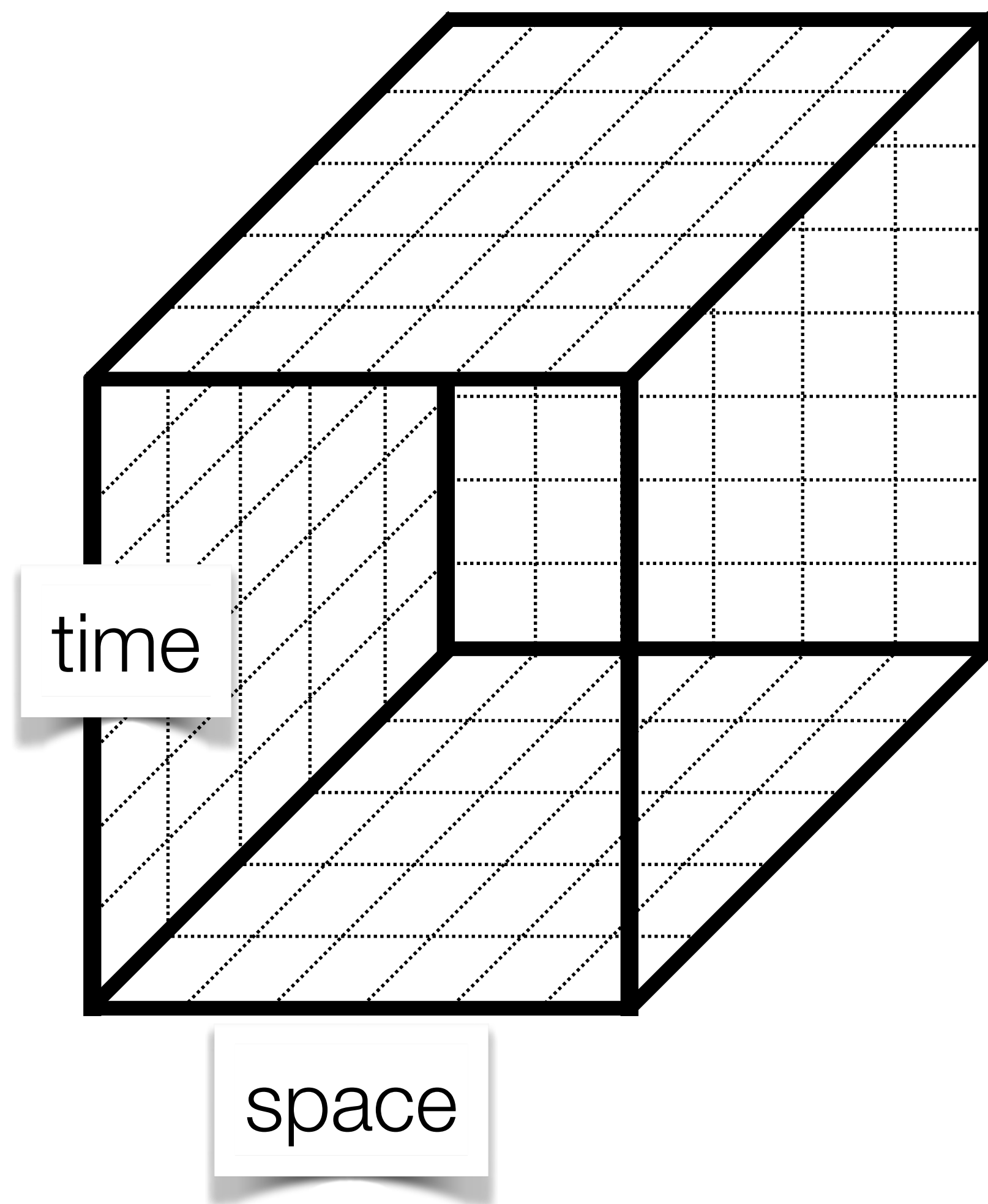
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$$= \frac{1}{\mathcal{Z}} \int \mathcal{D}U \det(\not{D} + M) e^{-S[U]} \mathcal{O}(t) \mathcal{O}^\dagger(0)$$

lattice

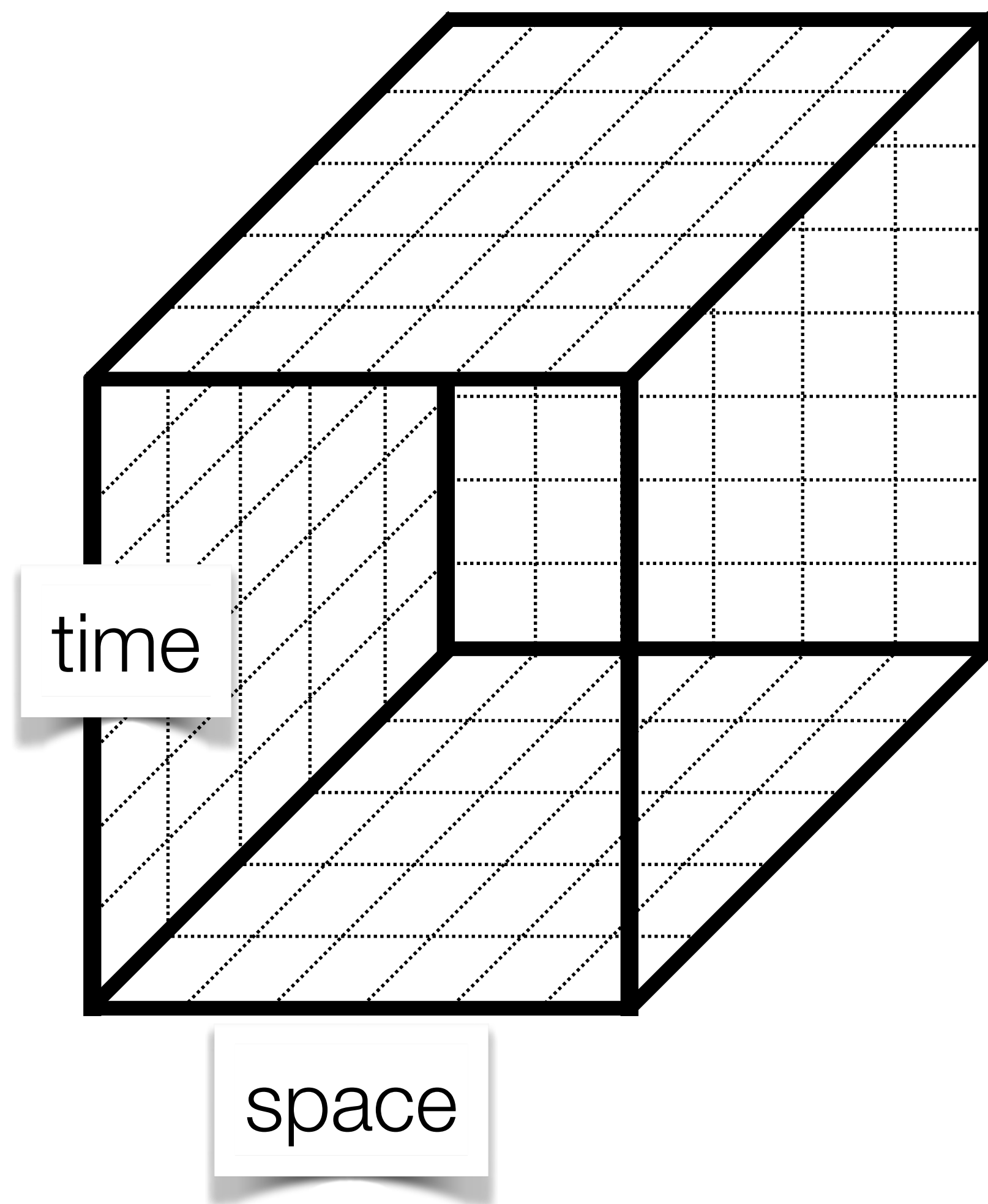
finite volume

Introduction to LQCD



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Introduction to LQCD



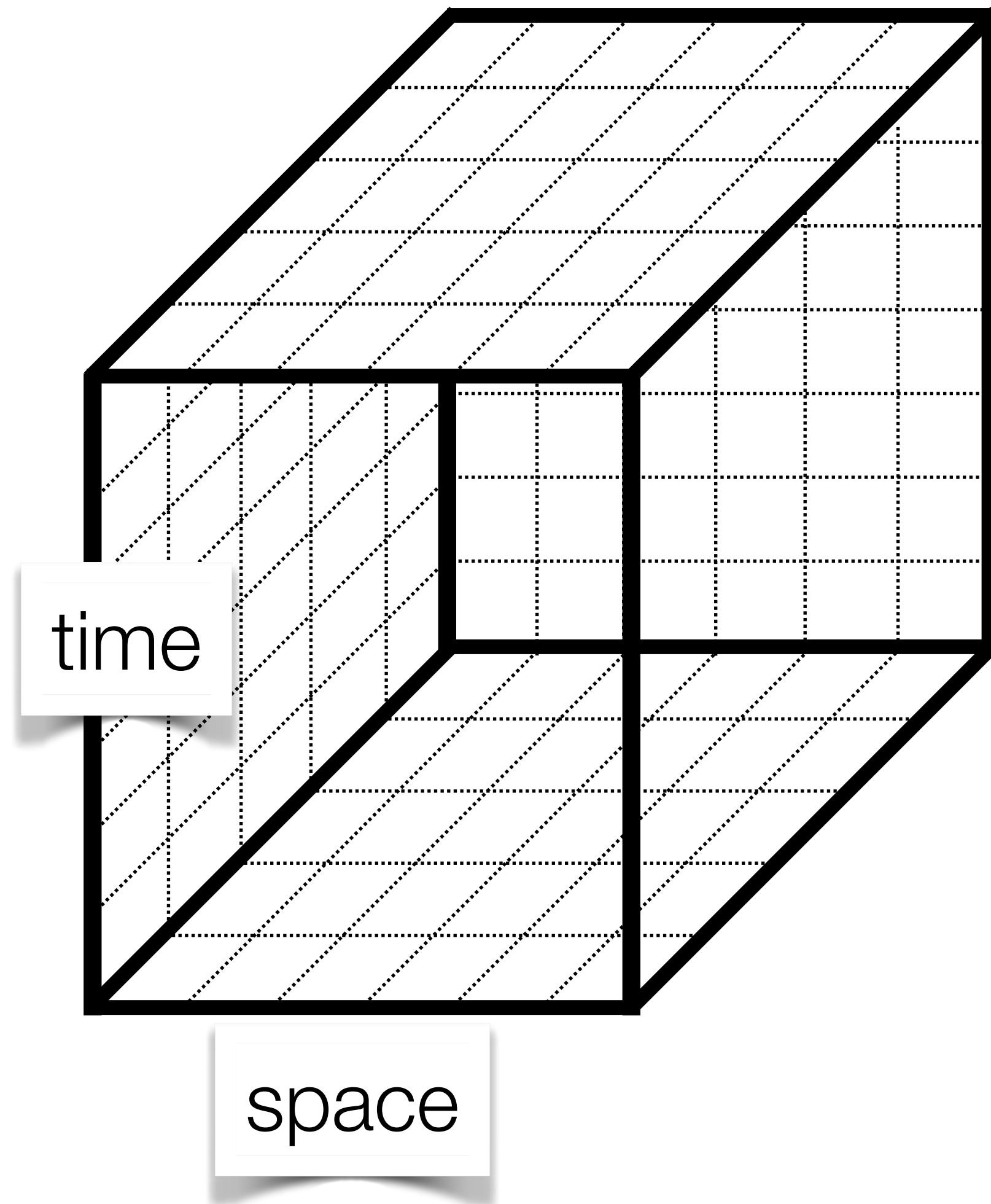
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Probability

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

Markov Chain Monte Carlo

Introduction to LQCD



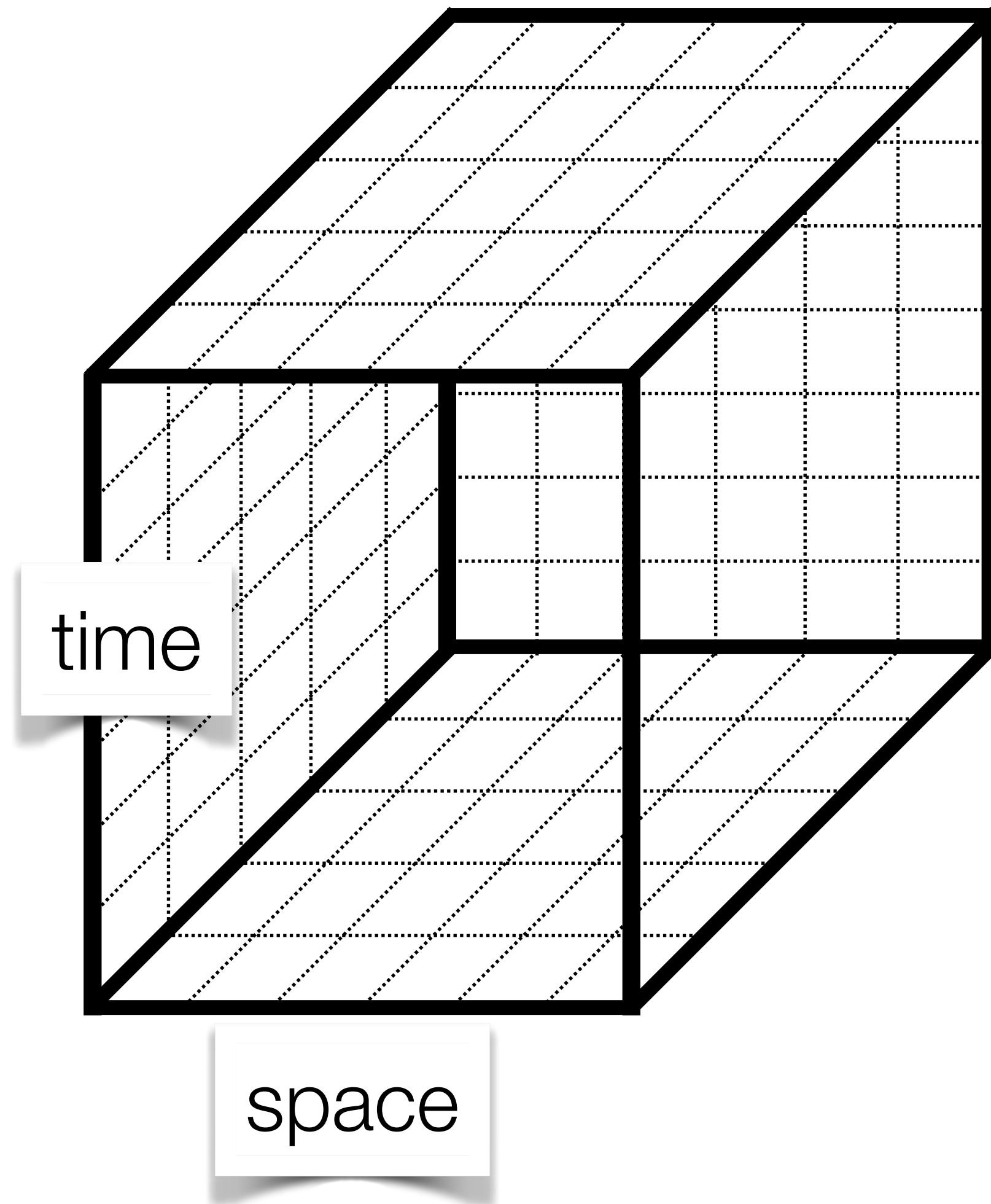
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$$\{U_1, U_2, U_3, \dots, U_N\}$$

Markov Chain Monte Carlo

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

Introduction to LQCD



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Probability

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

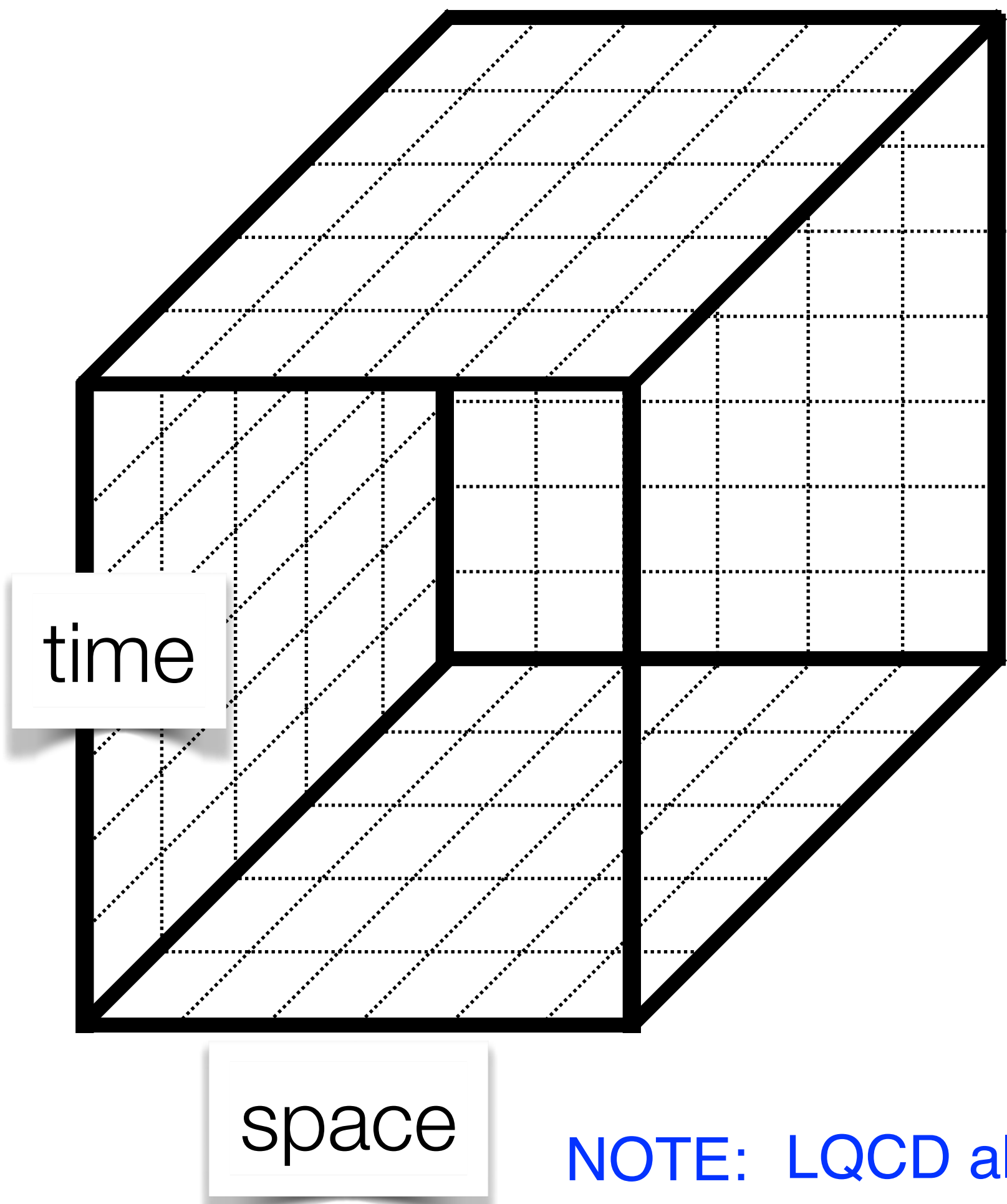
Markov Chain Monte Carlo

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

Introduction to LQCD

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

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Probability

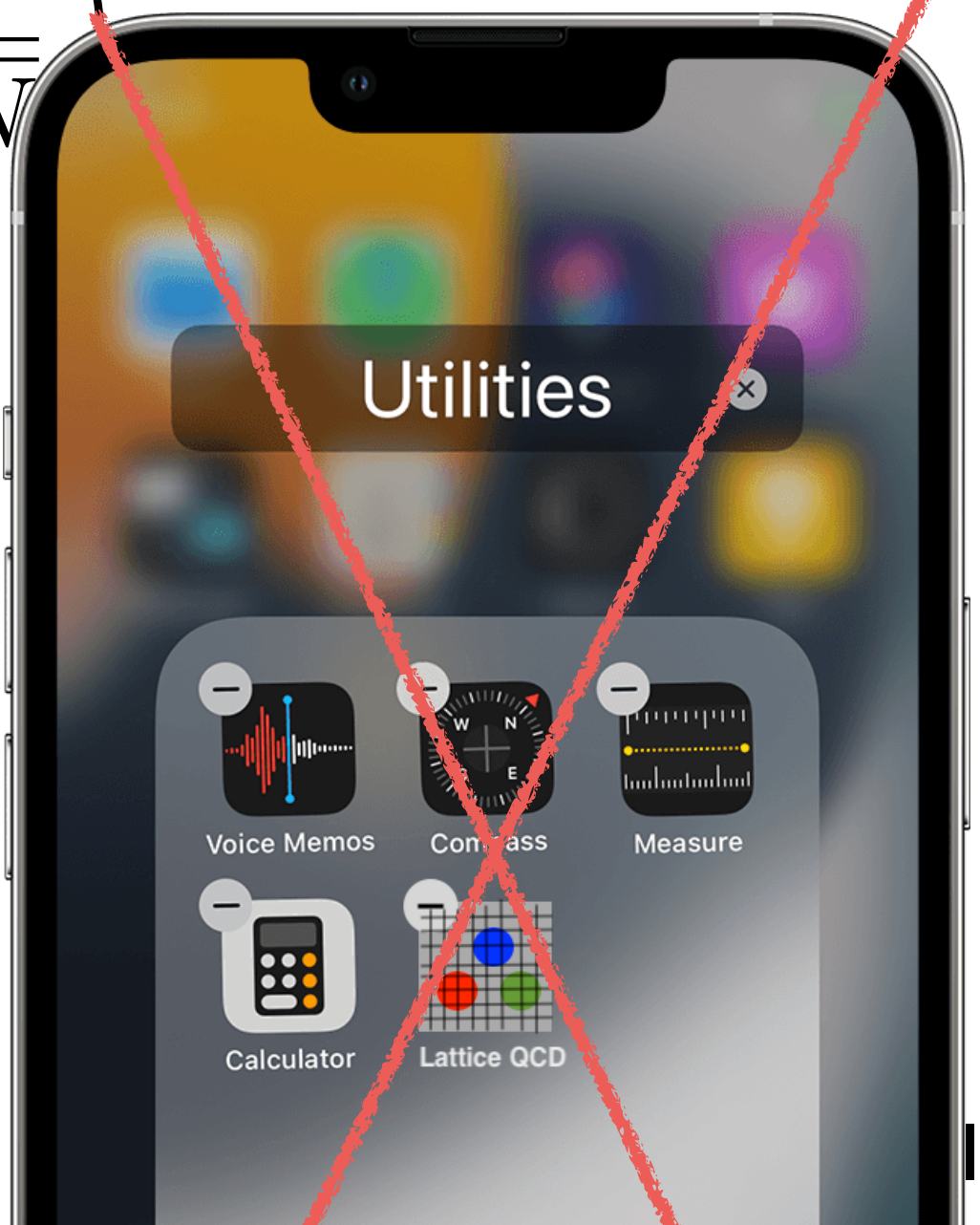
$$\{U_1, U_2, U_3, \dots, U_N\}$$

Markov Chain Monte Carlo

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

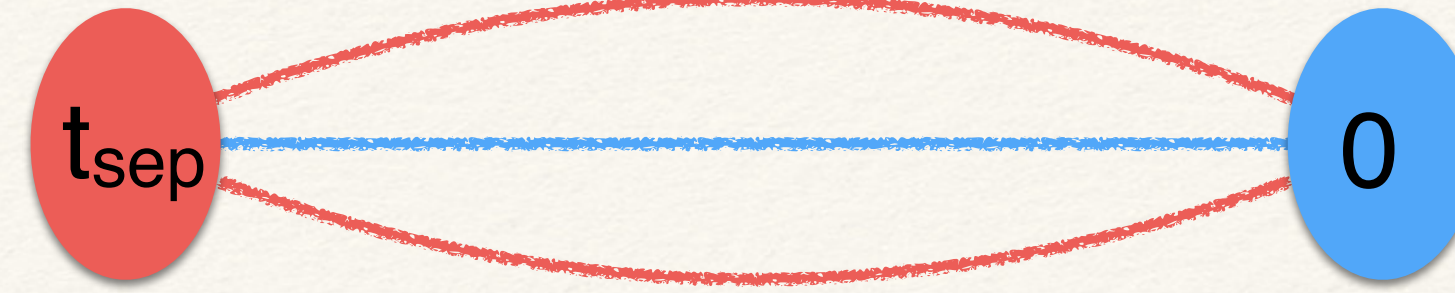
NOTE: LQCD allows us to compute Euclidean space, finite volume, correlation functions

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



LQCD: 2 point functions - proton

$$C_{\gamma\gamma'}(t_{\text{sep}}, \mathbf{z}) = \langle \Omega | N_{\gamma}(t_{\text{sep}}, \mathbf{z}) \bar{N}_{\gamma'}(0) | \Omega \rangle$$



$$N_{\gamma} = \epsilon_{ijk} P_{\gamma\rho} u_{\rho}^i (u_{\alpha}^j \Gamma_{\alpha\beta}^{snk} d_{\beta}^k)$$

$$\bar{N}_{\gamma'} = \epsilon_{i'j'k'} P_{\gamma'\rho'} \bar{u}_{\rho'}^{i'} (\bar{u}_{\alpha'}^{j'} \Gamma_{\alpha'\beta'}^{\dagger,src} \bar{d}_{\beta'}^{k'})$$

$$\begin{aligned} \mathbf{N} \subset \square \times \square \times \square &= \square \square \square \oplus \begin{array}{c} \square \square \\ \square \end{array} \\ &= 4 \oplus 2 \\ &= \Delta \oplus \mathbf{N} \end{aligned}$$

