Nuclear reactions from lattice QCD simulations

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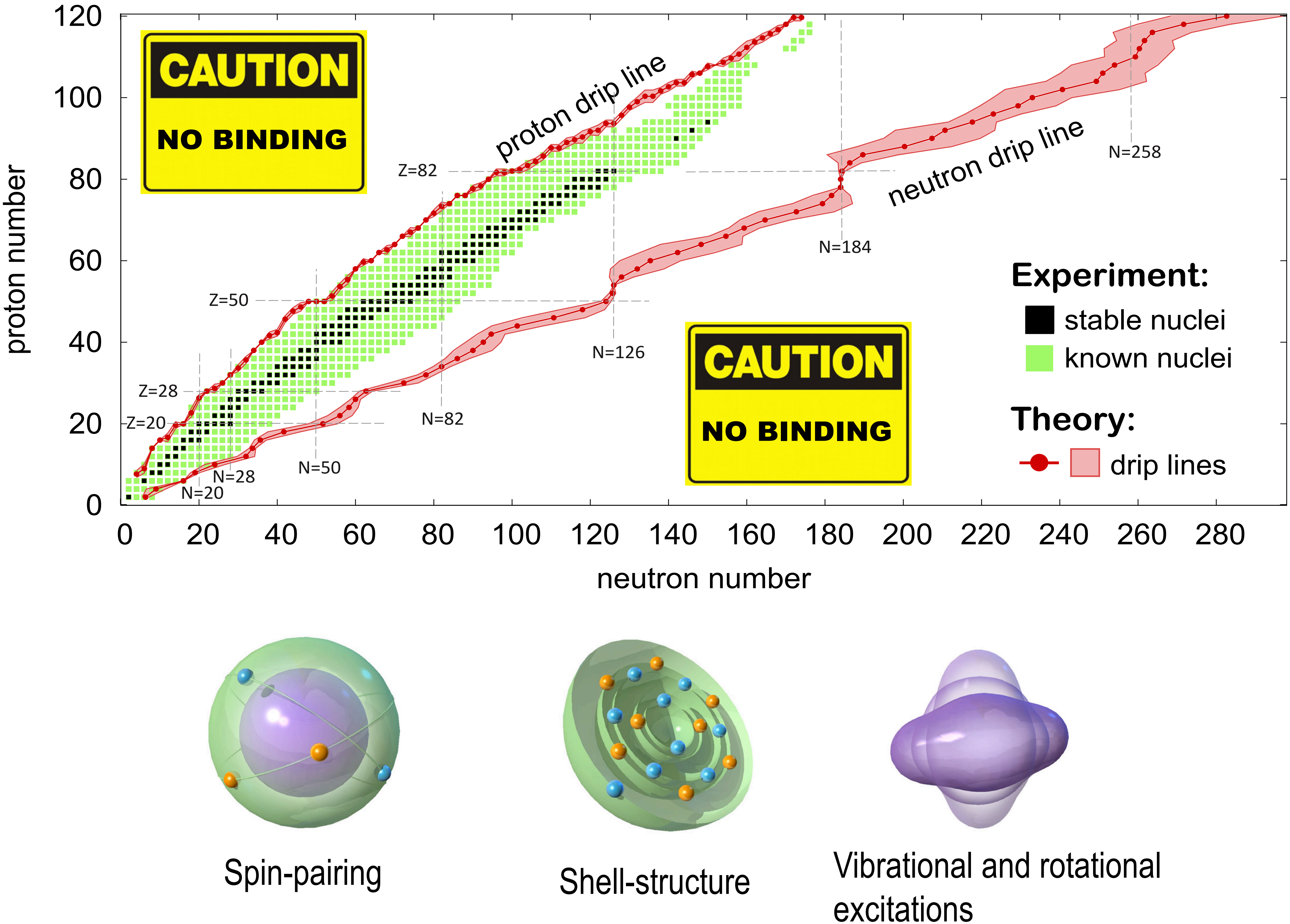
Erice 9/18/2018

NPLQCD: UNPHYSICAL NUCLEI

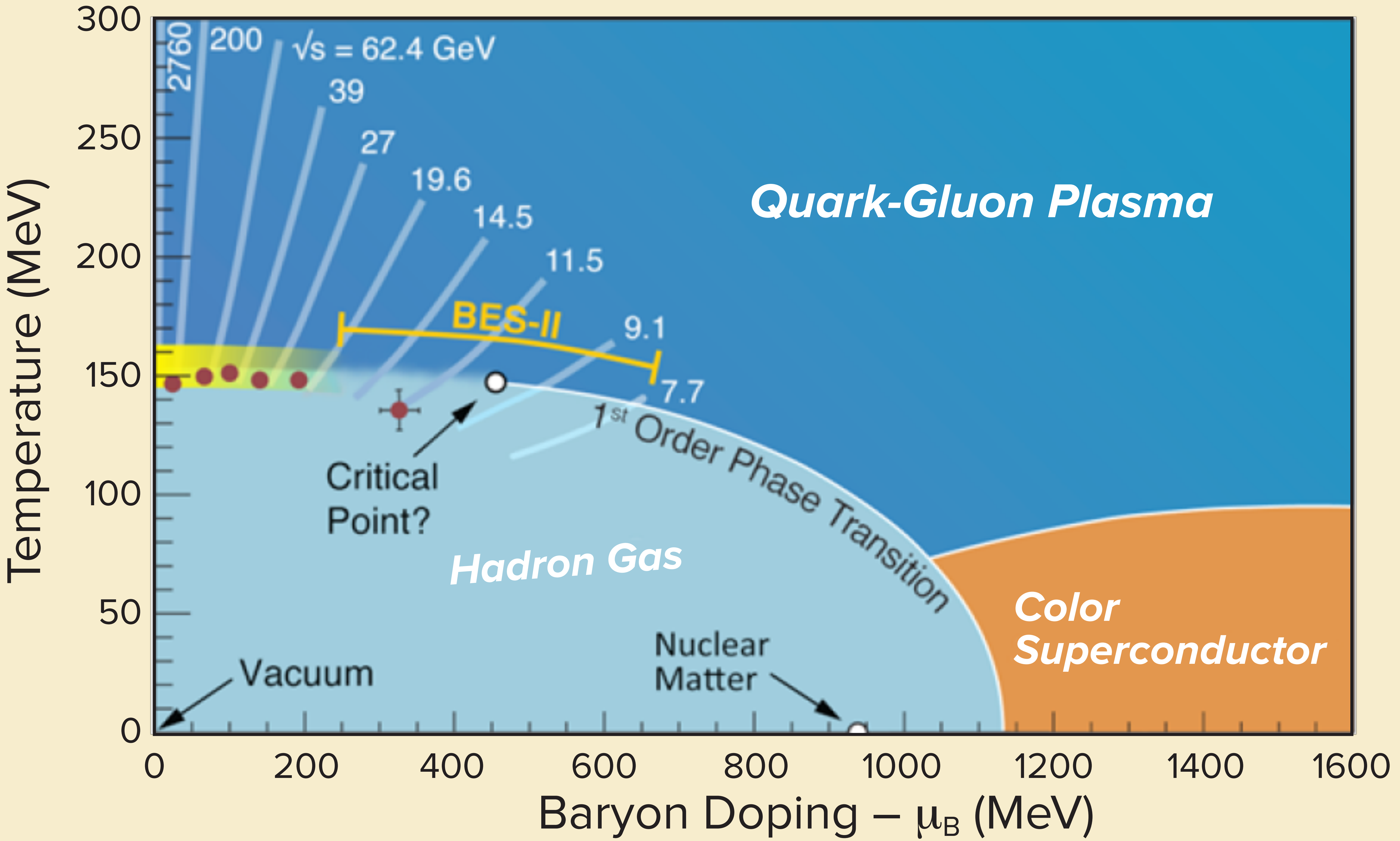
- Case study LQCD with unphysical quark masses (m_π~800 MeV, 450 MeV)

1. Spectrum and scattering of light nuclei (A<5) [PRD 87 (2013), 034506]
2. Nuclear structure: magnetic moments, polarisabilities (A<5) [PRL **113**, 252001 (2014), PRL **116**, 112301 (2016)]
3. Nuclear reactions: np→dγ [PRL **115**, 132001 (2015)]
4. Gamow-Teller transitions: pp→deν, $g_A(^3H)$ [PRL **119** 062002 (2017)]
5. Double β decay: pp→nn [PRL **119**, 062003 (2017)]
6. Gluon structure (A<4) [PRD **96** 094512 (2017)]
7. Scalar/tensor currents (A<4) [PRL **120** 152002 (2018)]

★ Together with the electroweak theory, QCD underlies all the interesting nuclear and strong-interaction phenomena that we study.



