

Assorted topics in Lattice QCD

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Hadrons and Hadron Interactions in QCD 2024 (HHIQCD 2024)

Yukawa Institute of Theoretical Physics, Kyoto University

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Topics of the Talk

- ✦ Dibaryons with heavy quarks
 - ✦ Spin one - deuteron-like dibaryons
 - ✦ Spin zero dibaryons
- ✦ Continuous temperature simulation in Lattice QCD
 - ✦ General method
 - ✦ Simulate high temperature dependence of χ_{top}
- ✦ Precision scale setting at high temperatures
 - ✦ New method of relative scale setting
 - ✦ Subpercent precision

Heavy quark dibaryons

- ✦ Phys. Rev. Lett. 123, 162003 (2019)
- ✦ arXiv:2410.08519

The NN interaction

On the Neutron-Proton Interaction*

WILLIAM RARITA† AND JULIAN SCHWINGER

Department of Physics, University of California, Berkeley, California

(Received January 7, 1941)



$$S = 1, I = 0, \frac{1}{\sqrt{2}}(pn - np)$$

$$S = 0, I = 1, (pp, \sqrt{2}pn, nn)$$

❖ Deuteron

❖ Dineutron

❖ Only bound dibaryon system in Nature

❖ Still debated ...

❖ Wonder about heavy flavor extension ... ?

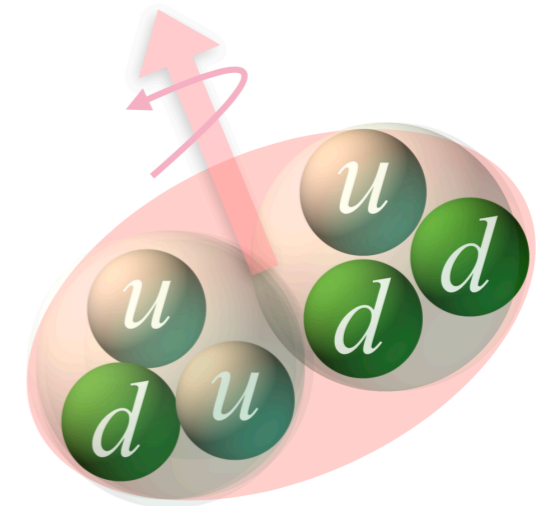
Spin-1 operators

❖ Construct deuteron operator :

$$D_{ud} = \frac{1}{\sqrt{2}} (N (C \gamma^j) P - P (C \gamma^j) N)$$

$$N_\alpha(x) = \epsilon_{abc} d_\alpha^a(x) (u_\mu^b(x) (C \gamma_5)_{\mu\nu} d_\nu^c(x))$$

$$P_\alpha(x) = \epsilon_{abc} u_\alpha^a(x) (u_\mu^b(x) (C \gamma_5)_{\mu\nu} d_\nu^c(x))$$



$$S = 1, \quad I = 0$$

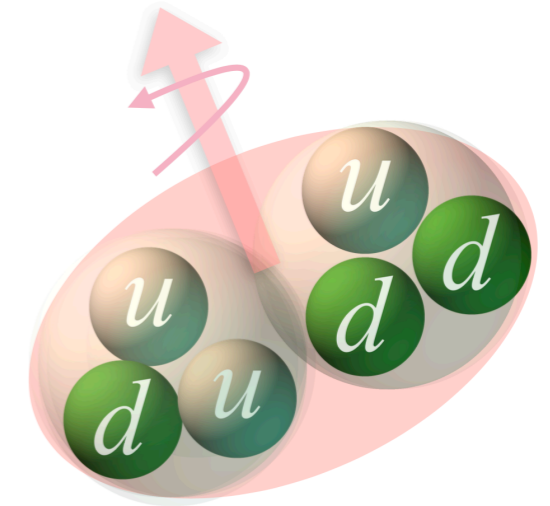
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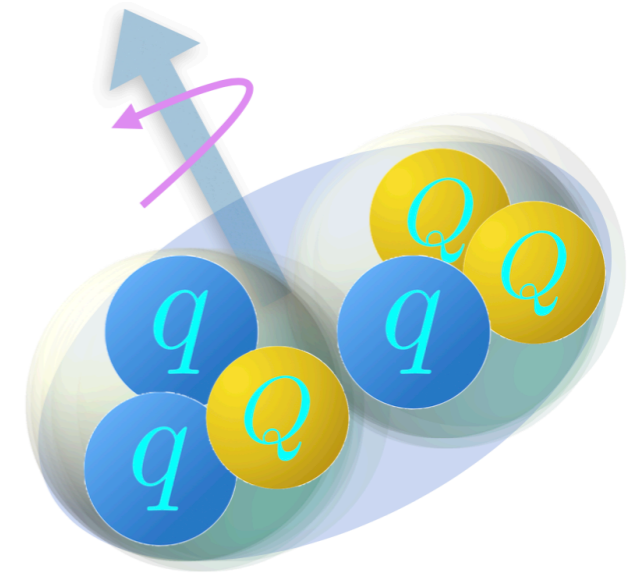
$$S = 1, \quad I = 0$$

❖ Deuteron-like heavy operator :

$$D_{qQ} = \frac{1}{\sqrt{2}} \left(\Omega_{qqQ} (C \gamma^j) \Omega_{QQq} - \Omega_{QQq} (C \gamma^j) \Omega_{qqQ} \right)$$

$$(\Omega_{qqQ})_\alpha = \epsilon^{abc} q_\alpha^a(x) q_\mu^b(x) (C \gamma_5)_{\mu\nu} Q_\nu^c(x)$$

$$(\Omega_{QQq})_\alpha = \epsilon^{abc} Q_\alpha^a(x) q_\mu^b(x) (C \gamma_5)_{\mu\nu} Q_\nu^c(x)$$



$$S = 1, \quad \text{FA}$$

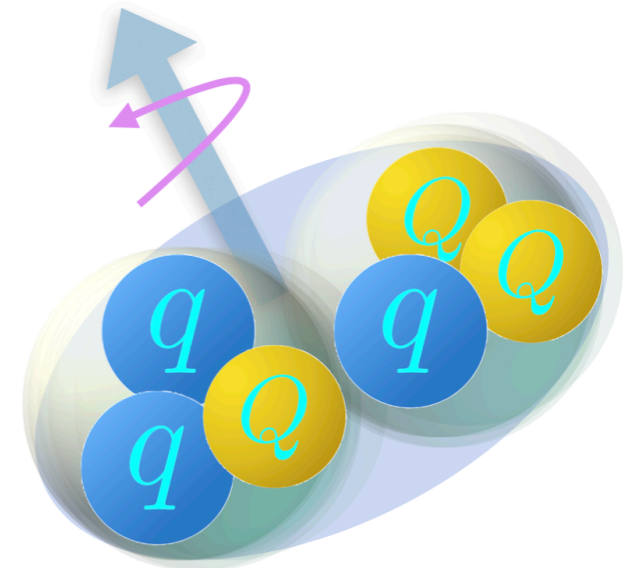
Spin-1 operators

❖ Deuteron-like heavy operator :

$$\mathcal{D}_{qQ} = \frac{1}{\sqrt{2}} \left(\Omega_{qqQ} (C\gamma^j) \Omega_{QQq} - \Omega_{QQq} (C\gamma^j) \Omega_{qqQ} \right)$$

$$(\Omega_{qqQ})_\alpha = \epsilon^{abc} q_\alpha^a(x) q_\mu^b(x) (C\gamma_5)_{\mu\nu} Q_\nu^c(x)$$

$$(\Omega_{QQq})_\alpha = \epsilon^{abc} Q_\alpha^a(x) q_\mu^b(x) (C\gamma_5)_{\mu\nu} Q_\nu^c(x)$$



$S = 1, \text{ FA}$

❖ Explore different flavor combinations

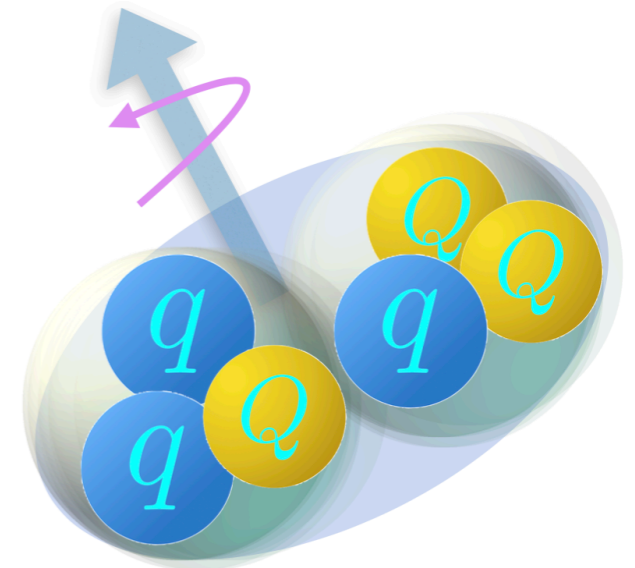
❖ Compute ground state and compare with non-interacting levels

\mathcal{D}_{Qq}	Interpolating fields
\mathcal{D}_{bc}	$\frac{1}{\sqrt{2}} (\Omega_{ccb} \Omega_{bbc} - \Omega_{bbc} \Omega_{ccb})$
\mathcal{D}_{bs}	$\frac{1}{\sqrt{2}} (\Omega_b \Omega_{bb} - \Omega_{bb} \Omega_b)$
\mathcal{D}_{cs}	$\frac{1}{\sqrt{2}} (\Omega_c \Omega_{cc} - \Omega_{cc} \Omega_c)$
\mathcal{D}_{bu}	$\frac{1}{\sqrt{2}} (\Sigma_b \Xi_{bb} - \Xi_{bb} \Sigma_b)$
\mathcal{D}_{cu}	$\frac{1}{\sqrt{2}} (\Sigma_c \Xi_{cc} - \Xi_{cc} \Sigma_c)$

Spin-0 operators

❖ Operators

$$(FS, S = 0) = \begin{cases} \Omega(l\bar{l}Q)_\alpha (C\gamma_5)_{\alpha\beta} \Omega(l\bar{l}Q)_\beta, \\ \sqrt{2} \Omega(l\bar{l}Q)_\alpha (C\gamma_5)_{\alpha\beta} \Omega(Q\bar{l}Q)_\beta, \\ \Omega(Q\bar{l}Q)_\alpha (C\gamma_5)_{\alpha\beta} \Omega(Q\bar{l}Q)_\beta. \end{cases}$$



$$S = 0, FS$$

❖ Explore different flavor combinations

❖ Compute ground state and compare with non-interacting levels

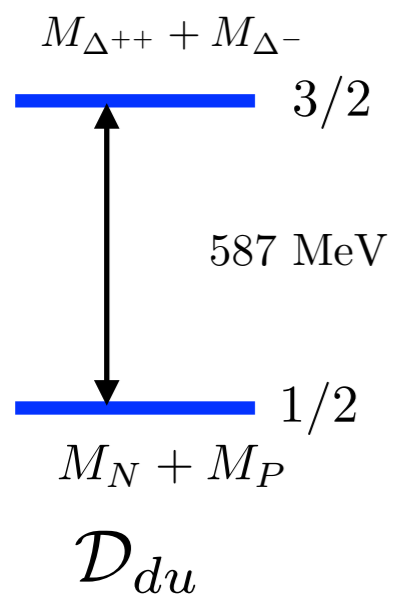
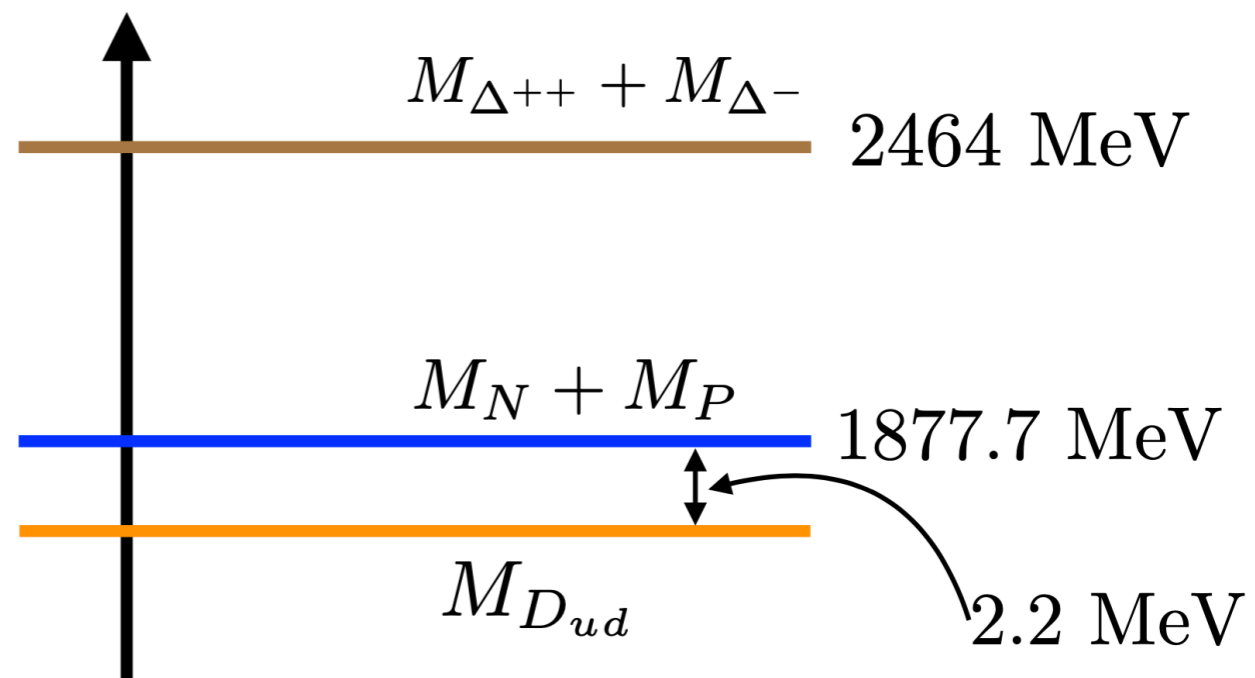
Dibaryon	Lowest NI state
$\Omega_{bcb}\Omega_{bcb}$	$\Omega_{ccb}^{\frac{3}{2}}, \Omega_{bbb}^{\frac{3}{2}}$
$\Omega_{ccb}\Omega_{bcb}$	$\Omega_{ccc}^{\frac{3}{2}}, \Omega_{bbb}^{\frac{3}{2}}$
$\Omega_{ccb}\Omega_{ccb}$	$\Omega_{ccc}^{\frac{3}{2}}, \Omega_{cbb}^{\frac{3}{2}}$
$\Omega_{bb}\Omega_{bb}$	$\Omega_b^{\frac{3}{2}}, \Omega_{bbb}^{\frac{3}{2}}$
$\Omega_b\Omega_{bb}$	$\Omega_{sss}^{\frac{3}{2}}, \Omega_{bbb}^{\frac{3}{2}}$
$\Omega_{cc}\Omega_{cc}$	$\Omega_{cc}^{\frac{1}{2}}, \Omega_{cc}^{\frac{1}{2}}$
$\Omega_c\Omega_{cc}$	$\Omega_c^{\frac{1}{2}}, \Omega_{cc}^{\frac{1}{2}}$

Non-interacting levels

❖ Consider deuteron energy spectrum

❖ Two levels spin 1/2 and 3/2

❖ Quark mass dependence of levels ?

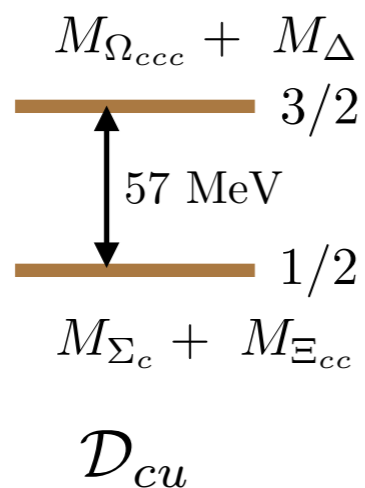
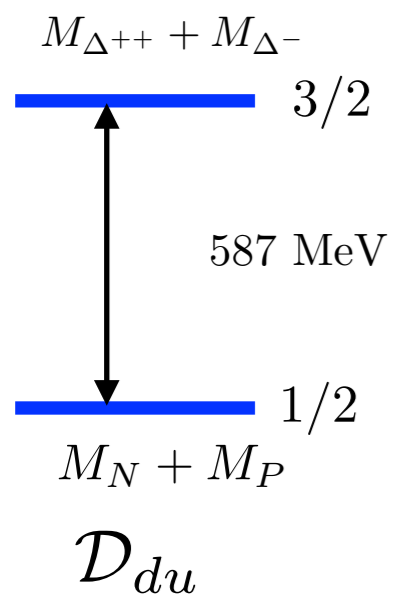
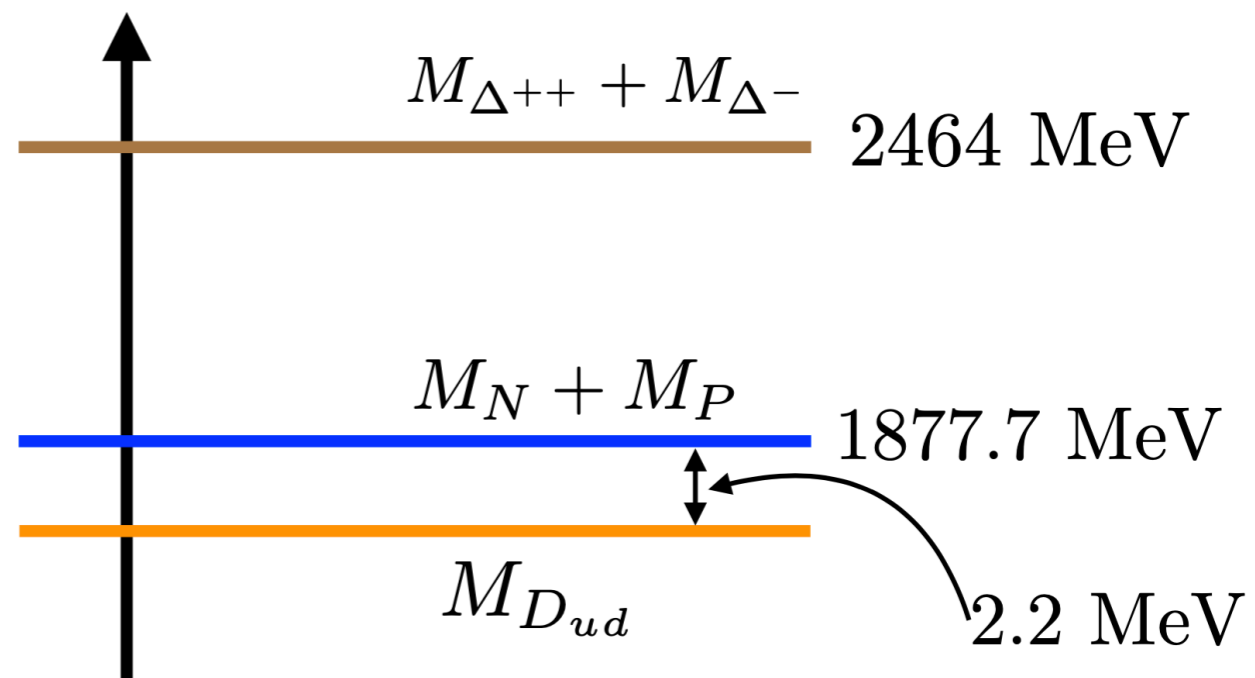


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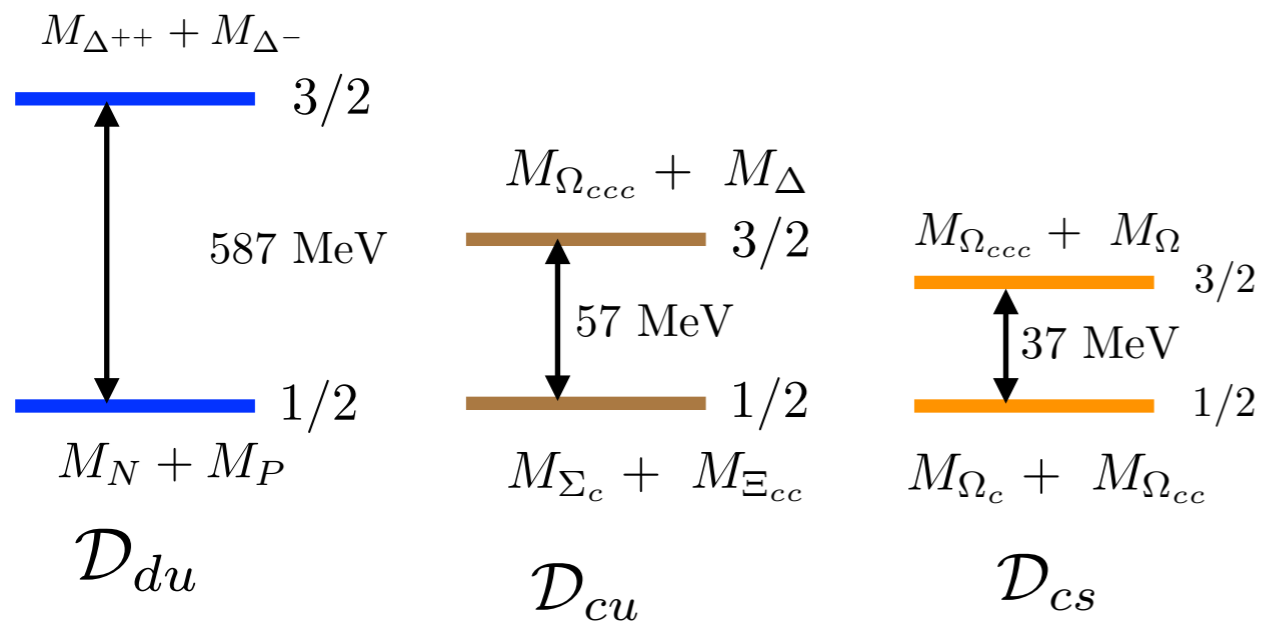
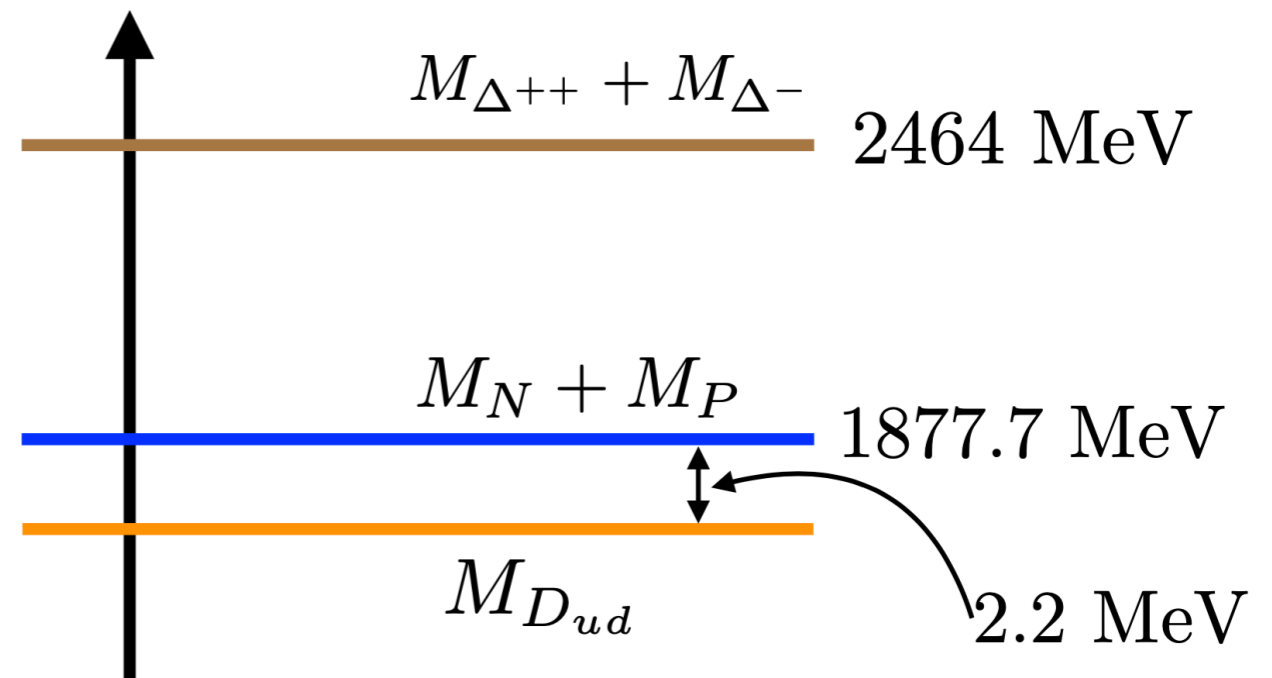