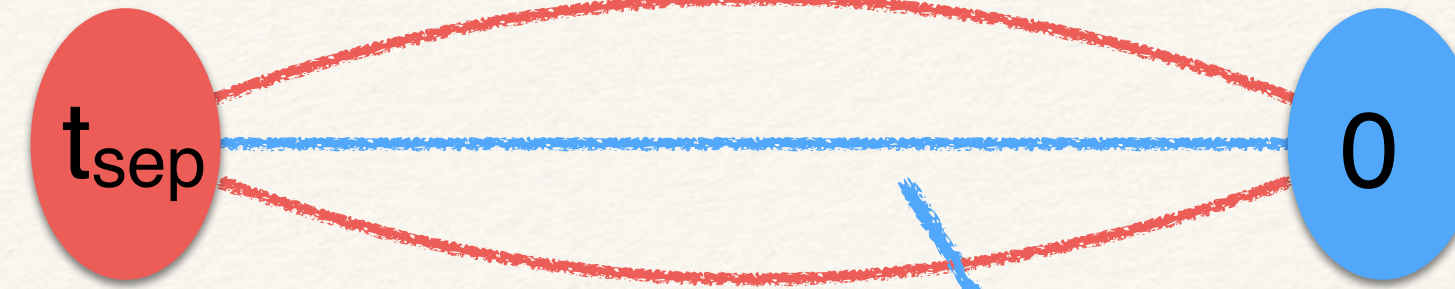
For the nucleon, 2 of the quarks must form a spin singlet

$$\Gamma_u = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

$$\begin{aligned} C_{\gamma\gamma'} &= \epsilon_{ijk} \epsilon_{i'j'k'} P_{\gamma\rho} P_{\gamma'\rho'} \langle 0 | u_{\rho}^i (u_{\alpha}^j \Gamma_{\alpha\beta}^{snk} d_{\beta}^k) \bar{u}_{\rho'}^{i'} (\bar{u}_{\alpha'}^{j'} \Gamma_{\alpha'\beta'}^{\dagger,src} \bar{d}_{\beta'}^{k'}) | 0 \rangle \\ &= -\epsilon_{ijk} \epsilon_{i'j'k'} P_{\gamma\rho} P_{\gamma'\rho'} \Gamma_{\alpha\beta}^{snk} \Gamma_{\alpha'\beta'}^{src} \left[-U_{\rho\rho'}^{ii'} U_{\alpha\alpha'}^{jj'} D_{\beta\beta'}^{kk'} + U_{\alpha\rho'}^{ji'} U_{\rho\alpha'}^{ij'} D_{\beta\beta'}^{kk'} \right] \\ &= \epsilon_{ijk} \epsilon_{i'j'k'} P_{\gamma\rho} P_{\gamma'\rho'} \Gamma_{\alpha\beta}^{snk} \Gamma_{\alpha'\beta'}^{src} \left[U_{\rho\rho'}^{ii'} U_{\alpha\alpha'}^{jj'} D_{\beta\beta'}^{kk'} + U_{\alpha\rho'}^{ii'} U_{\rho\alpha'}^{jj'} D_{\beta\beta'}^{kk'} \right] \\ &= \epsilon_{ijk} \epsilon_{i'j'k'} P_{\gamma'\rho'} \Gamma_{\alpha'\beta'}^{src} \left[P_{\gamma\rho} \Gamma_{\alpha\beta}^{snk} + P_{\gamma\alpha} \Gamma_{\rho\beta}^{snk} \right] U_{\rho\rho'}^{ii'} U_{\alpha\alpha'}^{jj'} D_{\beta\beta'}^{kk'}. \end{aligned}$$

LQCD: 2 point functions - proton

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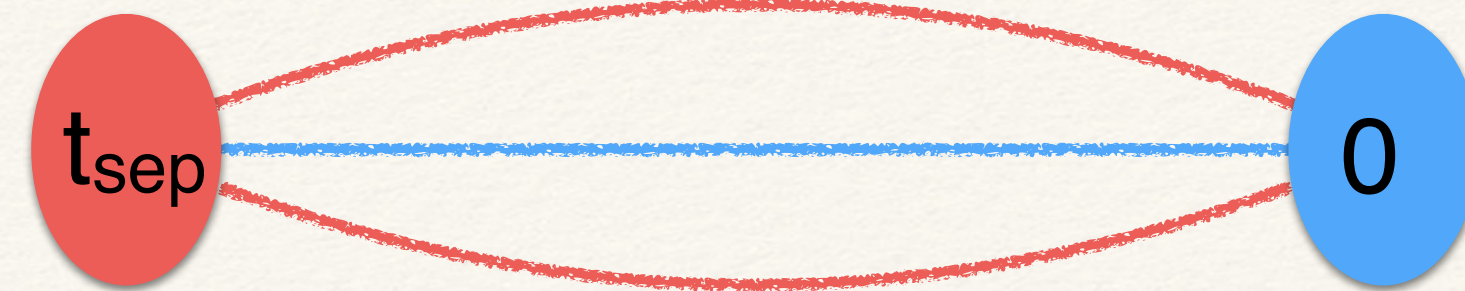
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LQCD: 2 point functions

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



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

focus on 0-momentum

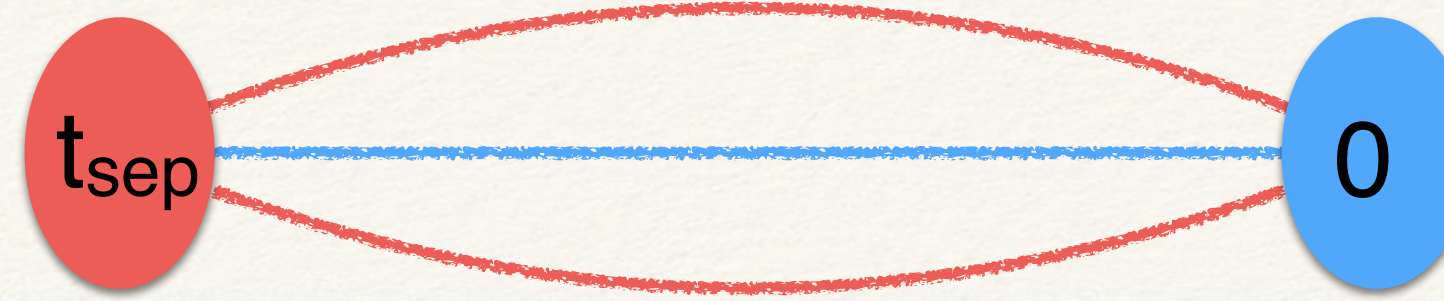
time-evolve operator

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

define vacuum to have 0-energy

sum of exponentials

LQCD: 2 point functions

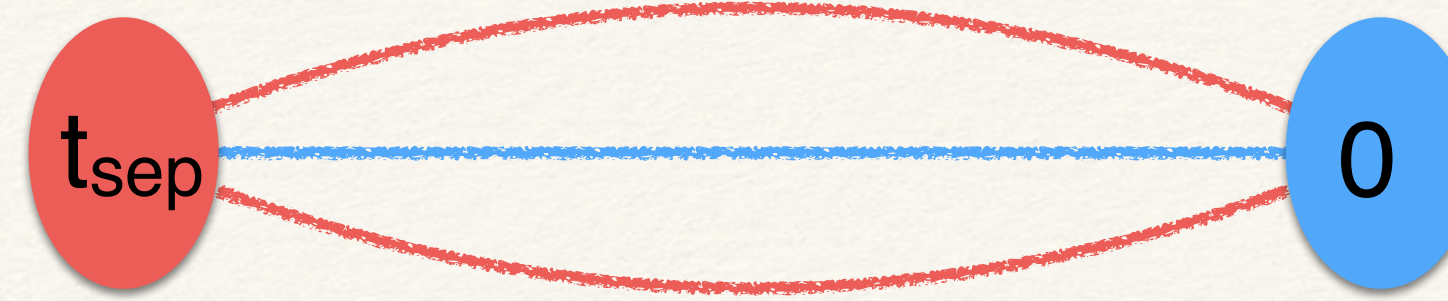


$$C(t, \mathbf{p} = 0) = \sum_{\mathbf{x}} \langle \Omega | N(t, \mathbf{x}) N^\dagger(0, \mathbf{0}) | \Omega \rangle$$
$$= A_0 e^{-E_0 t} \left(1 + \sum_{n>0} r_n e^{-\Delta_{n0} t} \right)$$
$$\Delta_{n0} = E_n - E_0$$

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

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

LQCD: 2 point functions



$$C(t, \mathbf{p} = 0) = \sum_{\mathbf{x}} \langle \Omega | N(t, \mathbf{x}) N^\dagger(0, \mathbf{0}) | \Omega \rangle$$

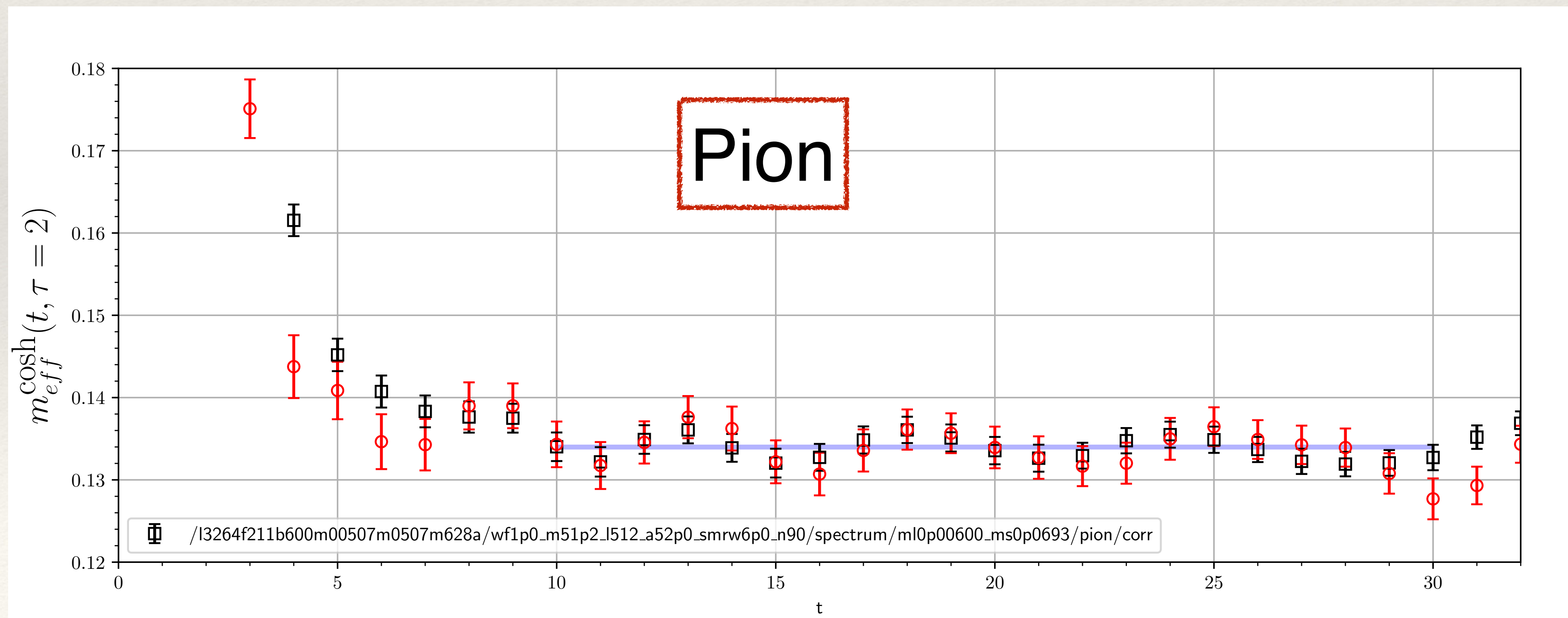
$$= A_0 e^{-E_0 t} \left(1 + \sum_{n>0} r_n e^{-\Delta_{n0} t} \right)$$

$$\Delta_{n0} = E_n - E_0$$

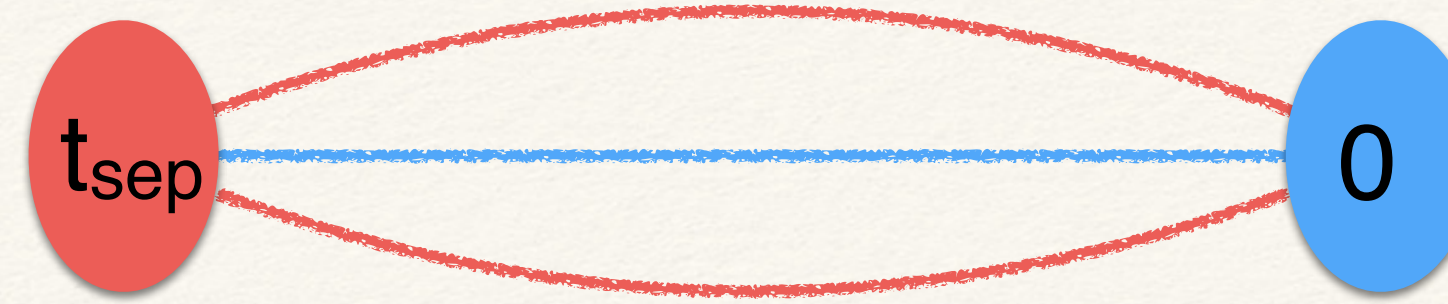
$$m_{\text{eff}}(t) = \ln \left(\frac{C(t)}{C(t+1)} \right) \xrightarrow{\text{large } t} E_0 + \sum_{n>0} r_n (e^{-\Delta_{n0} t} - e^{-\Delta_{n0} t+1})$$

NOTE: if the creation operator is conjugate to the annihilation operator

$$r_n \geq 0$$



LQCD: 2 point functions



$$C(t, \mathbf{p} = 0) = \sum_{\mathbf{x}} \langle \Omega | N(t, \mathbf{x}) N^\dagger(0, \mathbf{0}) | \Omega \rangle$$

$$= A_0 e^{-E_0 t} \left(1 + \sum_{n>0} r_n e^{-\Delta_{n0} t} \right)$$

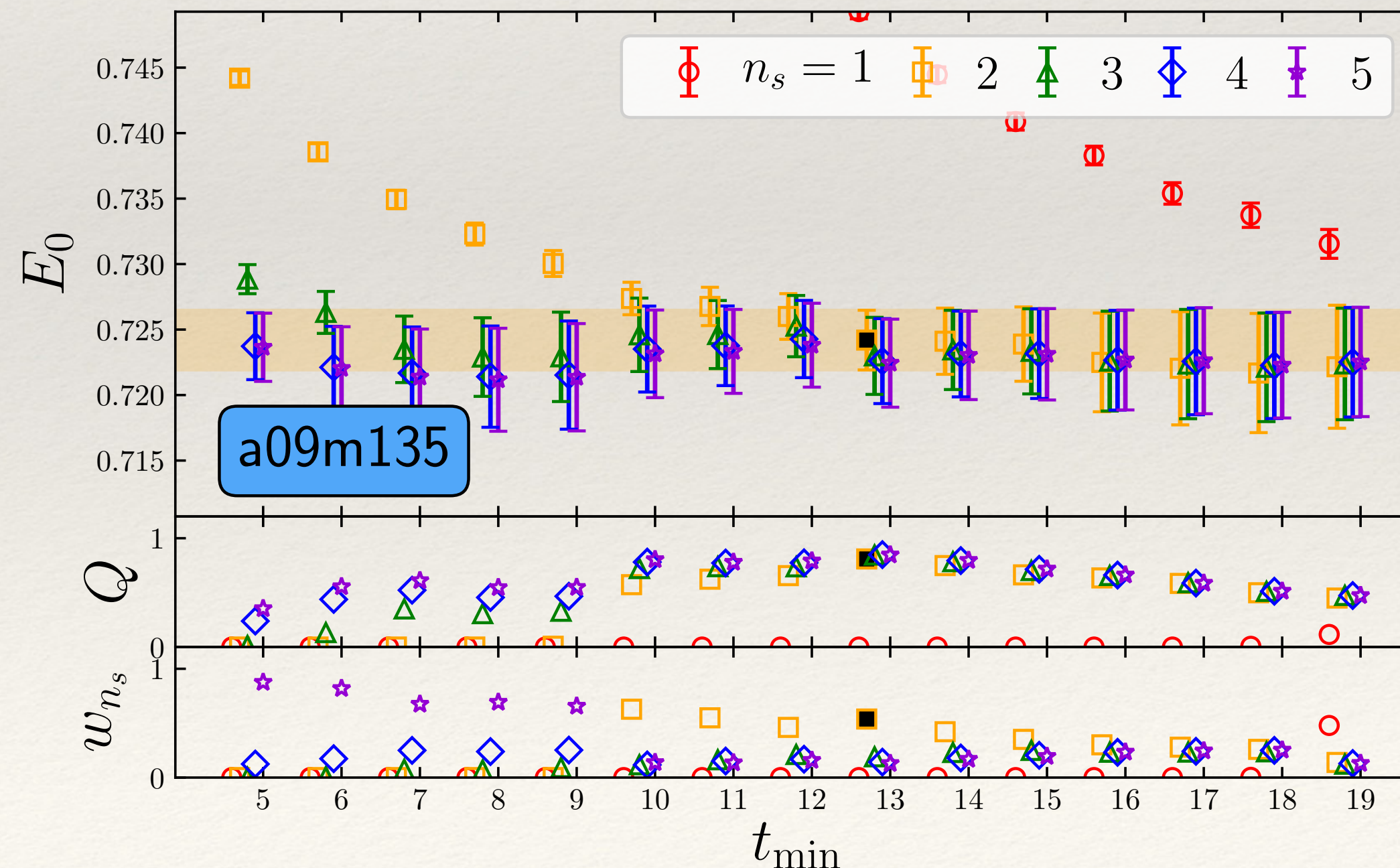
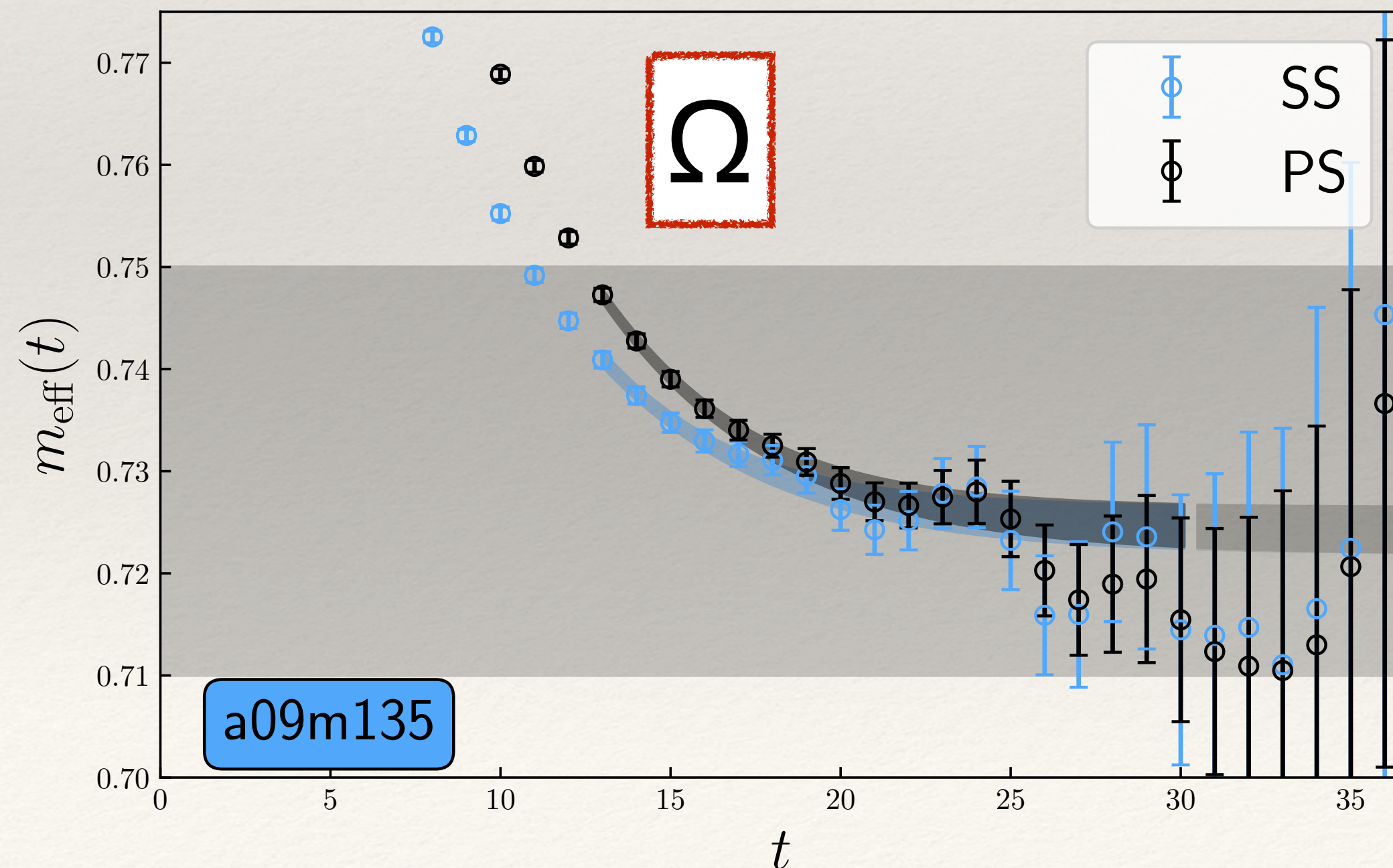
$$\Delta_{n0} = E_n - E_0$$

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

NOTE: if the creation operator is conjugate to the annihilation operator

$$r_n \geq 0$$

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



What does it mean to have a LQCD result?