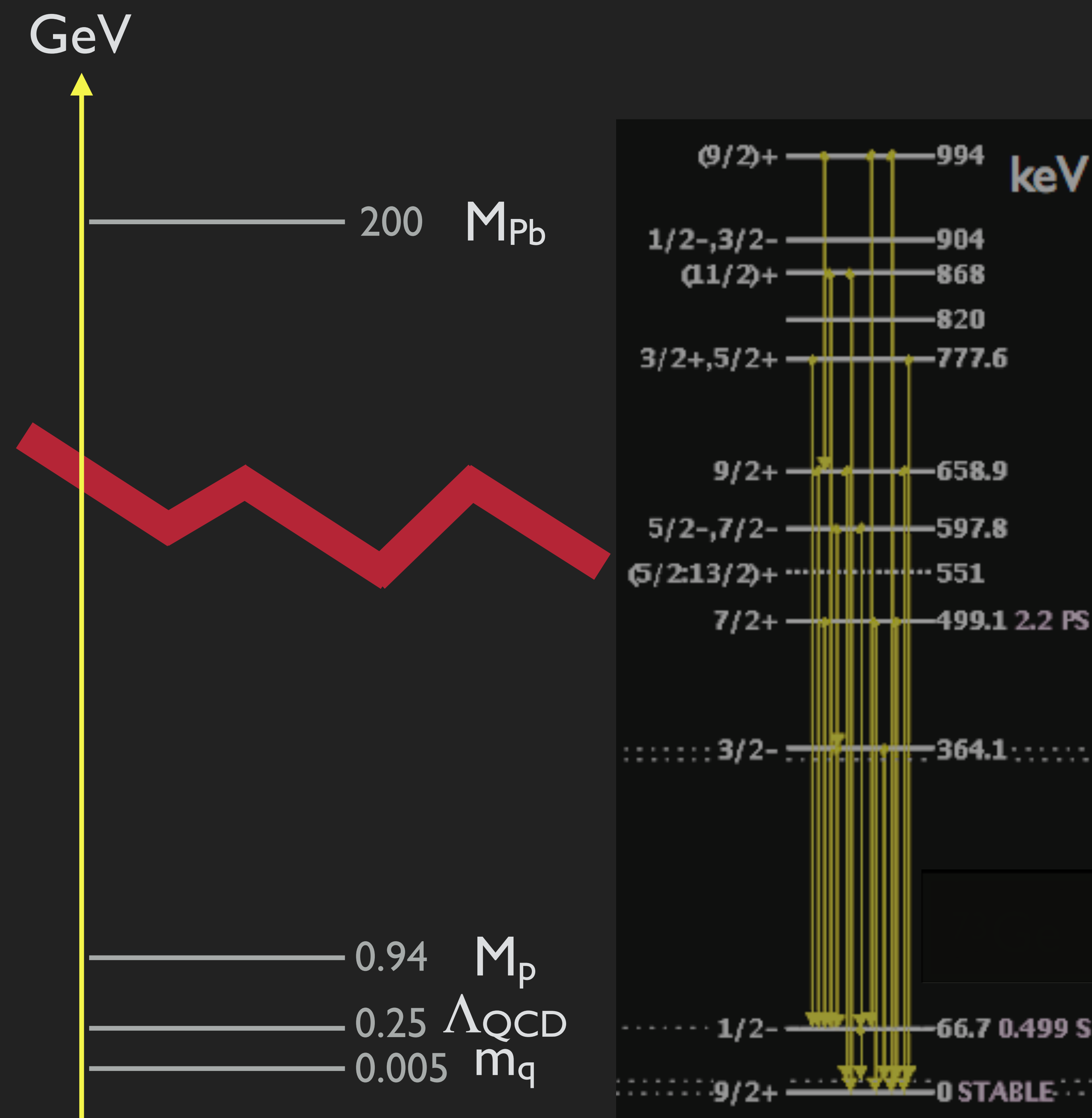
CAUTION
NO BINDING
CAUTION
NO BINDING
proton drip line
neutron drip line
Z=82
Z=50
Z=28
Z=20
N=20
N=28
N=50
N=82
N=126
N=184
N=258
proton number
neutron number
Experiment:
stable nuclei
known nuclei
Theory:
drip lines
Spin-pairing
Shell-structure
Vibrational and rotational excitations



Quark-Gluon Plasma
Hadron Gas
Color Superconductor
√s = 62.4 GeV
2760
200
39
27
19.6
14.5
11.5
9.1
7.7
BES-II
Critical Point?
1st Order Phase Transition
Nuclear Matter
Vacuum
Temperature (MeV)
Baryon Doping – μB (MeV)
300
250
200
150
100
50
0
0
200
400
600
800
1000
1200
1400
1600

In principle can calculate properties of any nucleus from QCD and EW

Multi-scale physics with at least two exponentially difficult computational challenges

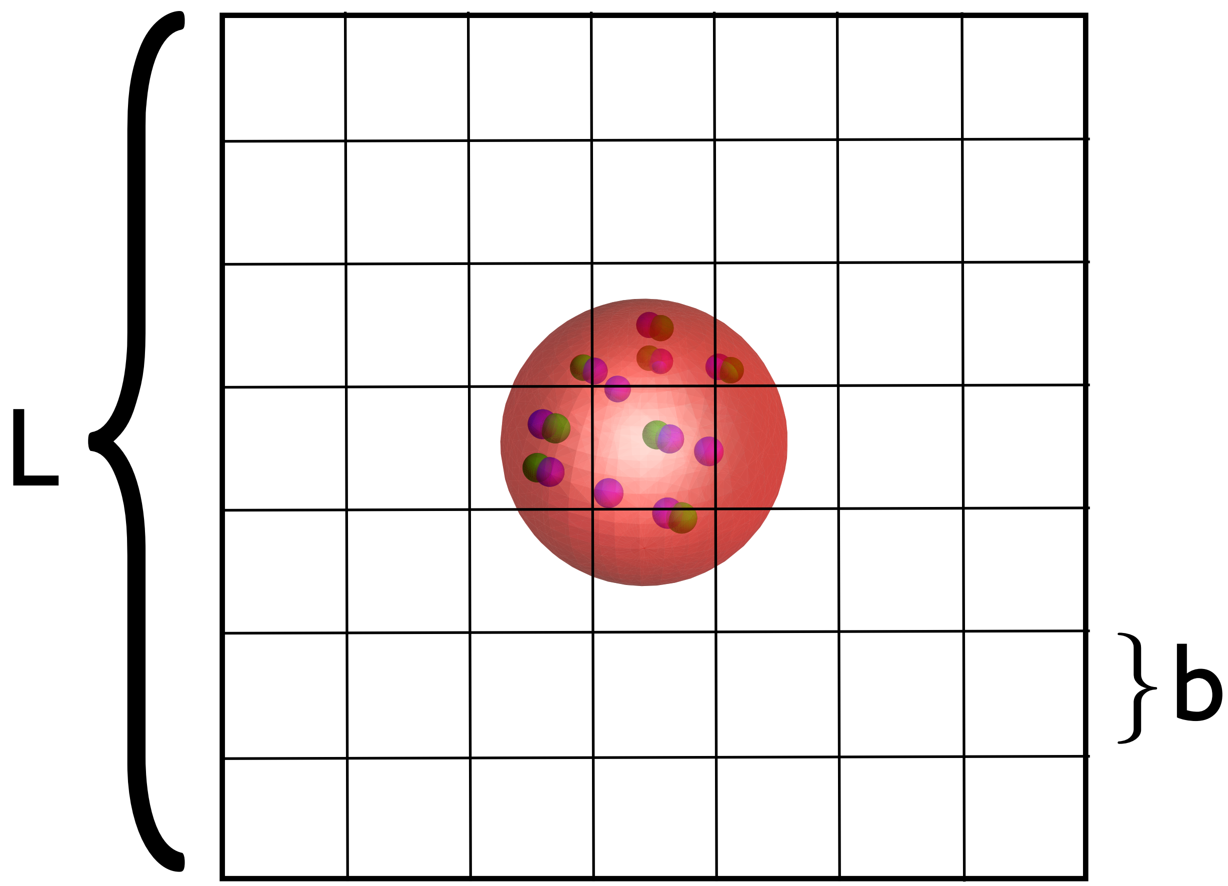


Outline

- Lattice QCD primer
- Bottlenecks: signal-to-noise
- Light nuclei and BB scattering
- External probes and nuclear reactions