Non-interacting levels

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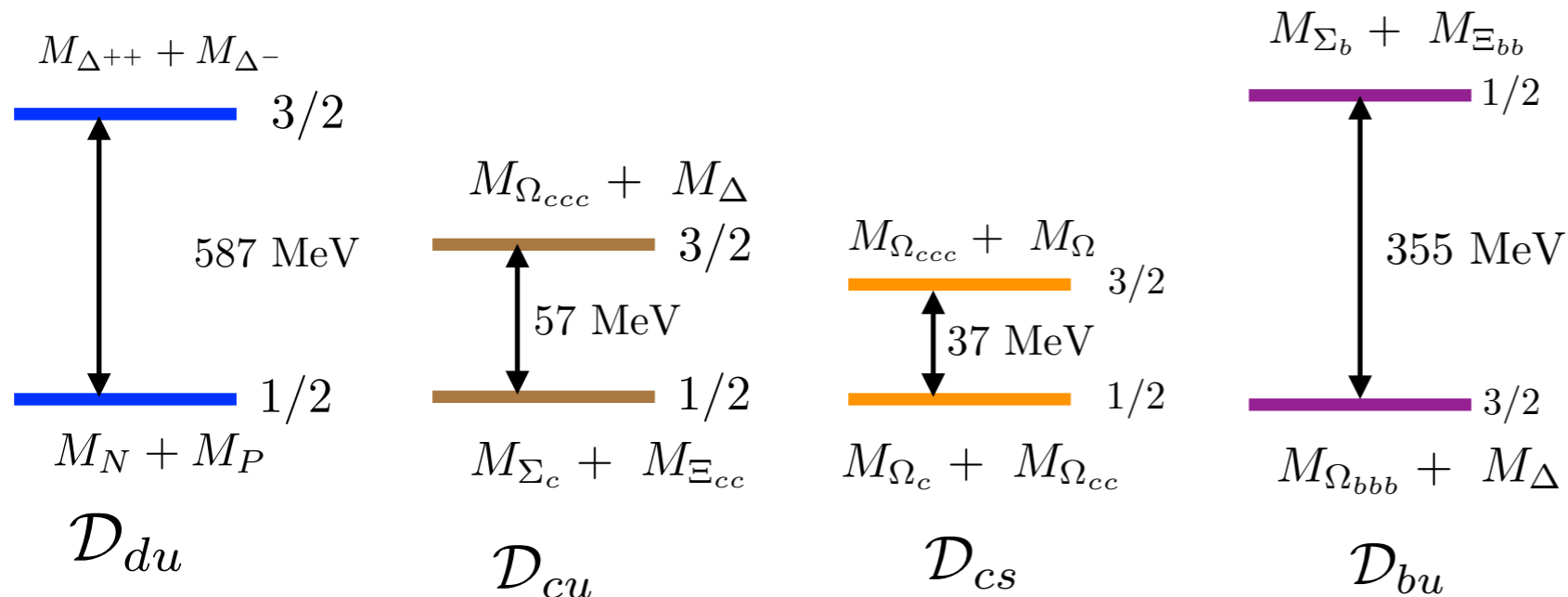
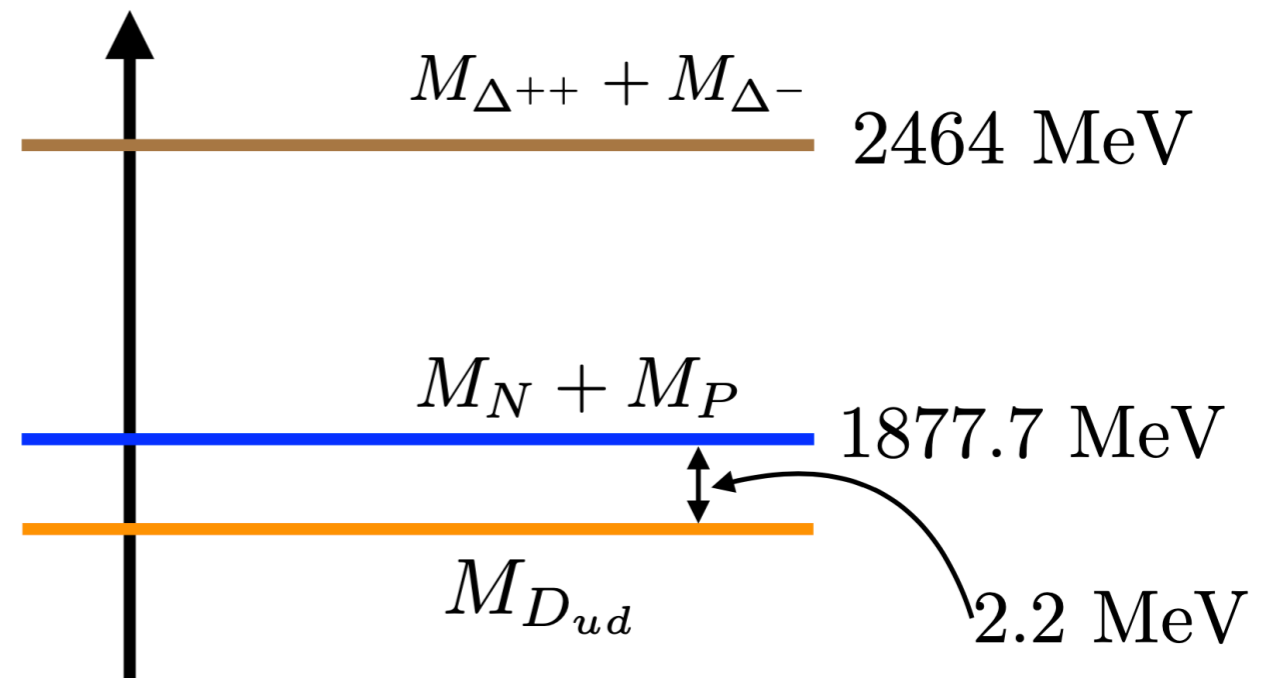
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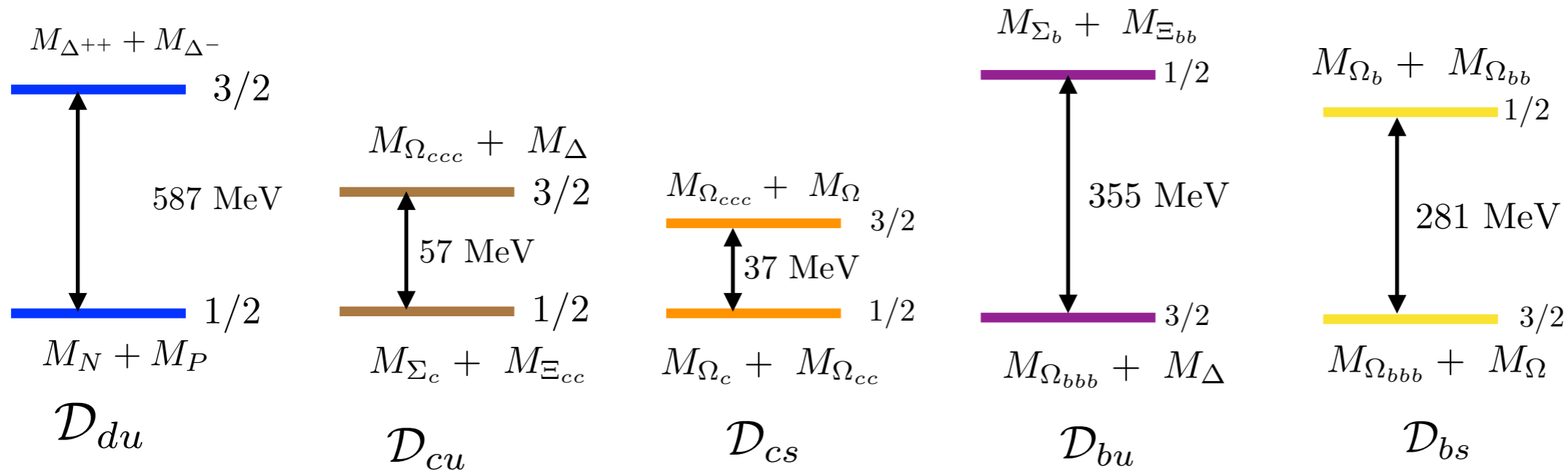
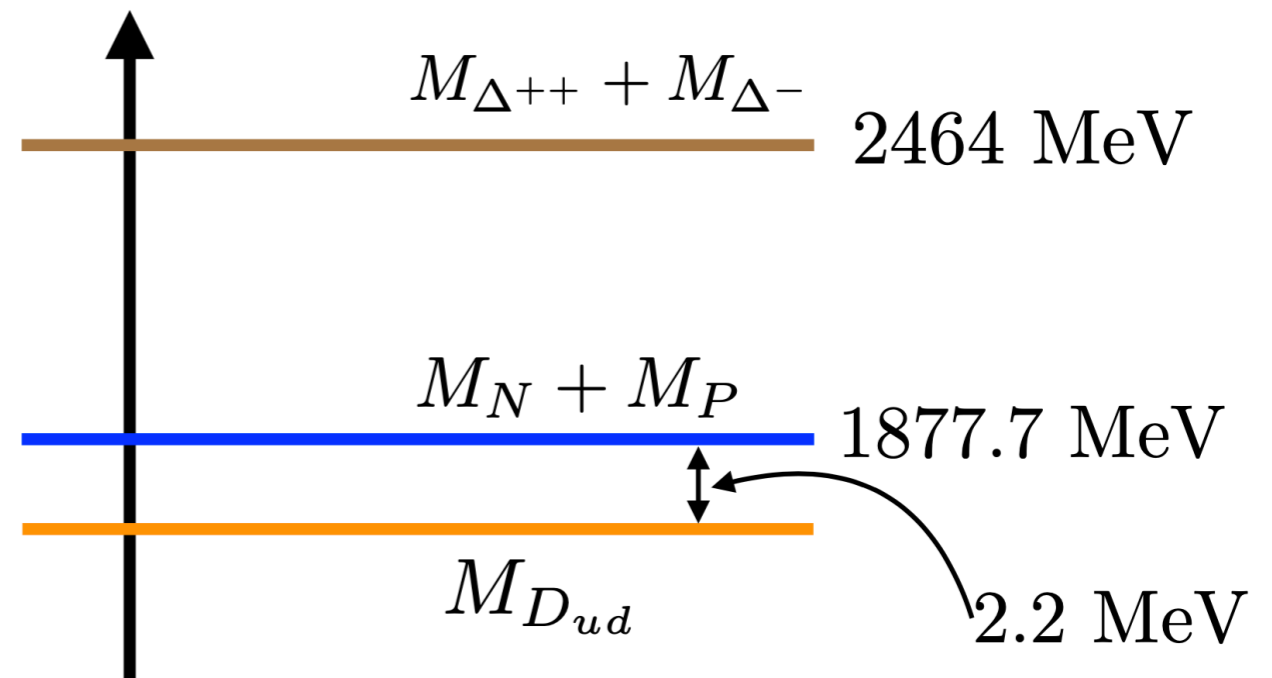
Non-interacting levels

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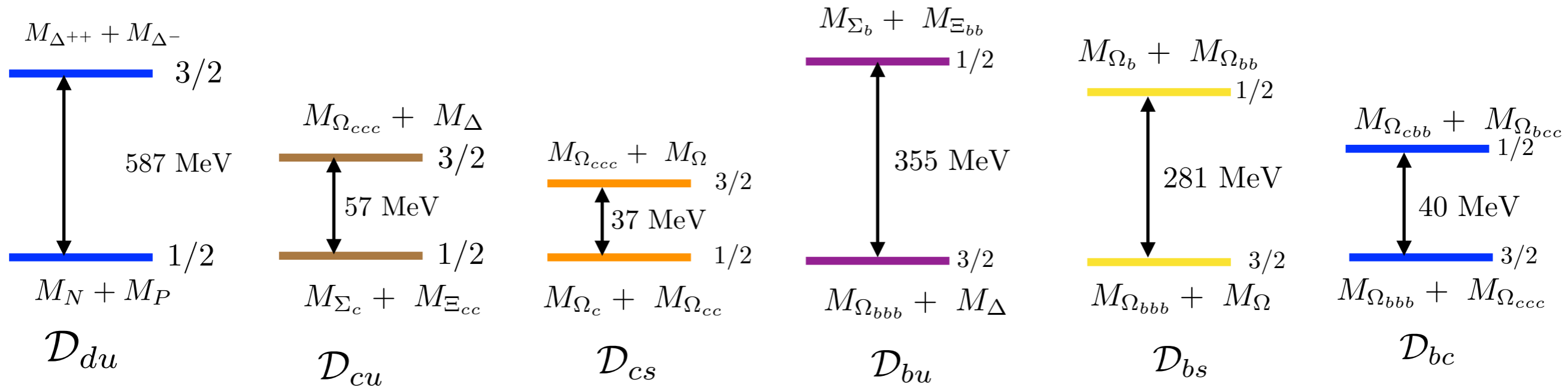
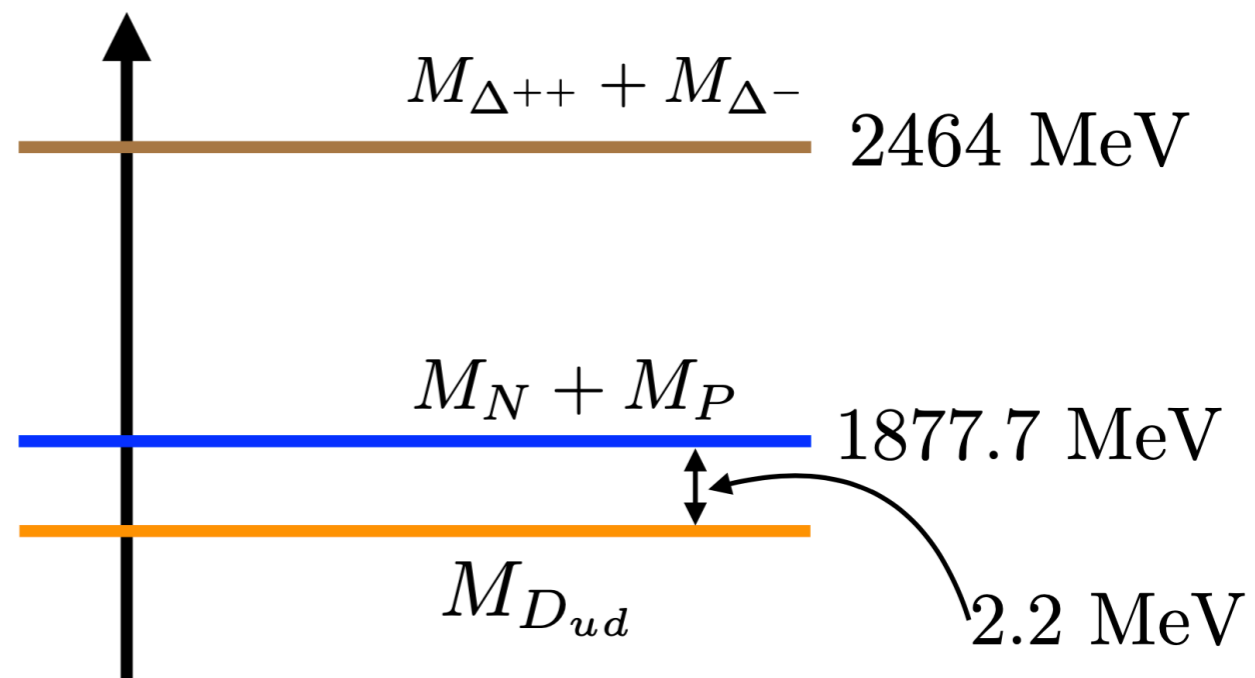
Non-interacting levels

- ❖ Consider deuteron energy spectrum
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Non-interacting levels

- ❖ Consider deuteron energy spectrum
- ❖ Two levels spin 1/2 and 3/2
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Lattice calculation

- ❖ We perform calculations at 3 lattice spacings

$L^3 \times T$	m_π^{sea} (MeV)	$m_\pi L$	a (fm)
$24^3 \times 64$	305.3	4.54	0.1207(11)
$32^3 \times 96$	312.7	4.50	0.0888(8)
$48^3 \times 144$	319.3	4.51	0.0582(5)

- ❖ Valence action DWF on MILC ensembles, NRQCD action for bottom
- ❖ Finest lattice spacing pion masses range from 0.3 - 1 GeV
- ❖ Compute dibaryon energy levels and compare them with NI levels

Results in spin-1 sector

✦ Fitted effective masses subtracted from N1 level

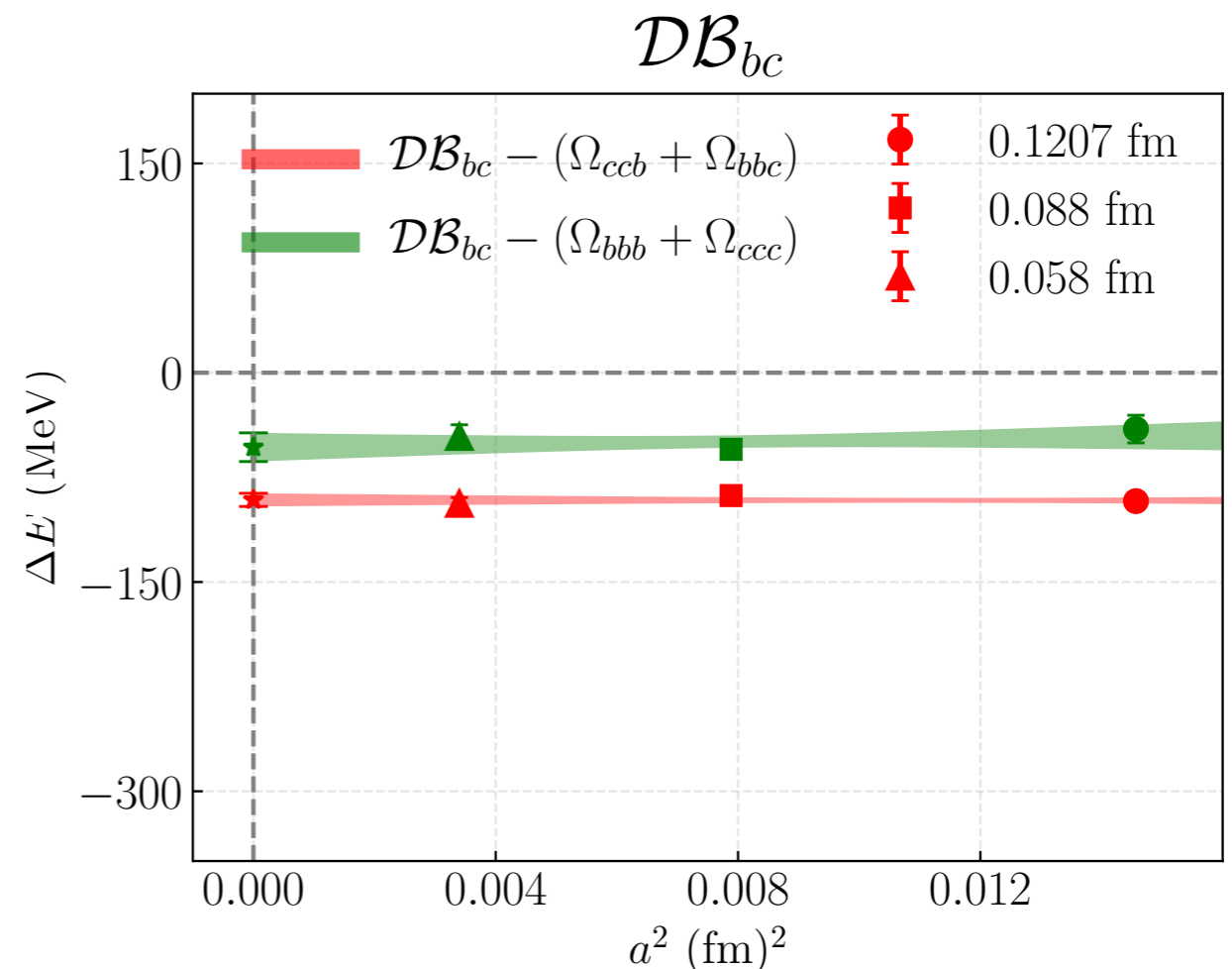
✦ Two relevant N1 levels

Spin - 1/2 - red

Spin - 3/2 - green

✦ Clear Indication of level below N1- Level

✦ No discretization effects



Phys. Rev. Lett. 123, 162003 (2019)