continuum limit

need 3 or more
lattice spacings

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

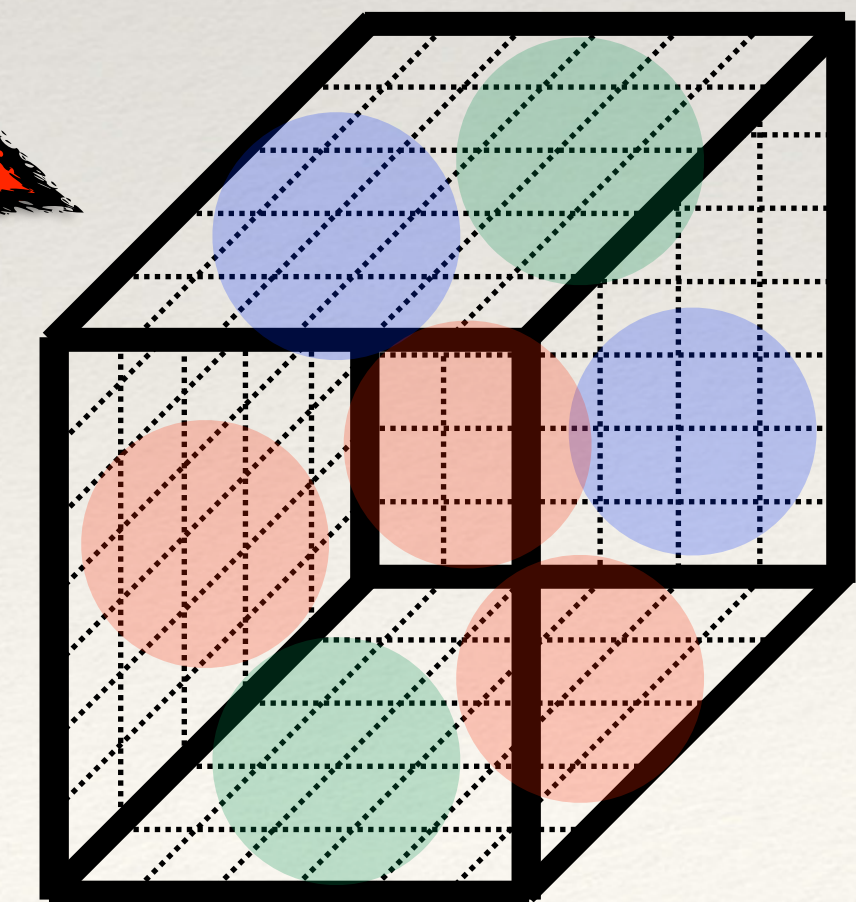
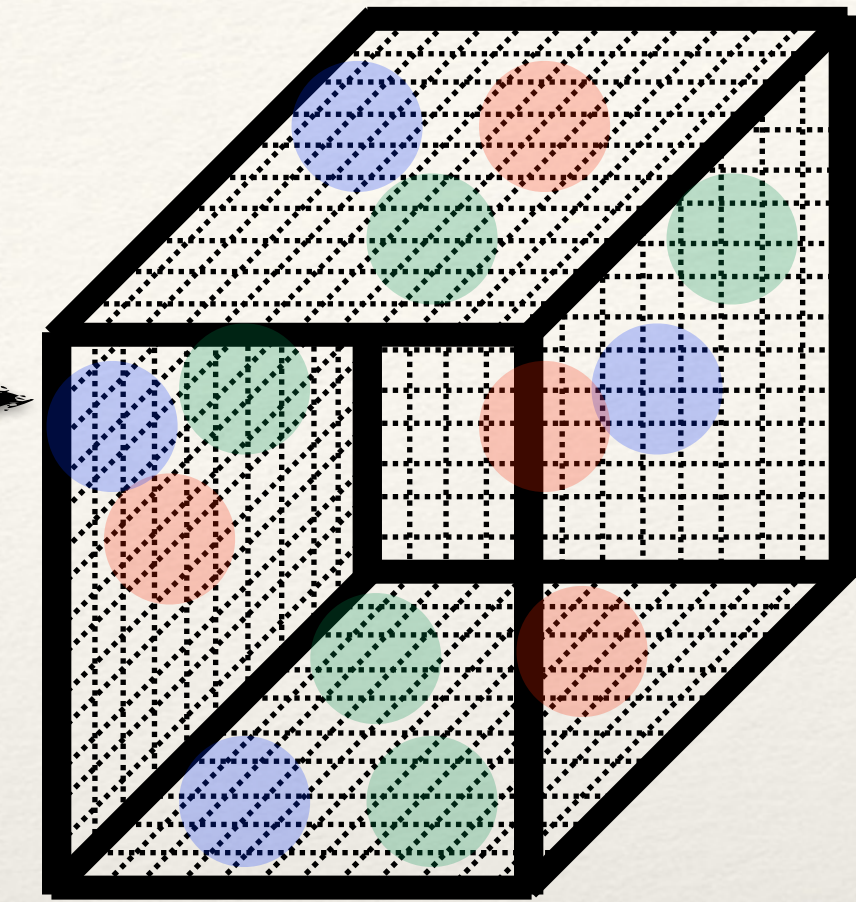
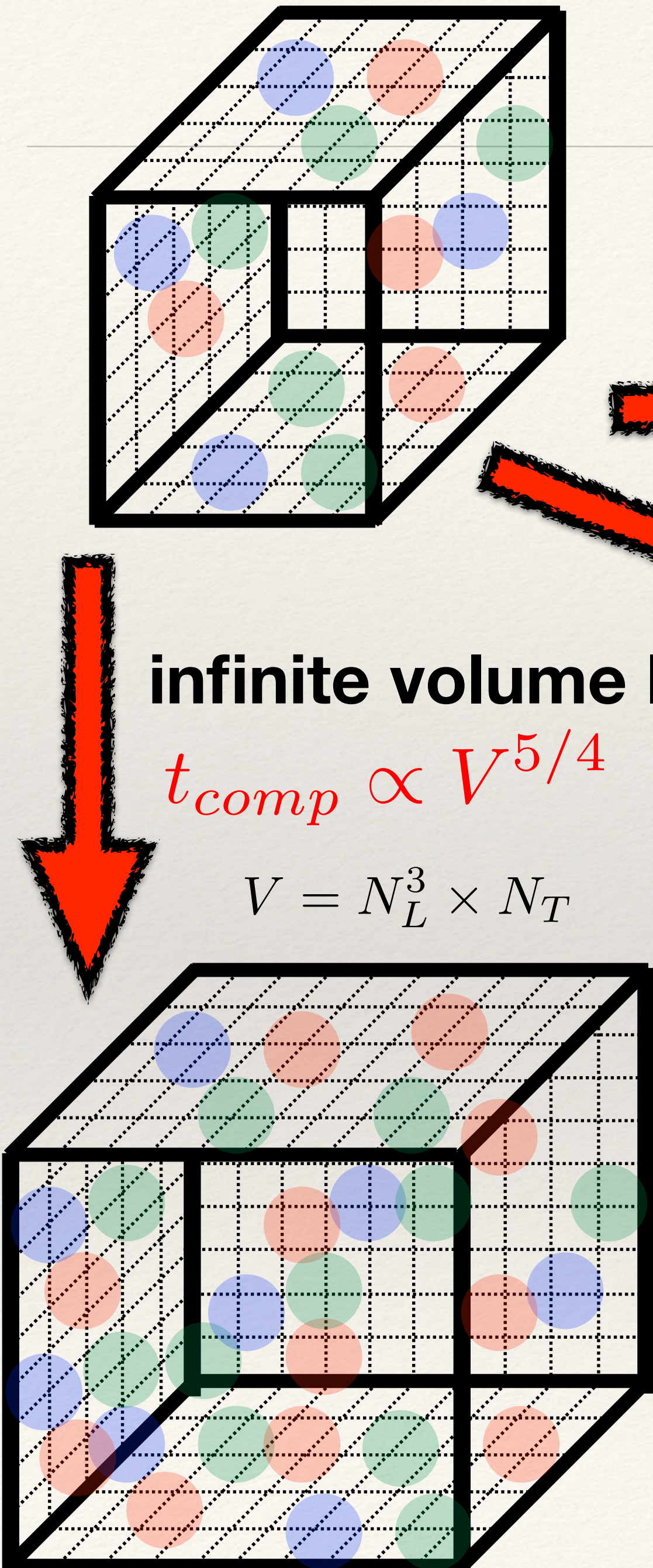
infinite volume limit

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

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

physical pion masses

exponentially bad
signal-to-noise problem



But what does this mean?

$$\begin{aligned} S &= a^4 \sum_n \bar{\psi}_n [D + m] \psi_n - \frac{1}{4g^2} G_{\mu\nu}(n) G_{\mu\nu}(n) \\ &= \sum_n (a^{3/2} \bar{\psi})_n [aD + am] (a^{3/2} \psi)_n - \frac{1}{4g^2} (a^2 G_{\mu\nu}(n)) (a^2 G_{\mu\nu}(n)) \end{aligned}$$

- ❑ The theory (the action, S), on the computer, is formulated in terms of dimensionless fields, dimensionless masses etc.
- ❑ The only parameters we chose are the dimensionless quark masses, am , and the dimensionless gauge coupling, g
- ❑ But quark masses are not observable/measurable, and neither is g , so how do we know what these choices correspond to?
- ❑ We have to pick values for am , g ,
run the Monte-Carlo,
“measure” some hadron correlation functions and extract the dimensionless masses
trade one experimental quantity for each input parameter
 $a(m_u + m_d) \longleftrightarrow M_\pi$ $am_s \longleftrightarrow M_K$ $aM_\Omega \longleftrightarrow \text{scale}$

Example Scale Setting: arXiv:2011.12166

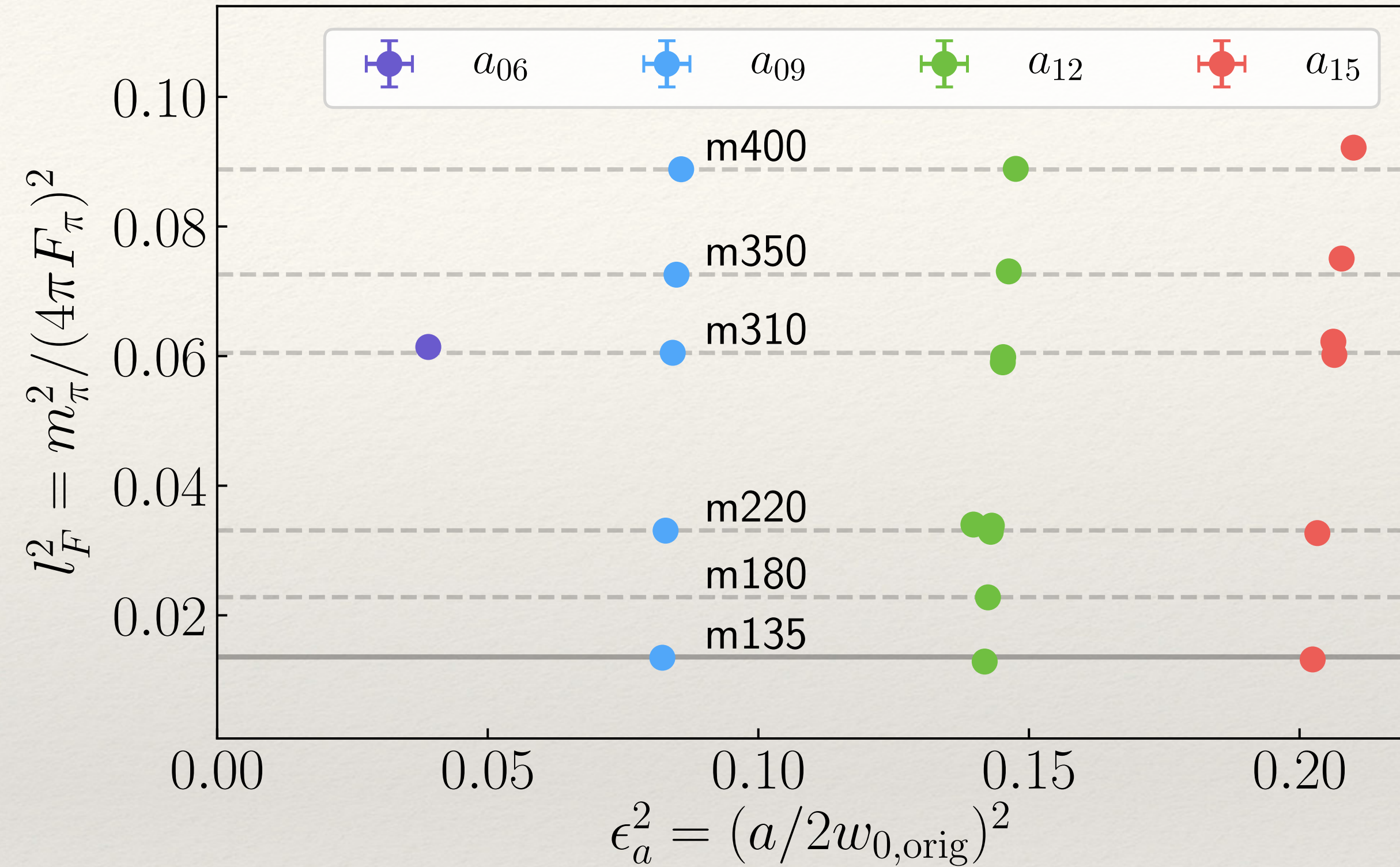
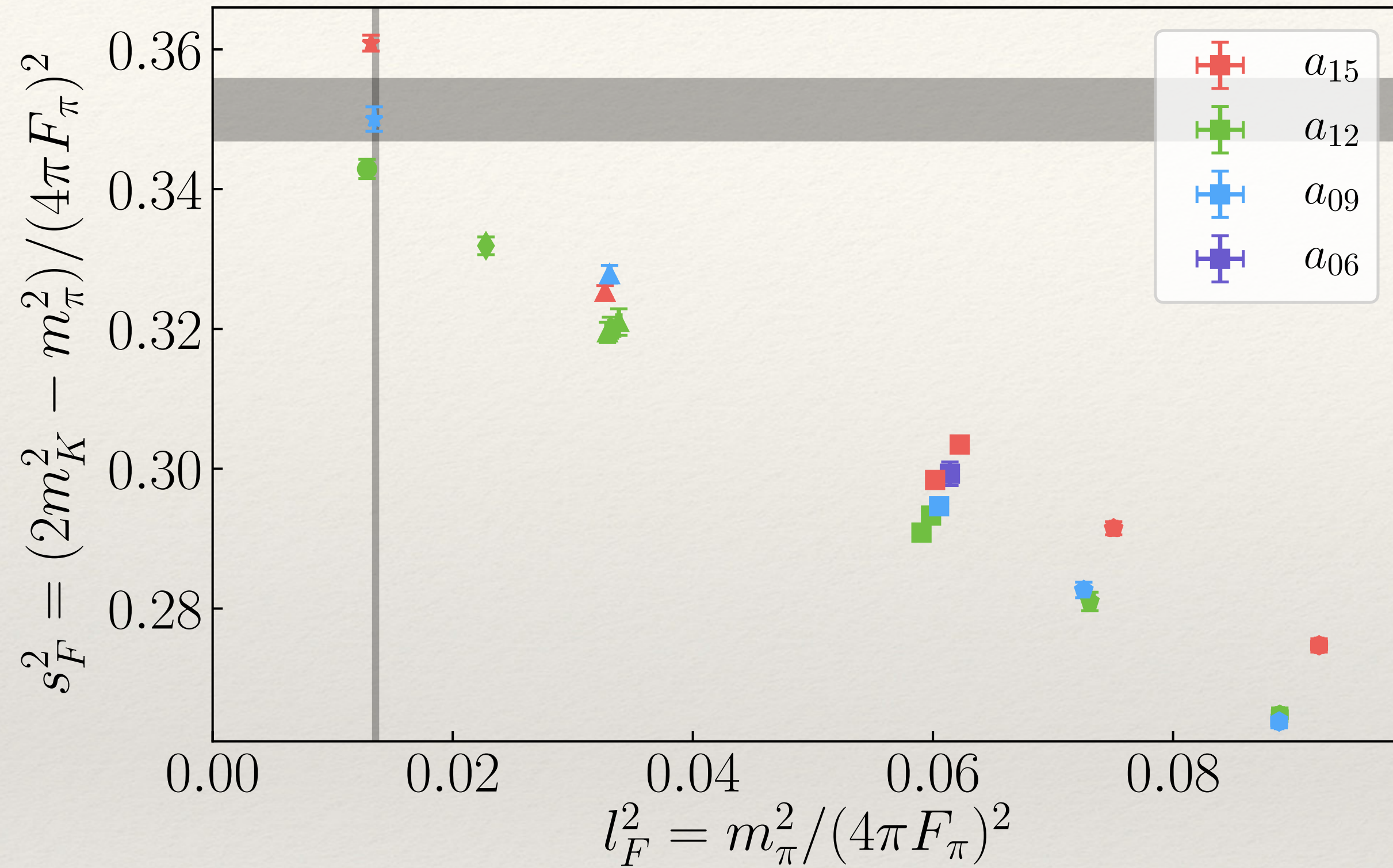
TABLE I. Input parameters for our lattice action. The abbreviated ensemble name [17] indicates the approximate lattice spacing in fm and pion mass in MeV. The S, L, XL which come after an ensemble name denote a relatively small, large and extra-large volume with respect to $m_\pi L = 4$.

ensemble	β	N_{cfg}	volume	am_l	am_s	am_c	L_5/a	aM_5	b_5, c_5	am_l^{val}	$am_l^{\text{res}} \times 10^4$	am_s^{val}	$am_s^{\text{res}} \times 10^4$	σ	N	N_{src}
a15m400 ^a	5.80	1000	$16^3 \times 48$	0.0217	0.065	0.838	12	1.3	1.50, 0.50	0.0278	9.365(87)	0.0902	6.937(63)	3.0	30	8
a15m350 ^a	5.80	1000	$16^3 \times 48$	0.0166	0.065	0.838	12	1.3	1.50, 0.50	0.0206	9.416(90)	0.0902	6.688(62)	3.0	30	16
a15m310	5.80	1000	$16^3 \times 48$	0.013	0.065	0.838	12	1.3	1.50, 0.50	0.0158	9.563(67)	0.0902	6.640(44)	4.2	45	24
a15m310L ^a	5.80	1000	$24^3 \times 48$	0.013	0.065	0.838	12	1.3	1.50, 0.50	0.0158	9.581(50)	0.0902	6.581(37)	4.2	45	4
a15m220	5.80	1000	$24^3 \times 48$	0.0064	0.064	0.828	16	1.3	1.75, 0.75	0.00712	5.736(38)	0.0902	3.890(25)	4.5	60	16
a15m135XL ^a	5.80	1000	$48^3 \times 64$	0.002426	0.06730	0.8447	24	1.3	2.25, 1.25	0.00237	2.706(08)	0.0945	1.860(09)	3.0	30	32
a12m400 ^a	6.00	1000	$24^3 \times 64$	0.0170	0.0509	0.635	8	1.2	1.25, 0.25	0.0219	7.337(50)	0.0693	5.129(35)	3.0	30	8
a12m350 ^a	6.00	1000	$24^3 \times 64$	0.0130	0.0509	0.635	8	1.2	1.25, 0.25	0.0166	7.579(52)	0.0693	5.062(34)	3.0	30	8
a12m310	6.00	1053	$24^3 \times 64$	0.0102	0.0509	0.635	8	1.2	1.25, 0.25	0.0126	7.702(52)	0.0693	4.950(35)	3.0	30	8
a12m310XL ^a	6.00	1000	$48^3 \times 64$	0.0102	0.0509	0.635	8	1.2	1.25, 0.25	0.0126	7.728(22)	0.0693	4.927(21)	3.0	30	8
a12m220S	6.00	1000	$24^4 \times 64$	0.00507	0.0507	0.628	12	1.2	1.50, 0.50	0.00600	3.990(42)	0.0693	2.390(24)	6.0	90	4
a12m220	6.00	1000	$32^3 \times 64$	0.00507	0.0507	0.628	12	1.2	1.50, 0.50	0.00600	4.050(20)	0.0693	2.364(15)	6.0	90	4
a12m220ms	6.00	1000	$32^3 \times 64$	0.00507	0.0304	0.628	12	1.2	1.50, 0.50	0.00600	3.819(26)	0.0415	2.705(20)	6.0	90	8
a12m220L	6.00	1000	$40^3 \times 64$	0.00507	0.0507	0.628	12	1.2	1.50, 0.50	0.00600	4.040(26)	0.0693	2.361(19)	6.0	90	4
a12m180L ^a	6.00	1000	$48^3 \times 64$	0.00339	0.0507	0.628	14	1.2	1.75, 0.75	0.00380	3.038(13)	0.0693	1.888(11)	3.0	30	16
a12m130	6.00	1000	$48^3 \times 64$	0.00184	0.0507	0.628	20	1.2	2.00, 1.00	0.00195	1.642(09)	0.0693	0.945(08)	3.0	30	32
a09m400 ^a	6.30	1201	$32^3 \times 64$	0.0124	0.037	0.44	6	1.1	1.25, 0.25	0.0160	2.532(23)	0.0491	1.957(17)	3.5	45	8
a09m350 ^a	6.30	1201	$32^3 \times 64$	0.00945	0.037	0.44	6	1.1	1.25, 0.25	0.0121	2.560(24)	0.0491	1.899(16)	3.5	45	8
a09m310	6.30	780	$32^3 \times 96$	0.0074	0.037	0.44	6	1.1	1.25, 0.25	0.00951	2.694(26)	0.0491	1.912(15)	6.7	167	8
a09m220	6.30	1001	$48^3 \times 96$	0.00363	0.0363	0.43	8	1.1	1.25, 0.25	0.00449	1.659(13)	0.0491	0.834(07)	8.0	150	6
a09m135 ^a	6.30	1010	$64^3 \times 96$	0.001326	0.03636	0.4313	12	1.1	1.50, 0.50	0.00152	0.938(06)	0.04735	0.418(04)	3.5	45	16
a06m310L ^a	6.72	1000	$72^3 \times 96$	0.0048	0.024	0.286	6	1.0	1.25, 0.25	0.00617	0.225(03)	0.0309	0.165(02)	3.5	45	8