Lattice QCD = QCD on a grid or lattice

Non-perturbative definition of QCD



volume: $M_\pi L \gg 1$

infrared cutoff

lattice spacing: $b \ll M_N^{-1}$

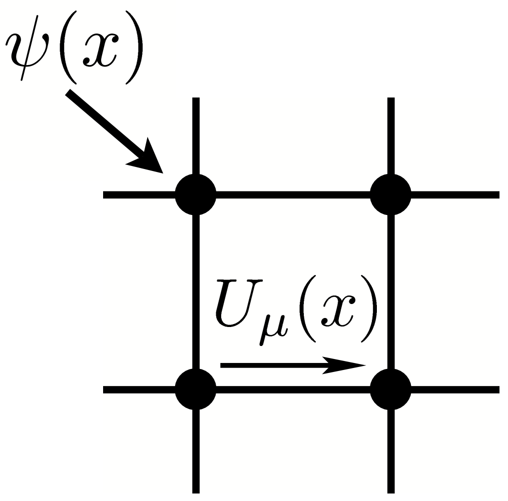
ultraviolet cutoff

Can use Effective Field Theory to extrapolate in L and b!

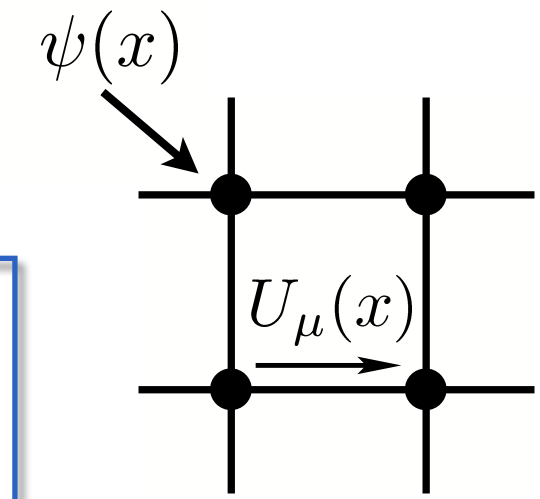
(systematic uncertainties from lattice artifacts are controlled)

QCD path integral with Montecarlo

$$\langle \mathcal{O} \rangle \sim \int dU_\mu \, d\bar{\psi} \, d\psi \; \mathcal{O}\left(U, \psi, \bar{\psi}\right) \; e^{-S_g(U) - \bar{\psi} D(U) \psi}$$



QCD path integral with Montecarlo



$$\langle \mathcal{O} \rangle \sim \int dU_\mu \, d\bar{\psi} \, d\psi \; \mathcal{O}\left(U, \psi, \bar{\psi}\right) \; e^{-S_g(U) - \bar{\psi} D(U) \psi}$$

propagators
(detector)

N gauge configurations
(accelerator)

$$\langle \mathcal{O} \rangle \sim \int dU_\mu \, \mathcal{O}(D(U)^{-1}) \;\; \det\left(f(U)\right) \;\; e^{-S_g(U)}$$

$$= \lim_{N \to \infty} \frac{1}{N} \sum_{i=1}^{N} \mathcal{O}(D(U_i)^{-1})$$

Estimate of $\mathcal{O}$ with $\sigma_{\mathcal{O}} \sim 1/\sqrt{N}$

Correlators in Euclidean Space

$$\pi^+(\mathbf{x},t) = \overline{u}(\mathbf{x},t)\gamma_5 d(\mathbf{x},t)$$

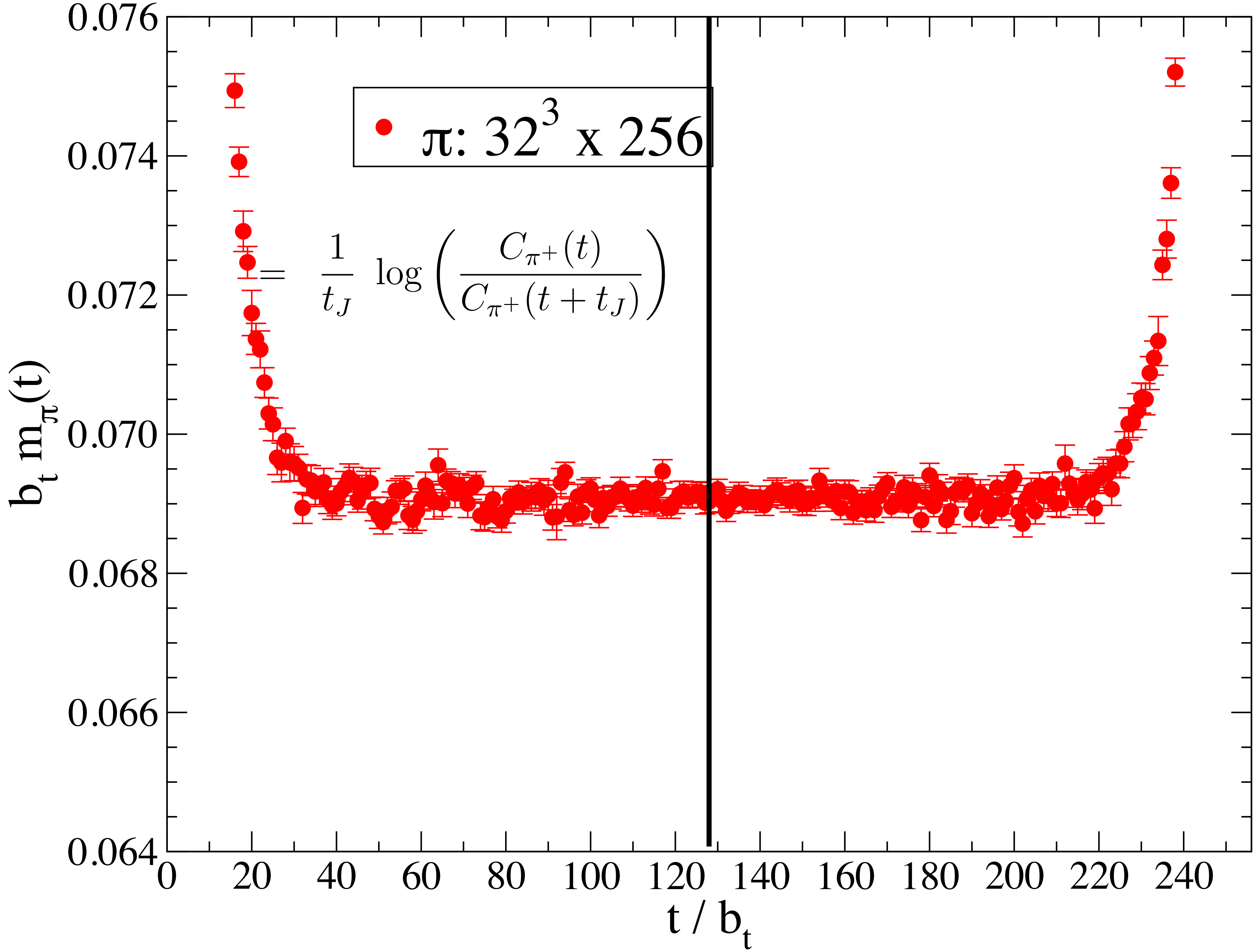
$$C_{\pi^+}(t) \;=\; \sum_{\mathbf{x}} \langle 0|\ \pi^-(\mathbf{x},t)\ \pi^+(\mathbf{0},0)\ |0\rangle$$

$$\pi^+(\mathbf{x},t) = e^{\hat{H}t}\pi^+(\mathbf{x},0)e^{-\hat{H}t}$$

$$C_{\pi^+}(t) \;=\; \sum_n \frac{e^{-E_n t}}{2E_n} \sum_{\mathbf{x}} \langle 0|\ \pi^-(\mathbf{x},0)|n\rangle\langle n|\pi^+(\mathbf{0},0)|0\rangle \;\rightarrow\; A_0\ \frac{e^{-m_\pi t}}{2m_\pi}$$