Results in spin-1 sector

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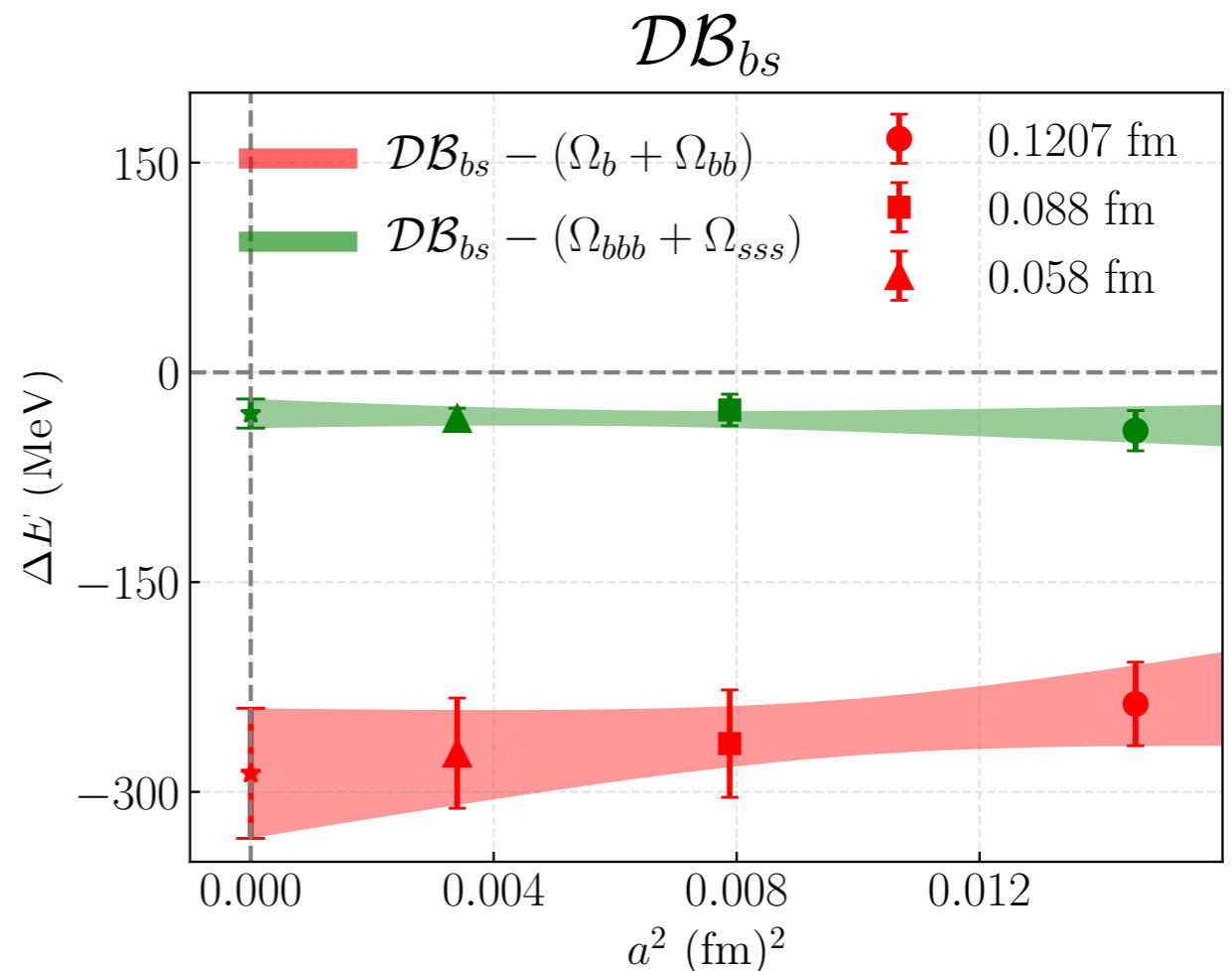
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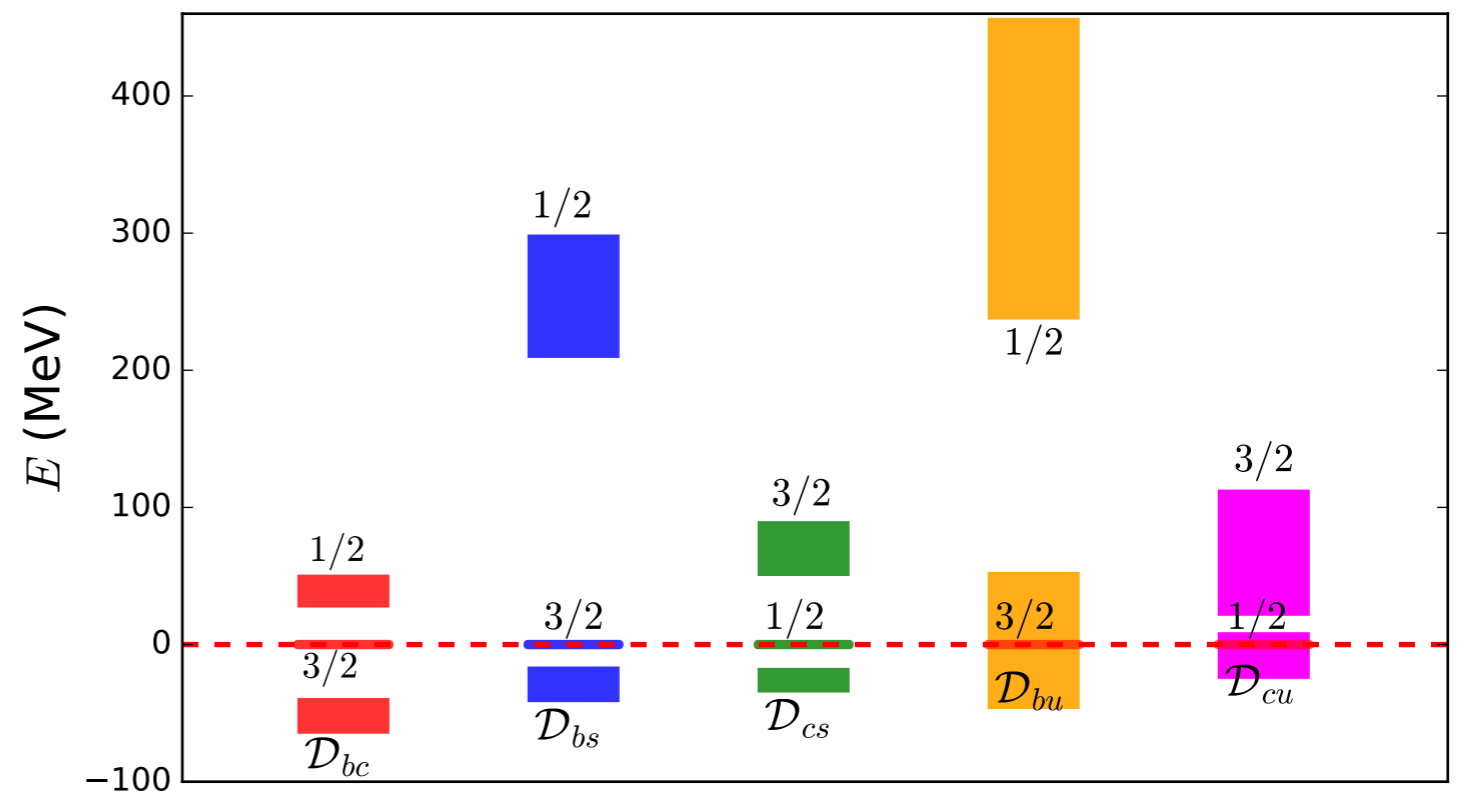
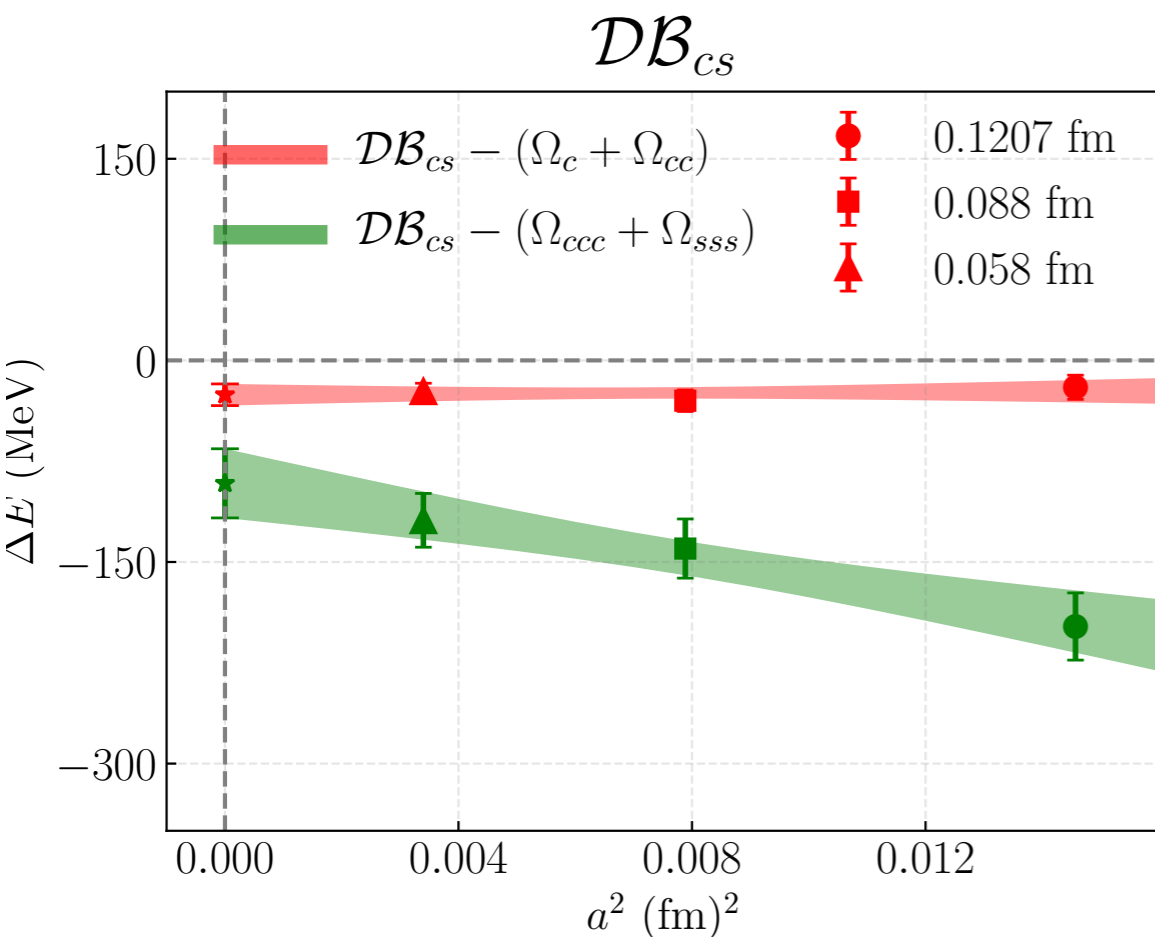
✦ No discretization effects



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Results in spin-1 sector

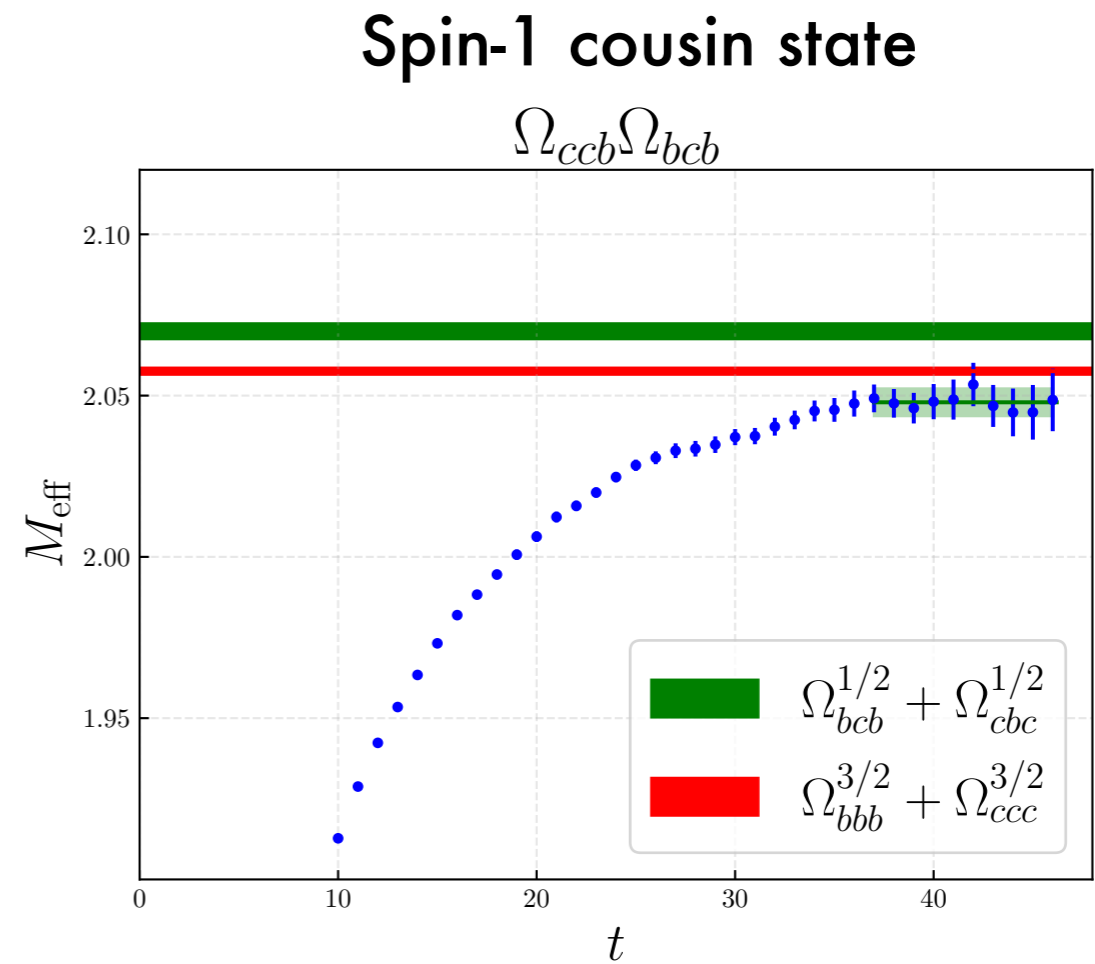
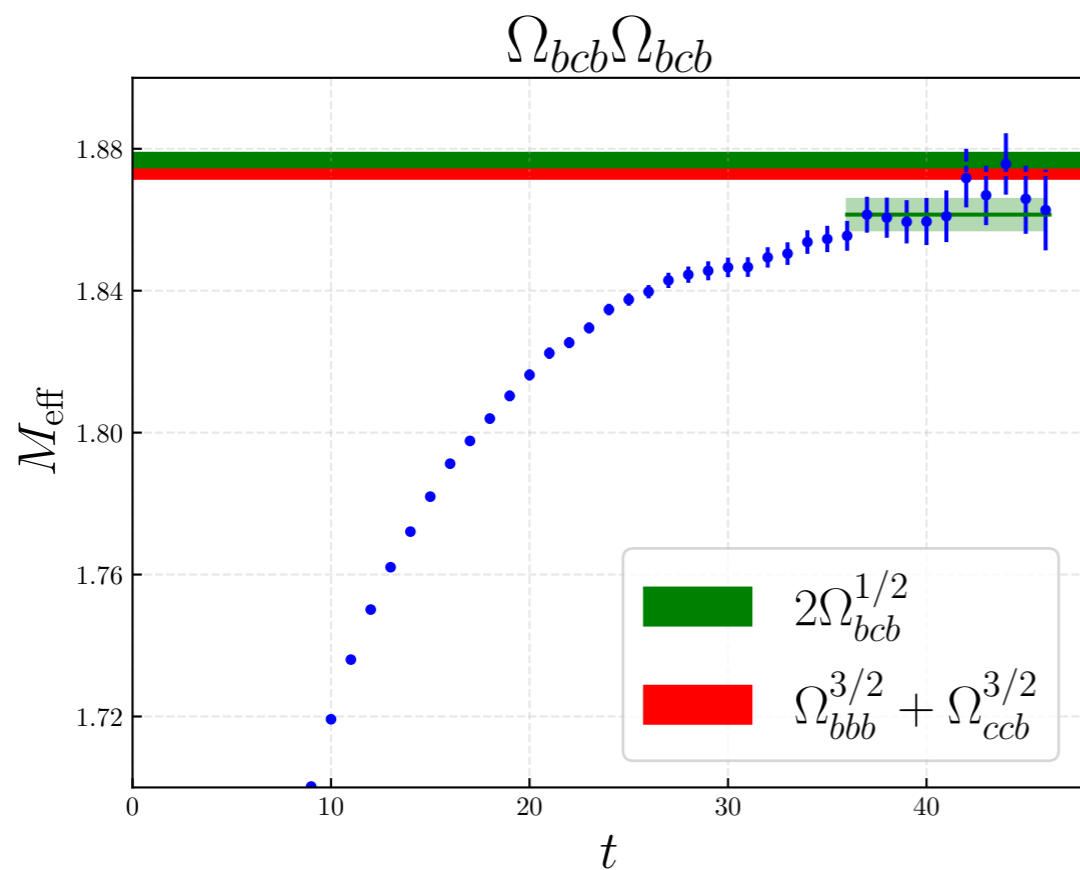
✿ Mild discretization for spin - 1/2 charm



✿ No conclusive results for \mathcal{D}_{bu} , \mathcal{D}_{cu}

Results in Singlet sector

✿ Flavor symmetric states in bottom-charm sector

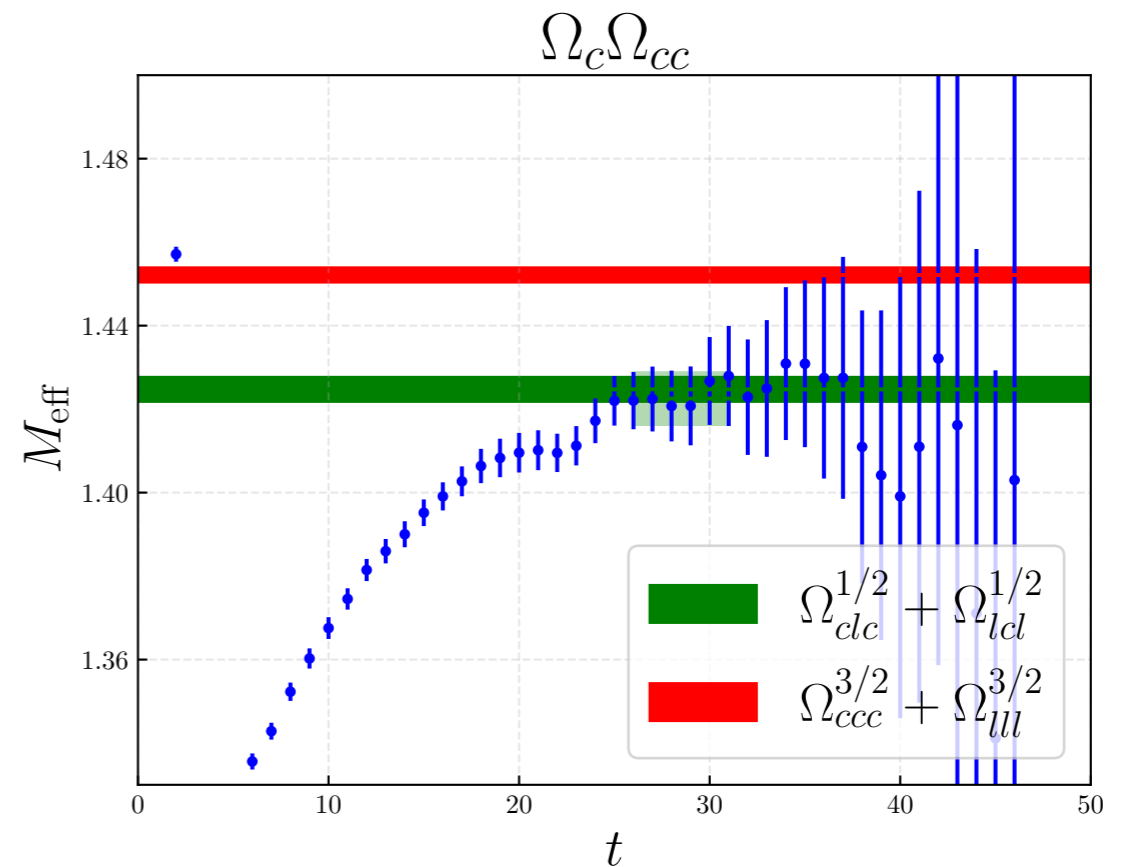
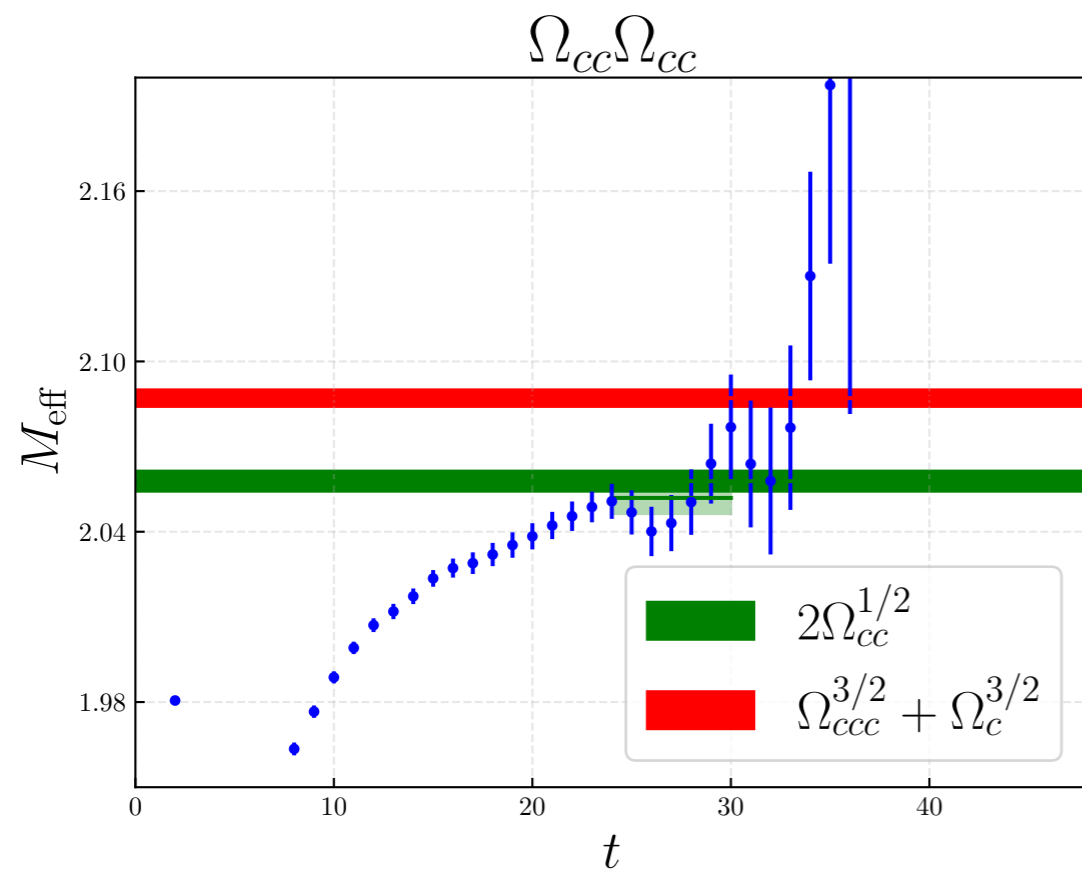


✿ Clear indication of level below N1-level

arXiv:2410.08519

Results in Singlet sector

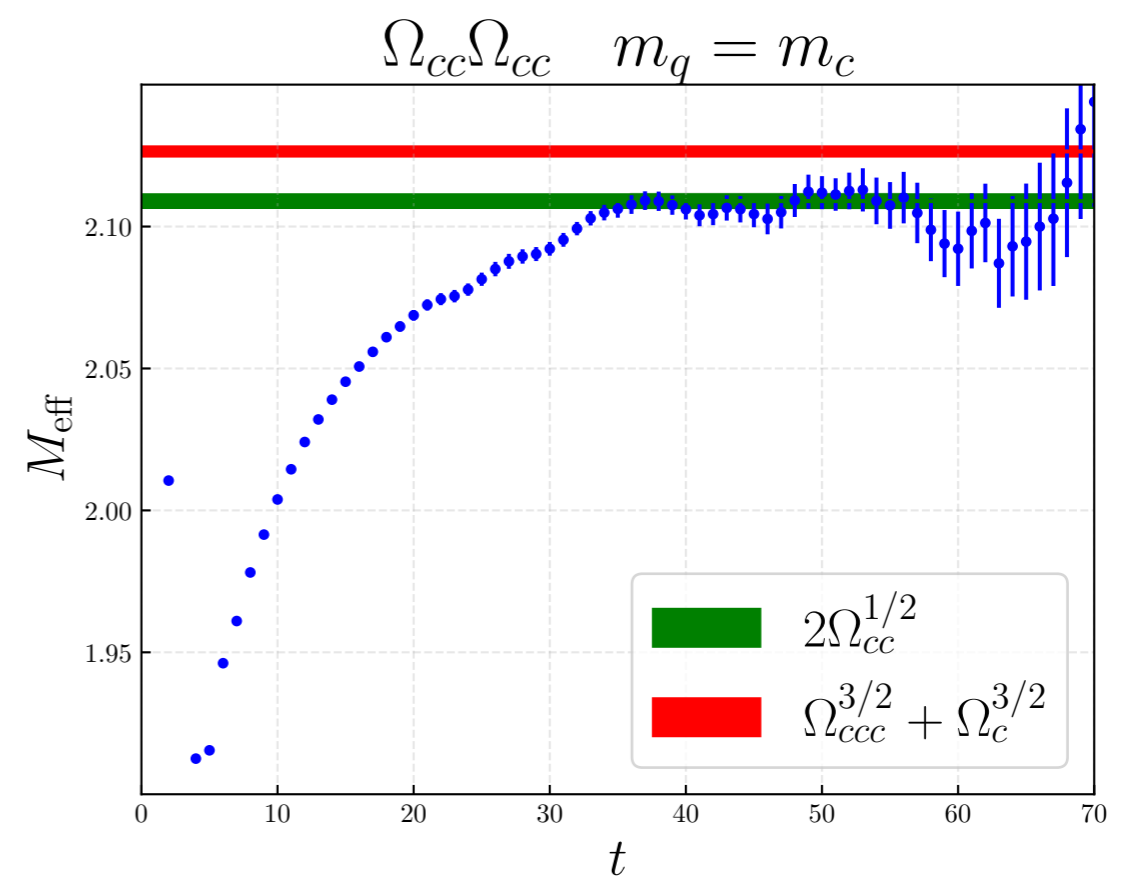
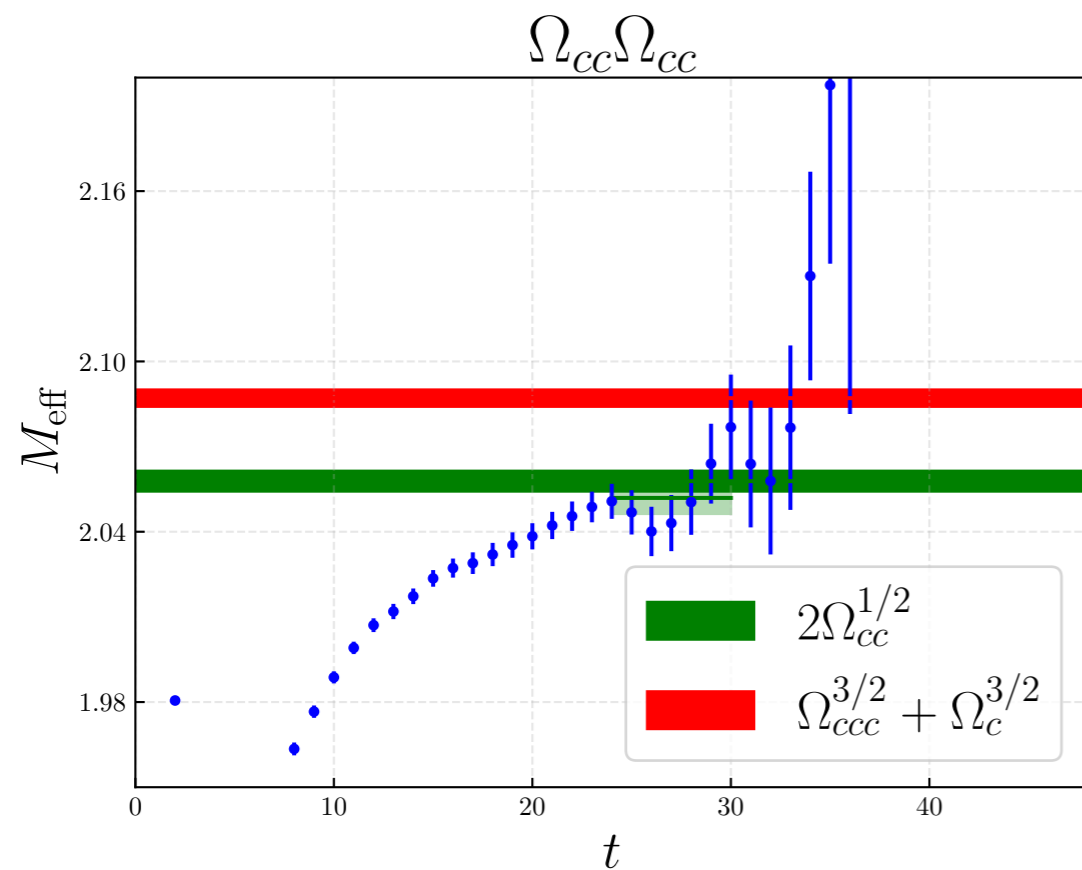
✿ Flavor symmetric states in charm-strange sector