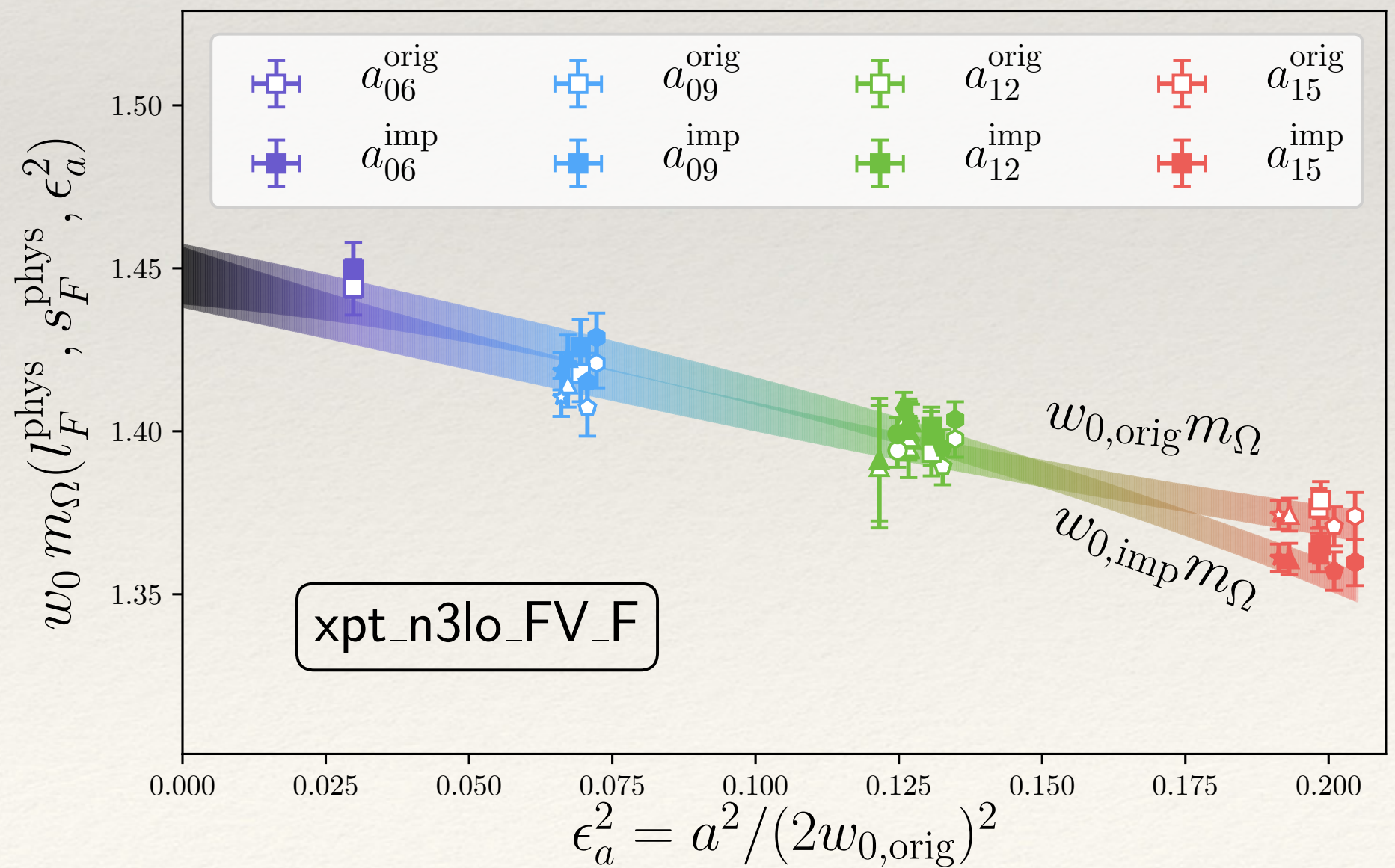
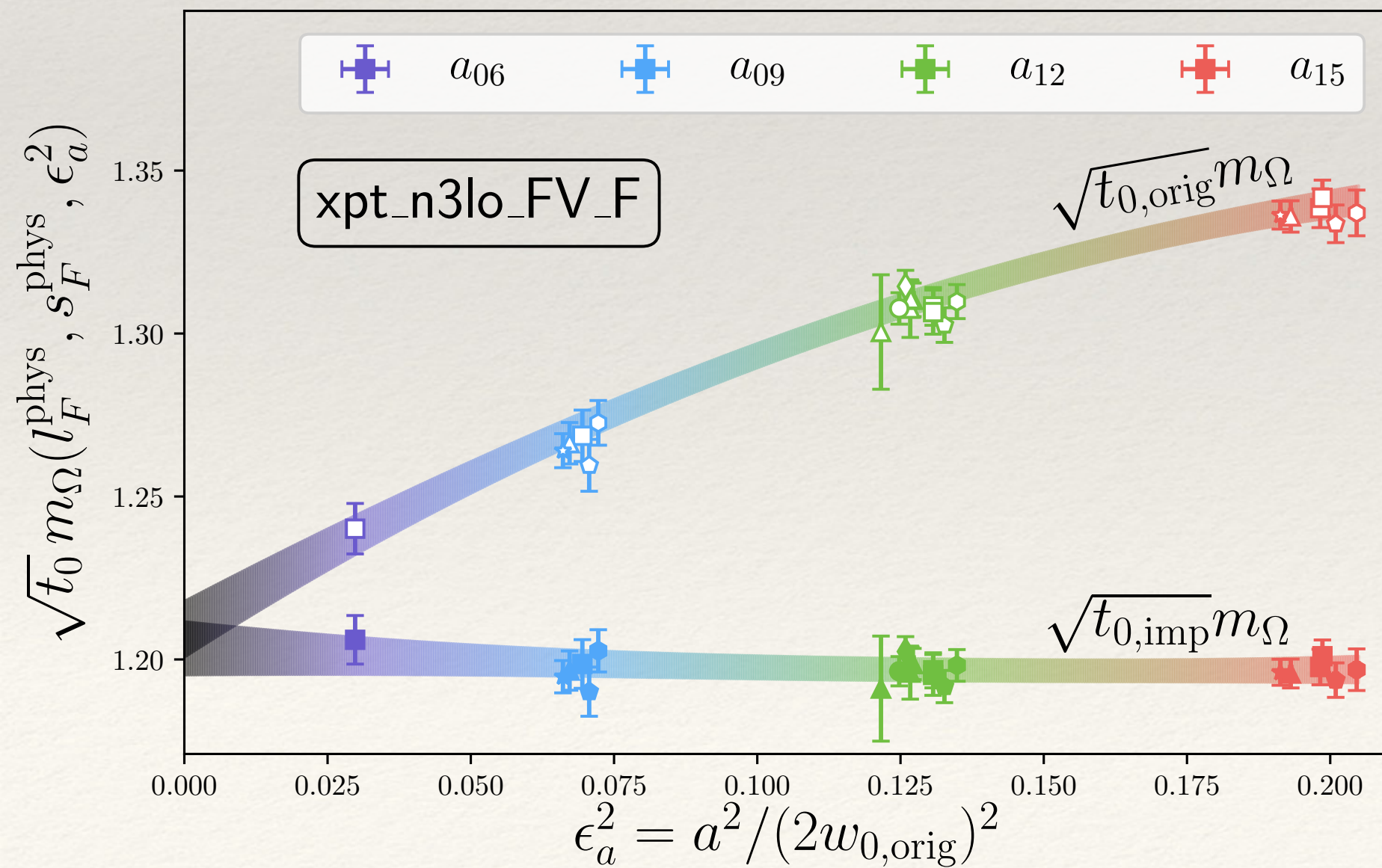
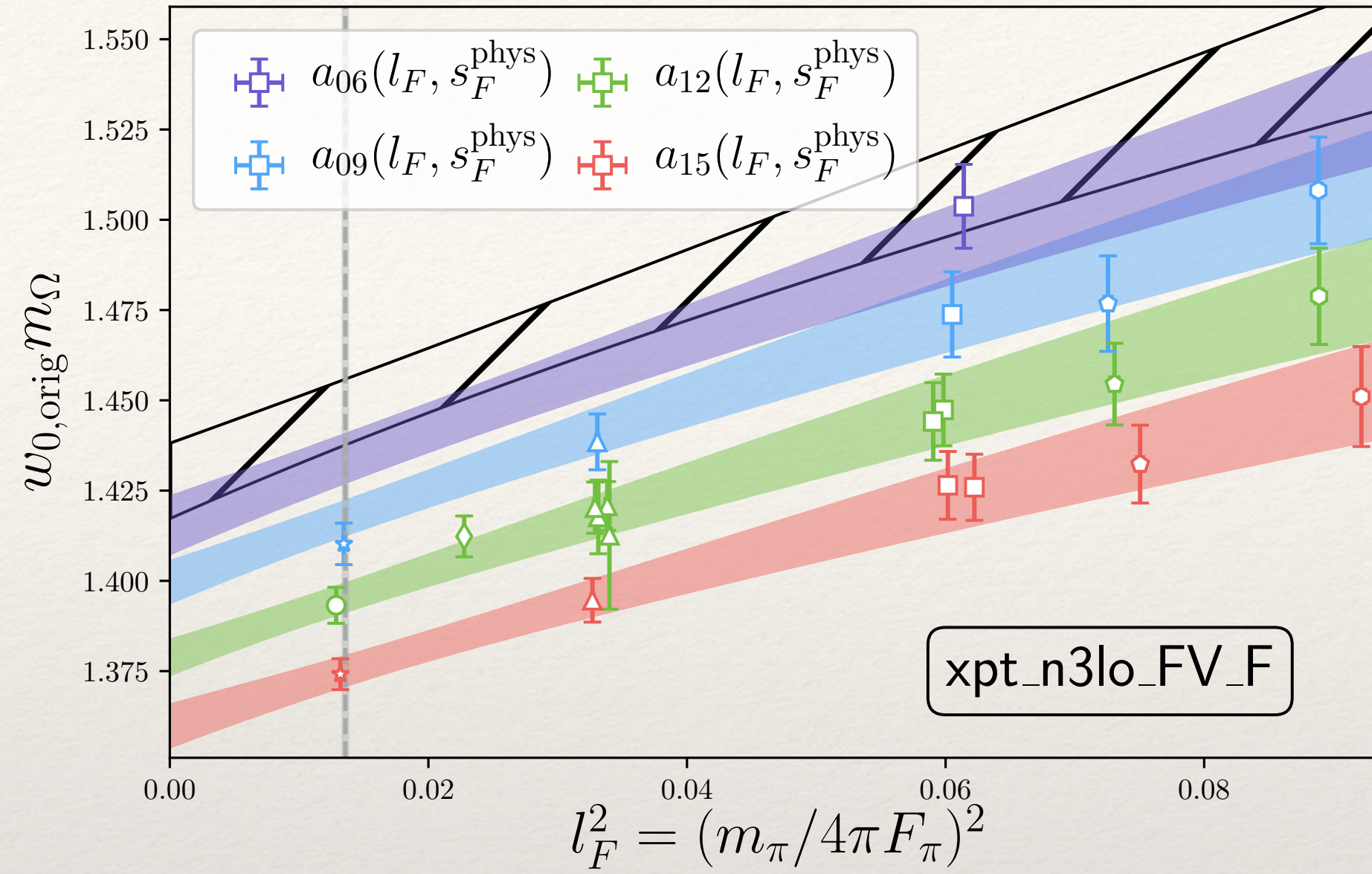
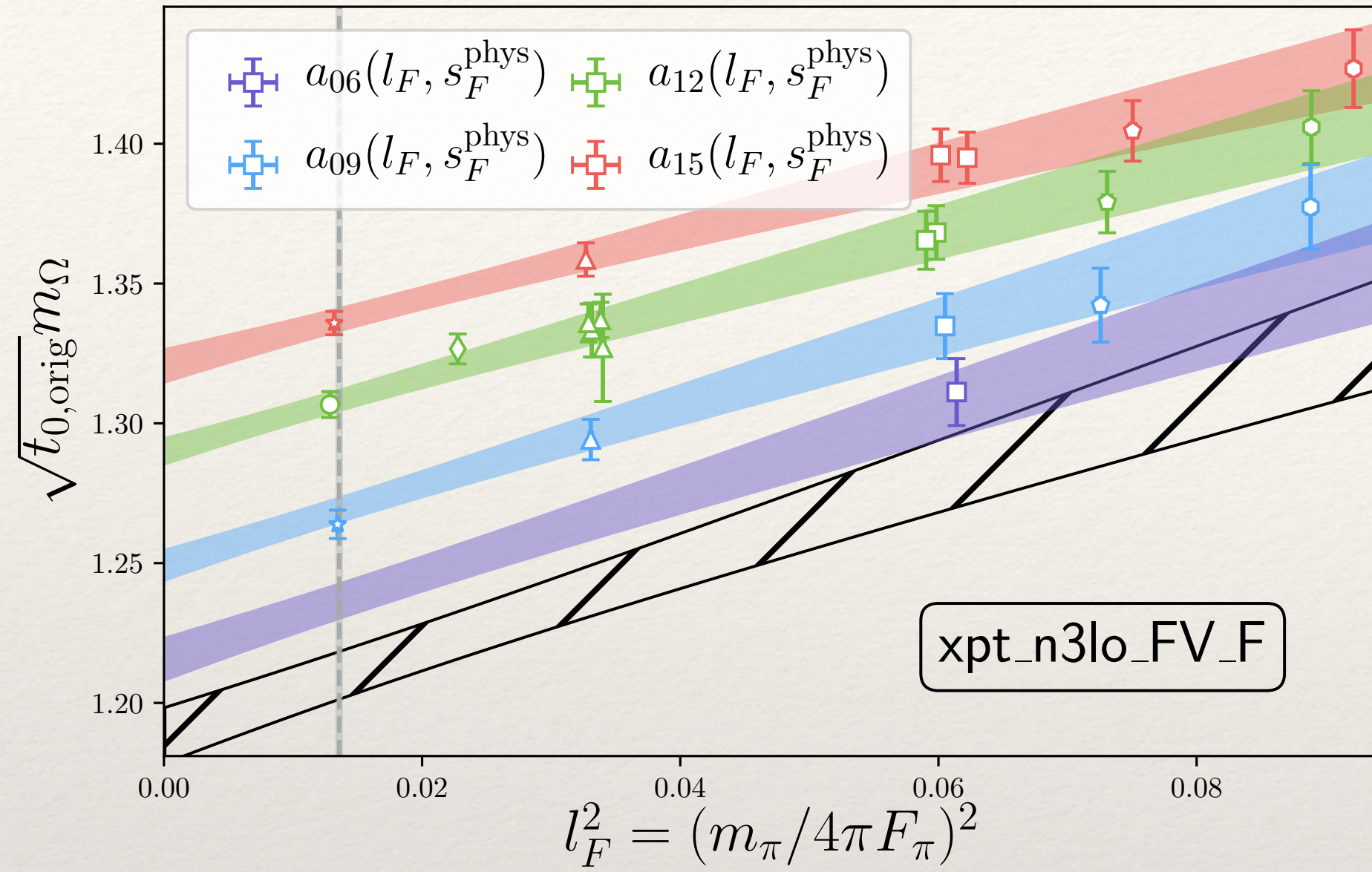
Example Scale Setting: arXiv:2011.12166

ensemble	am_Ω	$t_{0,\text{orig}}/a^2$	$t_{0,\text{imp}}/a^2$	$\sqrt{t_{0,\text{orig}}}m_\Omega$	$\sqrt{t_{0,\text{imp}}}m_\Omega$	$w_{0,\text{orig}}/a$	$w_{0,\text{imp}}/a$	$w_{0,\text{orig}}m_\Omega$	$w_{0,\text{imp}}m_\Omega$
a15m400	1.2437(43)	1.1905(15)	0.9563(11)	1.3570(47)	1.2162(42)	1.1053(12)	1.0868(14)	1.3747(49)	1.3516(50)
a15m350	1.2331(31)	1.2032(14)	0.9660(11)	1.3526(35)	1.2120(32)	1.1154(11)	1.0988(13)	1.3754(37)	1.3550(38)
a15m310L	1.2287(31)	1.2111(07)	0.9720(05)	1.3521(34)	1.2113(30)	1.1219(06)	1.1066(07)	1.3784(35)	1.3596(35)
a15m310	1.2312(36)	1.2121(09)	0.9727(07)	1.3555(40)	1.2143(36)	1.1230(07)	1.1079(09)	1.3826(41)	1.3640(41)
a15m220	1.2068(26)	1.2298(08)	0.9861(07)	1.3383(30)	1.1984(27)	1.1378(07)	1.1255(08)	1.3731(31)	1.3582(31)
a15m135XL	1.2081(19)	1.2350(04)	0.9897(03)	1.3425(21)	1.2018(19)	1.1432(03)	1.1319(04)	1.3811(22)	1.3674(22)
a12m400	1.0279(25)	1.6942(11)	1.4172(10)	1.3380(33)	1.2237(30)	1.3616(07)	1.3636(08)	1.3997(35)	1.4017(35)
a12m350	1.0139(26)	1.7091(14)	1.4298(12)	1.3255(35)	1.2124(32)	1.3728(10)	1.3755(11)	1.3918(38)	1.3946(38)
a12m310XL	1.0072(41)	1.7221(07)	1.4407(06)	1.3217(54)	1.2089(50)	1.3831(05)	1.3865(06)	1.3930(58)	1.3964(58)
a12m310	1.0112(32)	1.7213(19)	1.4398(17)	1.3267(42)	1.2134(39)	1.3830(13)	1.3863(12)	1.3985(46)	1.4019(46)
a12m220ms	0.8896(92)	1.7891(15)	1.4977(13)	1.190(12)	1.089(11)	1.4339(12)	1.4406(12)	1.276(13)	1.282(13)
a12m220S	0.9970(26)	1.7466(20)	1.4614(17)	1.3177(35)	1.2053(32)	1.4021(15)	1.4069(16)	1.3980(39)	1.4027(39)
a12m220L	0.9944(30)	1.7489(09)	1.4633(08)	1.3150(40)	1.2028(37)	1.4041(06)	1.4090(07)	1.3962(43)	1.4010(43)
a12m220	0.9924(60)	1.7498(14)	1.4641(12)	1.3127(80)	1.2007(73)	1.4047(10)	1.4096(11)	1.3940(85)	1.3988(86)
a12m180L	0.9924(26)	1.7553(05)	1.4686(05)	1.3148(35)	1.2026(32)	1.4093(05)	1.4145(05)	1.3985(38)	1.4037(38)
a12m130	0.9801(26)	1.7628(07)	1.4749(06)	1.3013(34)	1.1903(31)	1.4155(05)	1.4211(06)	1.3873(37)	1.3928(37)
a09m400	0.7716(23)	2.9158(42)	2.6040(33)	1.3176(41)	1.2451(38)	1.8602(26)	1.8686(27)	1.4353(48)	1.4418(48)
a09m350	0.7561(35)	2.9455(37)	2.6301(34)	1.2977(61)	1.2262(58)	1.8810(25)	1.8900(26)	1.4222(69)	1.4291(70)
a09m310	0.7543(36)	2.9698(32)	2.6521(29)	1.2998(63)	1.2283(59)	1.8970(22)	1.9066(22)	1.4308(71)	1.4381(71)
a09m220	0.7377(30)	3.0172(16)	2.6952(15)	1.2814(53)	1.2111(50)	1.9282(12)	1.9388(12)	1.4224(59)	1.4302(60)
a09m135	0.7244(25)	3.0390(12)	2.7147(11)	1.2629(44)	1.1936(42)	1.9450(10)	1.9563(11)	1.4091(50)	1.4172(50)
a06m310L	0.5069(21)	6.4079(45)	6.0606(44)	1.2830(54)	1.2478(52)	2.8958(20)	2.9053(20)	1.4678(62)	1.4726(62)

Example Scale Setting: arXiv:2011.12166

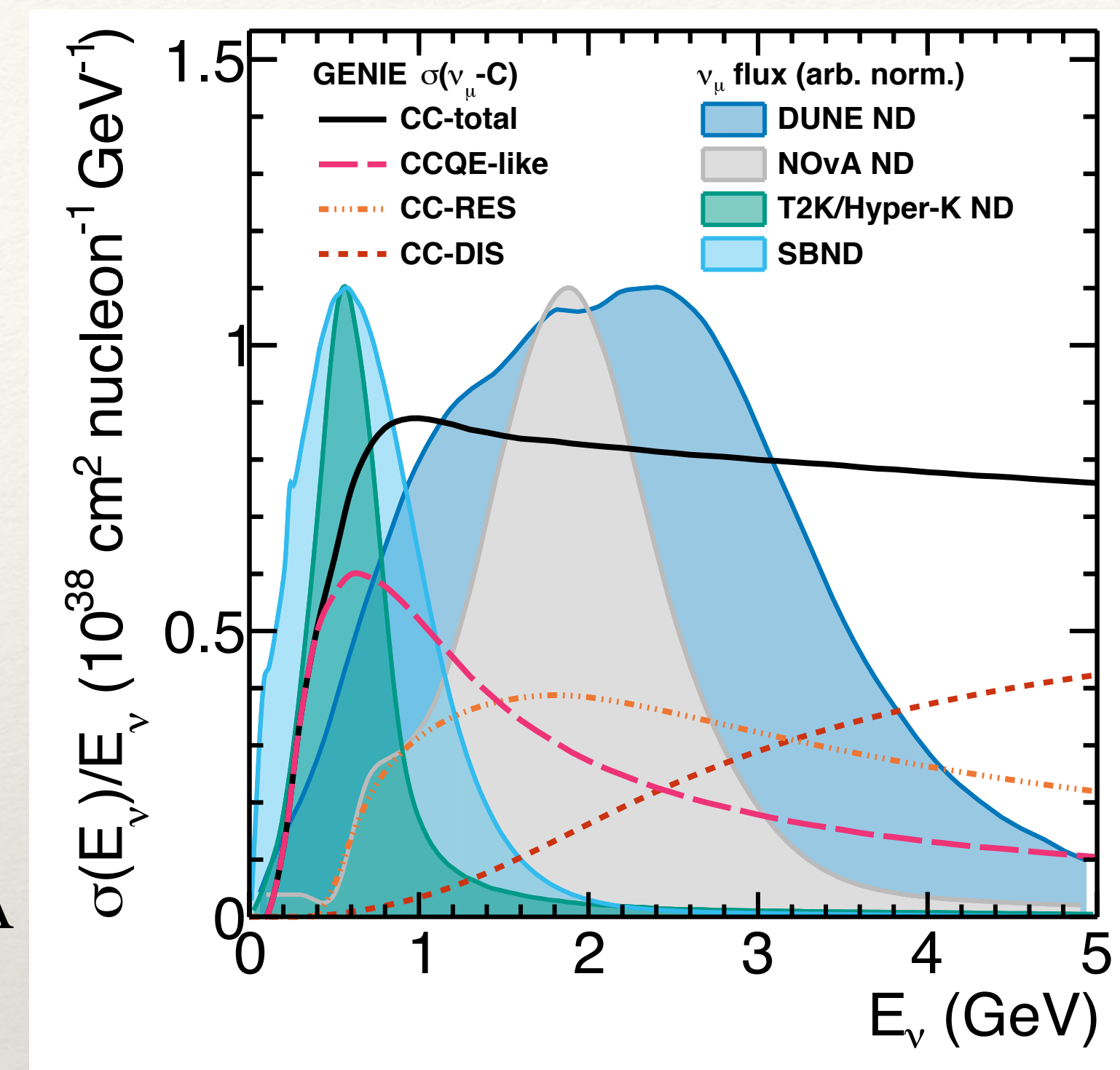
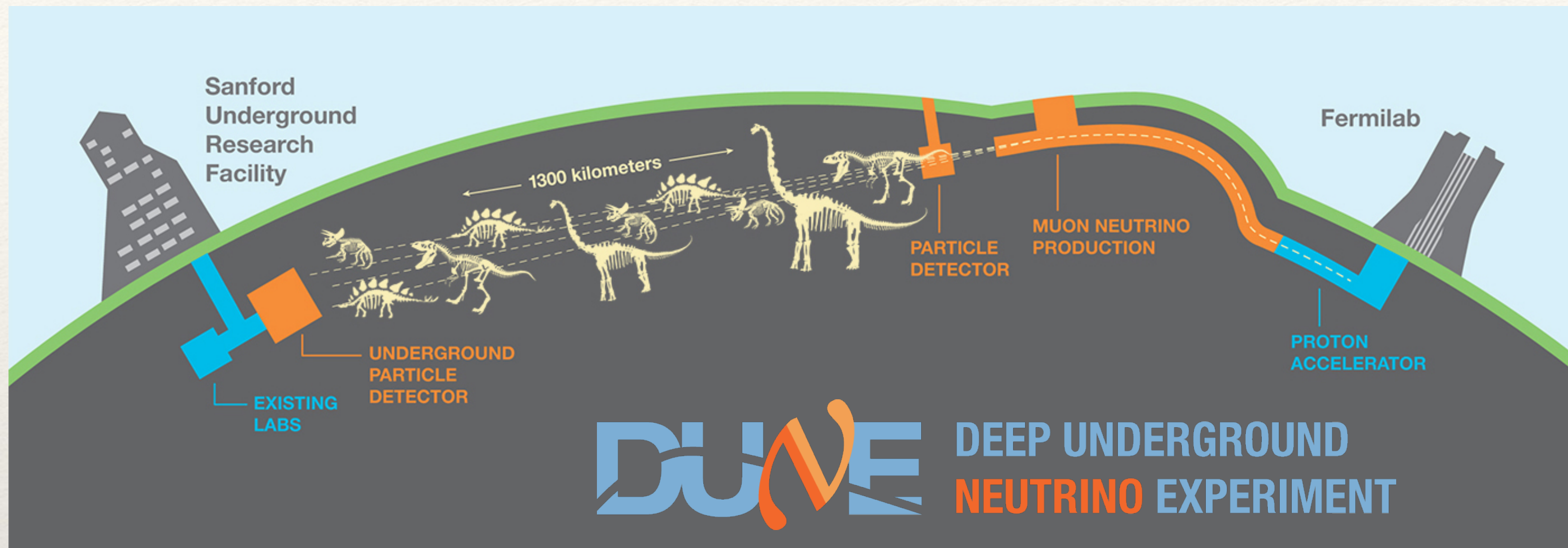


Example Scale Setting: arXiv:2011.12166



scheme	a_{15}/fm	a_{12}/fm	a_{09}/fm	a_{06}/fm
$t_{0,\text{orig}}/a^2$	0.1284(10)	0.10788(83)	0.08196(64)	0.05564(44)
$t_{0,\text{imp}}/a^2$	0.1428(10)	0.11735(87)	0.08632(65)	0.05693(44)
$w_{0,\text{orig}}/a$	0.1492(10)	0.12126(87)	0.08789(71)	0.05717(51)
$w_{0,\text{imp}}/a$	0.1505(10)	0.12066(88)	0.08730(70)	0.05691(51)