Infinite sum of exponentials: $E_0 = m_\pi = \frac{1}{t_J}\log\left(\frac{C_{\pi^+}(t)}{C_{\pi^+}(t+t_J)}\right)$

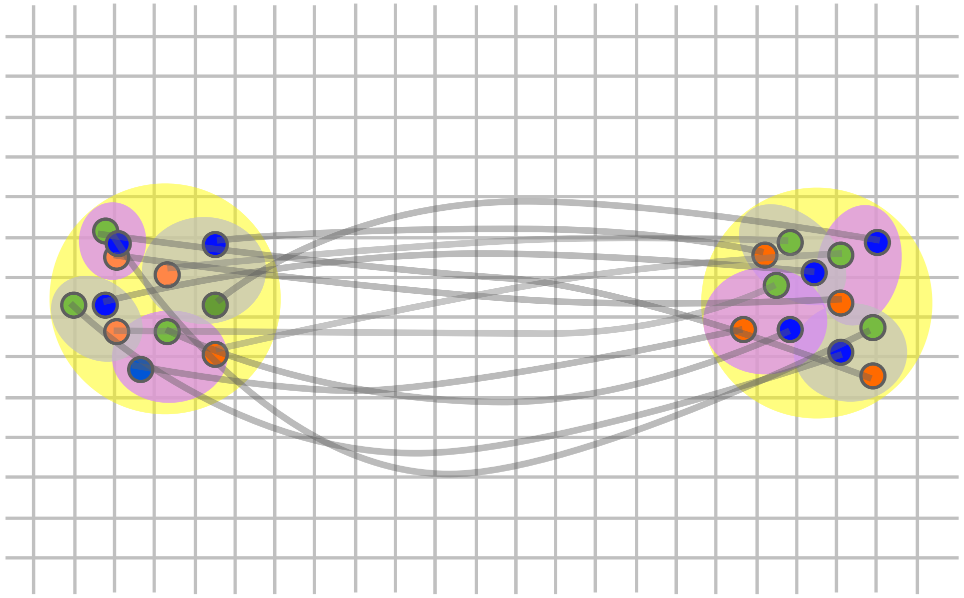
$$C_{\pi^+}(t) \;=\; \sum_{\mathbf{x}} \langle 0|\ \pi^-(\mathbf{x},t)\ \pi^+(\mathbf{0},0)\ |0\rangle \;\longrightarrow e^{-m_\pi t}\ \ \ldots$$



Why is lattice QCD for nuclear physics hard ?

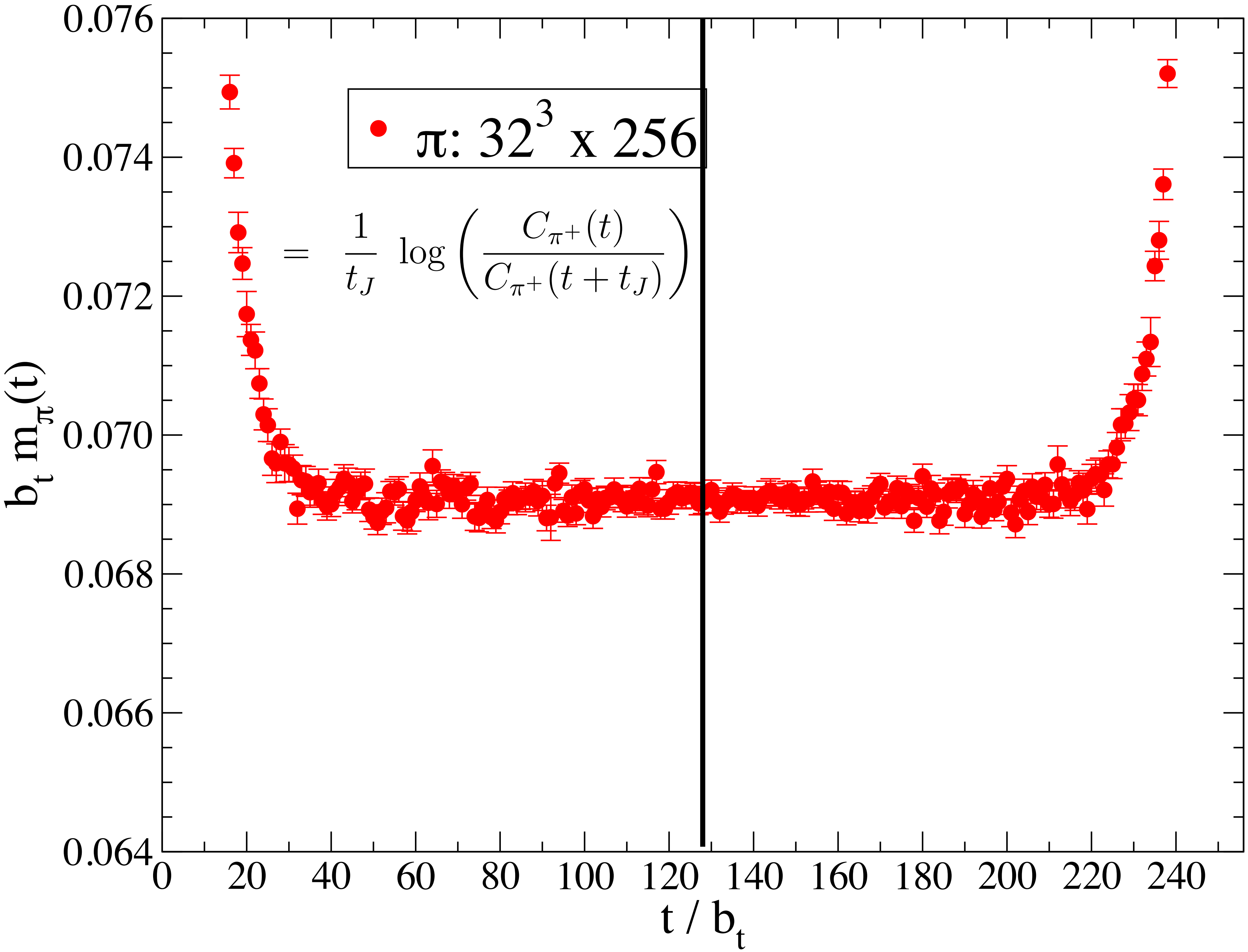
- Signal/noise (sign problem) and statistics
- Number of contractions

[Detmold,Orginos(2012),Doi,Endres(2012)]