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Results in Singlet sector

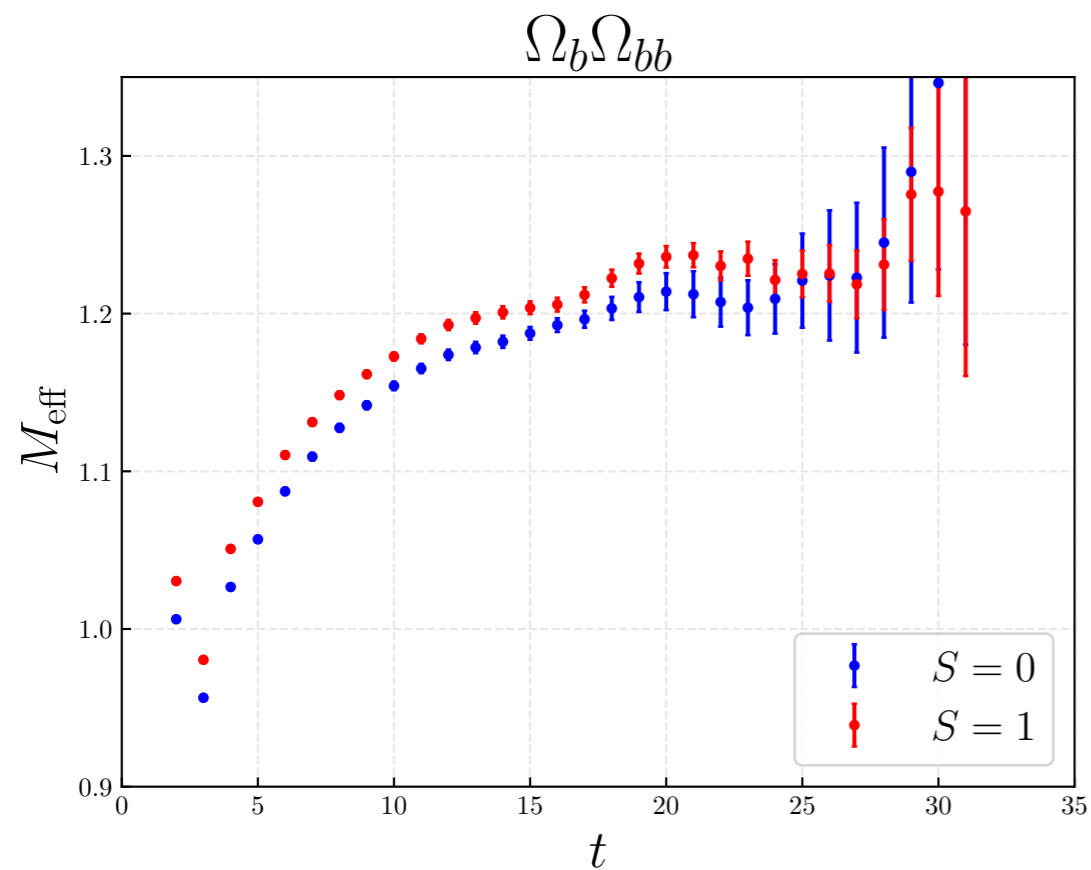
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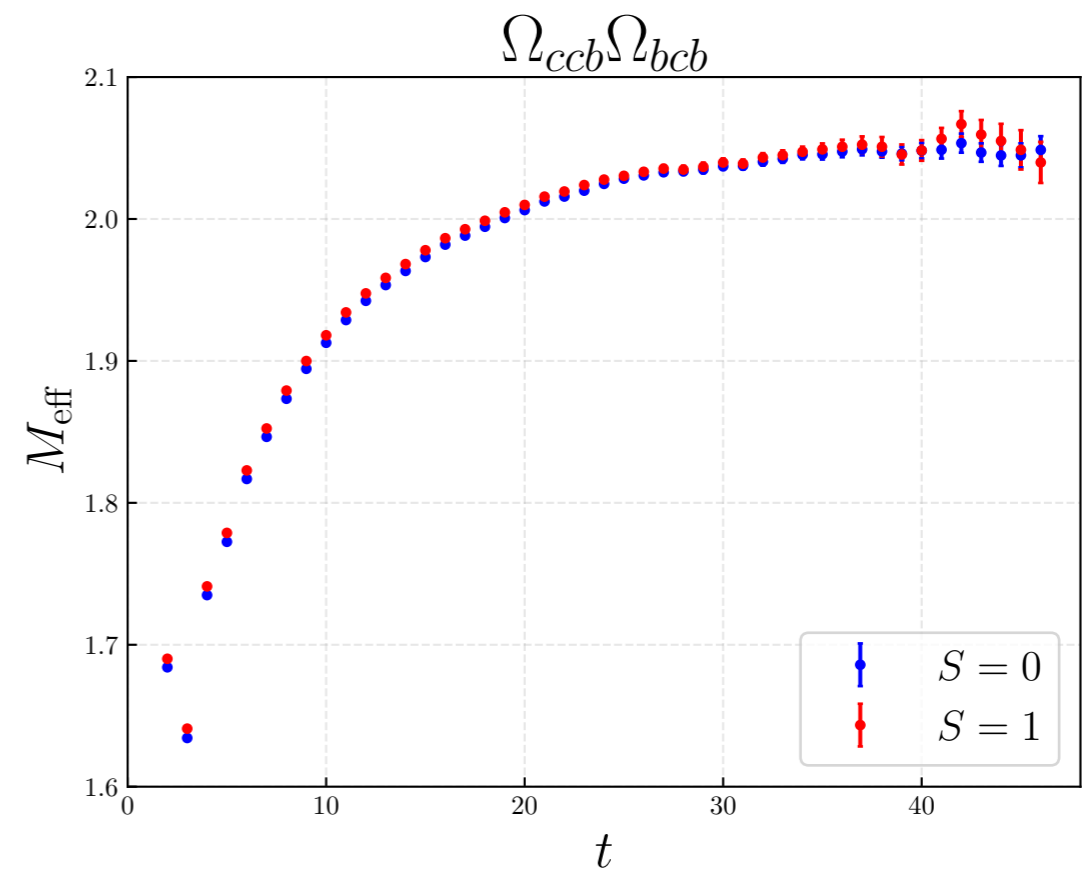
✿ No Clear indication of level below N1-level

Heavy quark spin symmetry

- ✿ Compare of correlation functions of : $S = 0, \quad S = 1$
- ✿ Consistent pattern $S = 1 > S = 0$



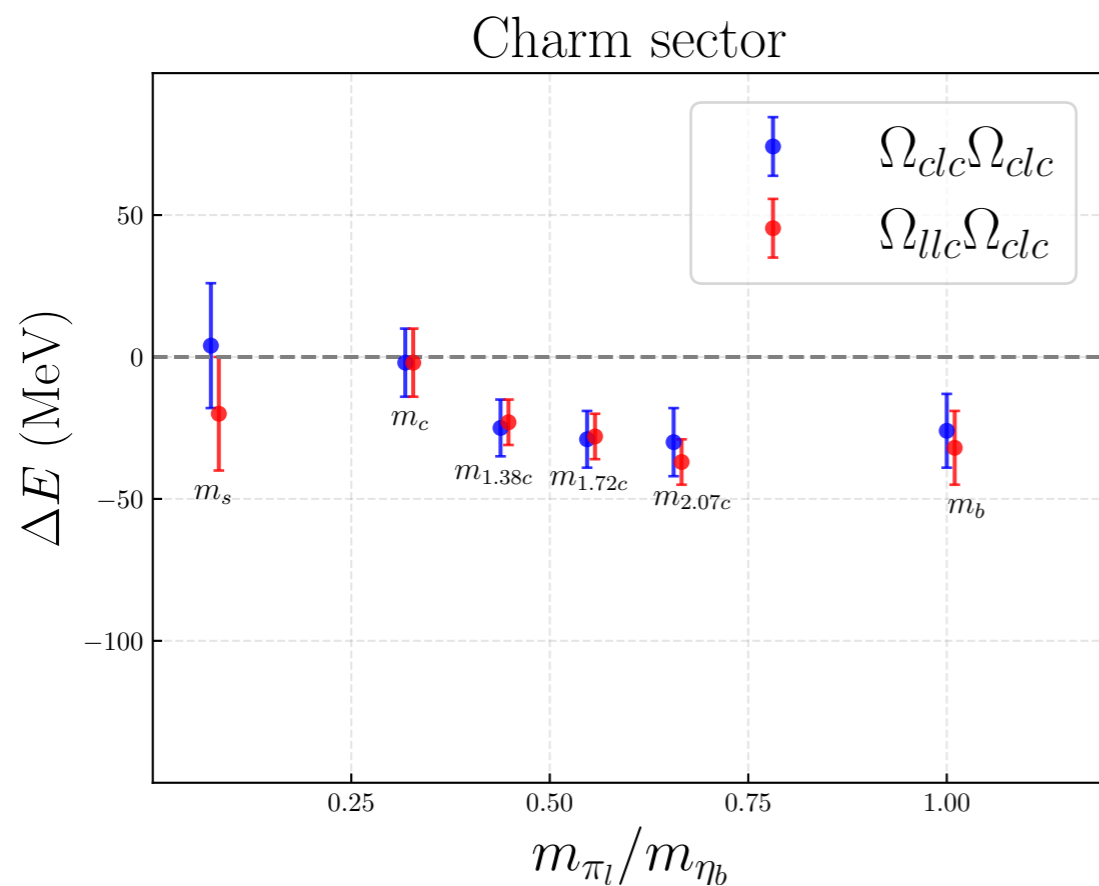
$$M_{\Omega_{bb}\Omega_b}^{S=1} - M_{\Omega_{bb}\Omega_b}^{S=0} = 70(30) \text{ MeV.}$$



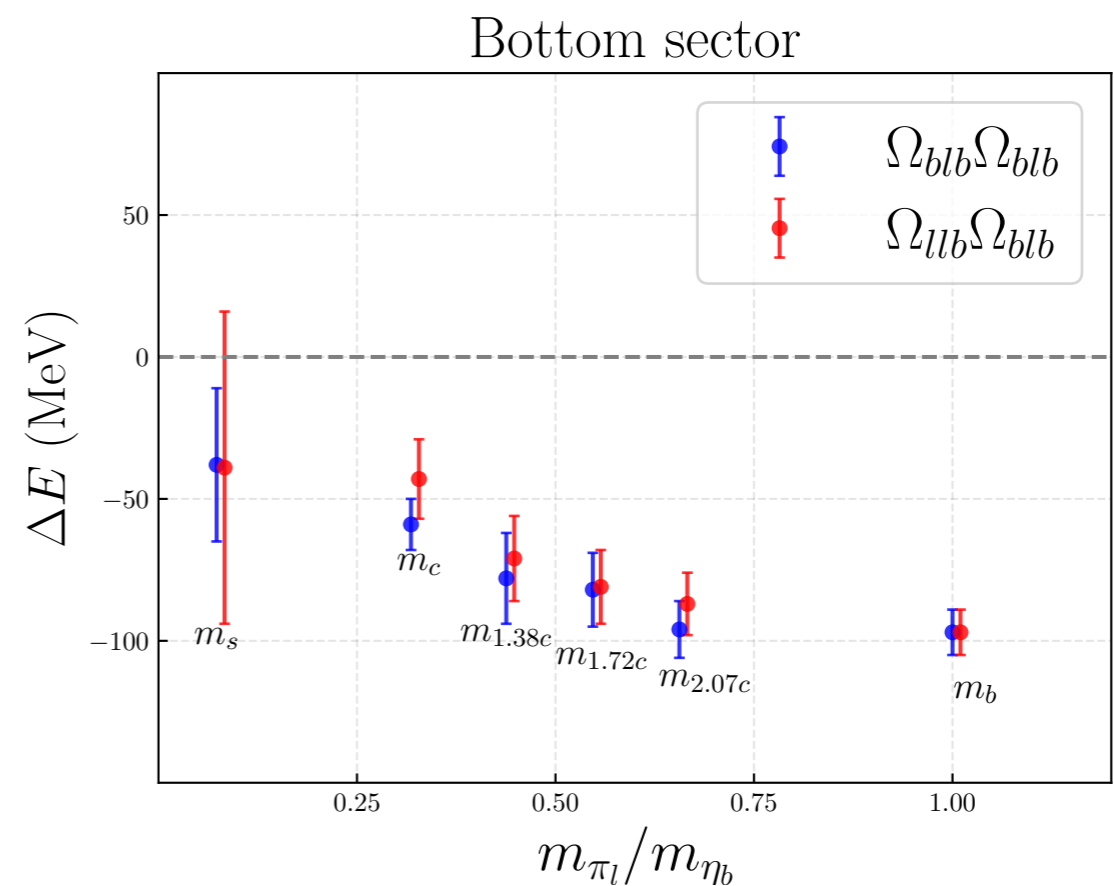
$$M_{\Omega_{ccb}\Omega_{bcb}}^{S=1} - M_{\Omega_{ccb}\Omega_{bcb}}^{S=0} = 2(6) \text{ MeV.}$$

New phenomenology ?

✿ Binding energy at unphysically heavy charm quarks



✿ Deepening of binding energy as bottom quark becomes heavier



✿ Indicative of new mechanism of binding for heavy quarks ?

Outlook

- ✦ Bound states in spin-1 and spin-0 states of charm-bottom

$$\Delta\mathcal{D}_{bc} = -52(13) \text{ MeV}$$

$$\Delta\mathcal{D}_{bs} = -29(13) \text{ MeV}$$

$$\Delta E_{\Omega_{bcb}\Omega_{bcb}} = -66(11) \text{ MeV}$$

$$\Delta E_{\Omega_{ccb}\Omega_{bcb}} = -48(13) \text{ MeV}$$

- ✦ No clear indication in bottom-strange and charm-strange
- ✦ Trend of deepening of binding energy with heavy quark mass
- ✦ Perhaps evidence of new phenomenology ... ?

Continuous temperature sampling in Lattice QCD

Phys. Rev. D 104, 014502 (2021)

Motivation

- ❖ Consider a lattice calculation of $\langle \mathcal{O}_\beta \rangle$

$$\langle \mathcal{O}_\beta \rangle = \frac{1}{\mathcal{Z}} \int \mathcal{D}U e^{-\beta S[U]} \mathcal{O}[U]$$

Single coupling
corresponds to a
single temperature

- ❖ We are interested in the temperature and cutoff dependence

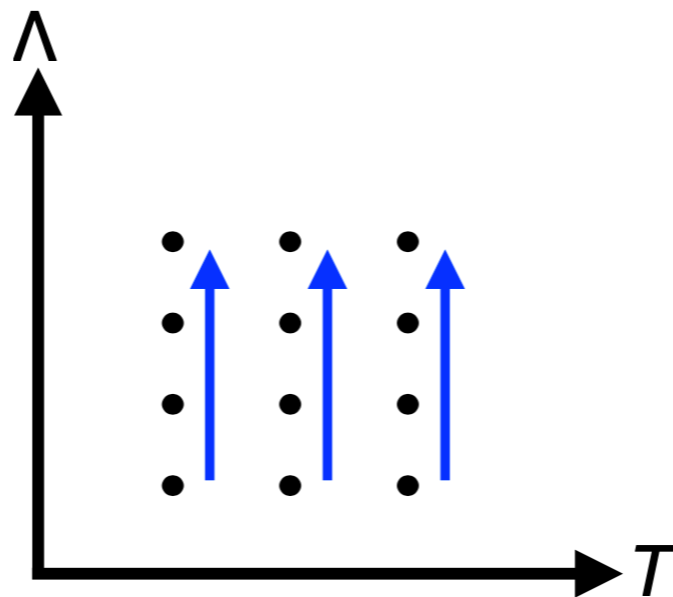
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Single coupling
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single temperature

Simulate at every
temperature and
cutoff

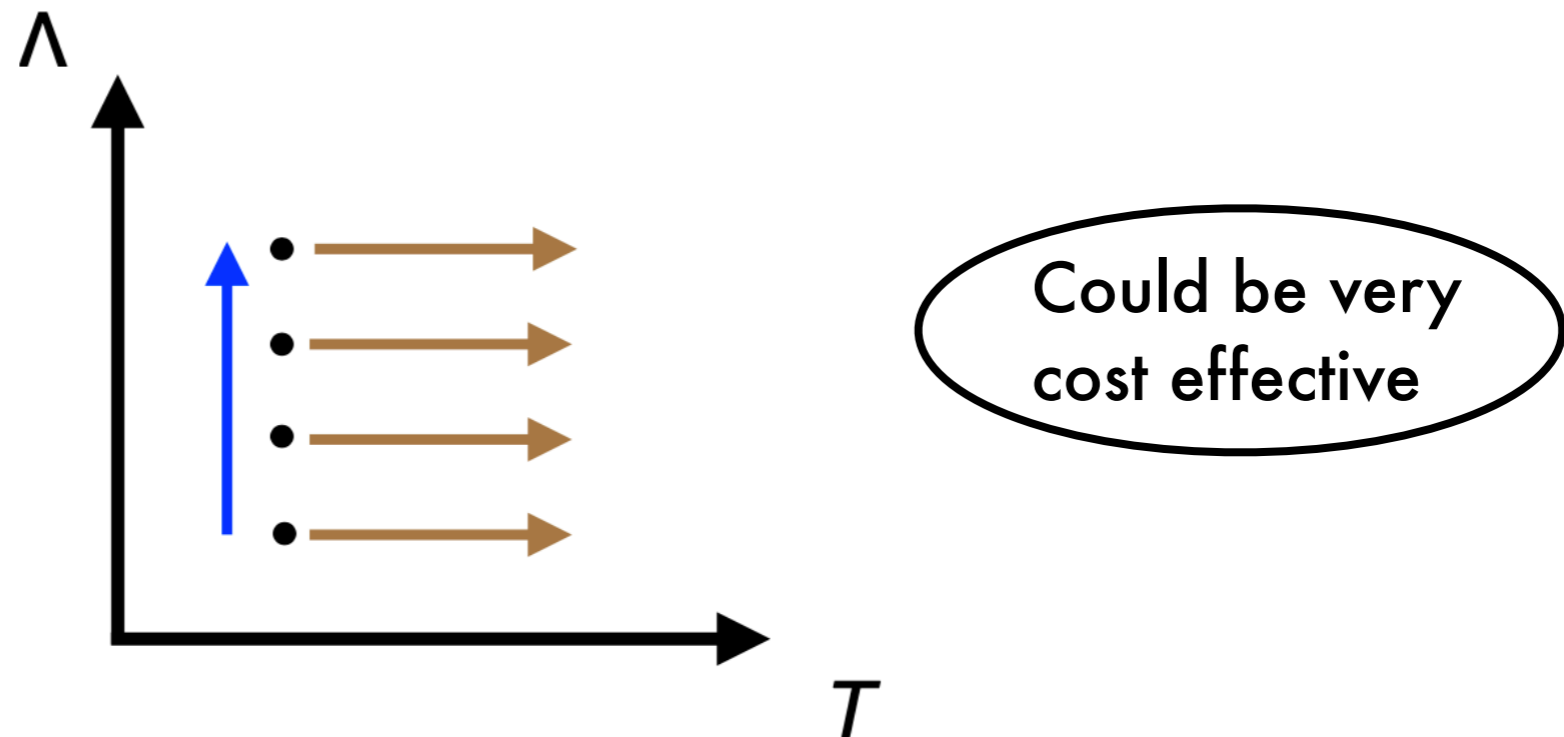


Could be
expensive if the
temperature range
is really large

Perhaps there is a better way ?