Nucleon Axial Form Factor



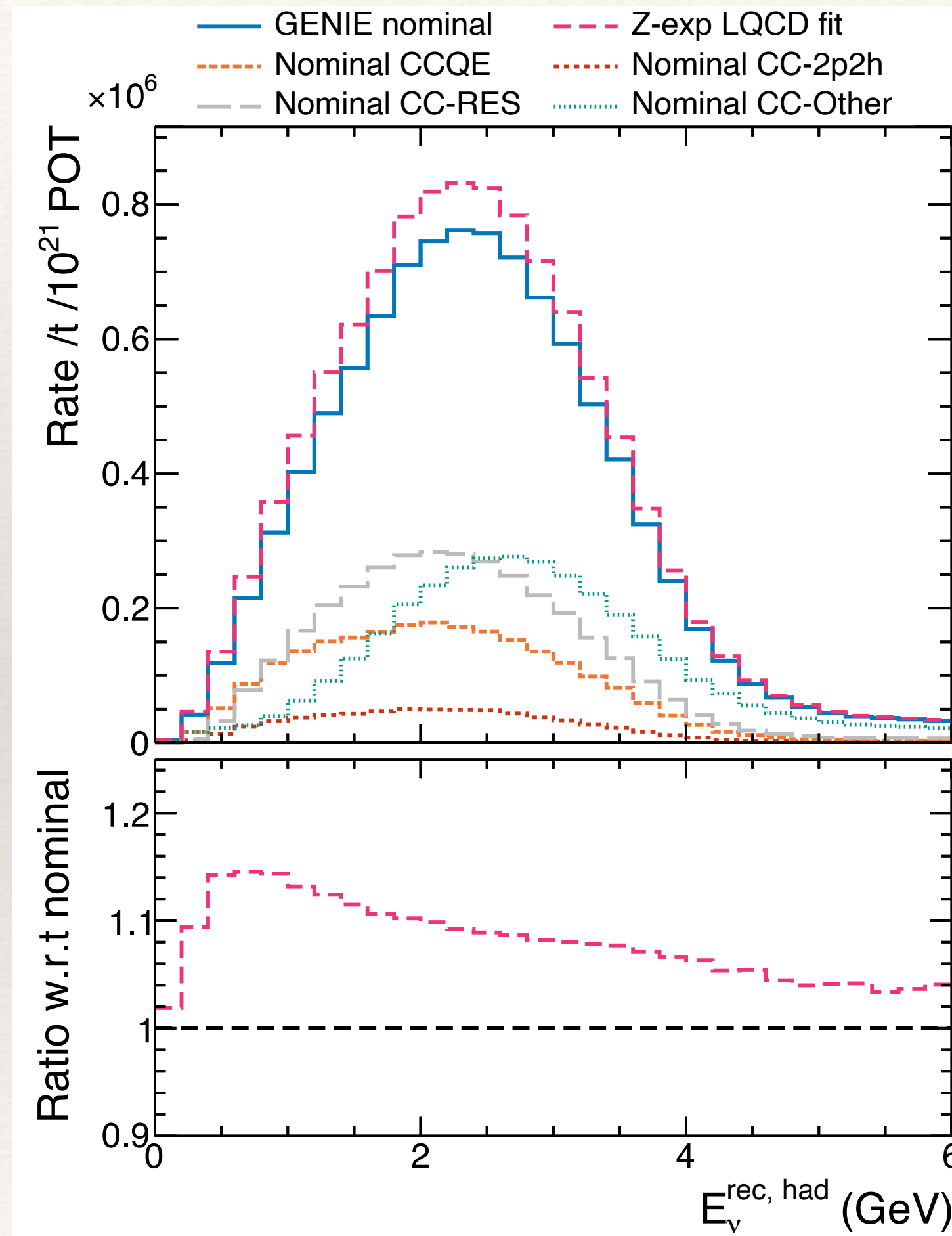
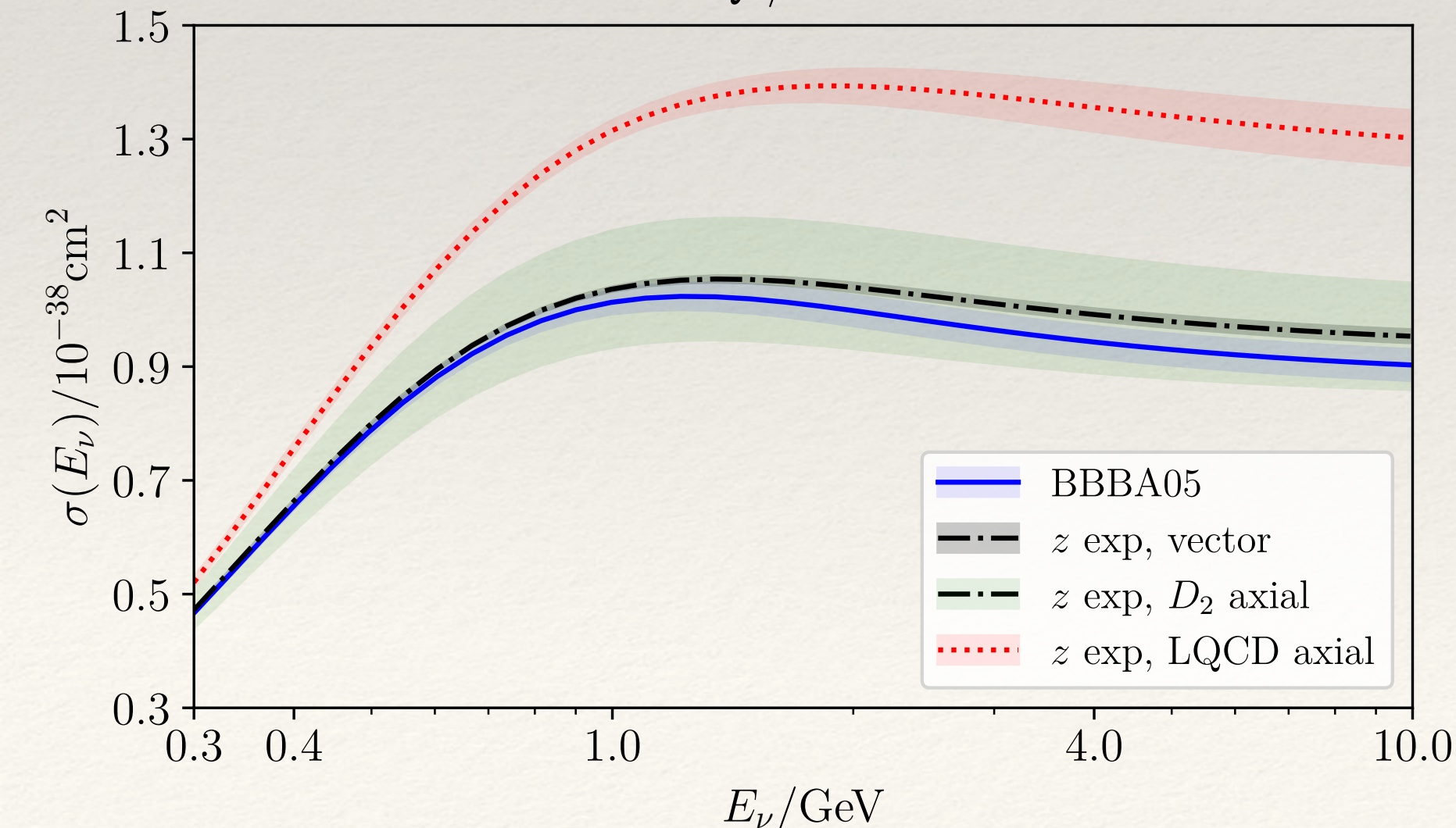
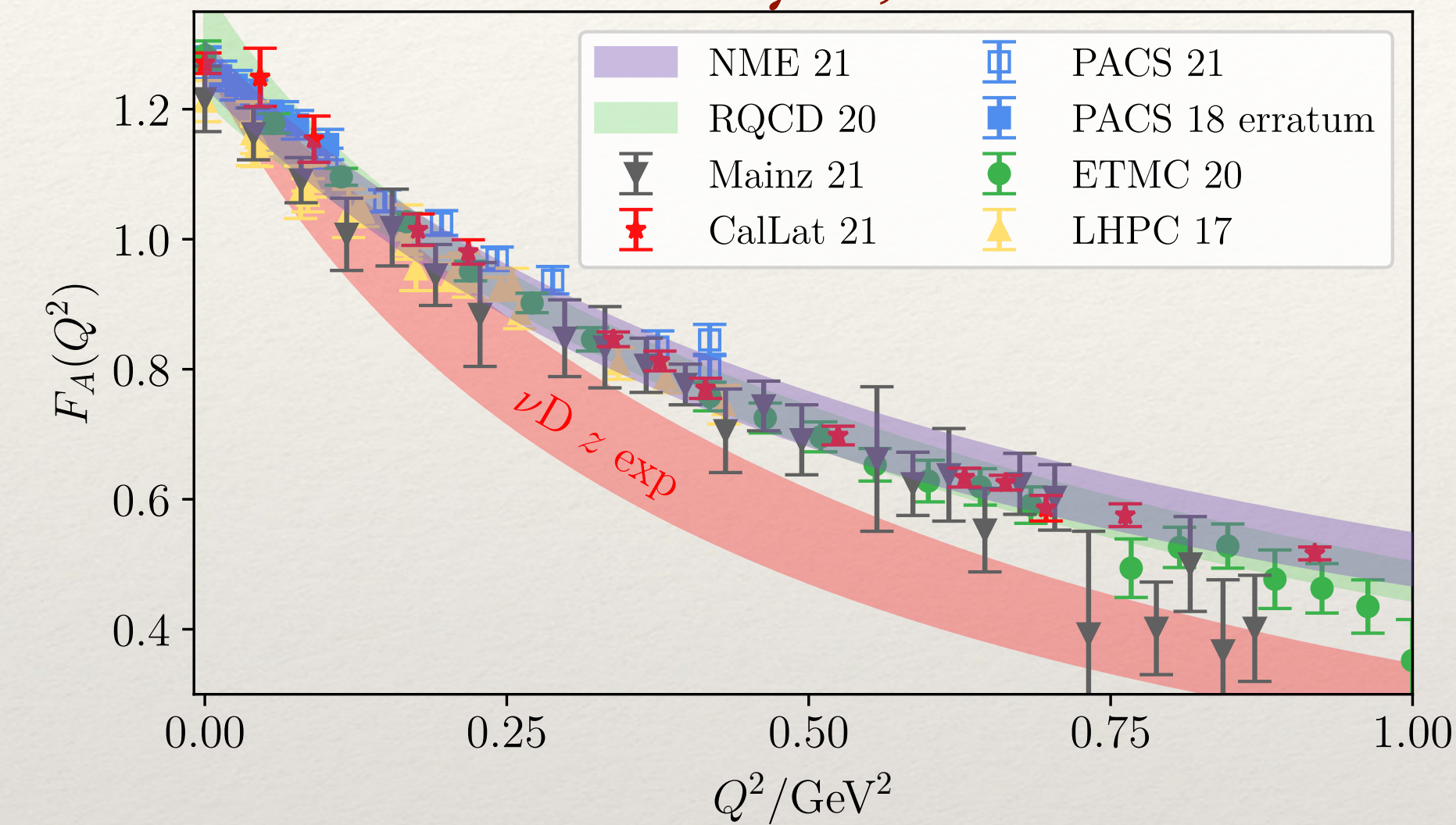
- DUNE and Hyper-K science goals reliant upon accurate and precise modeling of ν -A cross sections
- The 50-year old pion-production model that is currently used in event generators was described by its authors as *naive and obviously wrong in its simplicity* [FKR]
- No experimental path forward to improve these basic ν 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 ν -A mechanisms

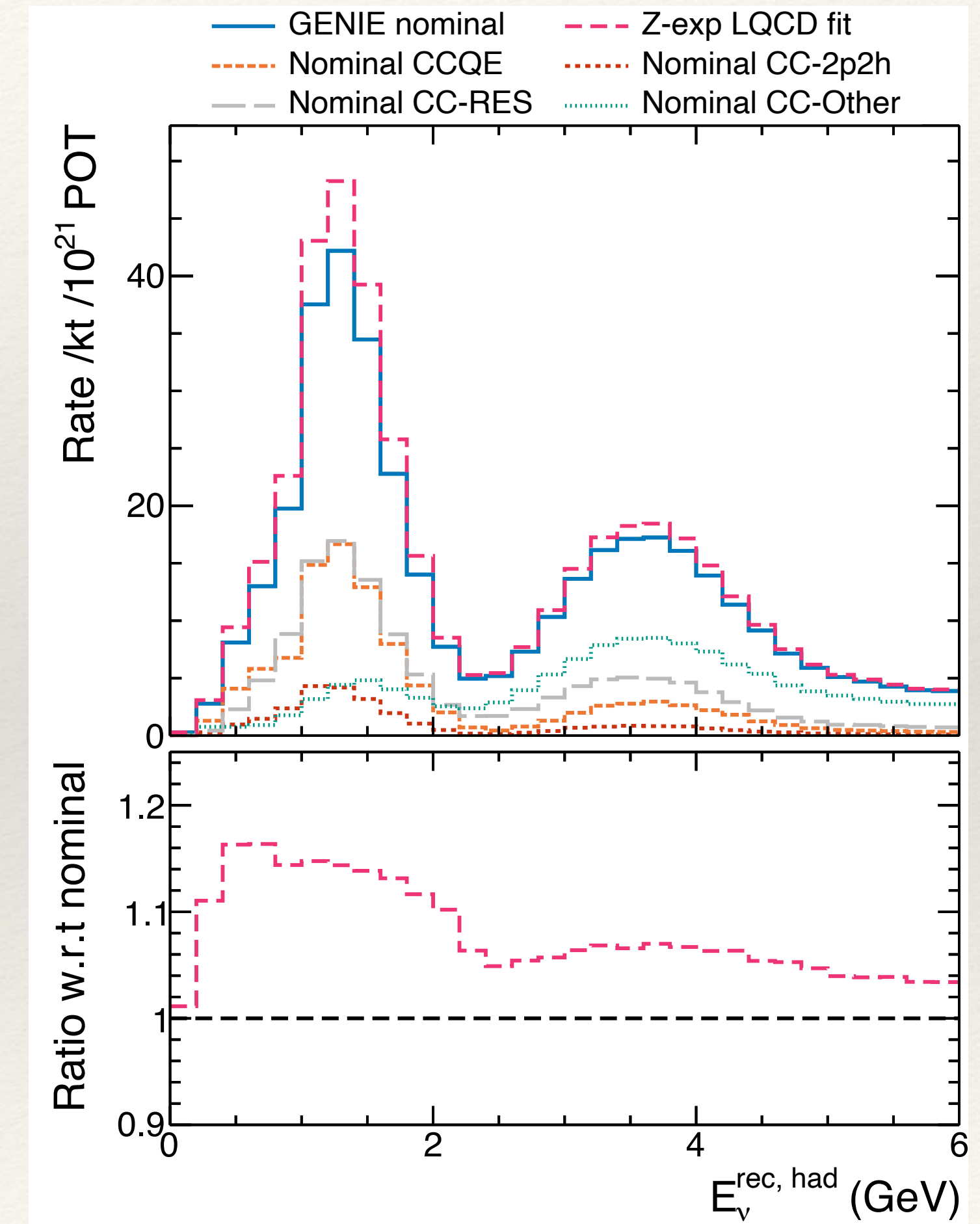
[FKR] Feynman, Kislinger, Ravndal
PRD 3 (1971)

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)*

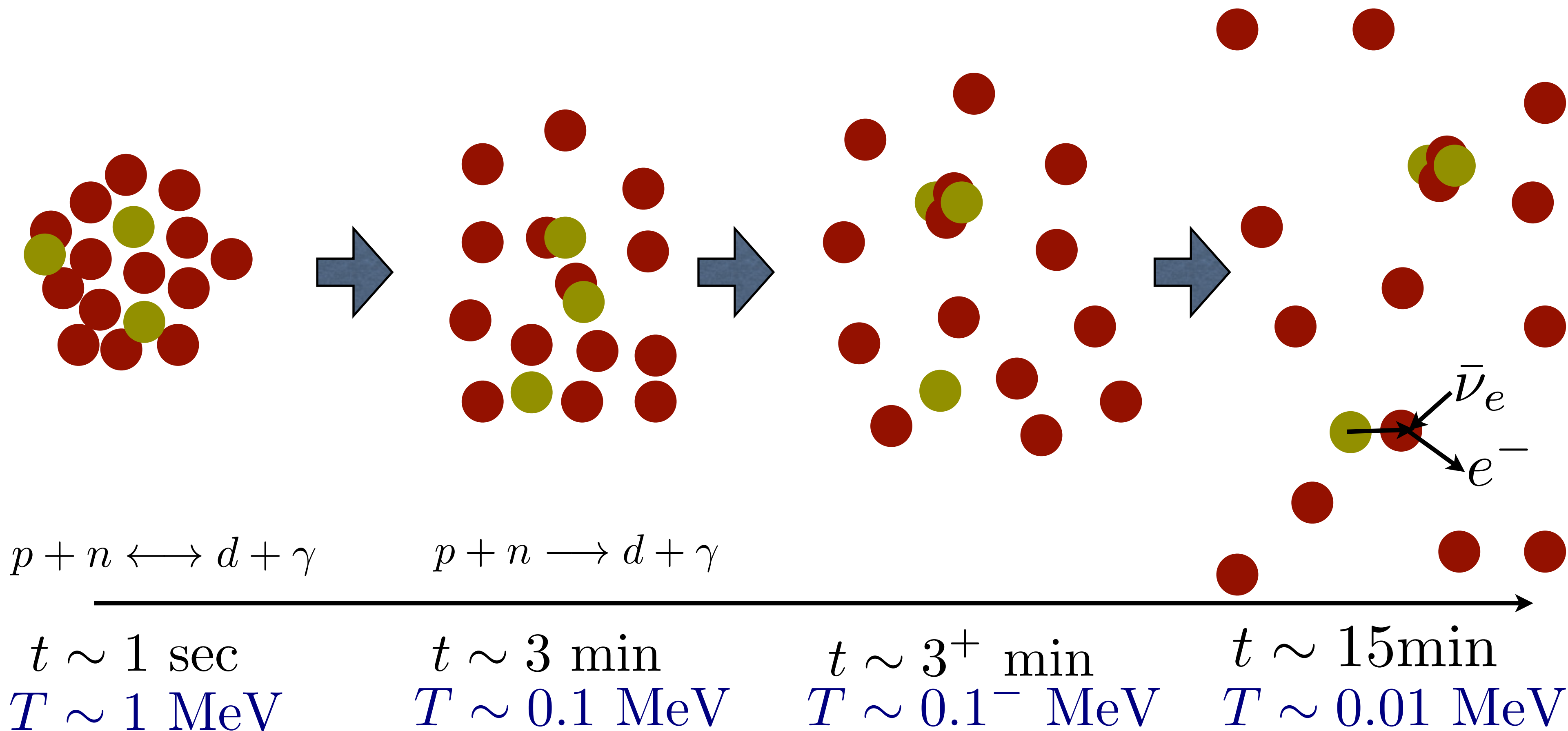


Near detector



Far detector

Primordial Abundance of Light Nuclei & Fine Tunings



Light Ion reactions in early universe produce primordial abundances of light nuclei

reactions dominated by radiation

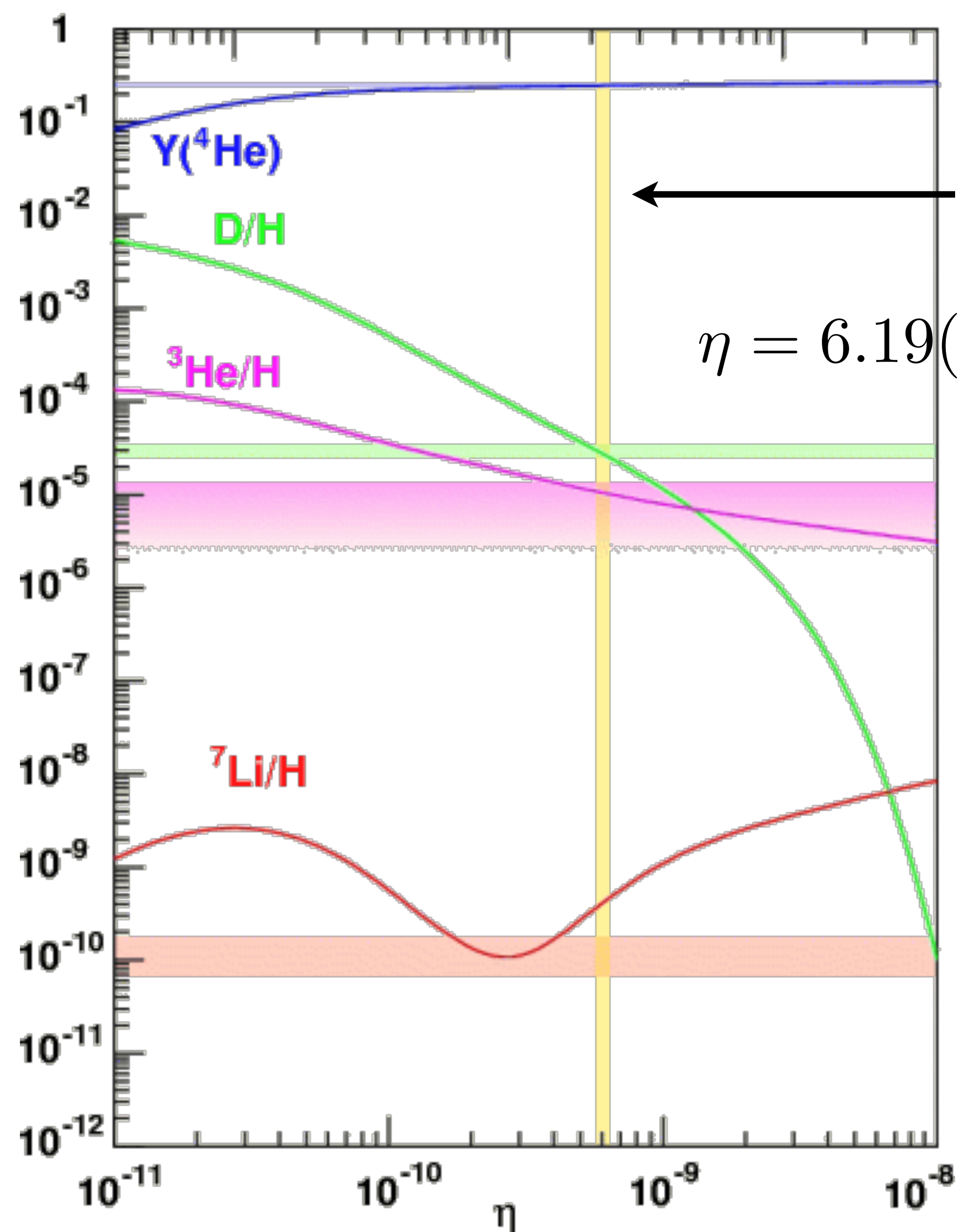
absence of bound $A=5,8$ nuclei limit synthesis (no ^{12}C)

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

Primordial Abundance of Light Nuclei & Fine Tunings

Primordial Universe
(Mass Fraction)

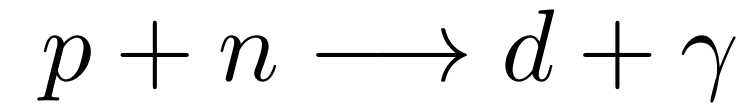
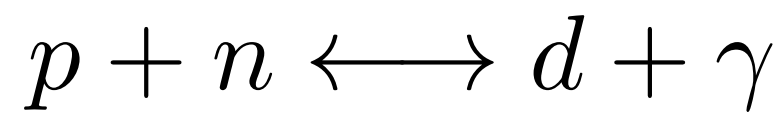
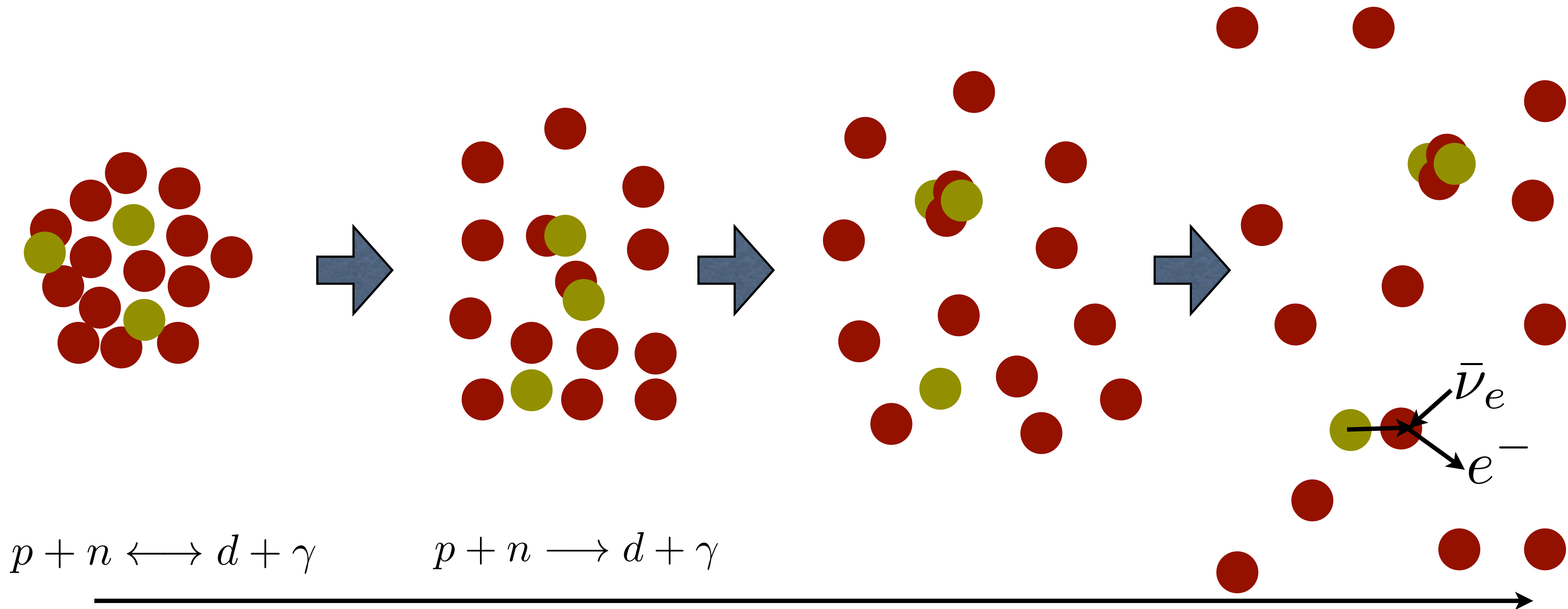
~75% H
~25% ^4He



$$\eta = 6.19(15) \times 10^{-10}$$

$$\eta \equiv \frac{X_N}{X_\gamma}$$

Primordial Abundance of Light Nuclei & Fine Tunings



$t \sim 1 \text{ sec}$
 $T \sim 1 \text{ MeV}$

$t \sim 3 \text{ min}$
 $T \sim 0.1 \text{ MeV}$

$t \sim 3^+ \text{ min}$
 $T \sim 0.1^- \text{ MeV}$

$t \sim 15 \text{ min}$
 $T \sim 0.01 \text{ MeV}$

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

Initial conditions

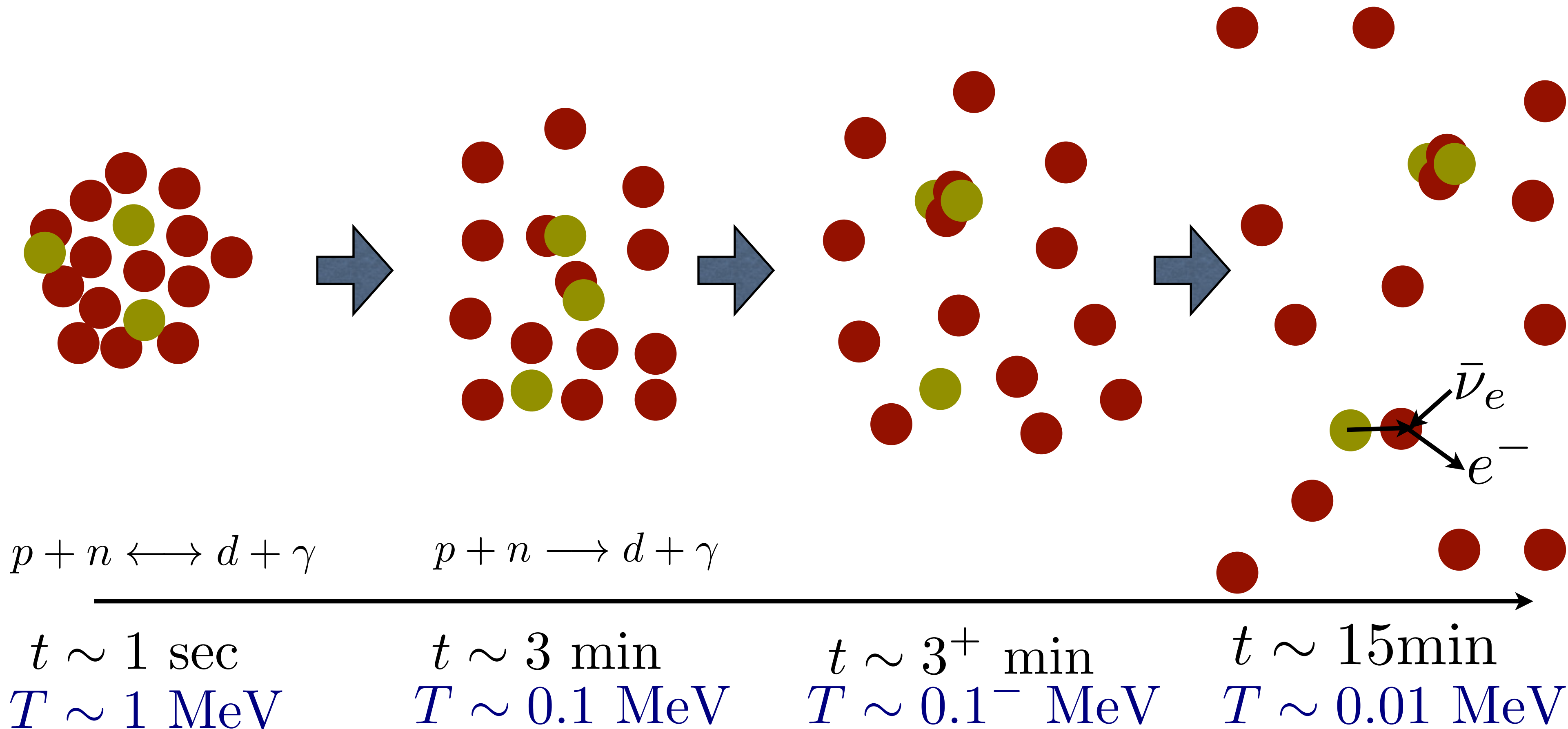
B_d

deuterium
binding energy

τ_n

neutron
lifetime

Primordial Abundance of Light Nuclei & Fine Tunings



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

Initial conditions

focus on leading
isospin breaking

τ_n

neutron
lifetime

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 ~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 > 0