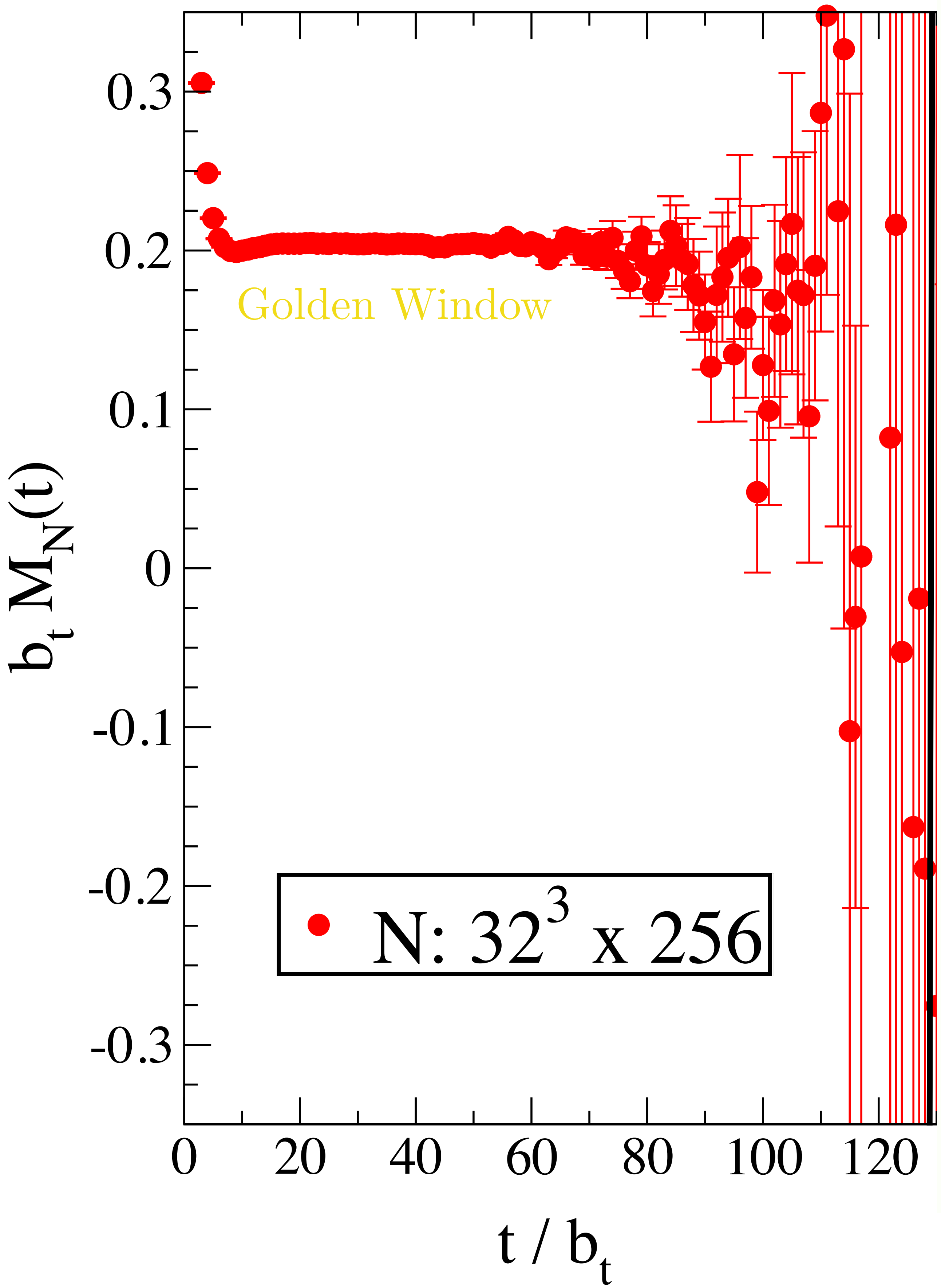


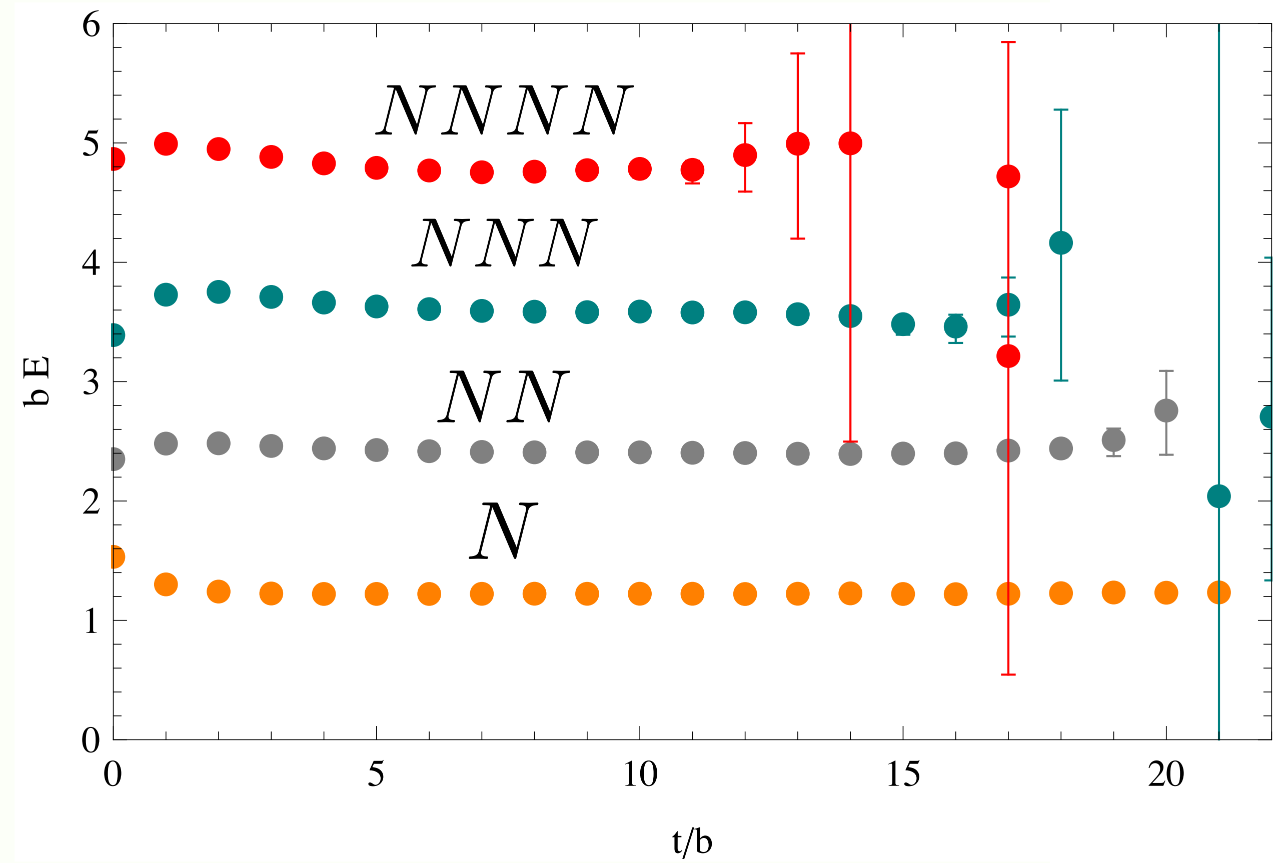
Signal/Noise Problem

$$C_{\pi^+}(t) \;=\; \sum_{\mathbf{x}} \langle 0|\; \pi^-(\mathbf{x},t)\; \pi^+(\mathbf{0},0)\; |0\rangle \longrightarrow e^{-m_\pi t} \quad \ldots$$



pions are easy! (i.e. cheap)