Temperature reweighting

- ❖ A novel way Sample temperatures continuously
- ❖ Employ a reweighting in temperature at a fixed cutoff



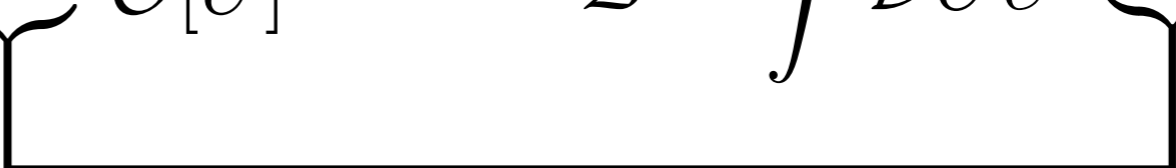
Temperature reweighting

❖ Consider a lattice calculation of $\langle \mathcal{O}_\beta \rangle$

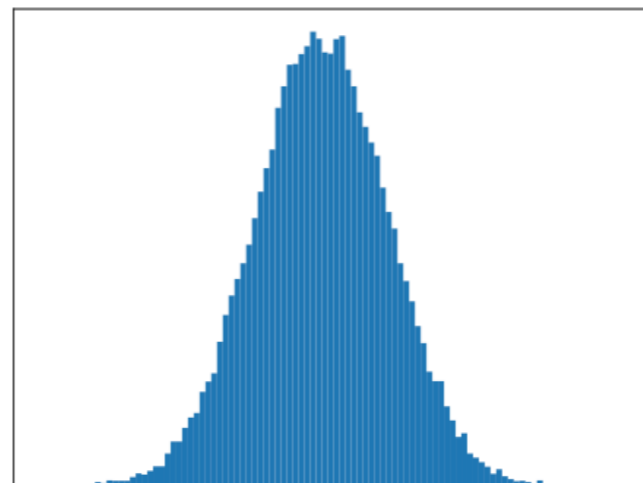
$$\langle \mathcal{O}_\beta \rangle = \frac{1}{\mathcal{Z}} \int \mathcal{D}U e^{-\beta S[U]} \mathcal{O}[U] \quad \mathcal{Z} = \int \mathcal{D}U e^{-\beta S[U]}$$

Temperature reweighting

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Single β simulates single temperature



Action histogram
approx gaussian

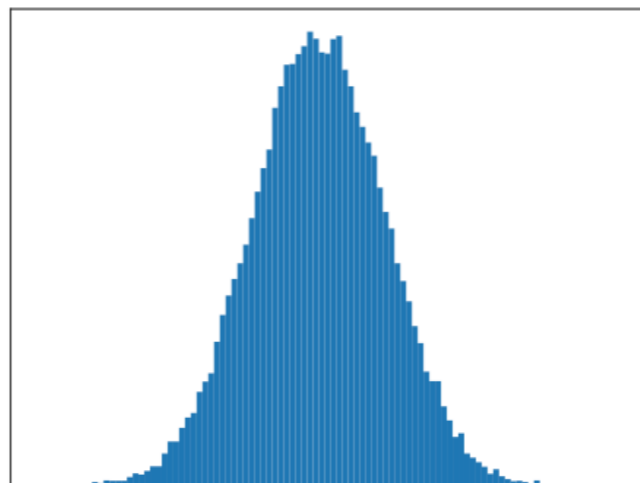
Temperature reweighting

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Single β simulates single temperature

To simulate continuous temperatures, simulate continuous β



Action histogram approx gaussian

Temperature reweighting

- ❖ Consider a lattice calculation of $\langle \mathcal{O}_\beta \rangle$

$$\langle \mathcal{O}_\beta \rangle = \frac{1}{\mathcal{Z}} \int \mathcal{D}U e^{-\beta S[U]} \mathcal{O}[U] \quad \mathcal{Z} = \int \mathcal{D}U e^{-\beta S[U]}$$

- ❖ Replace the weight βS

$$\mathcal{Z} = \int \mathcal{D}U e^{-\beta S[U]} \quad \downarrow$$
$$\int \mathcal{D}U e^{-W(S)}$$

$$W(S) = \beta S$$

$$W'(S) = \frac{dW(S)}{dS} = \beta$$

Continuous
temperatures



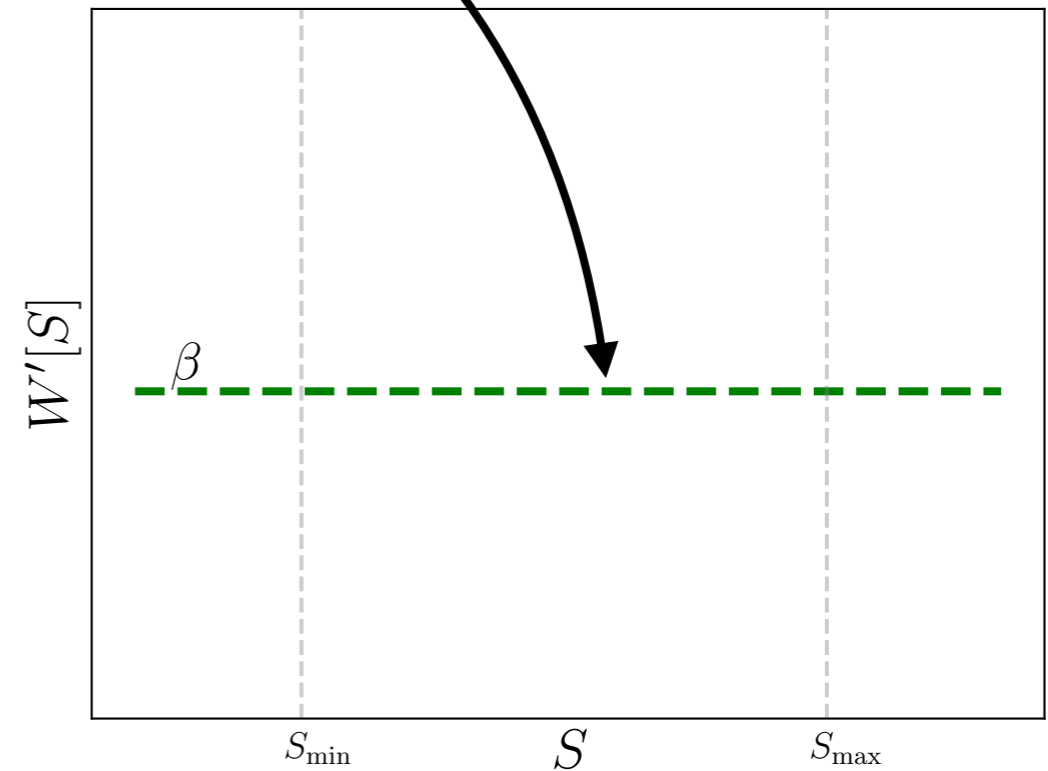
Continuous
gauge couplings



Continuous
 $W'(S)$

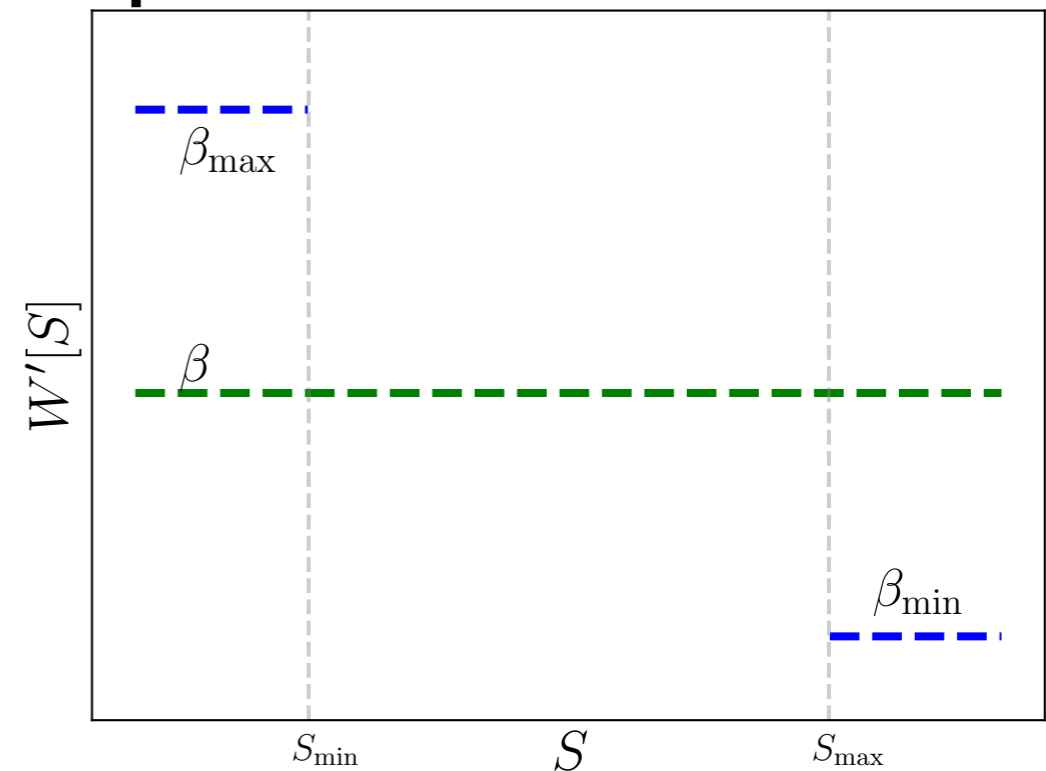
Temperature reweighting

❖ Single temperature/coupling MC



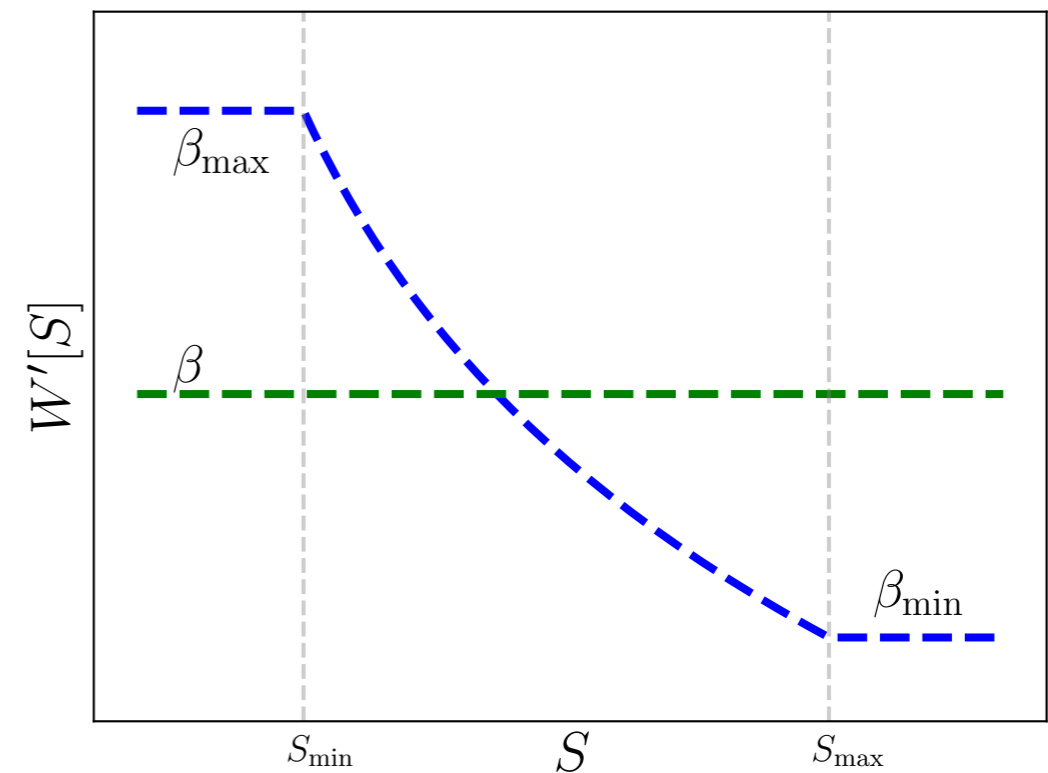
Temperature reweighting

- ❖ Single temperature/coupling MC
- ❖ Define a range of continuous temperatures



Temperature reweighting

- ❖ Single temperature/coupling MC
- ❖ Continuous sampling of S , then samples continuous β

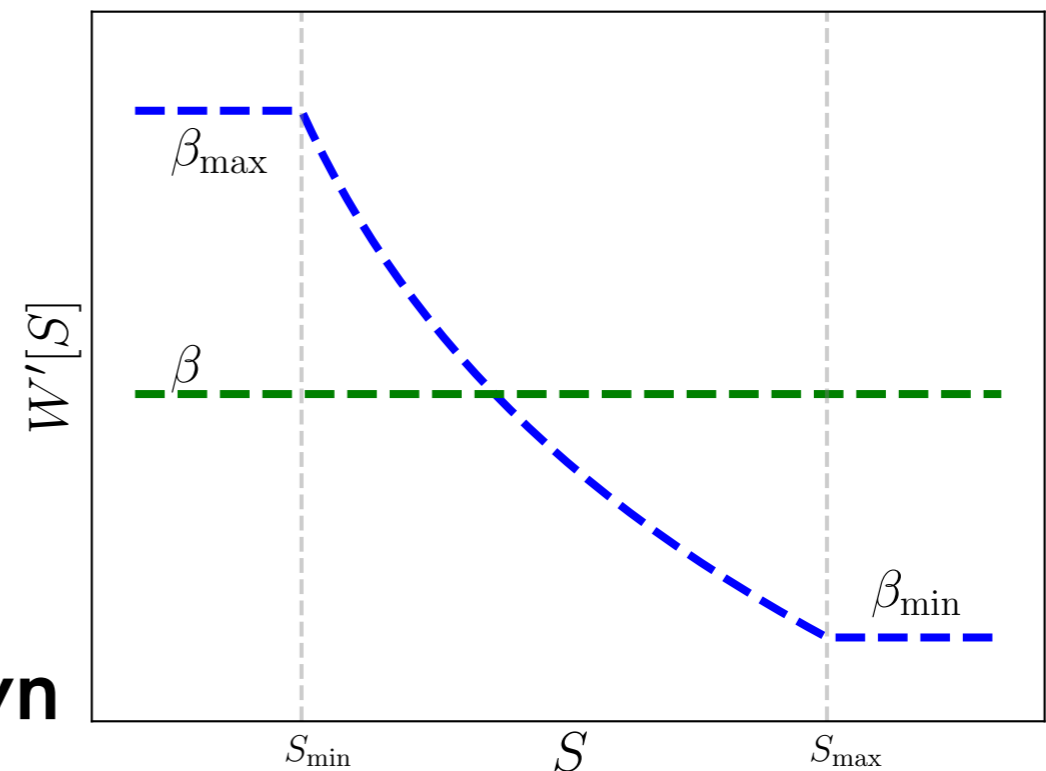


Temperature reweighting

- ❖ Single temperature/coupling MC

- ❖ Computing $\mathcal{Z}(\beta_0)$ from $\int \mathcal{D}U e^{-W(S)}$ Assuming $W(s)$ is known

$$\mathcal{Z}(\beta_0) = \int \mathcal{D}U e^{-W(S)} e^{W(S) - \beta_0 S}$$
$$\propto \sum_i e^{W(S_i) - \beta_0 S_i}$$



- ❖ Overall normalization unknown

- ❖ Regularisation issues with $\mathcal{Z}(\beta_0)$

Topological Susceptibility

❖ Compute QCD $\chi_{\text{top}}(\beta)$ at high temperatures :

$$\chi_{\text{top}}(\beta)a^4(\beta) = \frac{1}{V_L} \frac{Z_1(\beta)}{Z_0(\beta)}$$

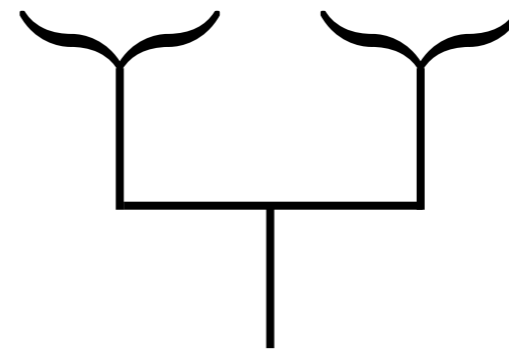
Topological Susceptibility

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$$\chi_{\text{top}}(\beta)a^4(\beta) = \frac{1}{V_L} \frac{Z_1(\beta)}{Z_0(\beta)}$$

- ❖ Computing ratios of $\chi_{\text{top}}(\beta)$

$$\frac{\chi_{\text{top}}(\beta_1)a^4(\beta_1)}{\chi_{\text{top}}(\beta_2)a^4(\beta_2)} = \frac{Z_1(\beta_1)}{Z_1(\beta_2)} \frac{Z_0(\beta_2)}{Z_0(\beta_1)}$$



Allows for two single topology simulations

Topological Susceptibility

- ❖ Compute QCD $\chi_{\text{top}}(\beta)$ at high temperatures :

$$\chi_{\text{top}}(\beta)a^4(\beta) = \frac{1}{V_L} \frac{Z_1(\beta)}{Z_0(\beta)}$$

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- ❖ Temperature reweighting :

$$\frac{\chi_{\text{top}}(\beta_1)a^4(\beta_1)}{\chi_{\text{top}}(\beta_2)a^4(\beta_2)} = \frac{\sum_{iQ} e^{W(S_{iQ}) - \beta_1 S_{iQ}}}{\sum_{iQ} e^{W(S_{iQ}) - \beta_2 S_{iQ}}} \frac{\sum_i e^{W(S_i) - \beta_1 S_i}}{\sum_i e^{W(S_i) - \beta_2 S_i}}$$

How to simulate continuous temperatures

❖ We would like to generate : $dP[U] = \frac{\mathcal{D}U e^{-W(S[U])}}{\int \mathcal{D}U e^{-W(S[U])}}$

❖ Construct an MD Hamiltonian :

$$\mathcal{H}(\pi, U) = \sum_{x, \mu} \frac{1}{2} \left((\pi_\mu(x))^2 + W(S[U]) \right)$$

How to simulate continuous temperatures

❖ We would like to generate : $dP[U] = \frac{\mathcal{D}U e^{-W(S[U])}}{\int \mathcal{D}U e^{-W(S[U])}}$

❖ Construct an MD Hamiltonian :

$$\mathcal{H}(\pi, U) = \sum_{x, \mu} \frac{1}{2} \left((\pi_\mu(x))^2 + W(S[U]) \right)$$

❖ Solve Hamilton's EOM :

$$\frac{dU}{dt} = i\pi U \quad \frac{d\pi}{dt} = iU^\dagger \frac{\partial W(S[U])}{\partial U} = iU^\dagger \frac{\partial W(S[U])}{\partial S[U]} \frac{\partial S[U]}{\partial U}$$

❖ Metropolis accept/reject :

$$\Delta H = \mathcal{H}(\pi_f, U_f) - \mathcal{H}(\pi_i, U_i)$$

How to compute $W(S)$

❖ $W(S)$ needs to be computed in a separate simulation :

❖ Initial $W(S)$ obtained from interpolation :

$$(\beta_{min}, \beta_{mid}, \beta_{max}) \longrightarrow (S_{max}, S_{mid}, S_{min})$$

❖ Action S is split in N intervals (S_1, S_2, \dots, S_N)

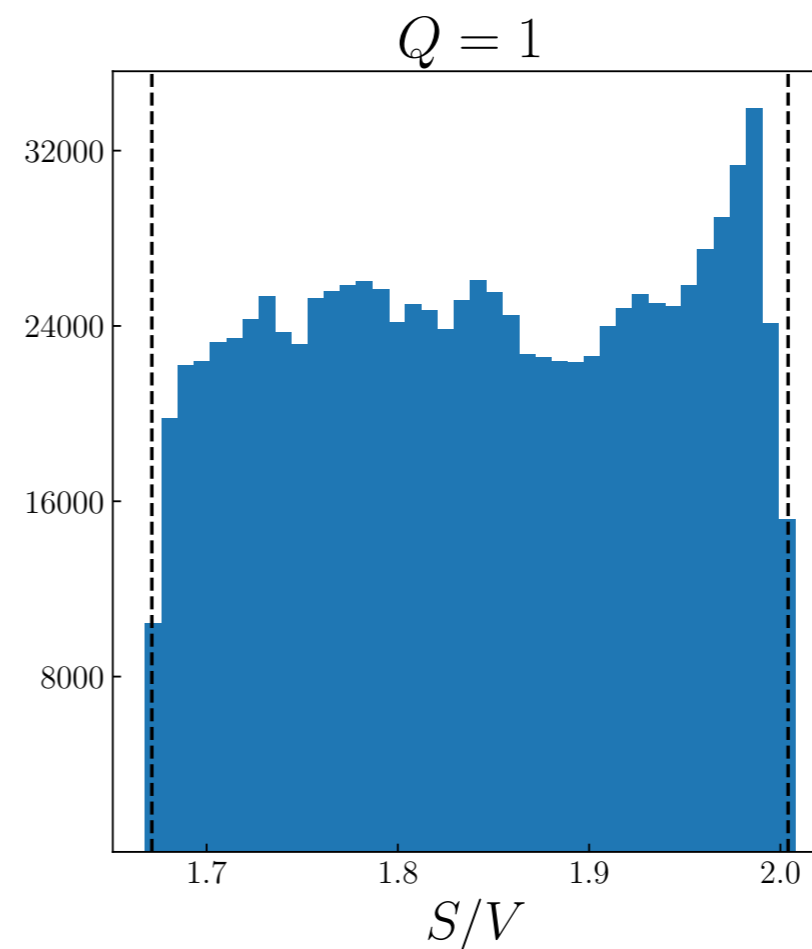
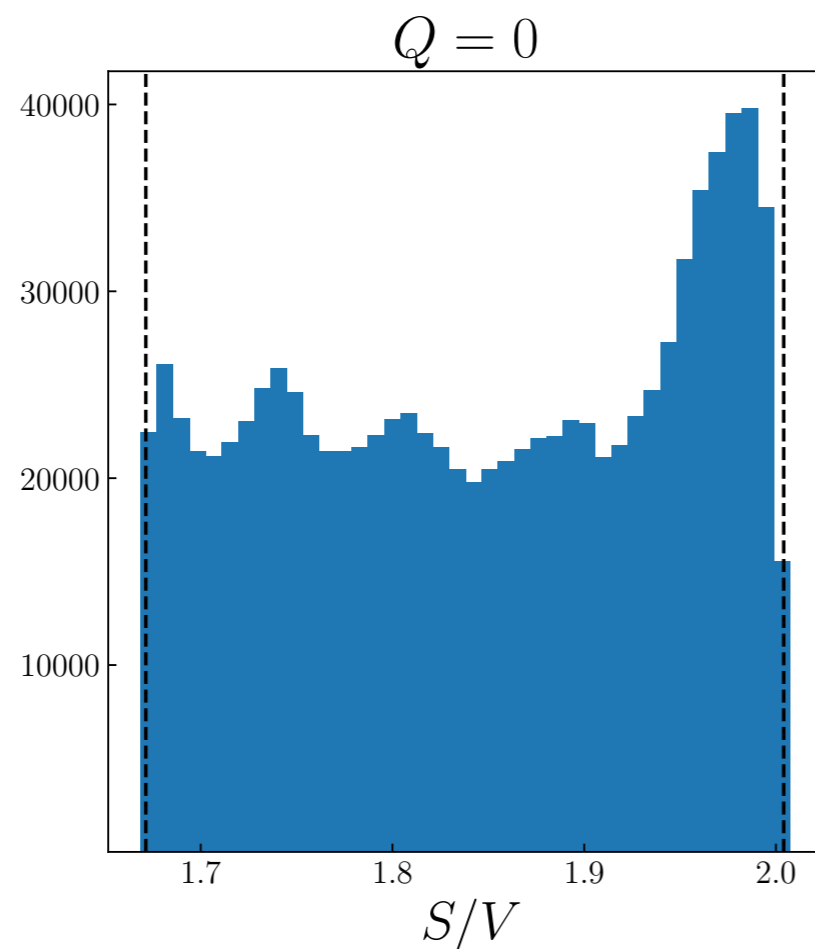
$$W(S) = \begin{cases} W_i + s_r x (W_{i+1} - W_i), & S_{max} < S_i < S_{min}, \\ \beta_{max} S, & S < S_{min} \\ \beta_{min} S, & S > S_{max} \end{cases} \quad x = \frac{S - S_i}{S_{i+1} - S_i}$$