Big Bang Nucleosynthesis and $M_n - M_p$

PRELIMINARY

$$\begin{aligned} M_n - M_p &= \delta M_{n-p}^\gamma + \delta M_{n-p}^{m_d - m_u} \\ &= -178(04)(64) \text{ MeV} \times \alpha_{f.s.} + 1.08(6)(9) \times (m_d - m_u) \\ &\hspace{15em} \text{(lattice average)} \end{aligned}$$

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

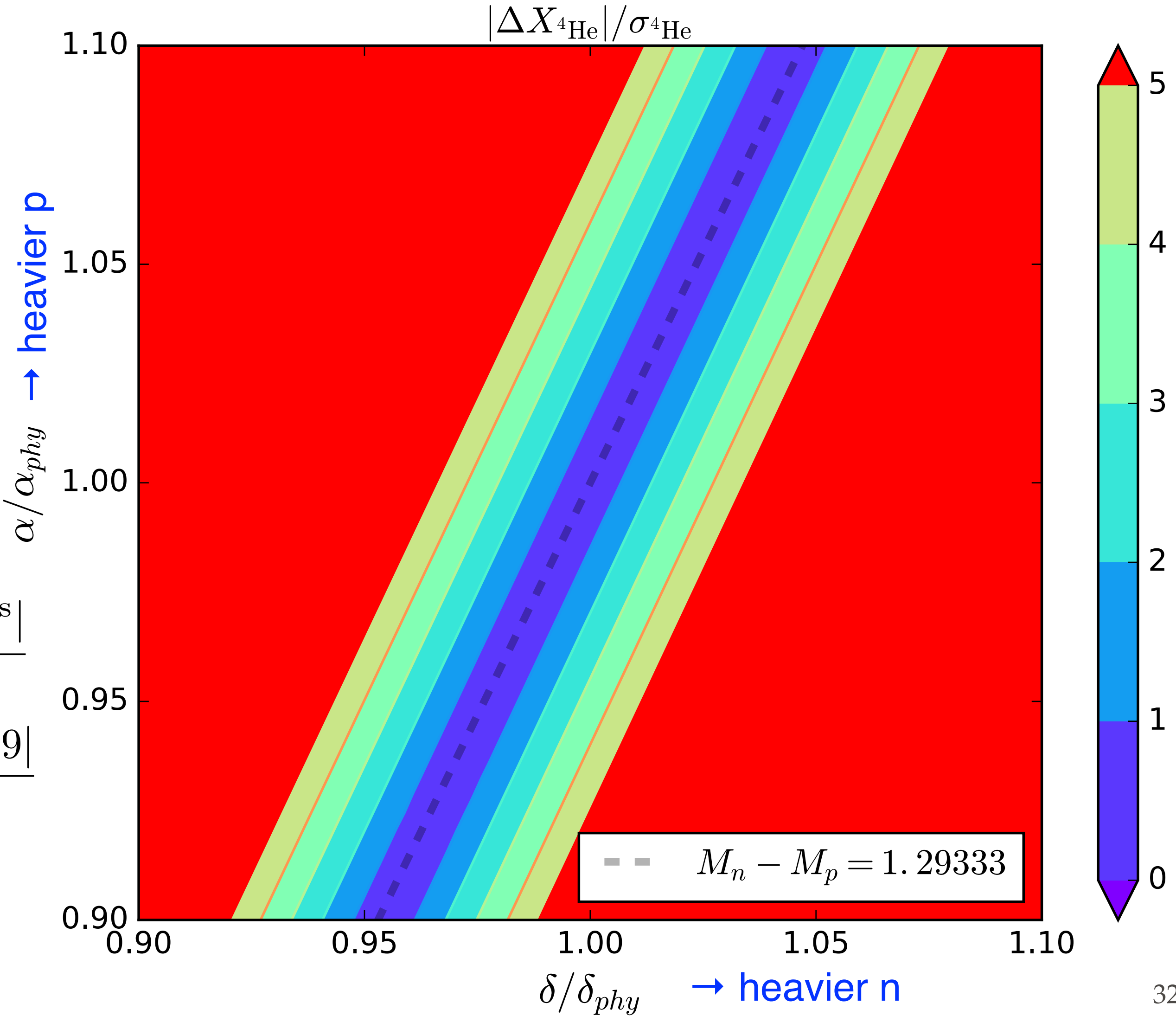
- Observe gas clouds with low metallicity (very few heavy elements).
- Assume these are representative of nuclear abundances shortly after the Big Bang (for some quantities, extrapolations are required)
- Run BBN code, changing input parameters connected to QCD, and compare predicted abundances to observed

$$\begin{aligned} {}^4\text{He} : \quad Y_p &= 0.2449 \pm 0.0040 \\ \left(\frac{\text{D}}{\text{H}} \right)_p &= (2.53 \pm 0.04) \times 10^{-5} \end{aligned}$$

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

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

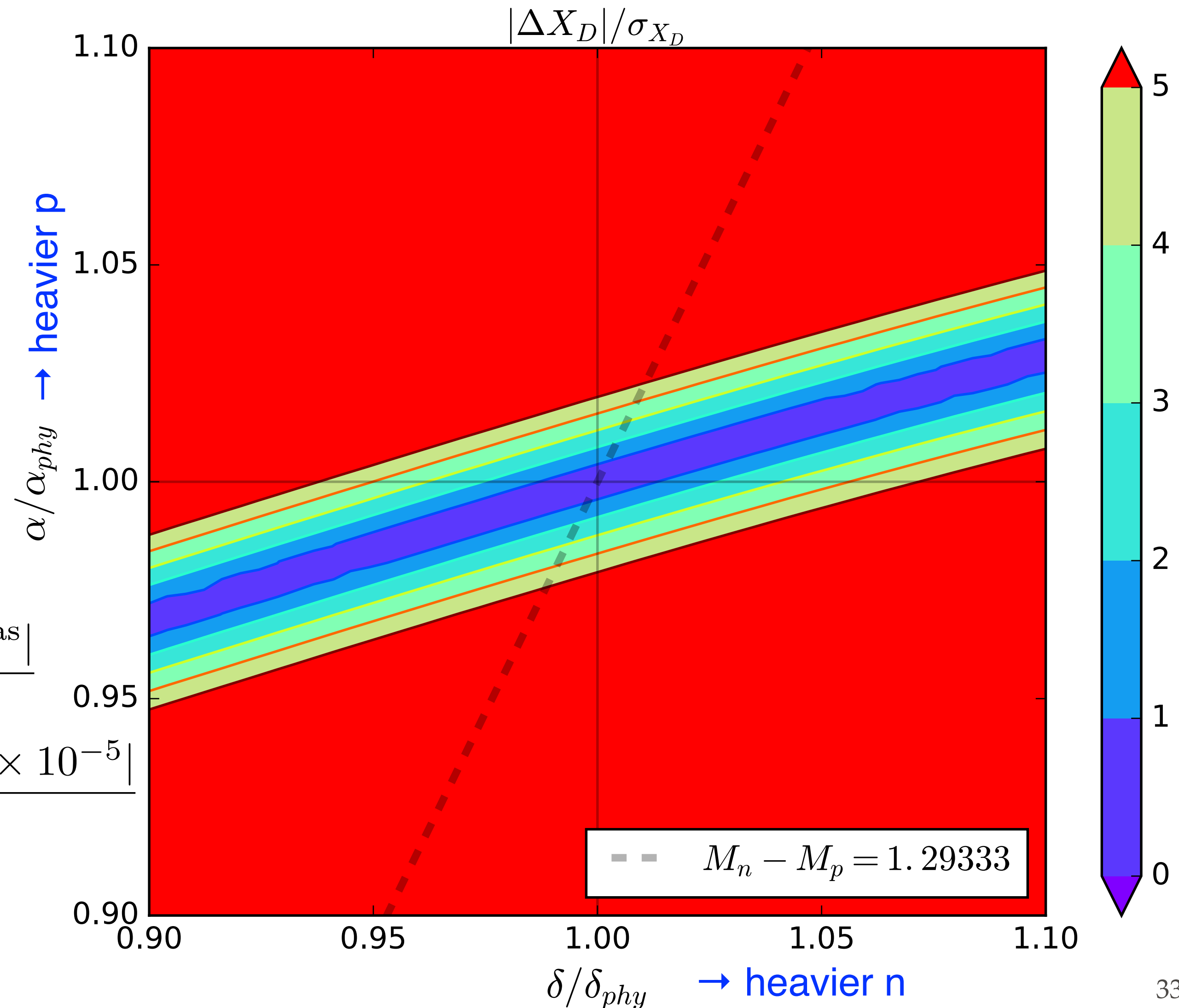
$$\frac{|\Delta X_{4\text{He}}|}{\sigma_{4\text{He}}} = \frac{|Y_p(\delta, \alpha_{f.s.}) - Y_p^{\text{meas}}|}{\sigma_{Y_p}} = \frac{|Y_p(\delta, \alpha_{f.s.}) - 0.2449|}{0.0040}$$



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

- ❑ 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 $M_n - M_p$

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

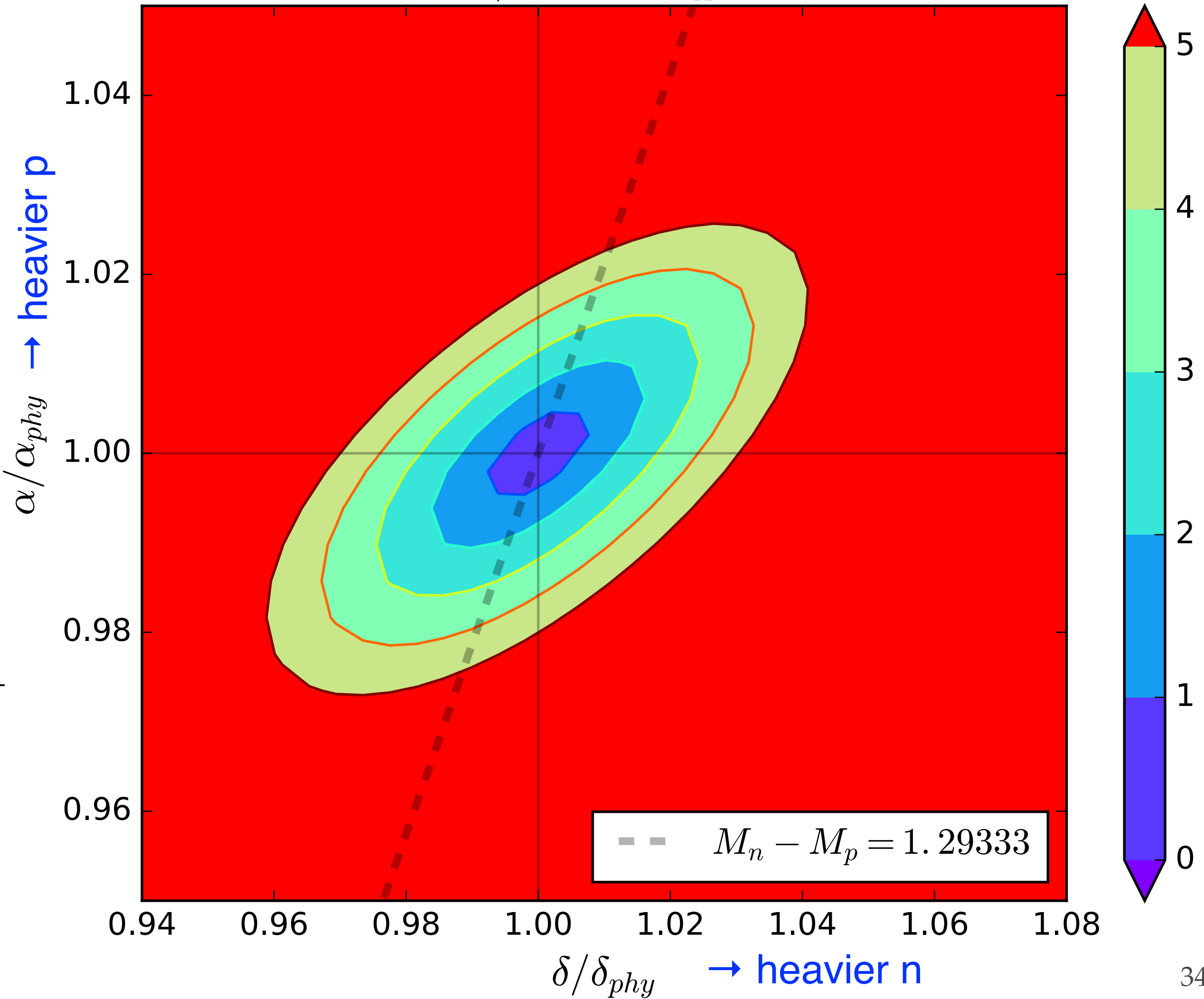


$$\delta M_{n-p} = \delta M_{n-p}^\delta + \delta M_{n-p}^\gamma = 2.39 \frac{\delta}{\delta_{\text{phys}}} - 1.10 \frac{\alpha_{f.s.}}{\alpha_{\text{phys}}} \text{ MeV}$$

$$\sqrt{\sum_X \Delta X^2 / \sigma_X^2}$$

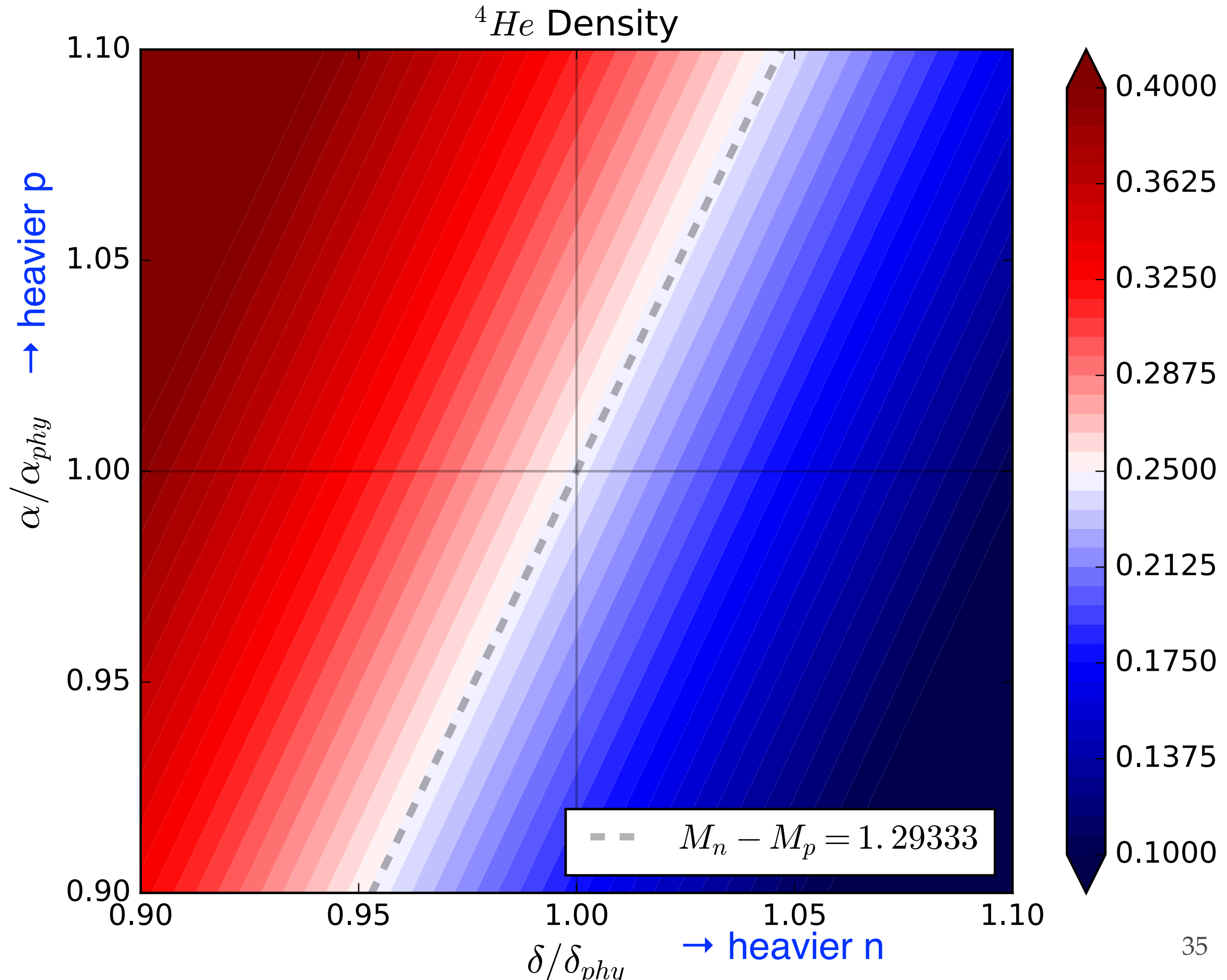
- The combined variation of D, ³He and ⁴He restrict possible primordial variations of isospin breaking to less than 2% at the 95% confidence level
- This places tight constraints on possible extensions of the Standard Model

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

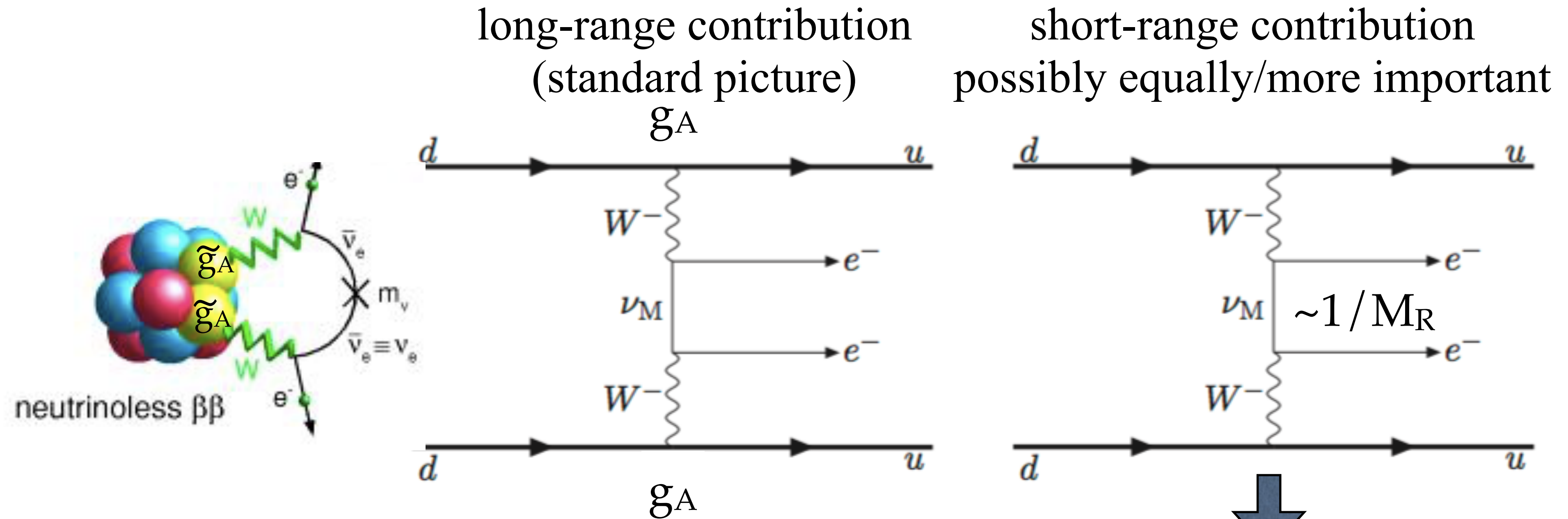


$$\delta M_{n-p} = \delta M_{n-p}^\delta + \delta M_{n-p}^\gamma = 2.39 \frac{\delta}{\delta_{\text{phys}}} - 1.10 \frac{\alpha_{f.s.}}{\alpha_{\text{phys}}} \text{ MeV}$$

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



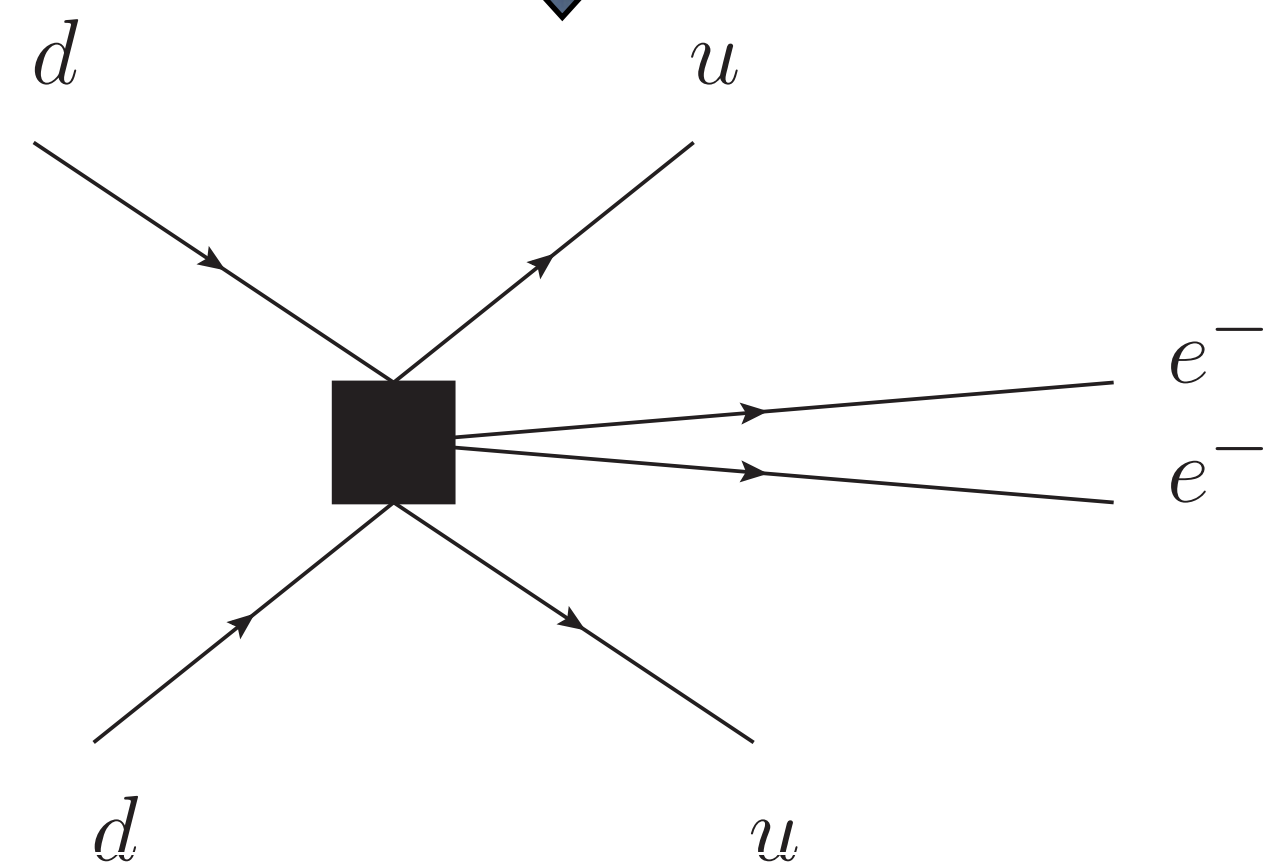
Neutrinoless Double Beta-Decay



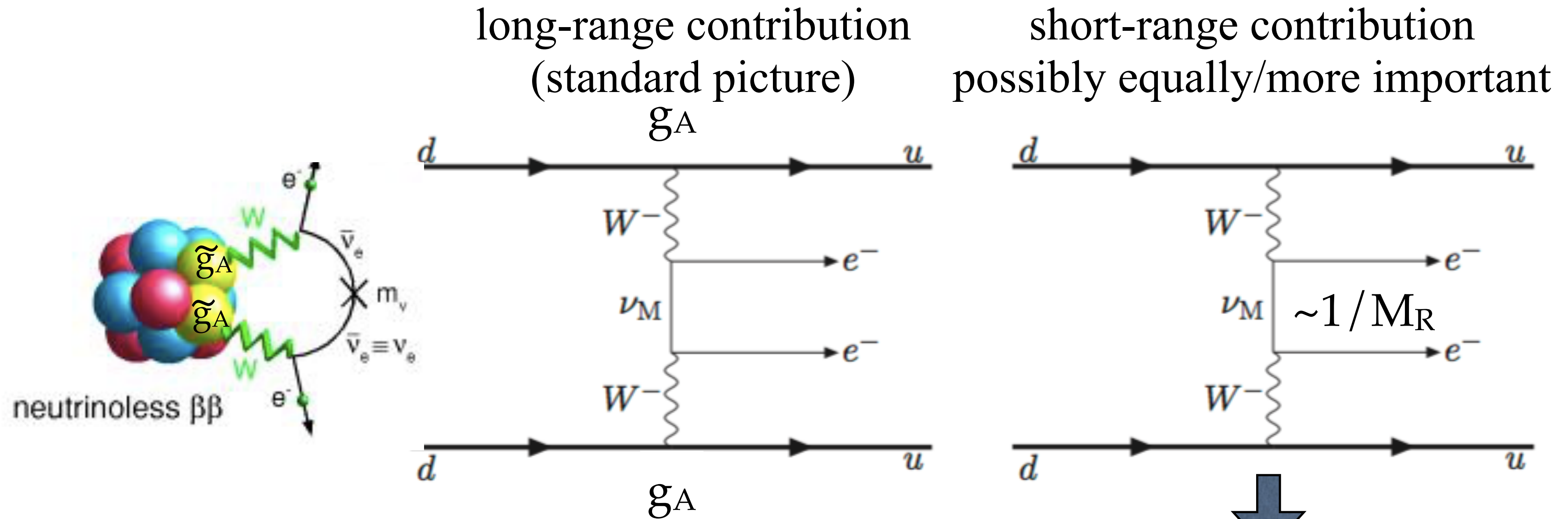
Short Range: lattice QCD is the ONLY theoretical tool we have to understand these contributions with quantified uncertainties