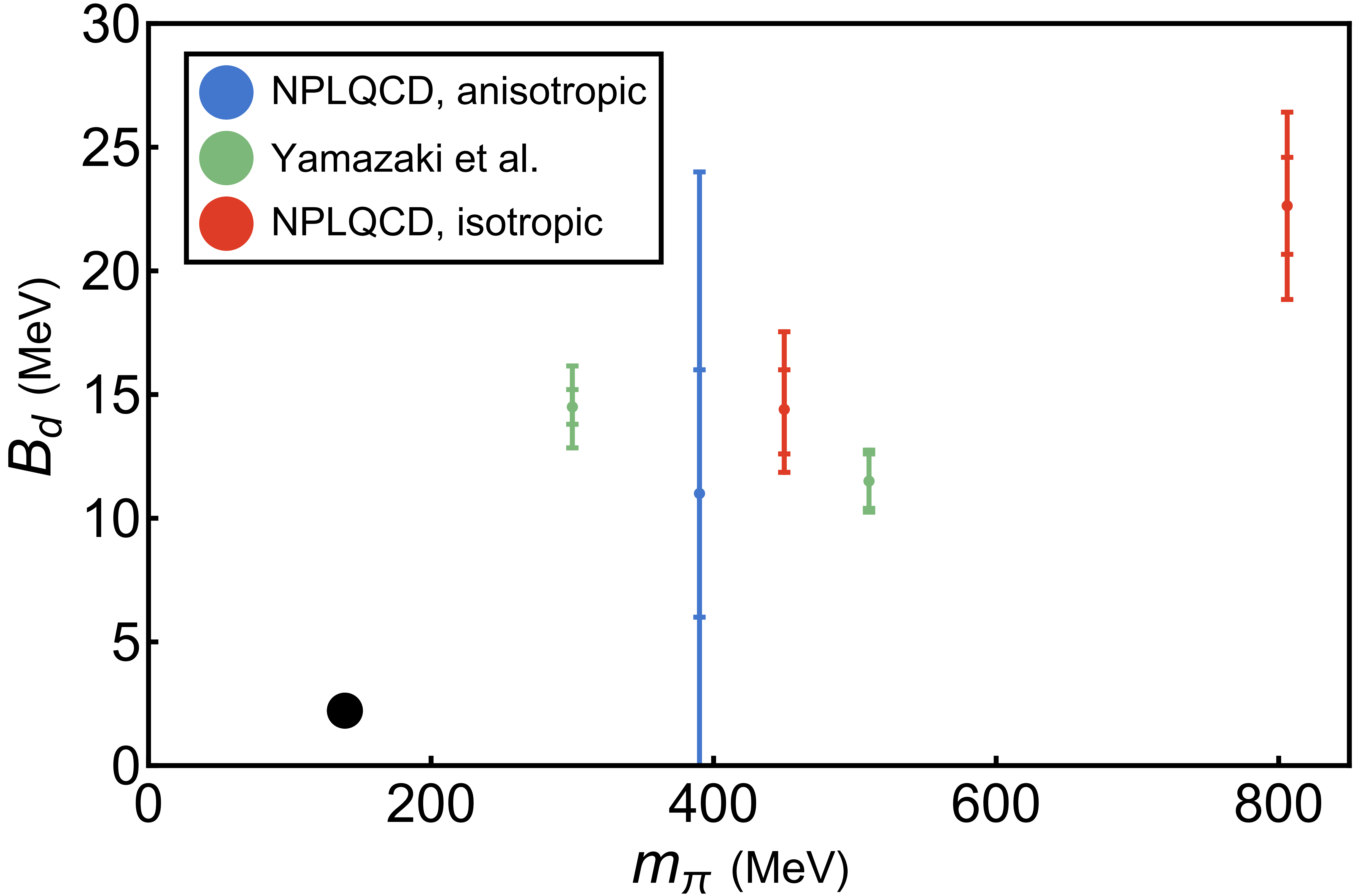


$$\frac{\text{noise}}{\text{signal}} \sim \frac{1}{\sqrt{N}}\; e^{A\left(m_p - \frac{3}{2}m_\pi\right)t}$$

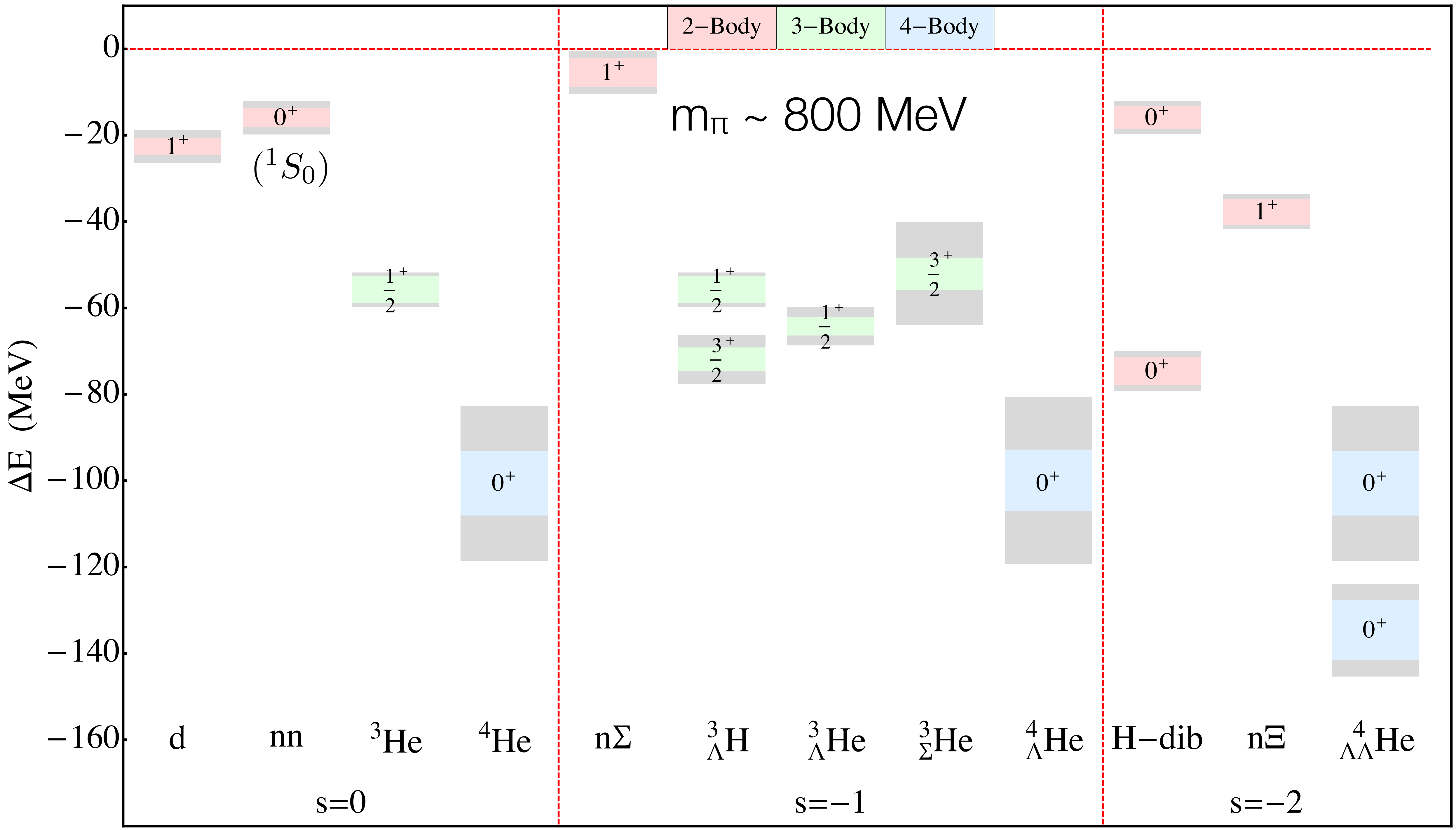
baryons are hard! (i.e. costly)

(Need quantum computers?)

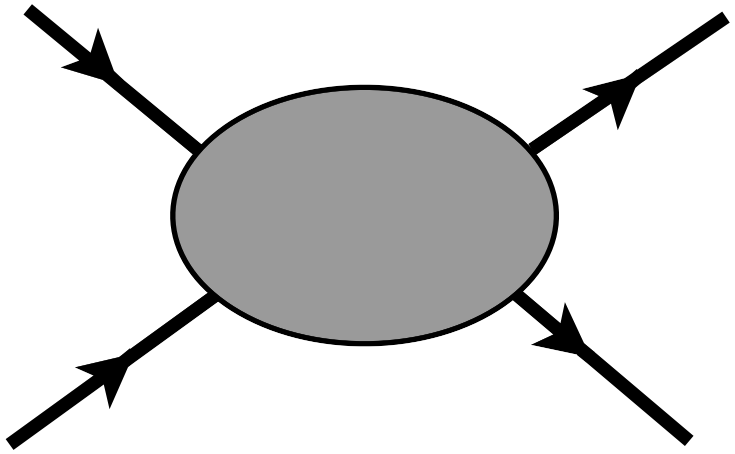
Deuteron binding energy from LQCD



Light (Hyper)Nuclei at SU(3) point



Nucleon-nucleon scattering



$$k \cot \delta \;=\; -\frac{1}{a} \;+\; \frac{1}{2} r |\mathbf{k}|^2 \;+\; P |\mathbf{k}|^4 \;+\; \mathcal{O}\left(|\mathbf{k}|^6\right)$$