❖ After S traverses all intervals and back, s_r is reduced

❖ Separate simulation needed for $Q=0,1$

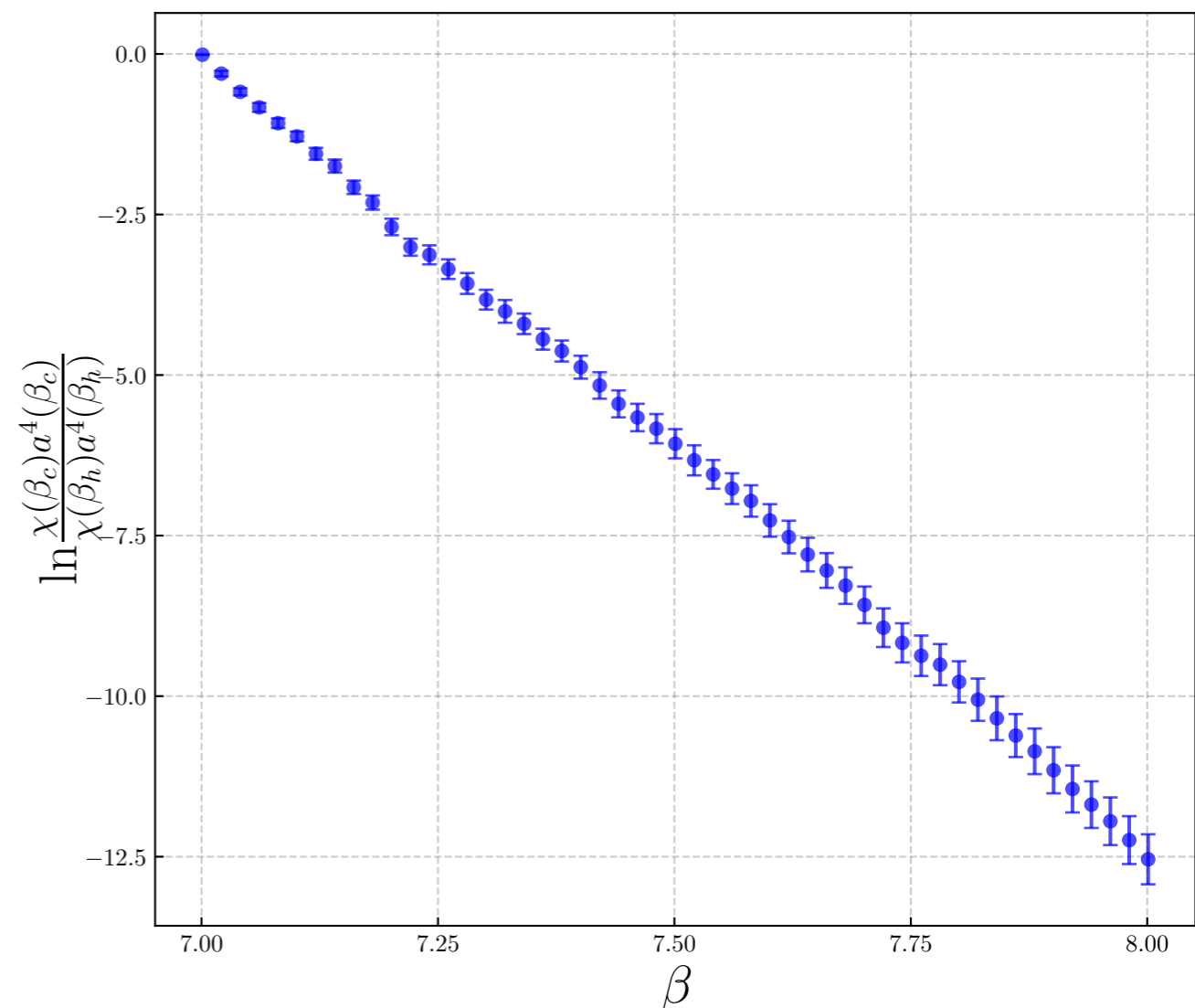
Results for action distribution

- ❖ Simulation with Wilson gauge action
- ❖ Temperature $2.5 T_c - 9.4 T_c$

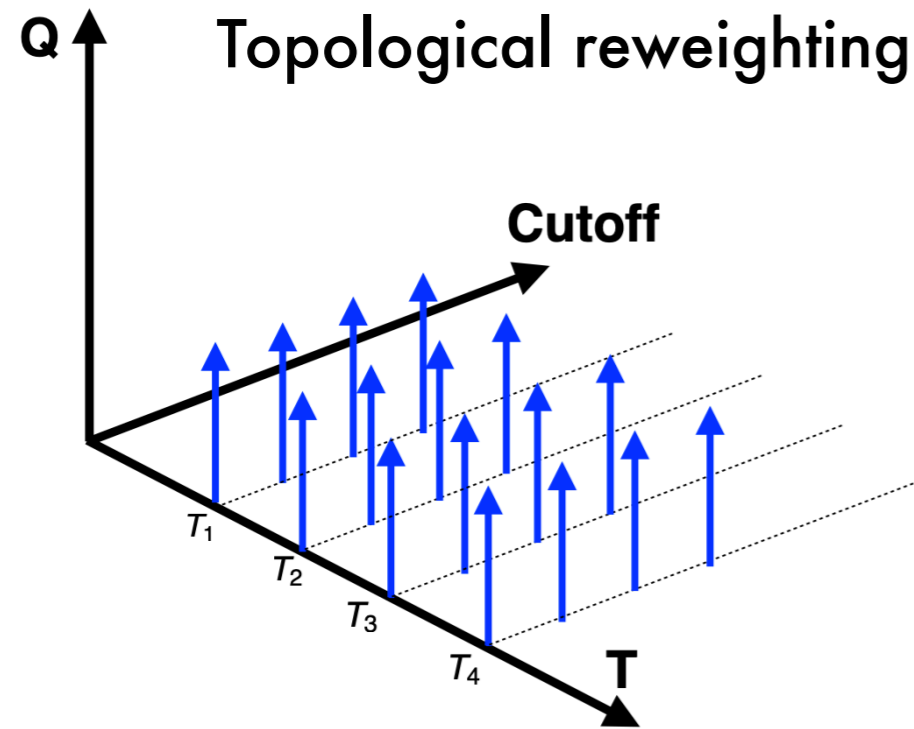


Results for Susceptibility

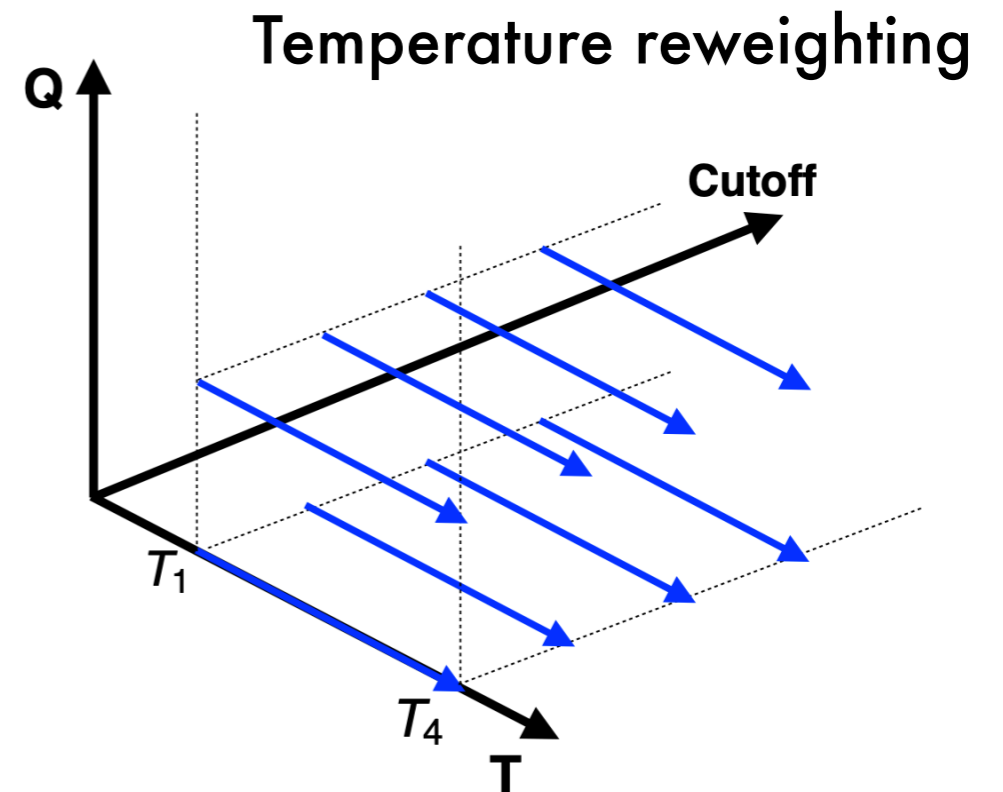
- ❖ Method accomplishes continuous sampling of temperatures.
- ❖ Results in agreement with topological reweighting.
- ❖ Scale agnostic determination.
- ❖ Method comparable to current methods for high statistics determination.
- ❖ Inefficient for less precise determination



Outlook



- ❖ Needs to be simulated at every cutoff and temperature.
- ❖ No of simulations = x
- ❖ Simulation for reweighting function cheap
- ❖ Cheaper for lower statistics



- ❖ Needs to be simulated at two topologies and every cutoff.
- ❖ No of simulations = $x/2$
- ❖ Simulation for reweighting function expensive
- ❖ Expensive for lower statistics

Scale setting at high temperature

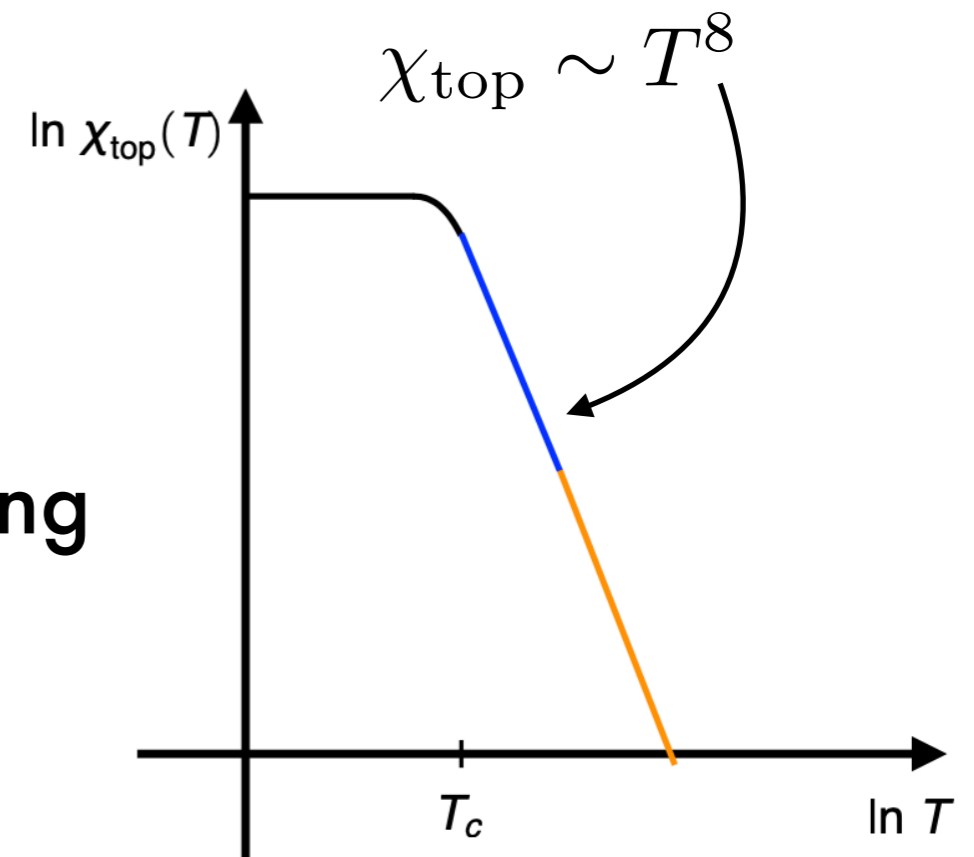
Phys.Rev.D 108 (2023) 7, 074512

Motivation

- ✦ Determine lattice cutoff – subpercent precision
 - very fine lattices ~ 0.015 fm
- ✦ Target – Full QCD determination of χ_{top}

Motivation

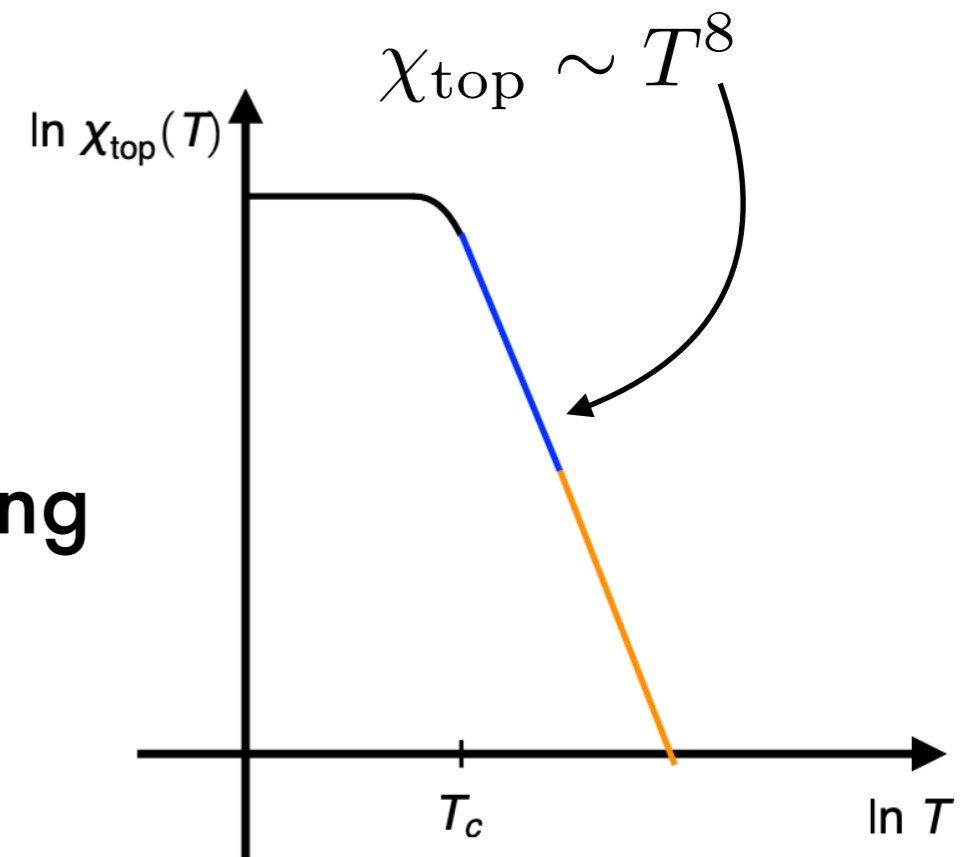
- ❖ Temperature dependence of χ_{top}
- ❖ Large power dependence on T
- ❖ Worse dependence on lattice spacing



$$\chi_{\text{top}} a^4 \sim a^{12}$$

Motivation

- ❖ Temperature dependence of χ_{top}
- ❖ Large power dependence on T
- ❖ Worse dependence on lattice spacing
- ❖ $2\% \sigma$ in $T \longrightarrow 24\% \sigma \chi_{\text{top}}$
- ❖ Need % level determination of a .
- ❖ Temp 1 GeV – Box size $N_t = 14 \longrightarrow a \sim 0.01$ fm



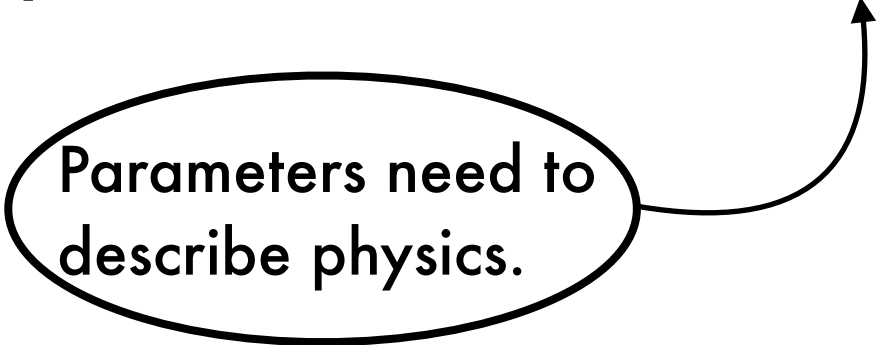
$$\chi_{\text{top}} a^4 \sim a^{12}$$

$$a \sim 0.01 \text{ fm}$$

Scale setting in Lattice QCD

❖ Lattice calculations use bare parameters (g_0, am_l, am_s, am_c)

Parameters need to describe physics.



Scale setting in Lattice QCD

- ✦ Lattice calculations use bare parameters (g_0, am_l, am_s, am_c)
- ✦ Determine the renormalized trajectory
- ✦ Determining the cutoff - "Set" the scale

Scale setting in Lattice QCD

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 - ✦ Tune bare parameters to physical observables
 - ✦ One observable for each parameter
 - ✦ Determine the Line of Constant Physics - Renormalised Trajectory
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Scale setting in Lattice QCD

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 - ✦ Lattice quantities computed as a ratio with the cutoff
 - ✦ Determines the overall precision

Scale setting in Lattice QCD

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 - ✦ Determines the overall precision
- ✦ Closer look at scale setting

Scale setting observables

- ✦ **Desirable properties** : *R.Sommer, arXiv:1401.3270v1*
- ✦ Low numerical effort
- ✦ Good statistical precision
- ✦ Small systematic error
- ✦ Weak quark mass dependence

Scale setting observables

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❖ **Classification of observables**

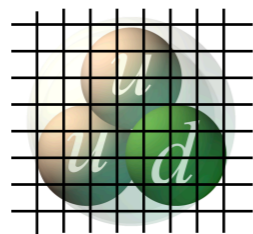
Phenomenological scales \longrightarrow Direct experimental observables

Theory scales \longrightarrow Observables defined from phenomenology.
Indirectly related to experiment.

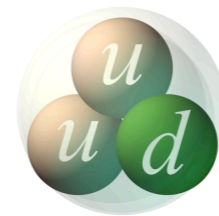
Phenomenological Scales

❖ Most Naive observable – Proton

Compute proton
mass on lattice



$$aM_N$$



$$M_N$$

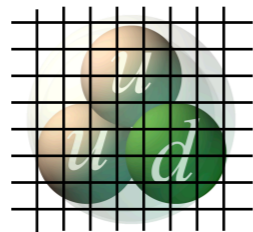
Compare it to
experiment

$$\mathcal{R} = \frac{aM_N}{M_N}$$

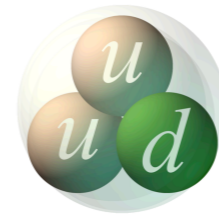
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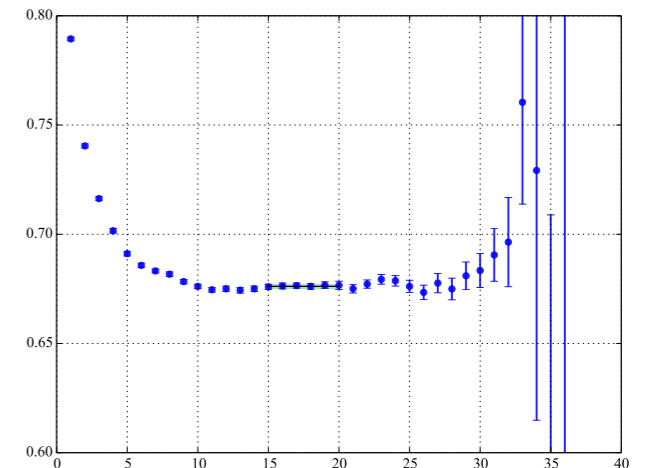
$$M_N$$

Compare it to experiment

$$\mathcal{R} = \frac{aM_N}{M_N}$$

- ✦ Highly sensitive to quark mass

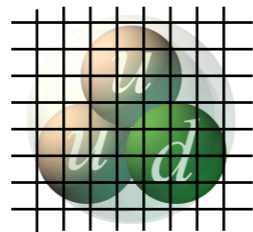
- ✦ Issue with precision – Low signal/noise



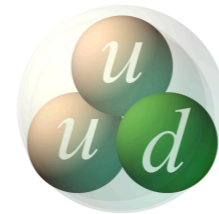
Phenomenological Scales

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$$aM_N$$

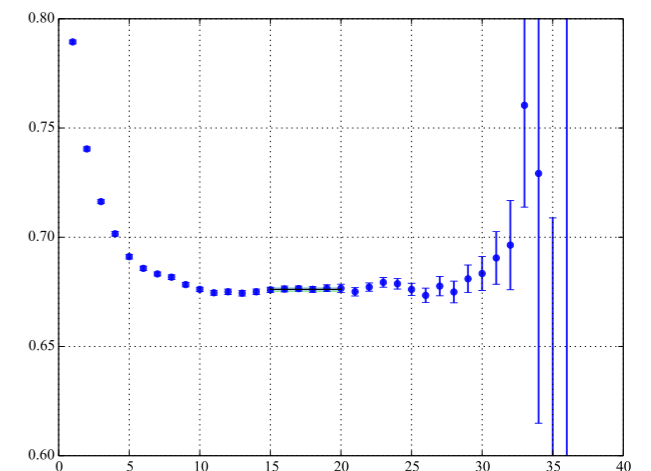


$$M_N$$

Compare it to experiment

$$\mathcal{R} = \frac{aM_N}{M_N}$$

- ✦ Highly sensitive to quark mass
- ✦ Issue with precision – Low signal/noise
- ✦ Use Omega baryon – scale setting



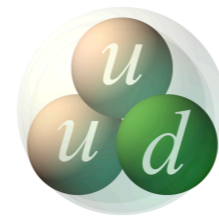
Phenomenological Scales

- ❖ Most Naive observable – Proton

Compute proton mass on lattice



$$aM_N$$



$$M_N$$

Compare it to experiment

$$\mathcal{R} = \frac{aM_N}{M_N}$$

- ❖ Pseudoscalar decay constants –

- ❖ Match lattice computations of f_π, f_K to experiment.

- ❖ Reliable lattice calculation – Good chiral behavior.

- ❖ Experimental results depend on precision of V_{ud}, V_{us}

Theory scales

- ❖ Observables defined from phenomenology

└──────────→ Indirectly related to experiment

- ❖ Sommer parameters : r_0, r_1

- ❖ Use static quark potential to define a hadronic scale.

- ❖ Defined as $r^2 F(r)|_{r=R(c)} = c$, choice $c = 1.65 \rightarrow r_0 = 0.5$ fm

- ❖ Related to the spectra of $\bar{b}b, \bar{c}c$ to Cornell potential

- ❖ Cheap computation, high statistical precision

- ❖ Gradient flow observables :

Gradient flow

❖ Gradient flow - smoothing procedure for gauge fields

$$\partial_t B_\nu(x, t) = D_\mu G_{\mu\nu}, \quad B_\mu(x, 0)|_{t=0} = A_\mu. \quad \text{Covariant diffusion equation}$$

LO in coupling - diffusion equation

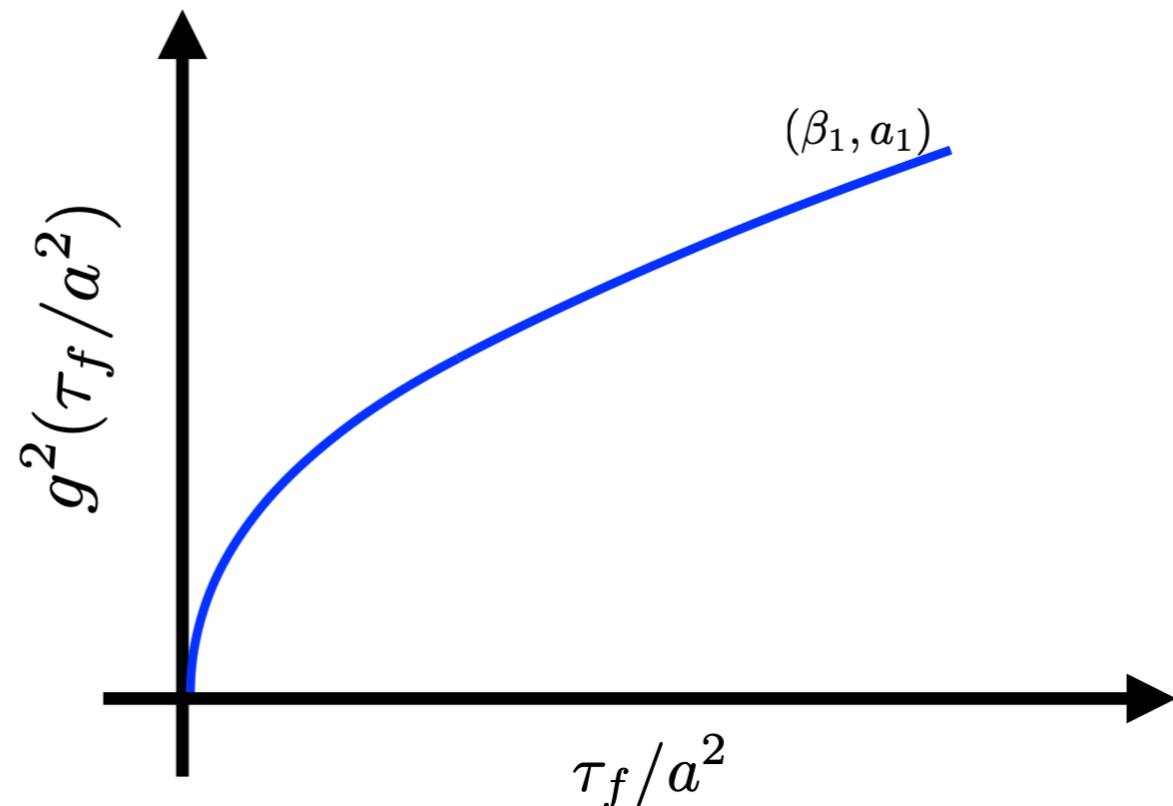
$$B_\mu(x, t) = \int d^4y \frac{e^{-(x-y)^2/4t}}{(4\pi t)^2} A_\mu(y)$$

Compute YM energy at LO

$$\langle E_t \rangle = \frac{24}{128\pi^2} \frac{g^2}{\tau_f^2}$$

Use this to define the coupling

$$g_{\text{flow}}^2(\tau_f) \equiv \frac{128\pi^2 \tau_f^2 \langle E_t(\tau_f) \rangle}{24}$$



Gradient flow observable

- ❖ Use simple prescriptions $\tau^2 \langle E_t \rangle |_{\tau=\tau_0} = c_1$, $\left(\tau \frac{d(\tau^2 \langle E_t \rangle)}{d\tau} \right)_{\tau=w_0^2} = c_2$

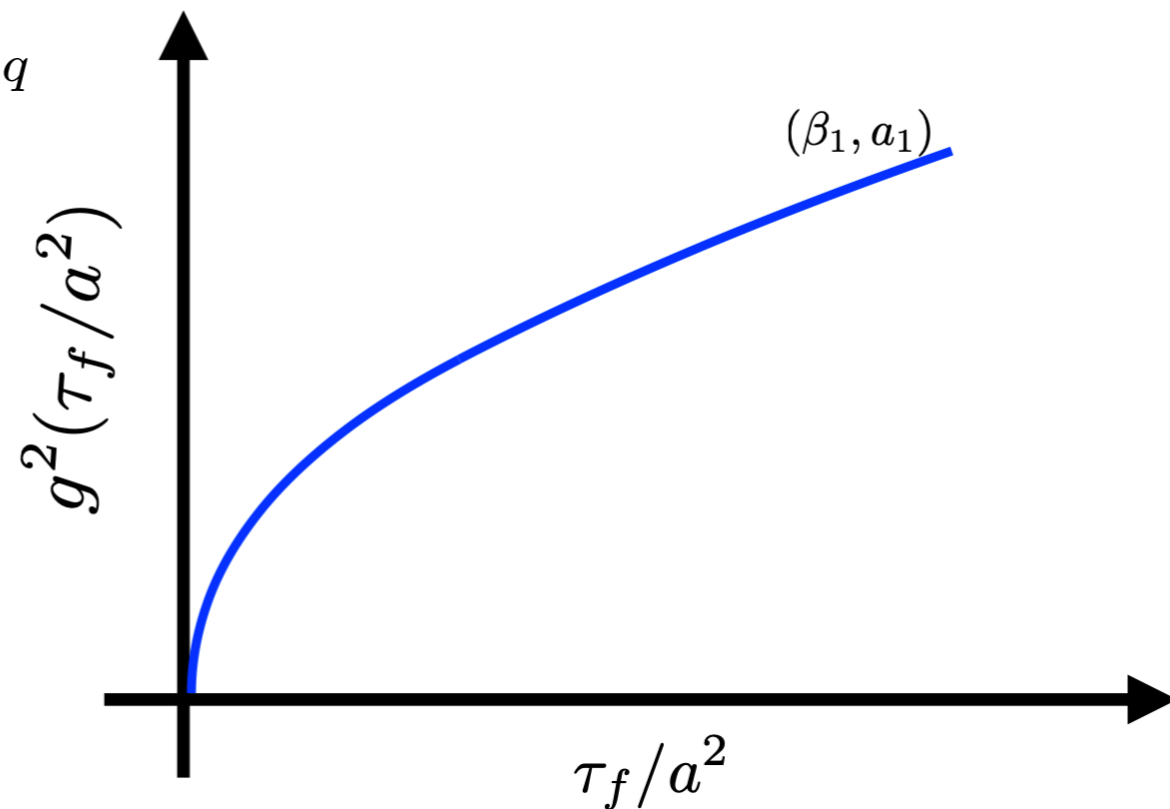
c_1, c_2 are chosen to reduce FV, discretization effects.