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)

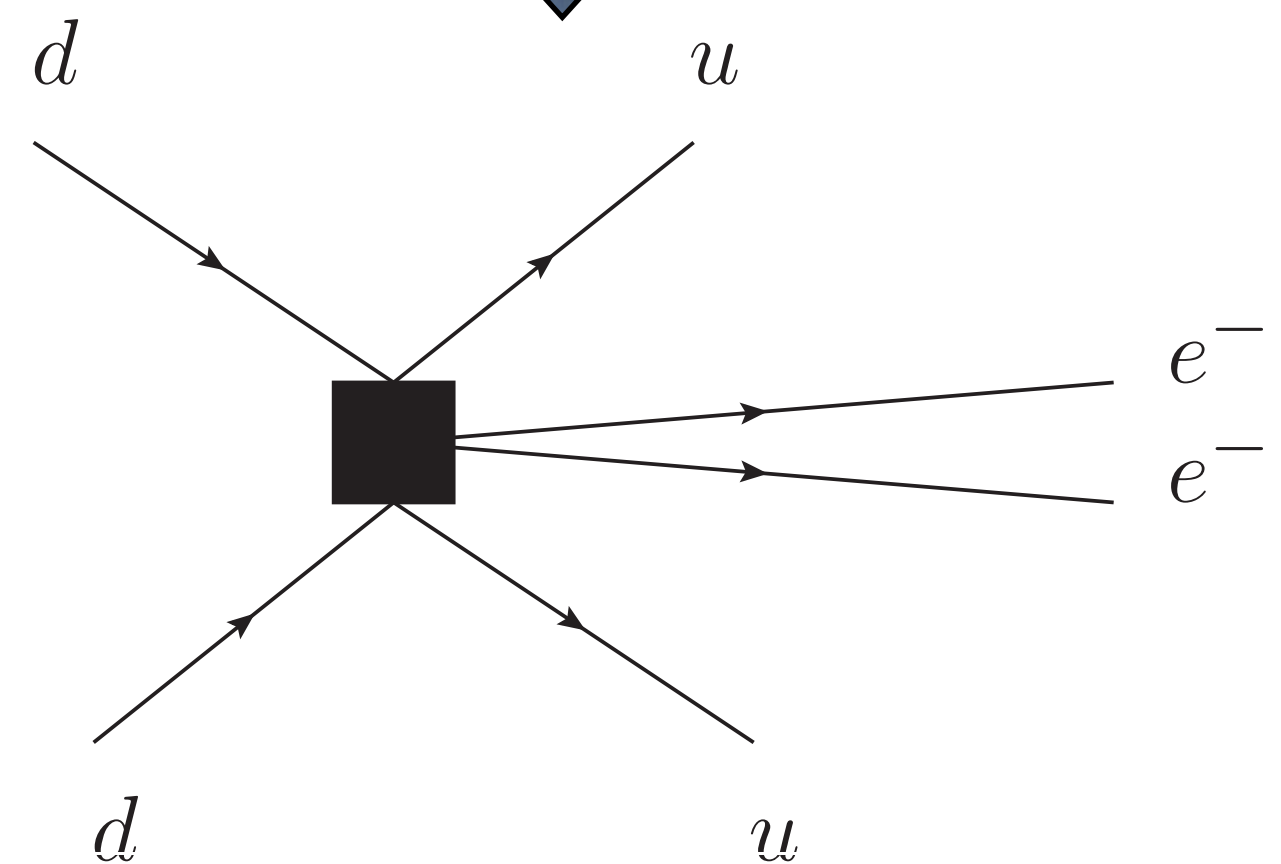


Neutrinoless Double Beta-Decay



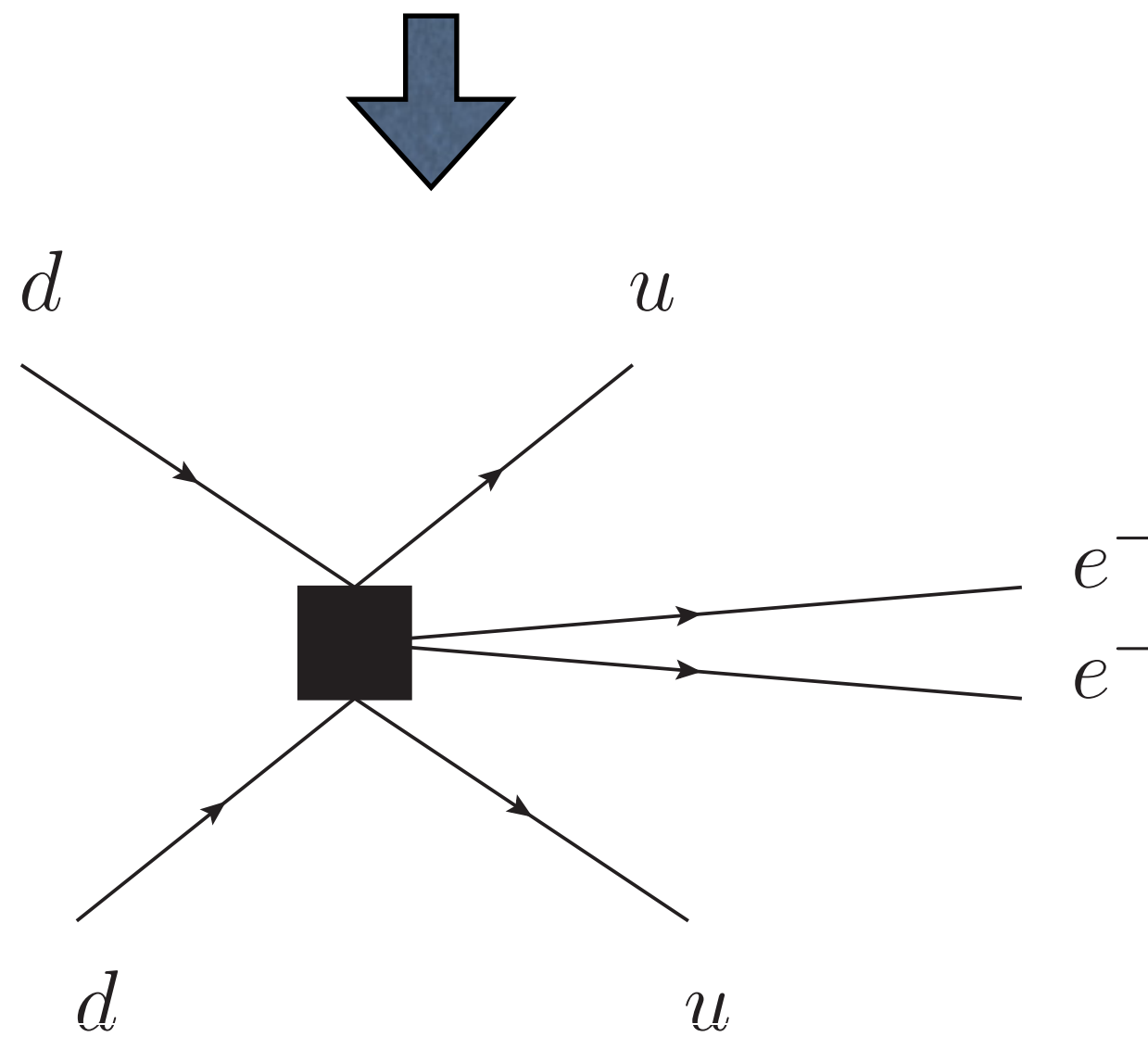
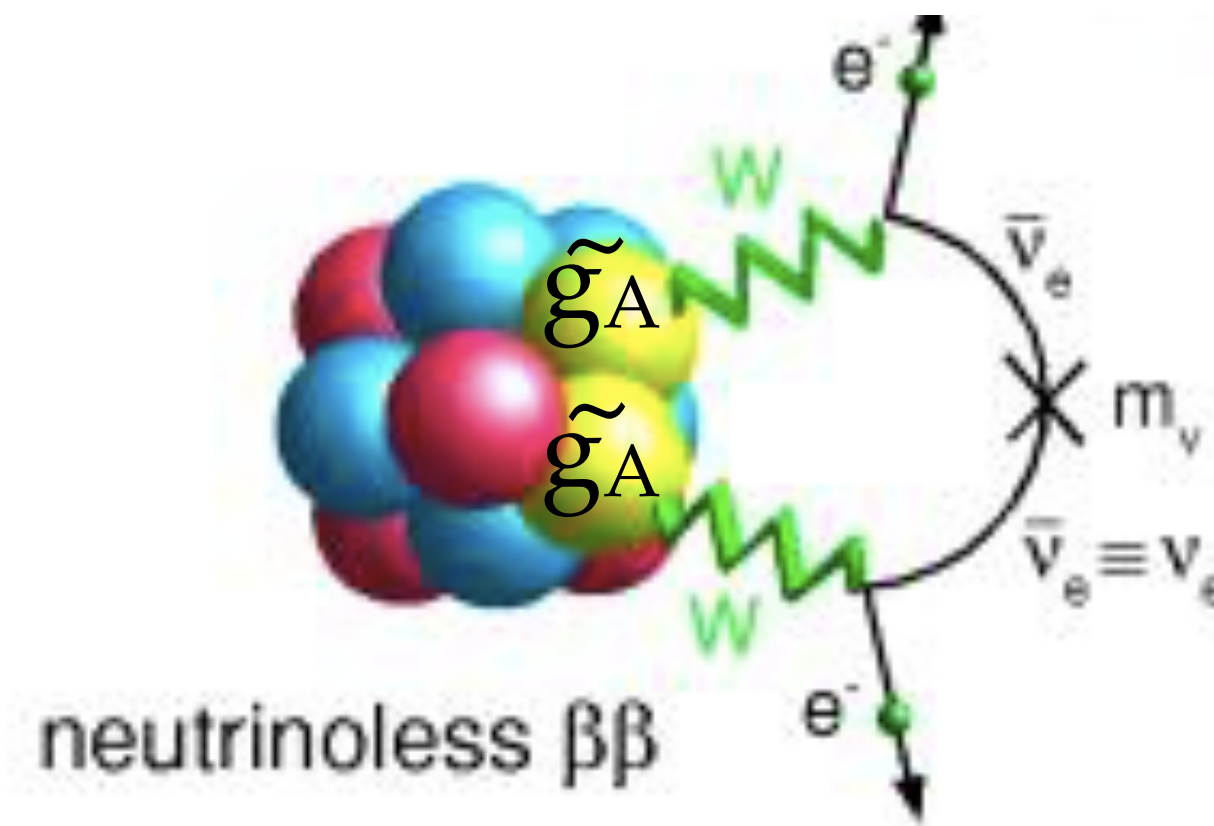
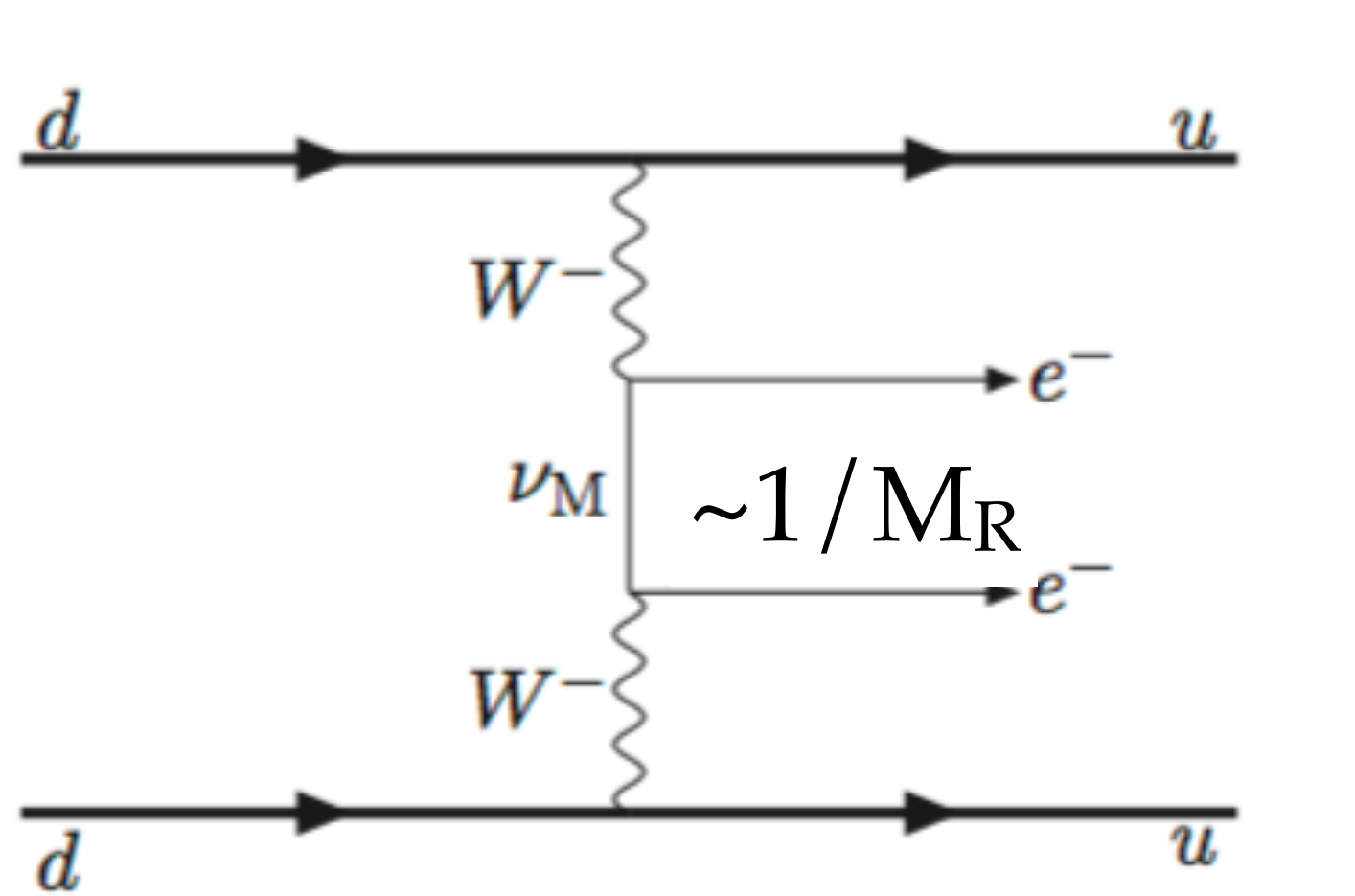
Short Range Contribution

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

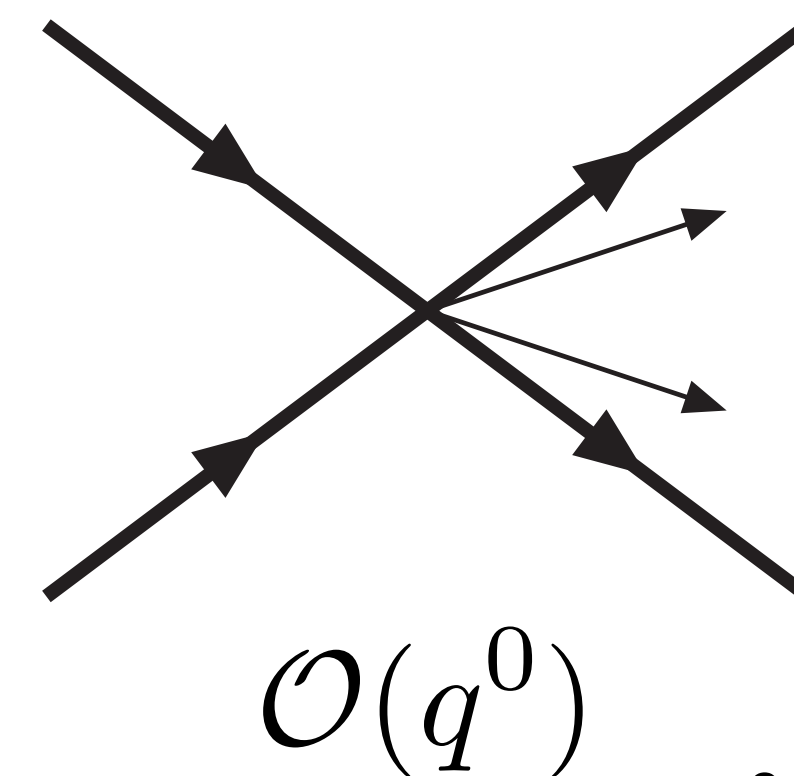
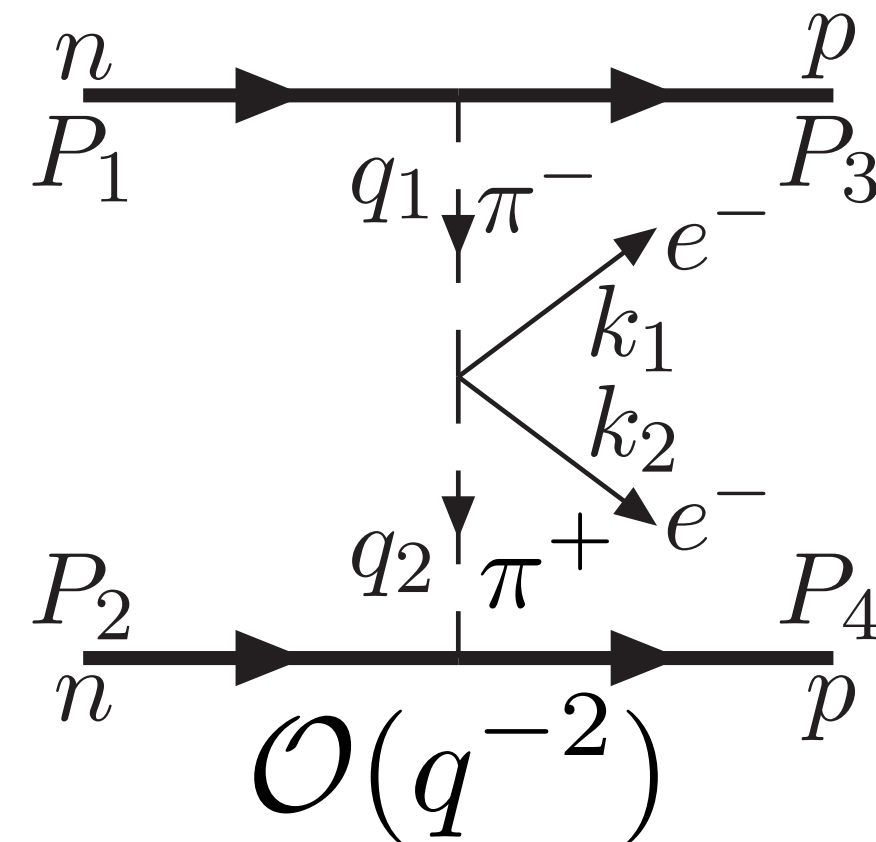