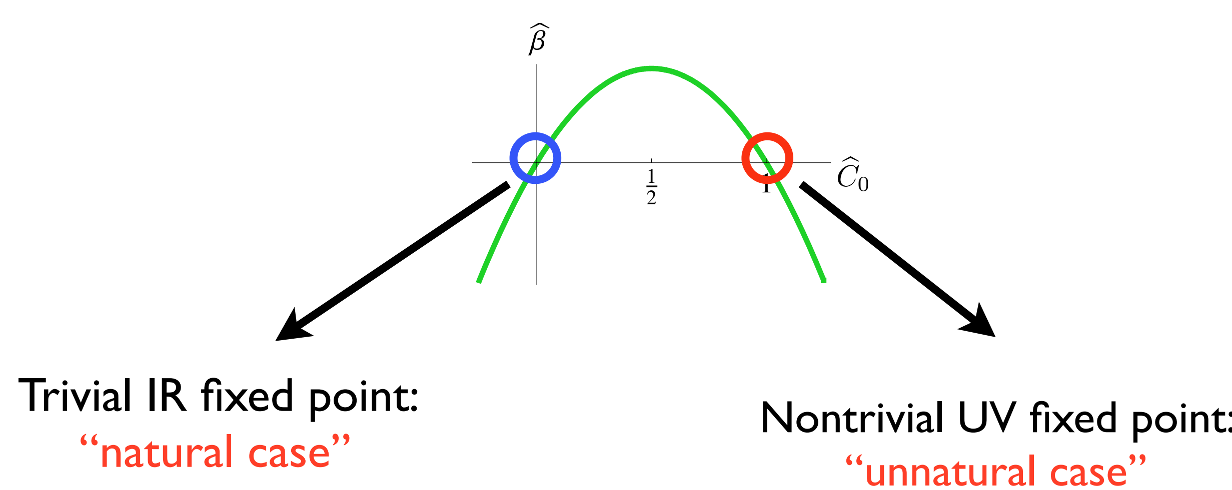
effective range: range of interaction

scattering length: unbounded

EXPERIMENT:

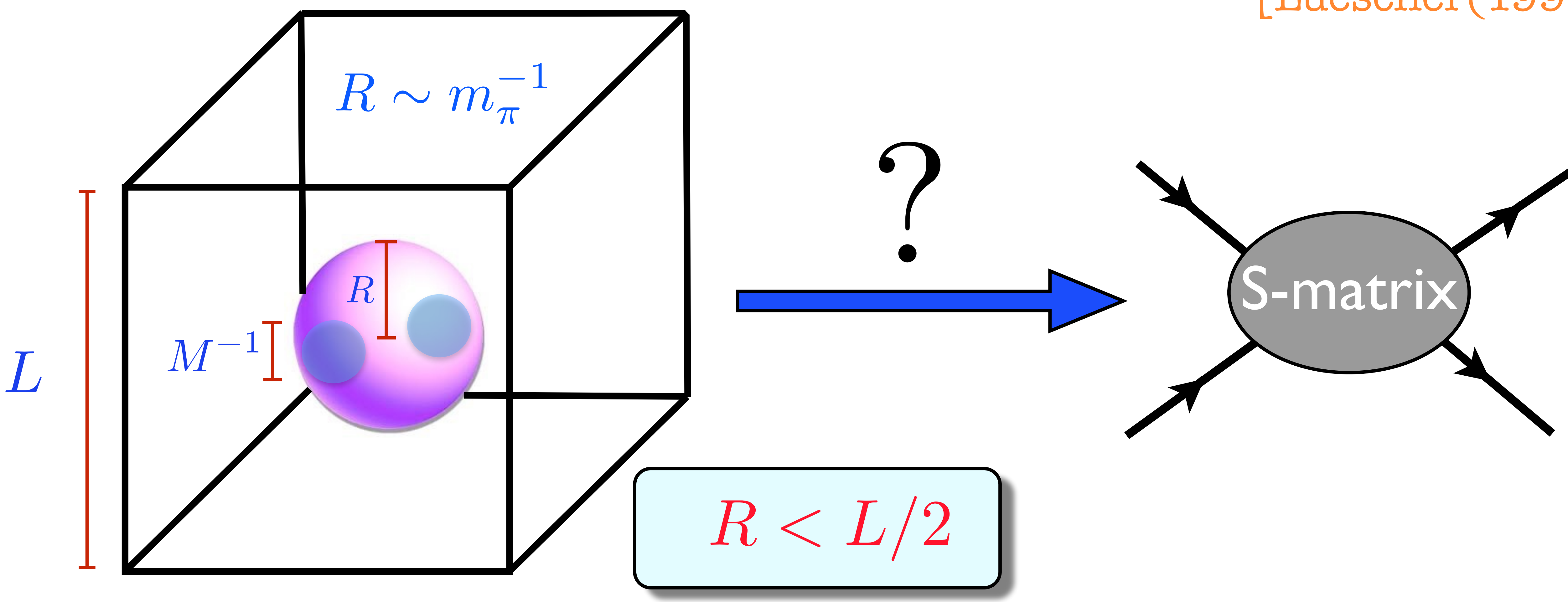
$a^{({}^1S_0)} = -23.71 \text{ fm}$		$a^{({}^3S_1)} = 5.43 \text{ fm}$	
$r^{({}^1S_0)} = 2.73 \text{ fm}$		$r^{({}^3S_1)} = 1.75 \text{ fm}$	