- ❖ At a given lattice spacing, measure $\sqrt{\tau_0}/a, w_0/a$ at different m_q

- ❖ Perform a χ^{PT} extrapolation

$\sqrt{\tau_0}_{\text{phys}}, (w_0)_{\text{phys}}$ Obtained from decay constants

- ❖ Compute scale by matching.



Issues with scale observables

❖ Phenomenological scales

❖ Decay constants : determined from weak processes $\pi \rightarrow l\nu$, $V_{ud}f_\pi$

Precision is depended on precision of V_{ud}

❖ Baryon masses : Signal/noise problem prohibits precision

❖ Theory scales :

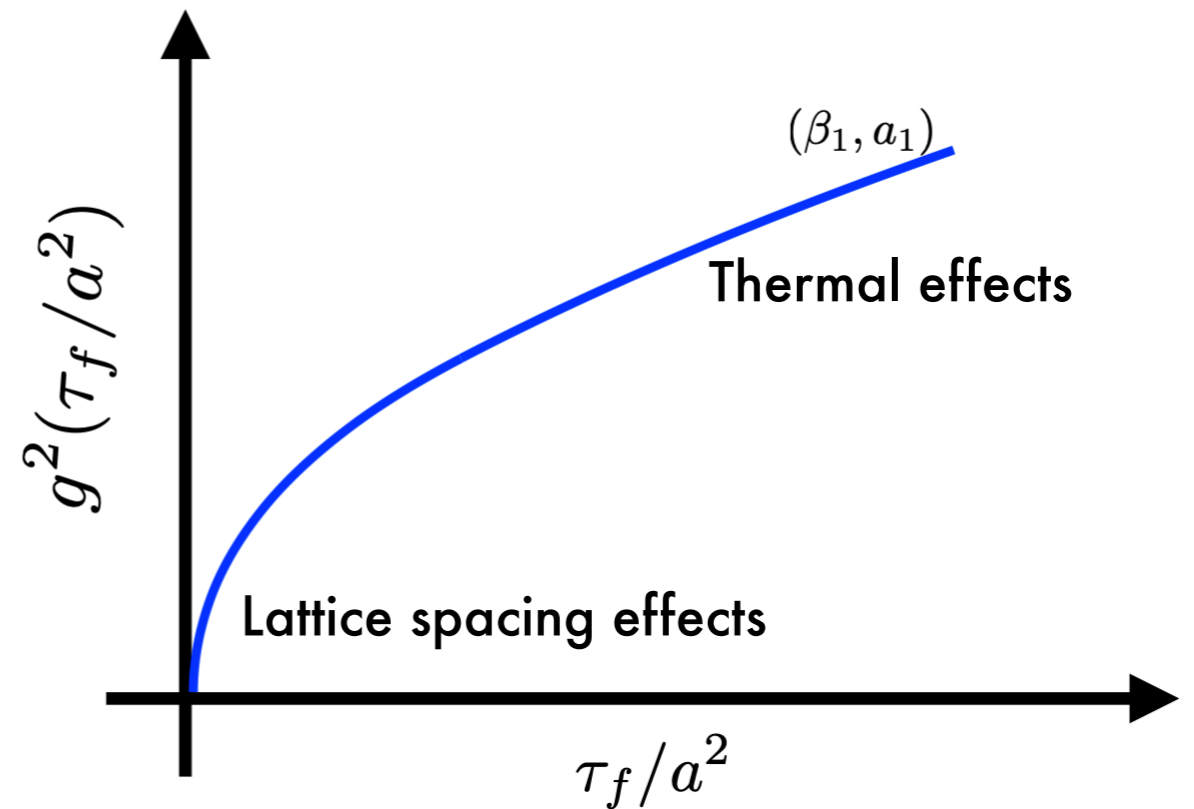
❖ Sommer parameter : poor behavior at fine lattice spacings - Small S/N

❖ Topological freezing problem at fine lattices with gradient flow

❖ New method : Relative scale setting with gradient flow

Systematics of coupling

❖ Lattice spacing effects :



❖ Thermal effects :

Systematics of coupling

❖ Lattice spacing effects :

$$\langle E_t \rangle_{\text{latt}} = \langle E_t \rangle_{\text{cont}} \left(1 + \frac{a^2}{\tau_f} C_1 + \frac{a^4}{\tau_f^2} C_2 + \mathcal{O} \left(\frac{a^6}{\tau_f^3} \right) \right) \quad R_{\text{latt}} \equiv \frac{\langle E_t \rangle_{\text{latt}}}{\langle E_t \rangle_{\text{cont}}}$$

C1 and C2 depend on lattice QCD action, flow type and observable

❖ Thermal effects :

Systematics of coupling

❖ Lattice spacing effects :

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C1 and C2 depend on lattice QCD action, flow type and observable

❖ Thermal effects :

$$\langle E_t \rangle(T) = \langle E_t \rangle(T=0) \sum_{n \in \mathbb{Z}} e^{-n^2/8\tau_f T^2} \quad R_T \equiv \frac{\langle E_t \rangle(T)}{\langle E_t \rangle(T=0)}$$

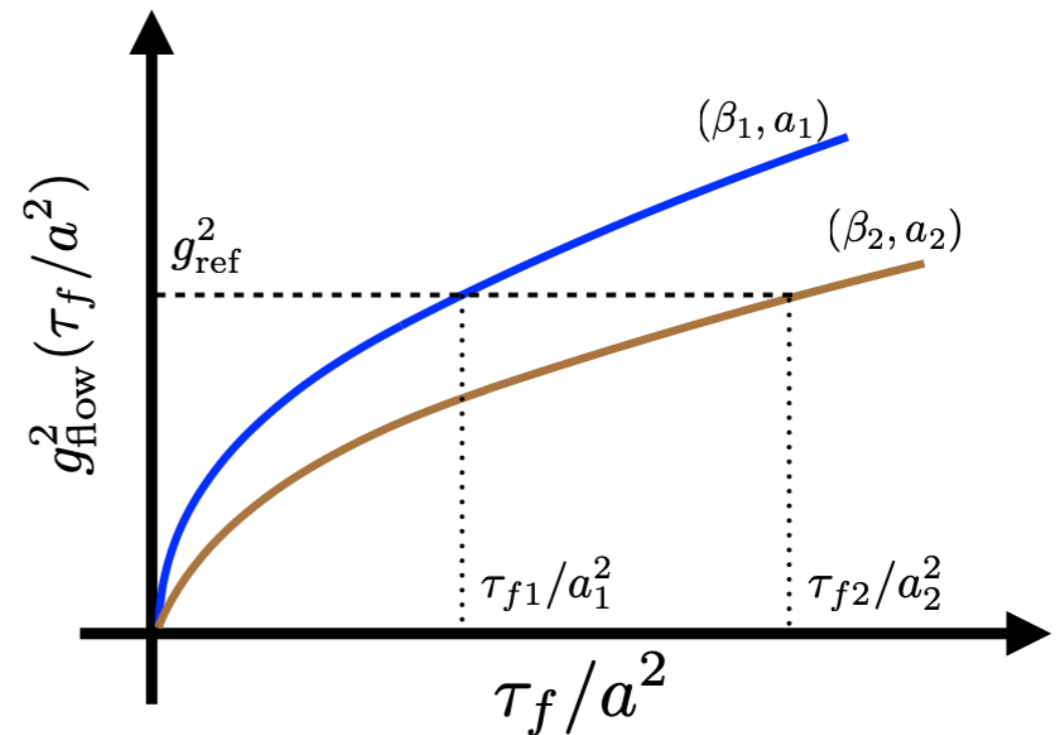
Computed from LO perturbative free theory

❖ Full coupling

$$g_{\text{flow}}^2(\tau_f) = \frac{128\pi^2}{24\tau_f^2} \frac{\langle E_t \rangle_{T,\text{latt}}}{R_{\text{latt}} R_T} + (\text{higher order}).$$

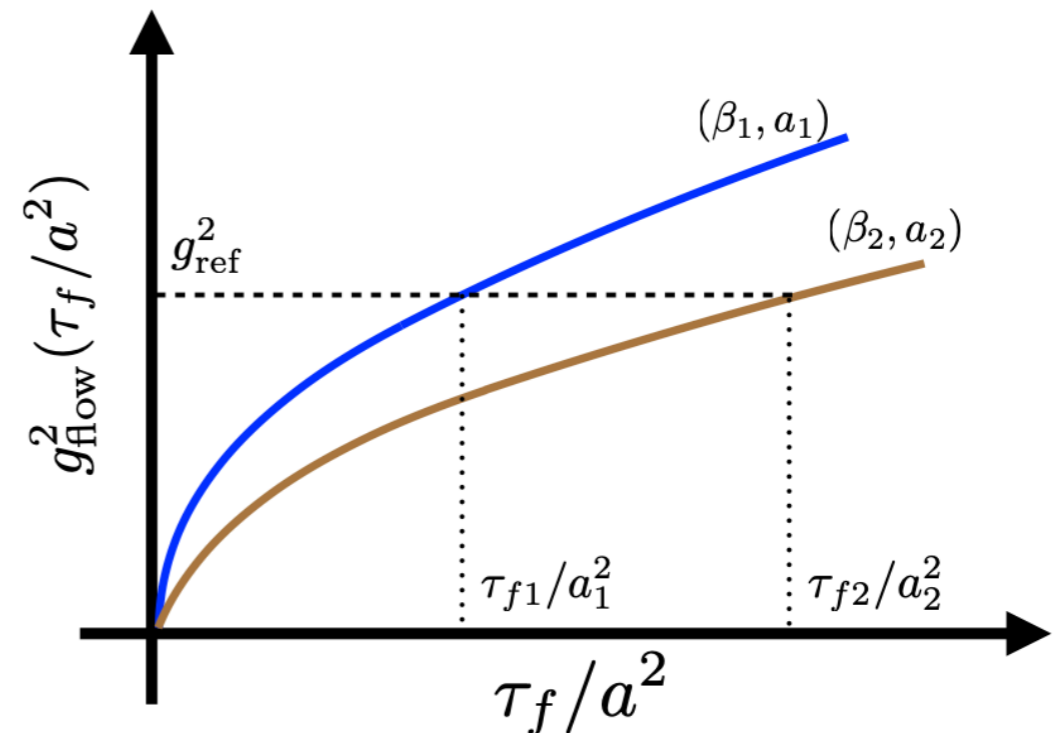
Relative Scale setting

- ❖ Two lattice ensembles at same temperature $T \begin{cases} (\beta_1, N_{\tau_1}, a_1) \\ (\beta_2, N_{\tau_2}, a_2) \end{cases}$



Relative Scale setting

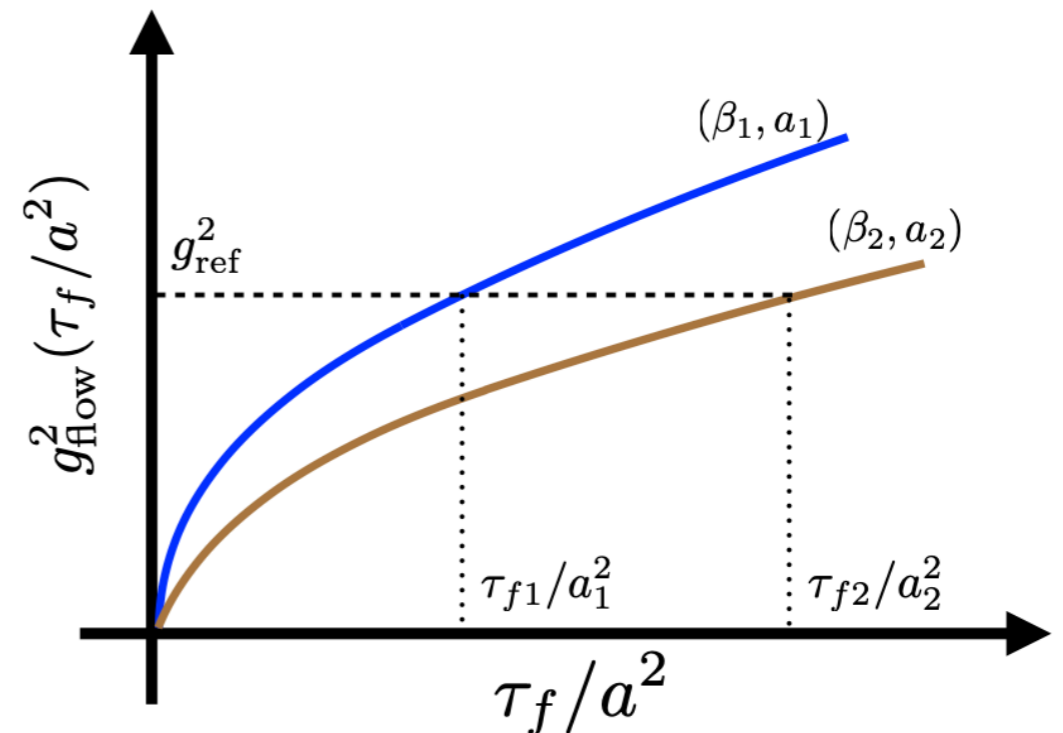
- ❖ Two lattice ensembles at same temperature $T \begin{cases} (\beta_1, N_{\tau_1}, a_1) \\ (\beta_2, N_{\tau_2}, a_2) \end{cases}$
- ❖ Relation between τ_{f1}/a_1^2 and τ_{f2}/a_2^2 for given



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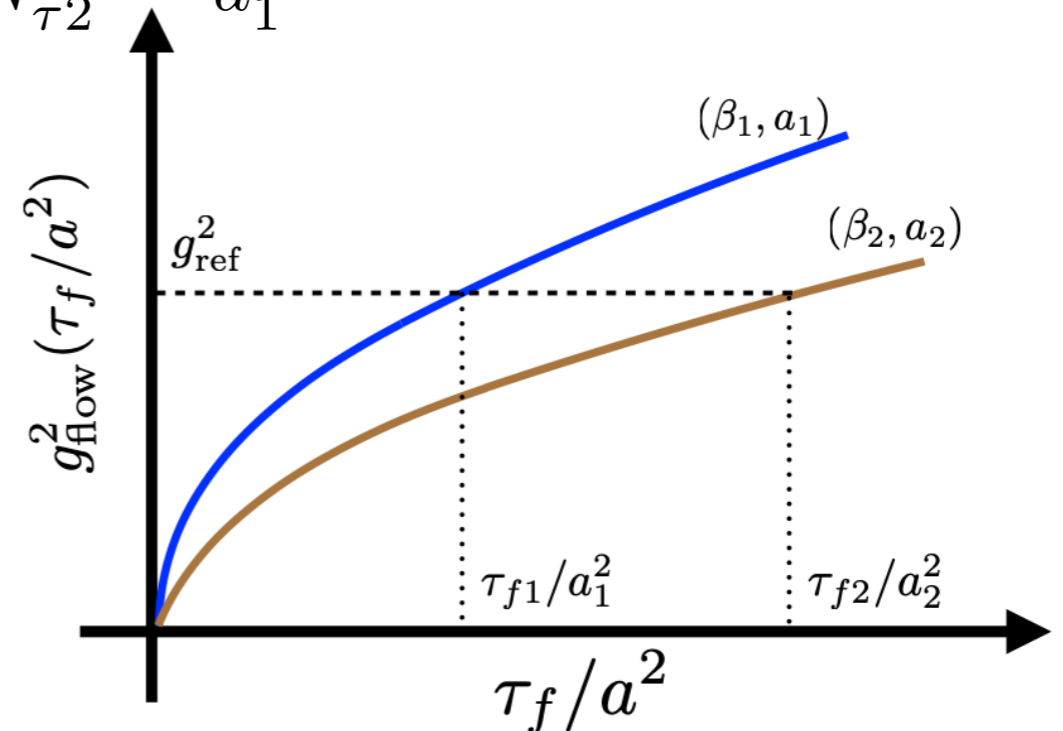
$$\frac{\tau_{f1}}{N_{\tau_1}^2 a_1^2} = \frac{\tau_{f2}}{N_{\tau_2}^2 a_2^2}$$



Relative Scale setting

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$$\frac{\tau_{f1}}{N_{\tau_1}^2 a_1^2} = \frac{\tau_{f2}}{N_{\tau_2}^2 a_2^2} \quad \frac{\tau_{f1}}{a_1^2} = s^2 \frac{\tau_{f2}}{a_2^2}, \quad s = \frac{N_{\tau_1}^2}{N_{\tau_2}^2} = \frac{a_2^2}{a_1^2}$$

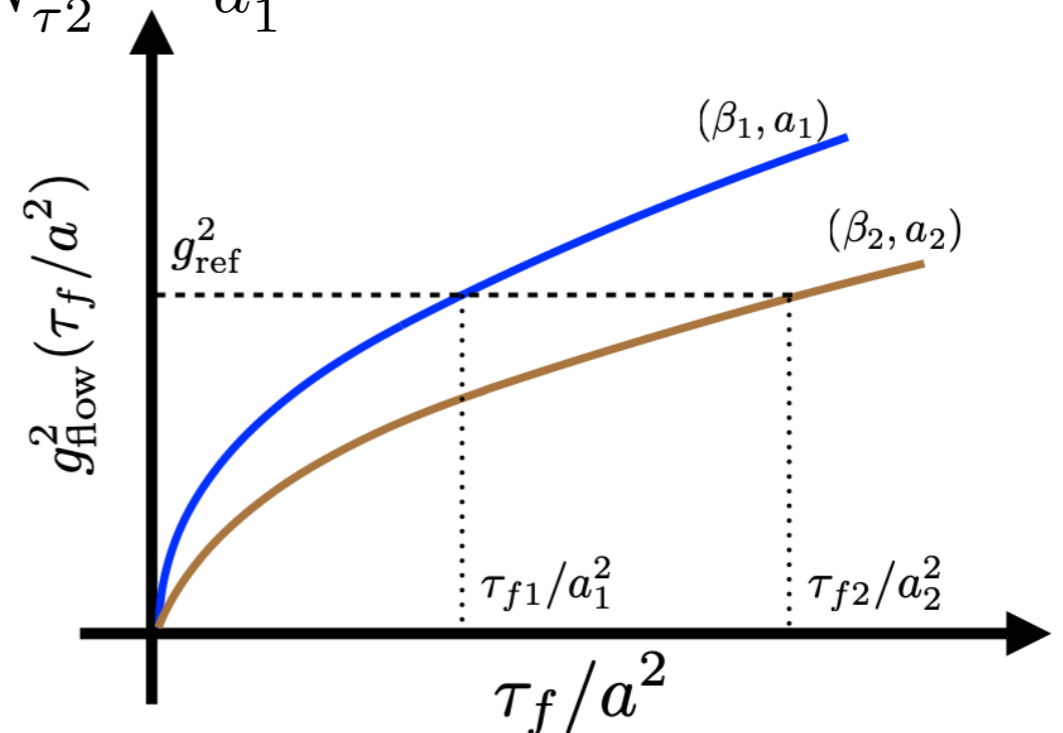


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- ❖ Can use this to set scale



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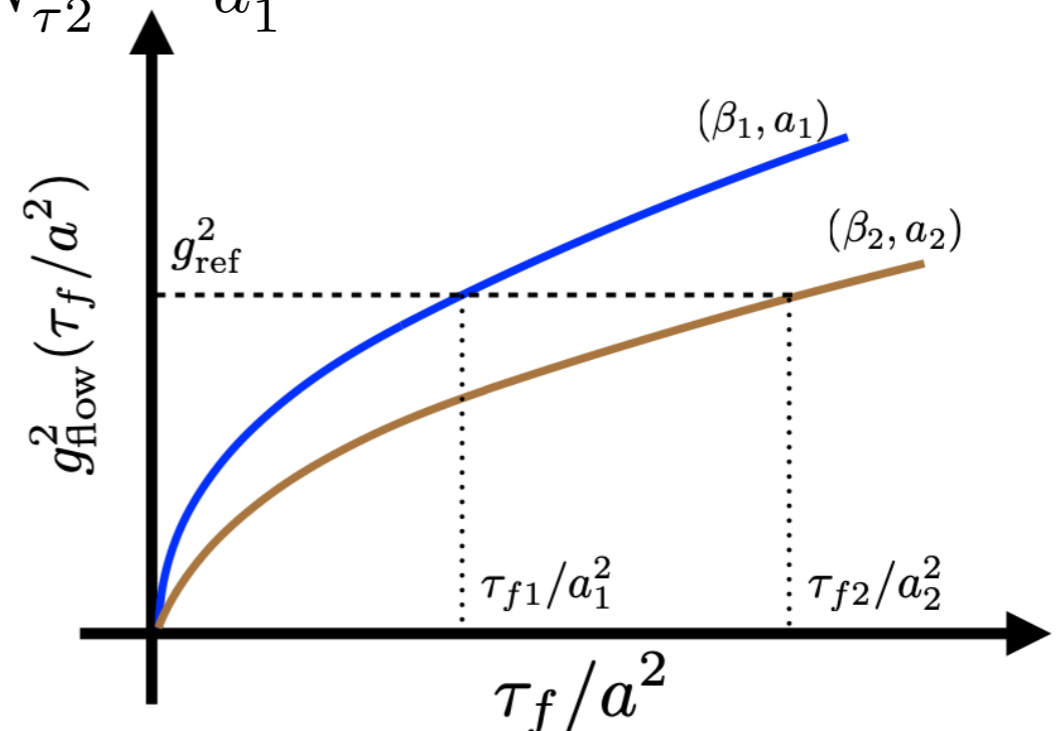
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- ❖ Can use this to set scale