Neutrinoless Double Beta-Decay

Short-range contribution: probe for heavy physics

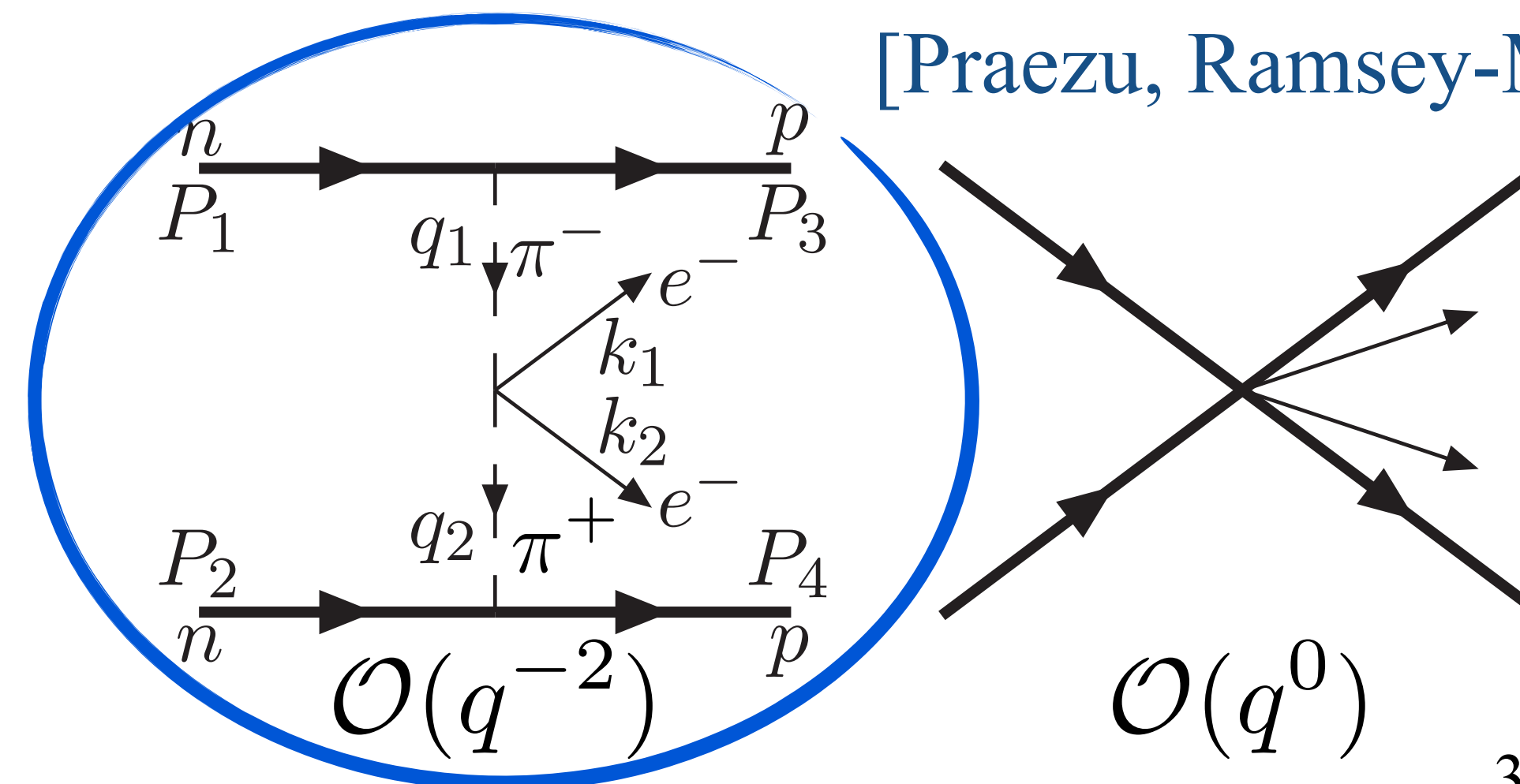
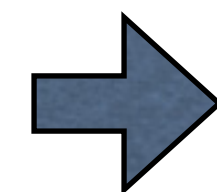
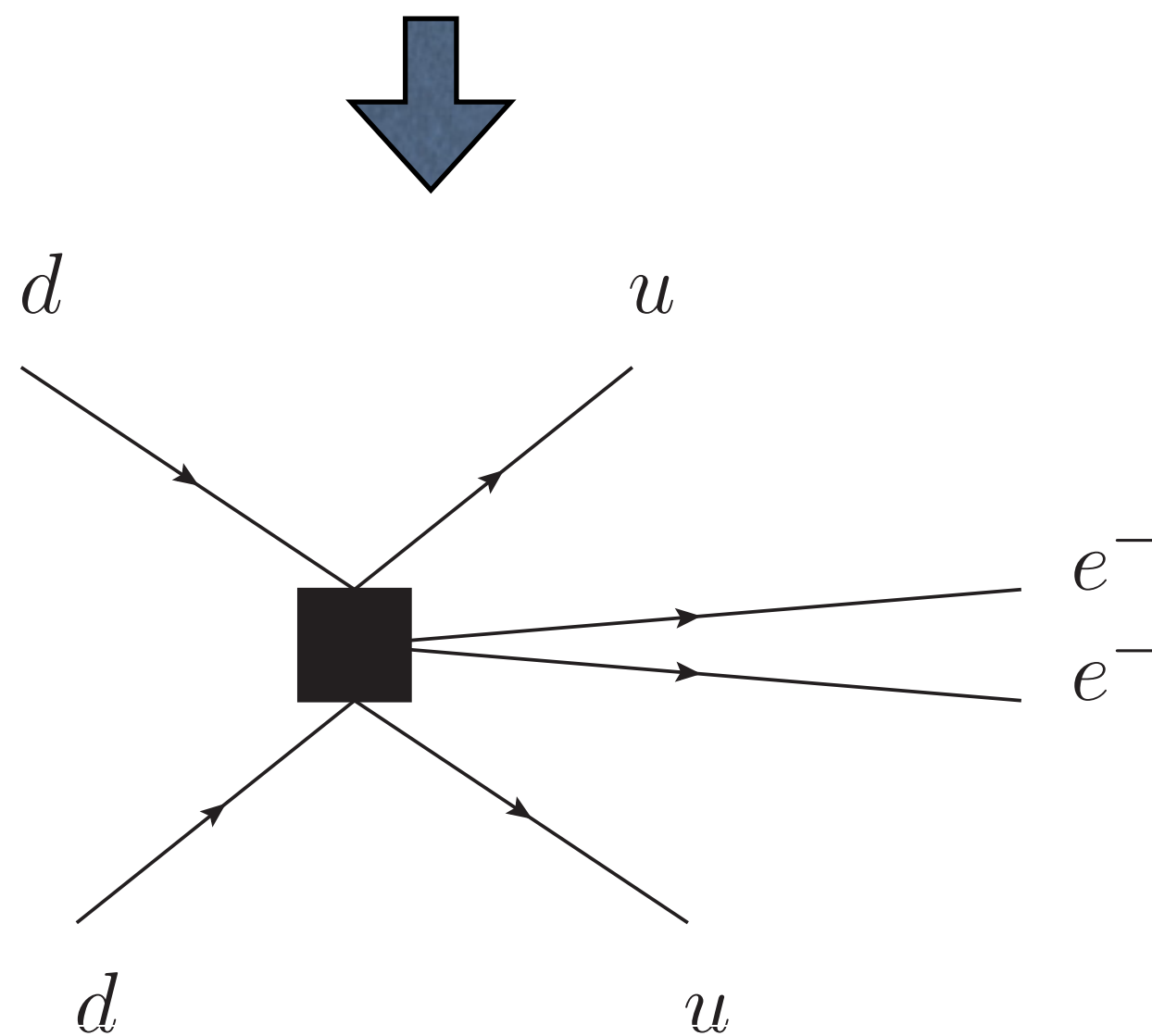
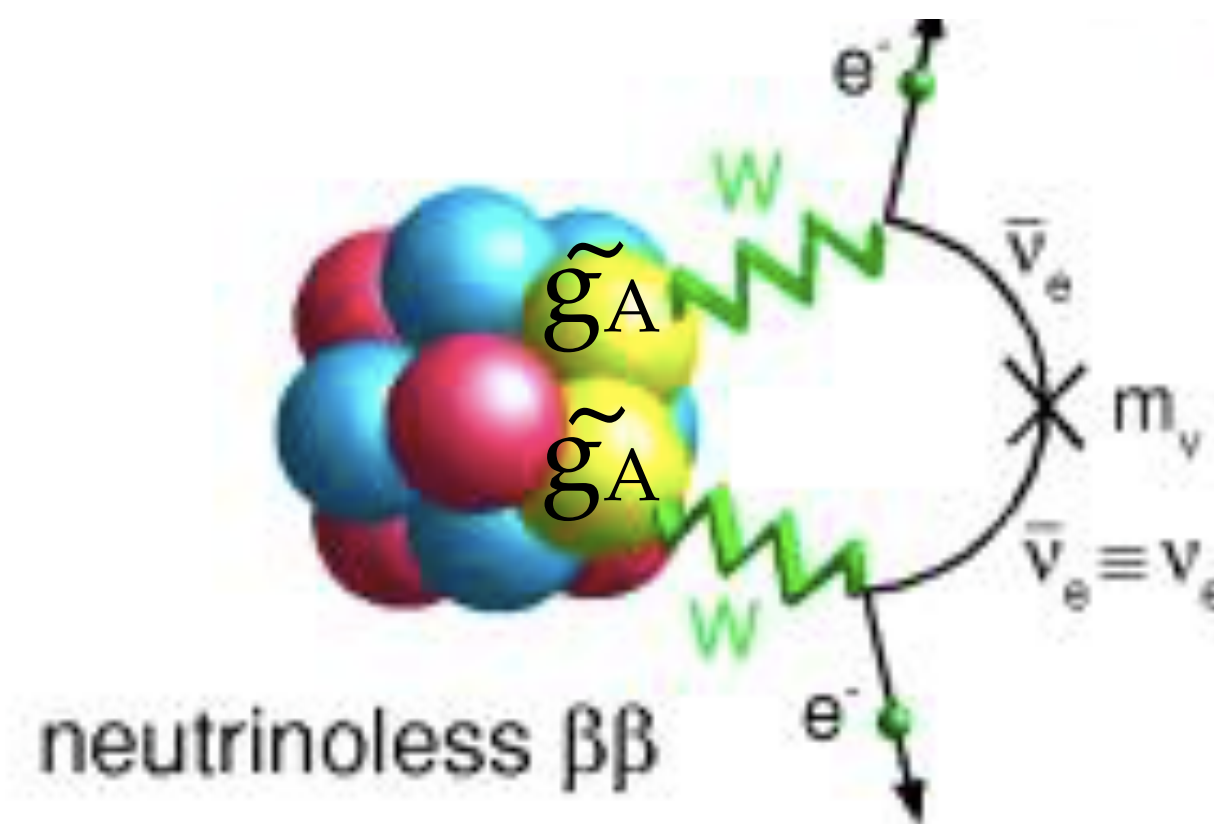
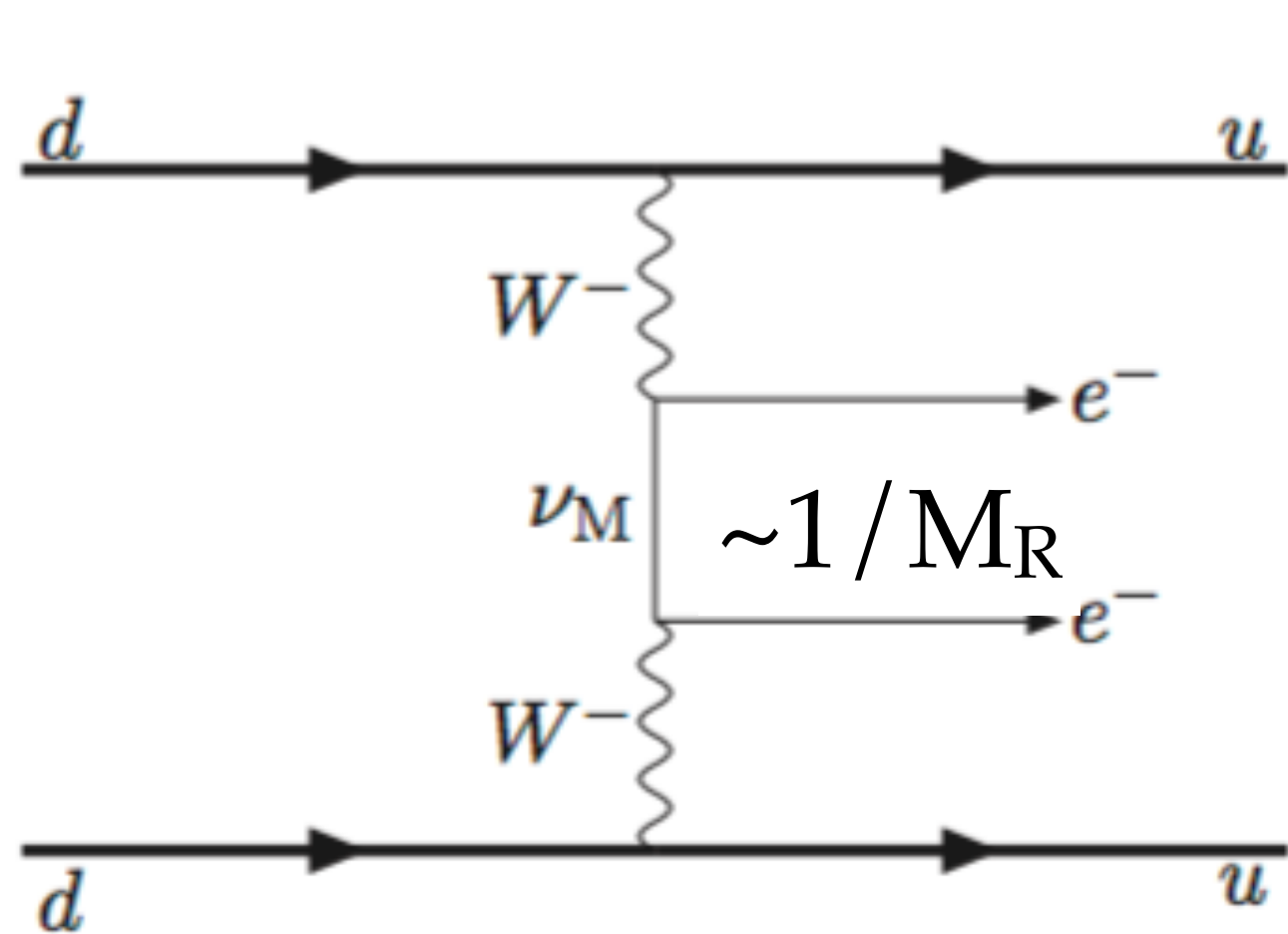


Effective Field Theory (π , N)
[Praezu, Ramsey-Musolf, Vogel]

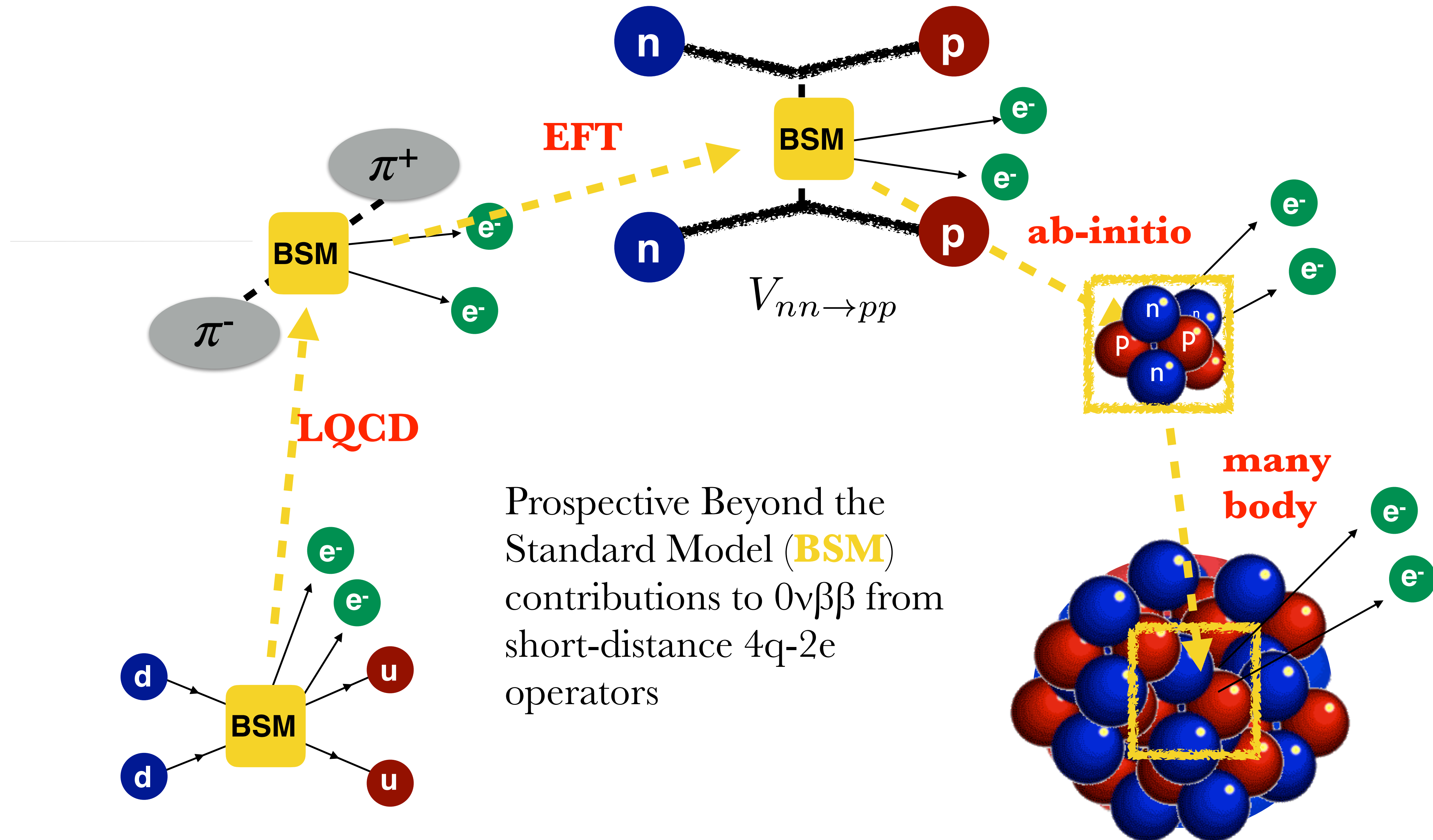


Neutrinoless Double Beta-Decay

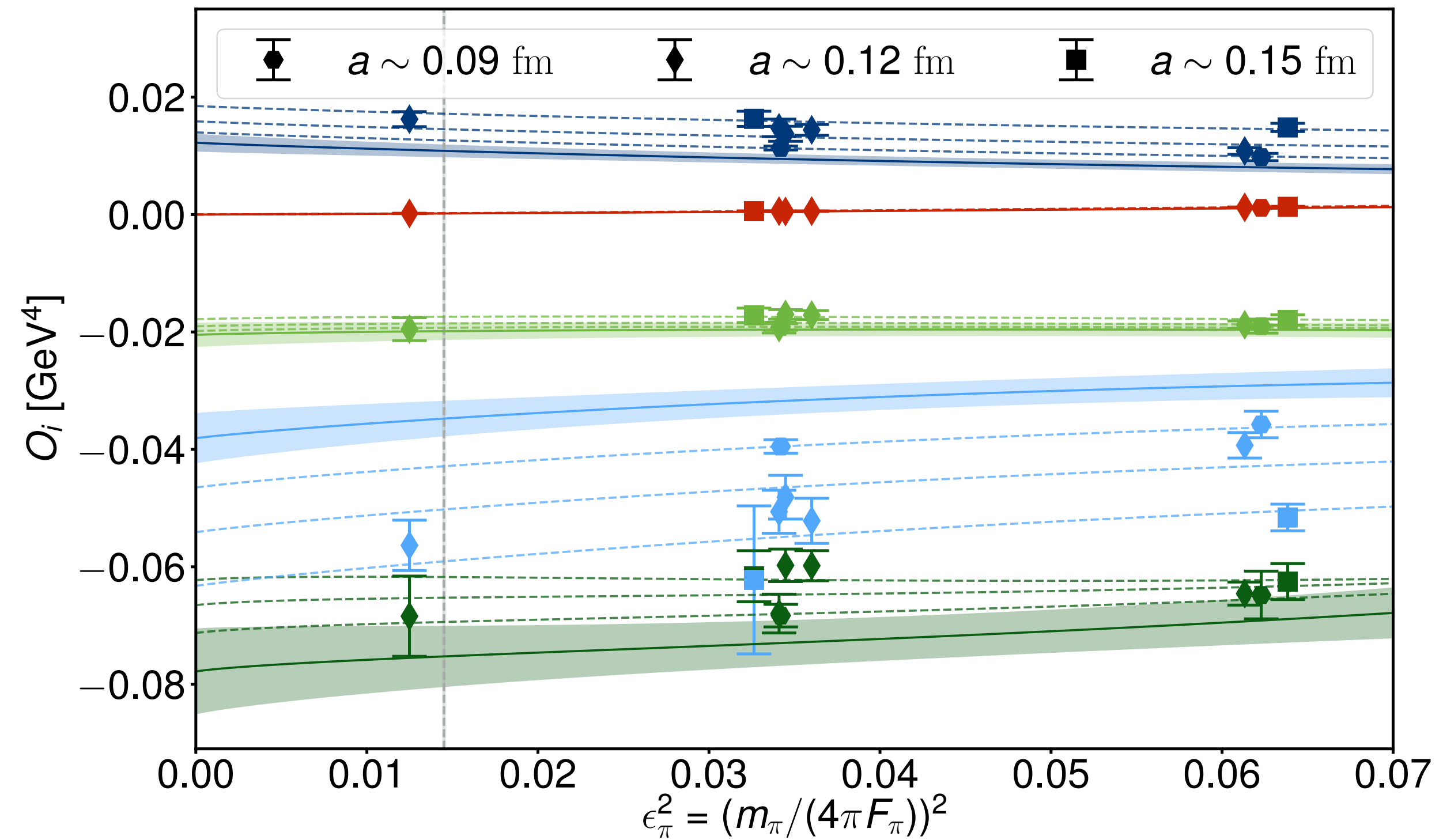
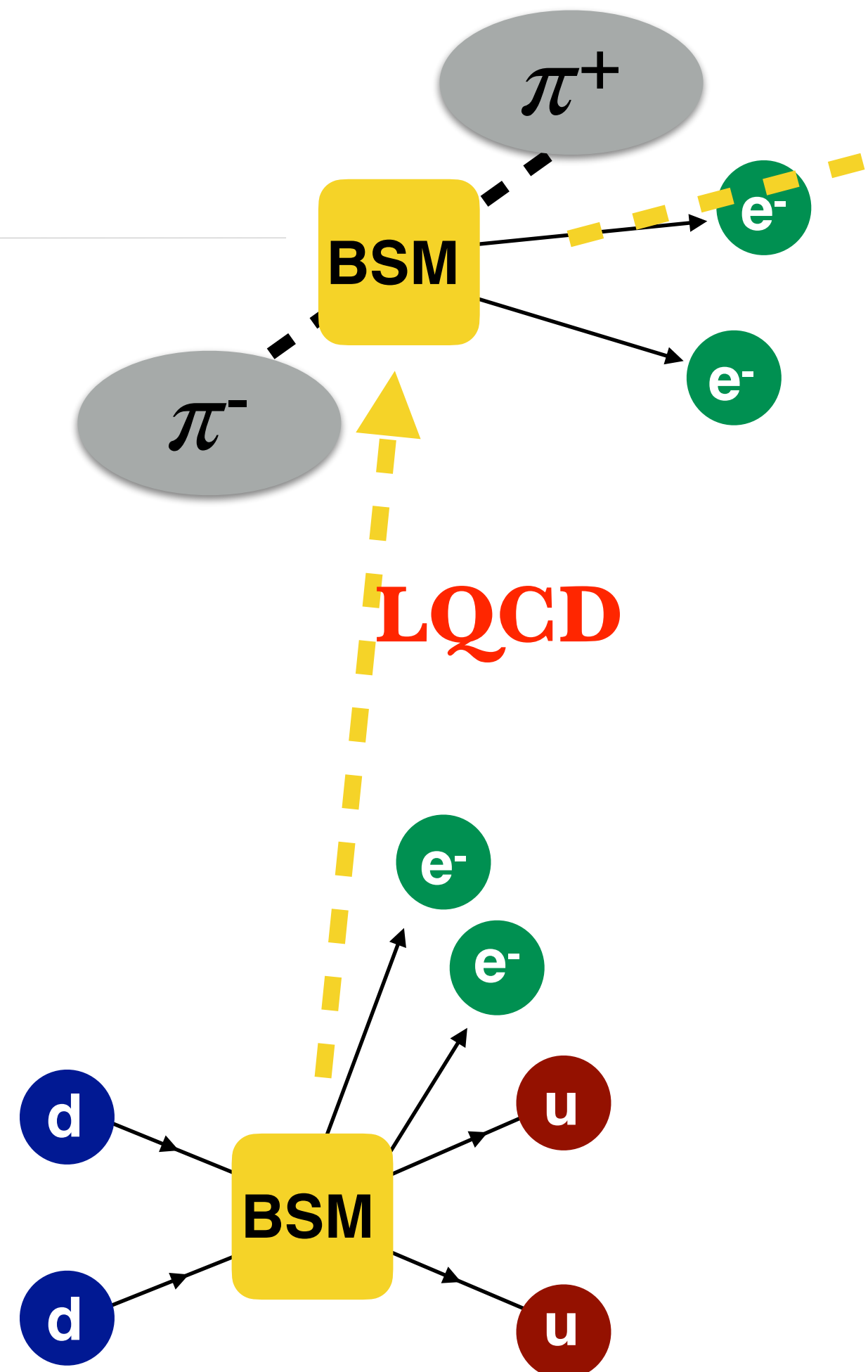
Short-range contribution: probe for heavy physics



Lattice QCD for Neutrinoless Double Beta-Decay



Lattice QCD for Neutrinoless Double Beta-Decay

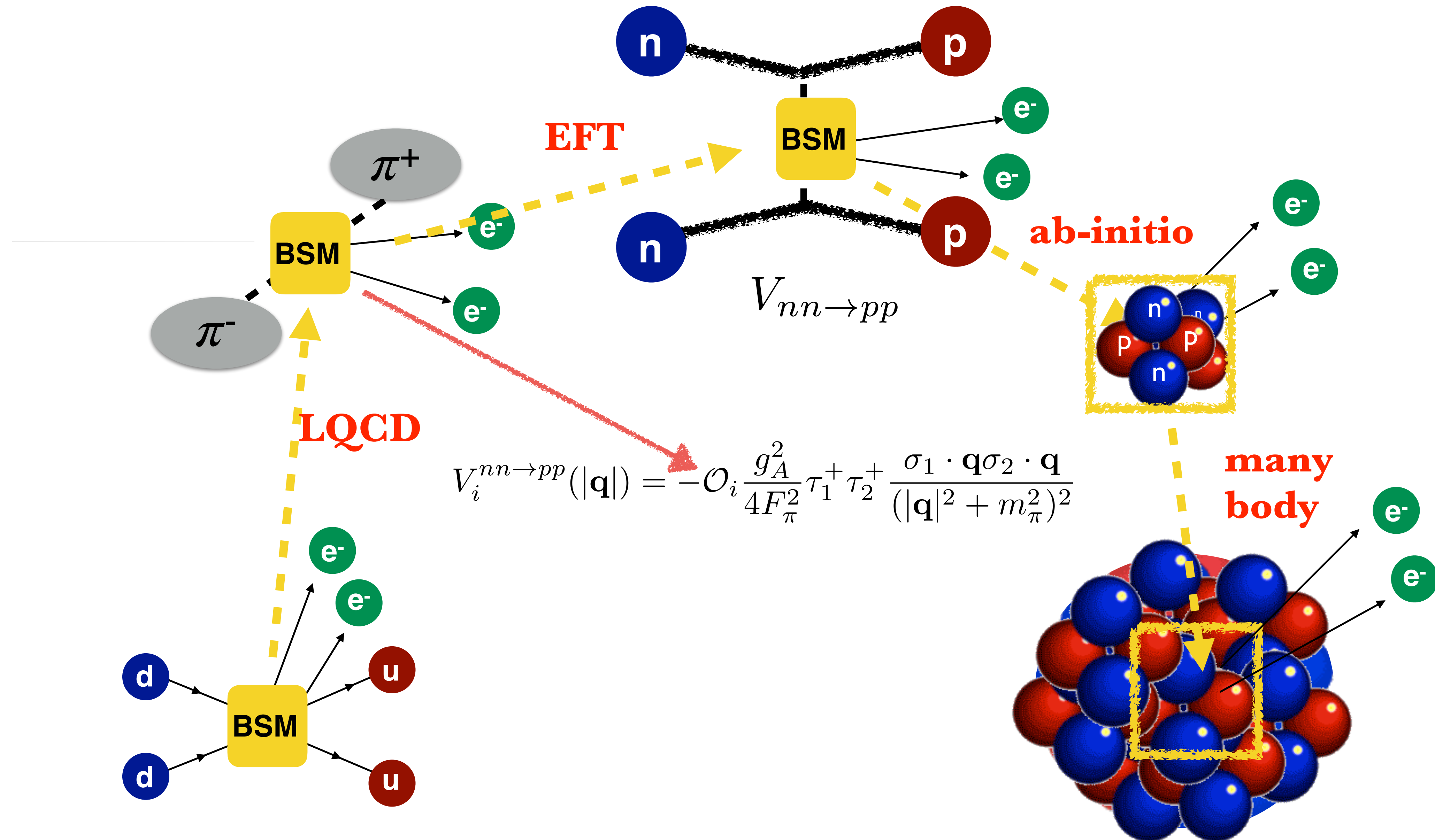


First (and complete) lattice QCD calculation of the $\pi^- \rightarrow \pi^+$ transition amplitude

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



Summary

- ❑ Lattice QCD is a formulation of QCD in Euclidean spacetime that enables the use of numerical methods to compute basic properties of nucleons and other hadrons
- ❑ Lattice QCD is the only non-perturbative regulator of QCD where we understand how to control all systematic uncertainties and provide fully quantified theoretical predictions for basic nuclear quantities
- ❑ Lattice QCD is essential to compute key quantities that are difficult or impossible to measure experimentally
 - ❑ $0\nu\beta\beta$ matrix elements
 - ❑ Hyperon-nucleon forces, three-nucleon forces
 - ❑ ...
- ❑ The calculations are very expensive — requiring significant time on the world's fastest supercomputers
- ❑ This is an exciting time to be involved as the growth of computing power has brought us to an era when LQCD is starting to impact our understanding of low-energy nuclear physics

Thank You