- ❖ Two Issues :

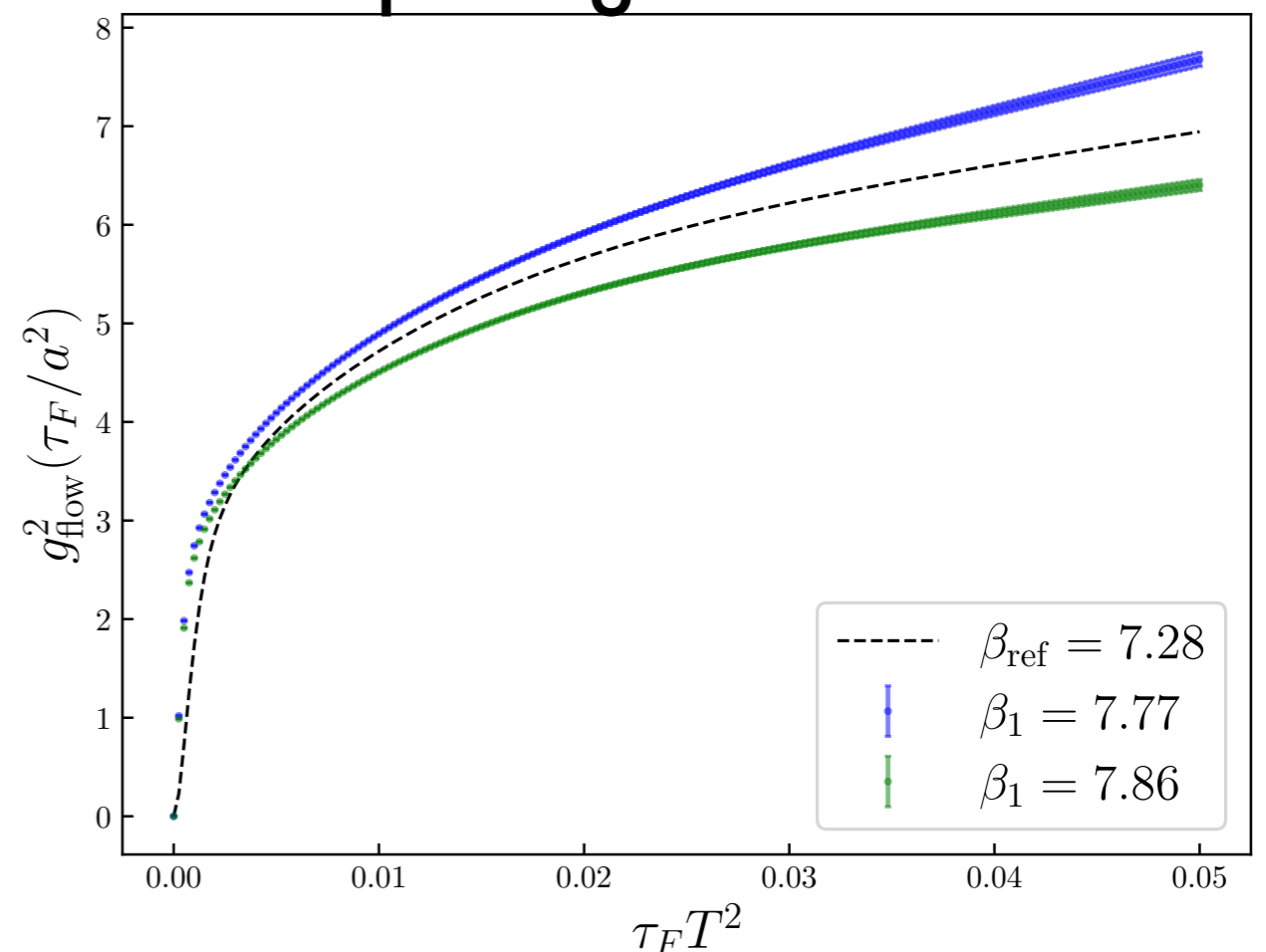
- ❖ Assumes β_2 is tuned

- ❖ Exists a procedure that accomplishes this



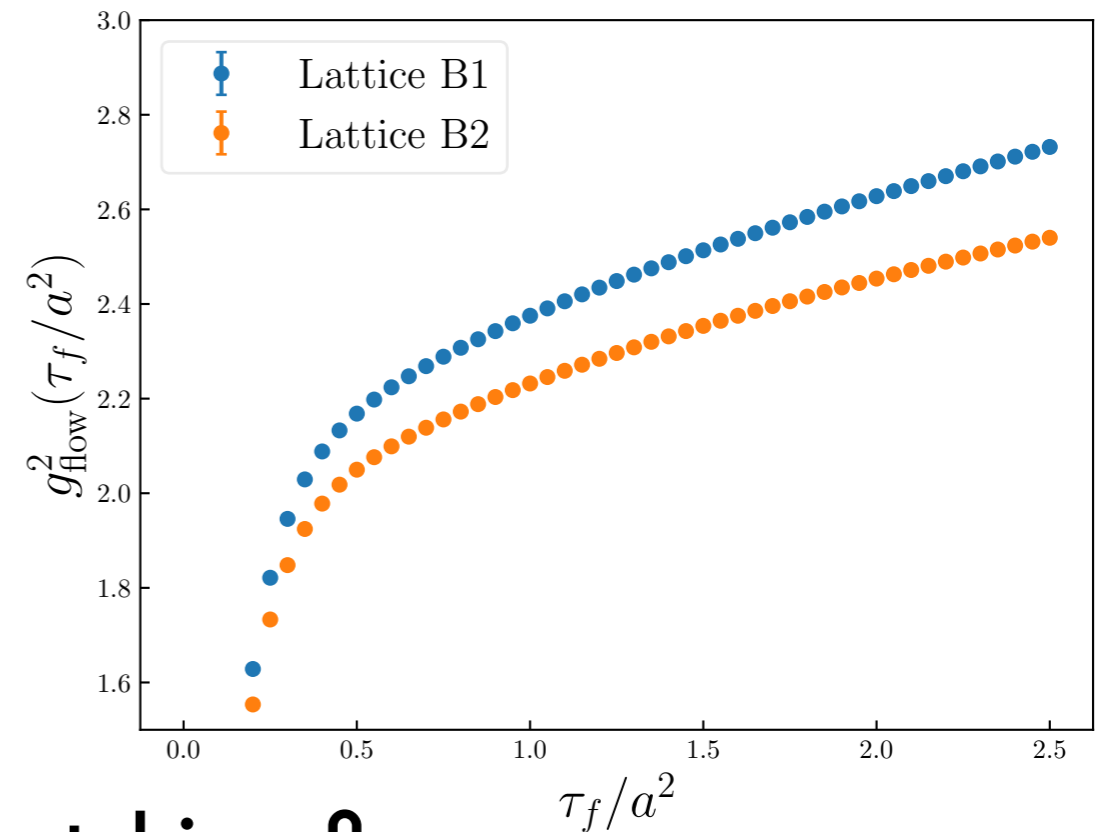
Gauge coupling tuning

- ✦ Relative scale setting implies prior knowledge of LCP
- ✦ MILC provides LCP data up to 0.04 fm
- ✦ Interpolate LCP data to target lattice spacing
- ✦ With 20% deviation, choose two couplings
- ✦ Interpolate in beta over several flow depths



Scale determination procedure

- ❖ Two gradient flows
 - ❖ B1 has well determined scale
 - ❖ Need to set the scale for tuned B2



- ❖ Would like to match two flows

- ❖ Chi-square like minimization for matching flows

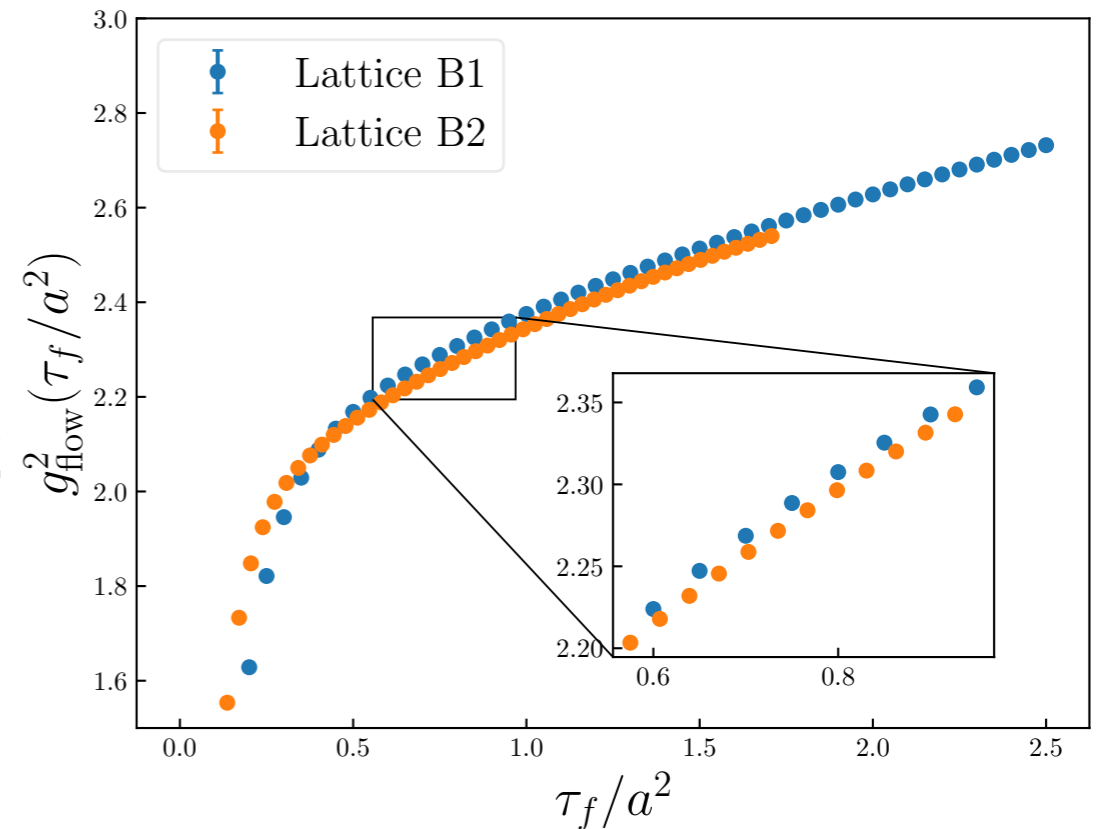
$$\Delta G(g_1^2(x_i), x_i, s) = \frac{1}{\sqrt{x_i}} (g_1^2(x_i) - p(x_i/s^2) \delta(A, B, x_i))$$

$$\chi^2(s, A, B, p(x)) = \Delta G(g_1^2(x_i), x_i, 1) C_{1,ij}^{-1} \Delta G(g_1^2(x_j), x_j, 1)$$

$$+ \Delta G(g_2^2(s x_l), s x_l, s) C_{2,lm}^{-1} \Delta G(g_2^2(s x_m), s x_m, s)$$

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$$+ \Delta G(g_2^2(s x_l), s x_l, s) C_{2,lm}^{-1} \Delta G(g_2^2(s x_m), s x_m, s)$$

Quark mass tuning

✦ Tune quark masses in $N_f = 2 + 1 + 1$ set up

✦ Tune only charm quarks and the rest from $m_l = \frac{m_s}{27.3}$, $m_s = \frac{m_c}{11.783}$

✦ Compute screening correlation functions of :

$$D_s(x) = \bar{c}_\alpha^j (\gamma_5)_{\alpha\beta} s_\beta^j(x)$$

$$D_c(x) = \bar{c}_\alpha^j (\gamma_5)_{\alpha\beta} c_\beta^j(x)$$

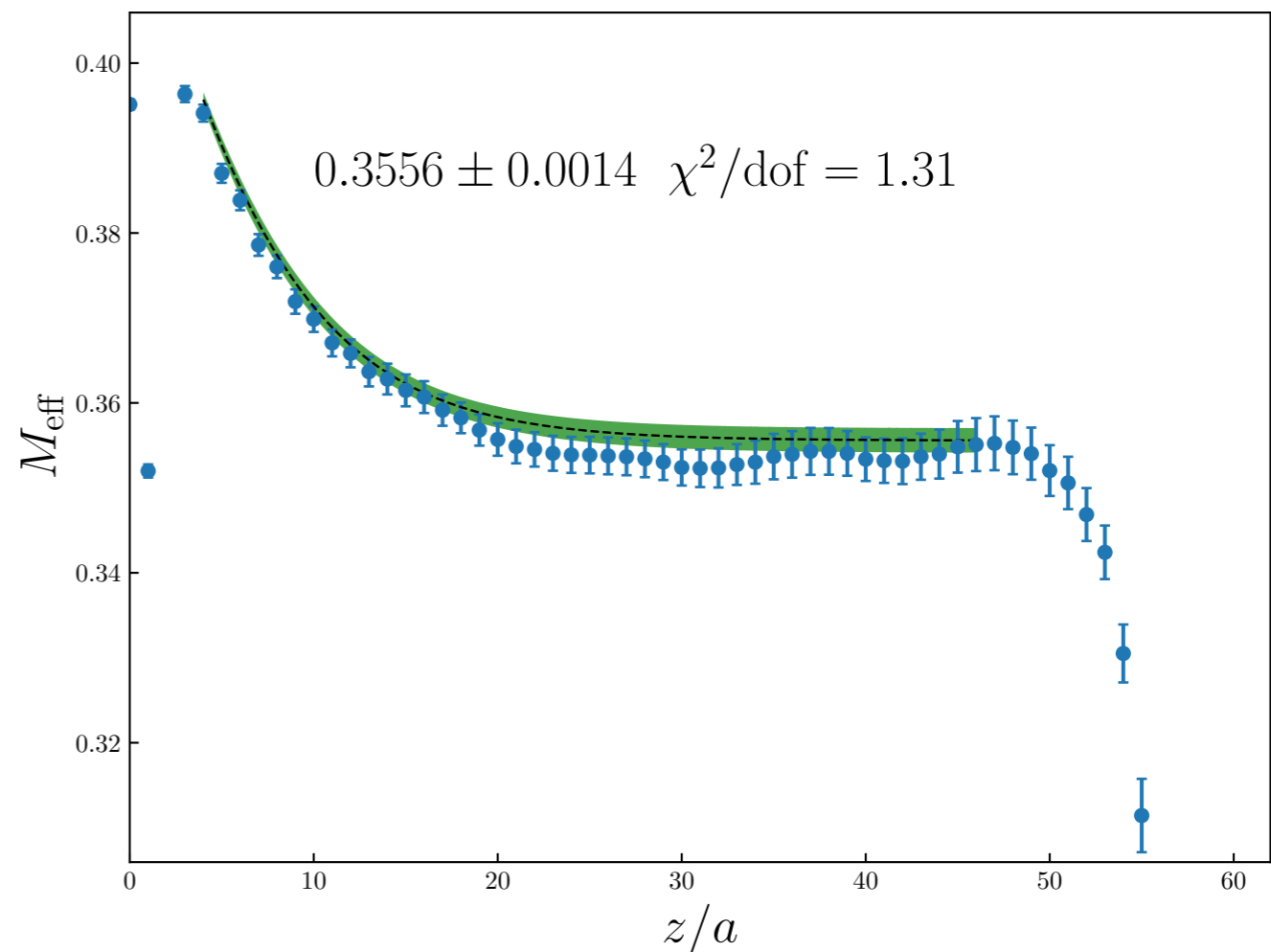
Complementary check

✦ Maintain z direction 6X longer than other spatial

✦ Generate 5 guesses with 20% deviation from original

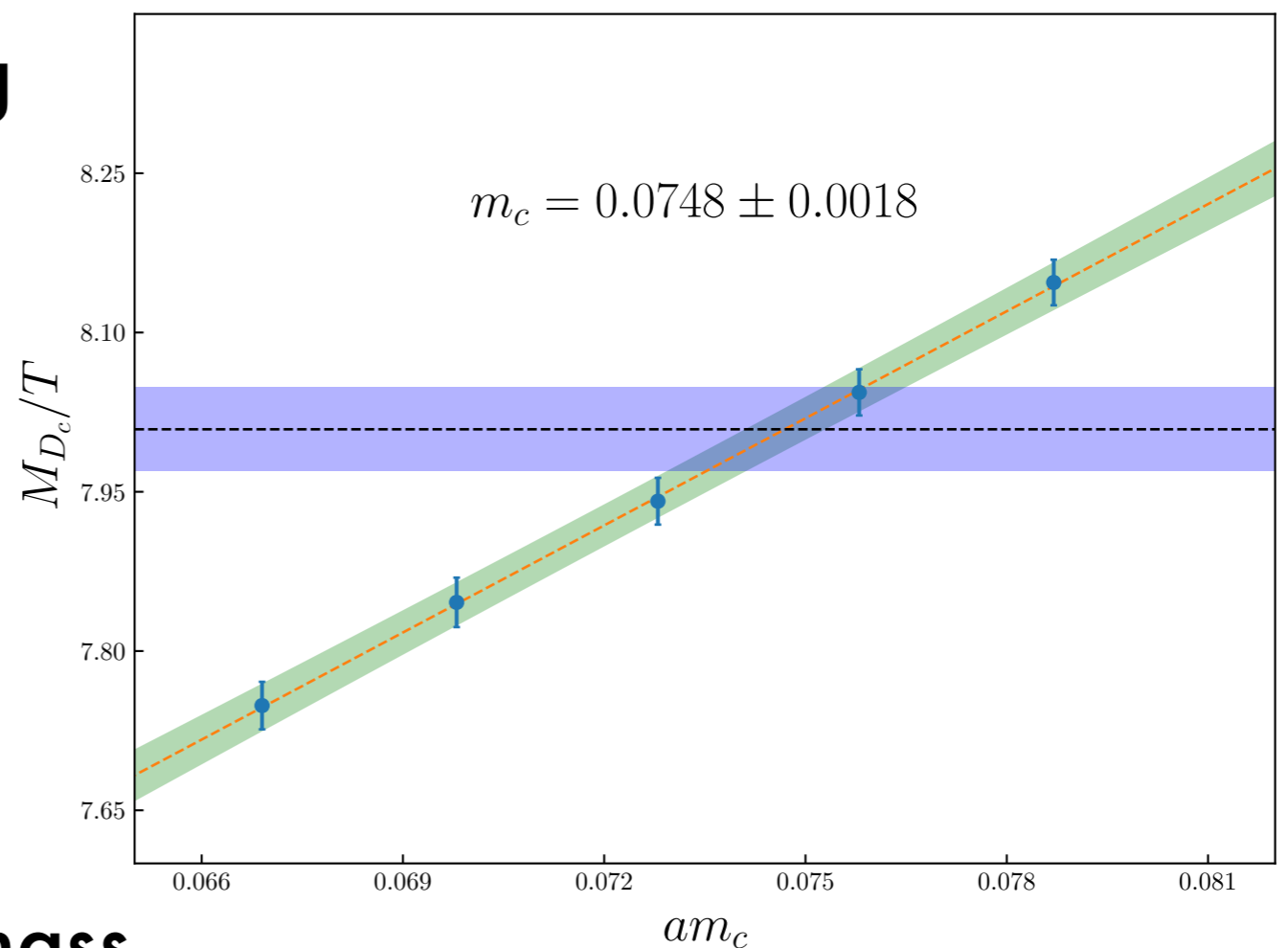
Quark mass tuning

- ❖ Momentum projected 12 equidistant sources
- ❖ Correlators averaged over sources
- ❖ Uncertainties account for autocorrelations
- ❖ Correlated two exponential fit.



Quark mass tuning

- ❖ Blue band – Screening mass corresponds to tuned quark mass
- ❖ Data points – Screening mass from each guess
- ❖ Green band – Linear fit to the data
- ❖ Shaded overlapping region – tuned quark mass



Final results

Extension of MILC scale to 0.013 fm

435 MeV

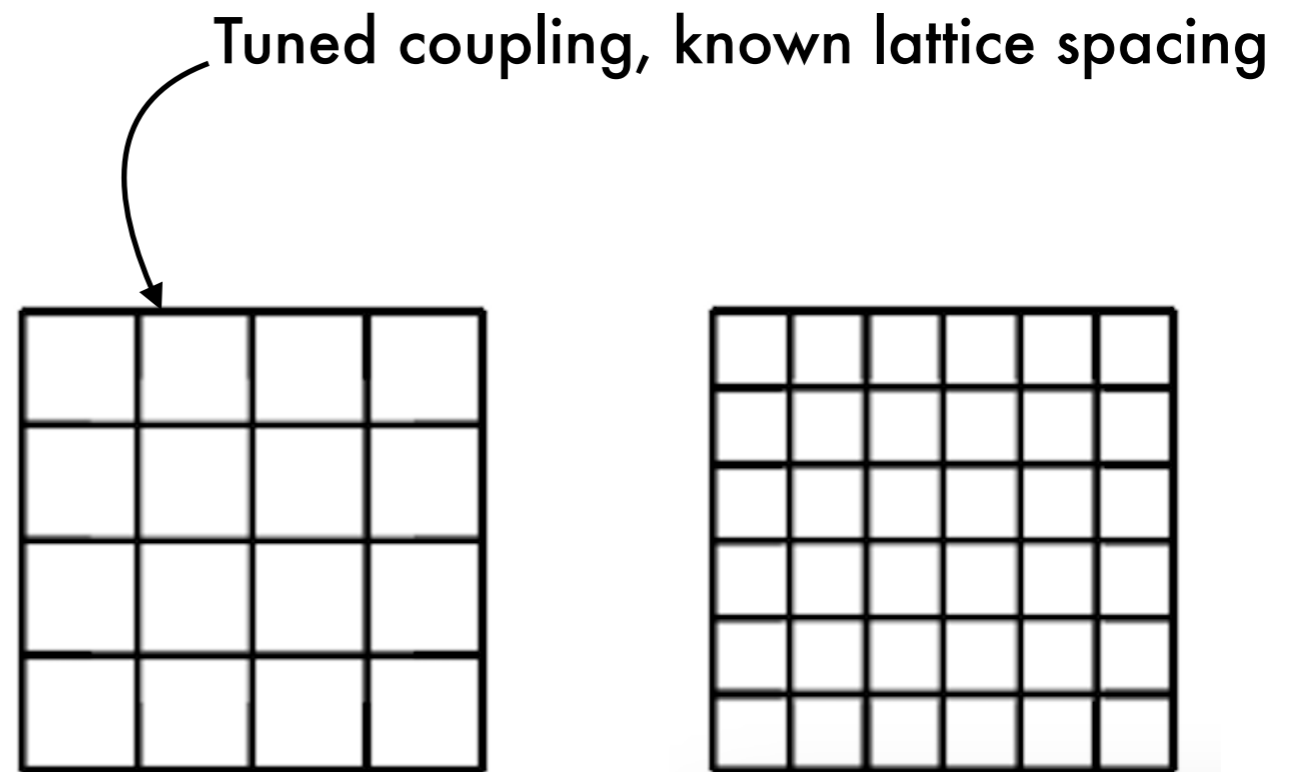
$$\beta = 6.72, a = 0.05662(13) \text{ fm}$$

341 MeV

$$\beta = 7.28, a = 0.03215(13) \text{ fm}$$

511 MeV

$$\beta = 7.28, a = 0.03215(13) \text{ fm}$$



Tune at finer lattice spacing

Final results

Extension of MILC scale to 0.013 fm

435 MeV

$$\beta = 6.72, a = 0.05662(13) \text{ fm}$$

$$\left\{ \begin{array}{l} \beta = 6.95, a = 0.04531(26) \text{ fm} \\ \beta = 7.13, a = 0.03786(12) \text{ fm} \end{array} \right.$$

341 MeV

$$\beta = 7.28, a = 0.03215(13) \text{ fm}$$

$$\left\{ \begin{array}{l} \beta = 7.15, a = 0.03626(9) \text{ fm} \\ \beta = 7.39, a = 0.02877(10) \text{ fm} \\ \beta = 7.715, a = 0.02084(15) \text{ fm} \end{array} \right.$$

511 MeV

$$\beta = 7.28, a = 0.03215(13) \text{ fm}$$

$$\left\{ \begin{array}{l} \beta = 7.60, a = 0.02400(4) \text{ fm} \\ \beta = 7.82, a = 0.01936(19) \text{ fm} \\ \beta = 8.045, a = 0.01599(18) \text{ fm} \\ \beta = 8.22, a = 0.01372(11) \text{ fm} \end{array} \right.$$

Thank you