$$a^{({}^1S_0)} \gg \Lambda_{QCD}^{-1}$$

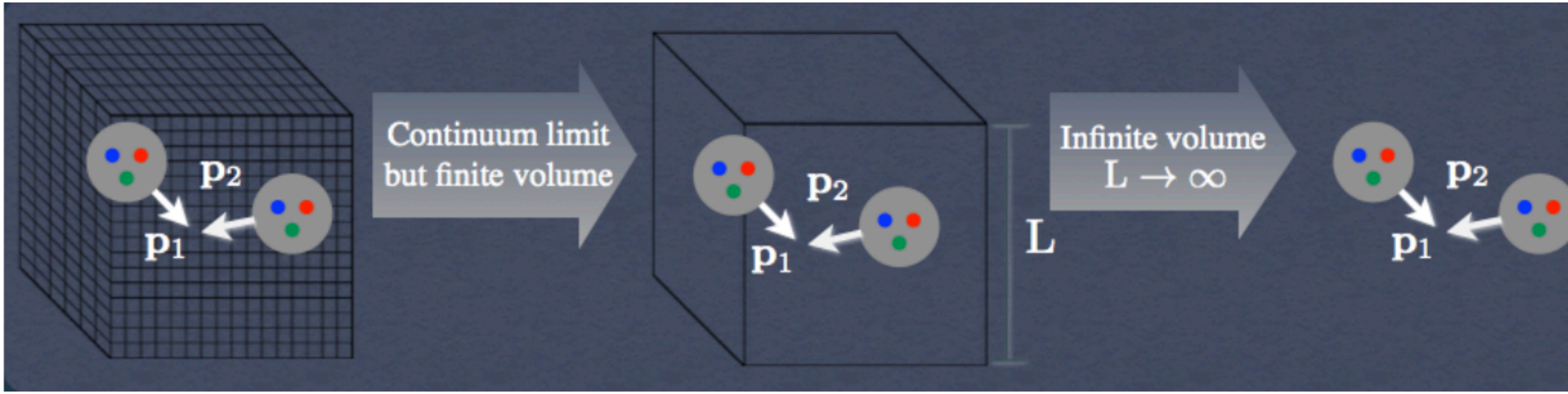


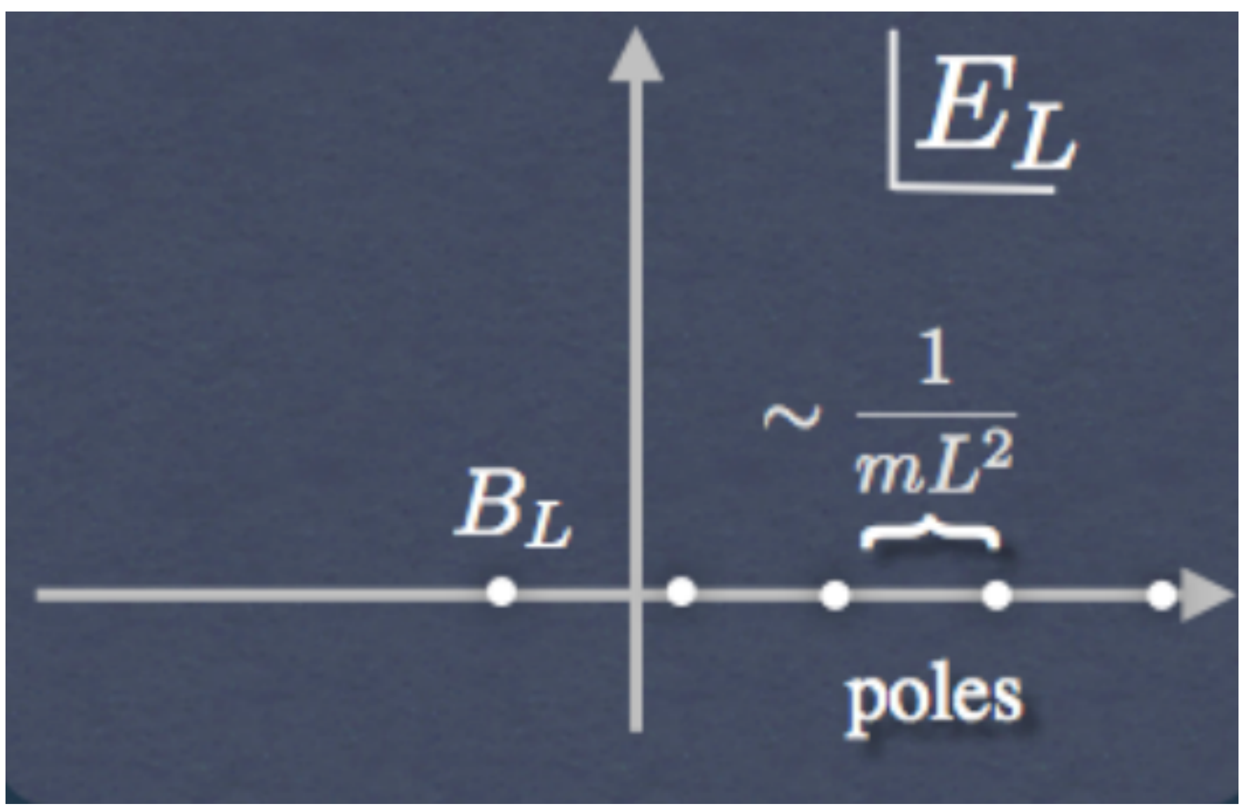
Scattering in a finite volume

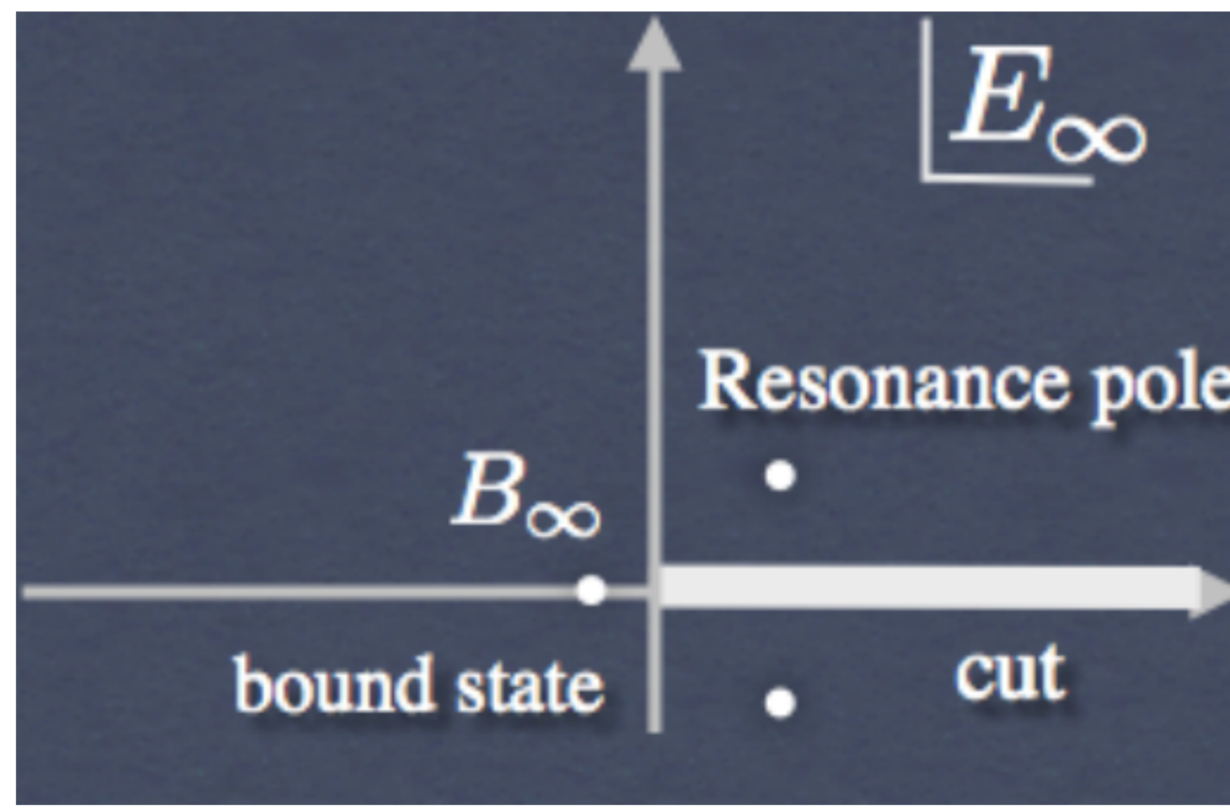
[Luescher(1990)]



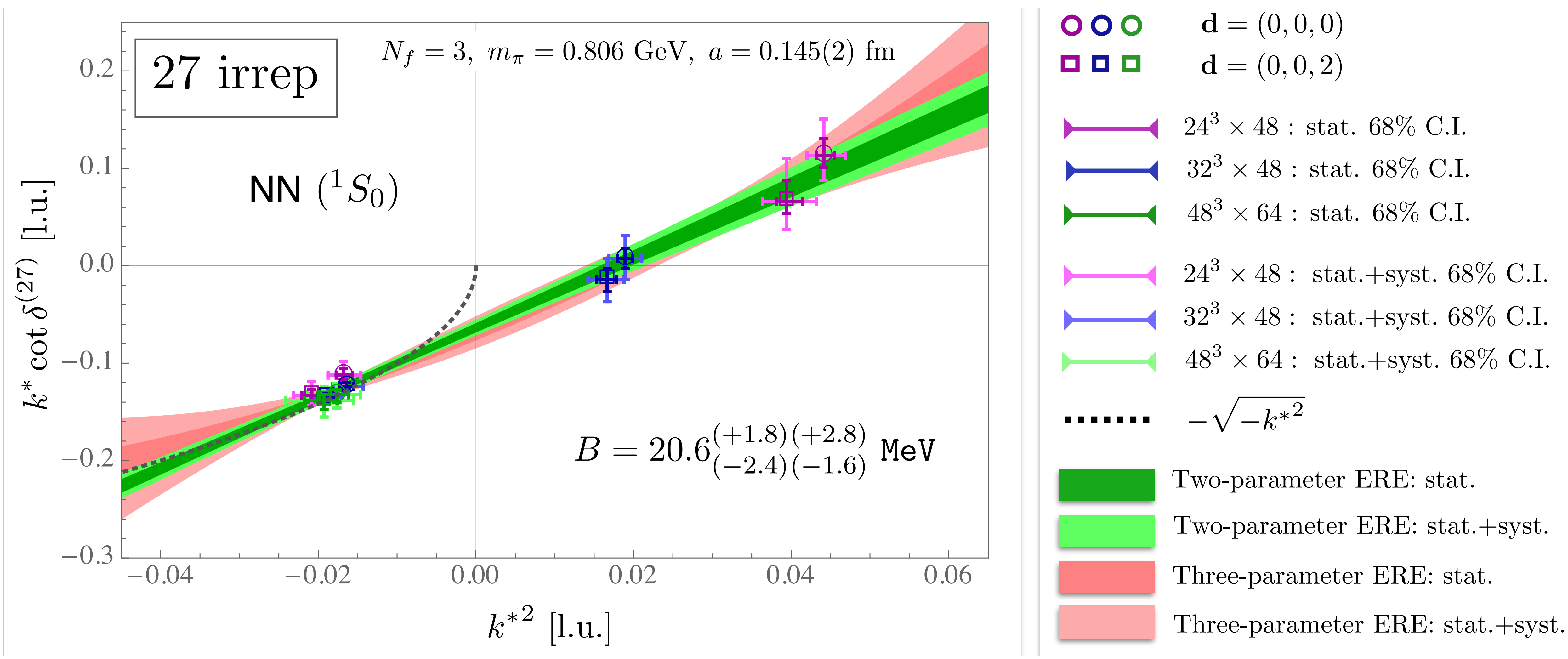
$$q \cot \delta(q) = \frac{1}{\pi L} \lim_{\Lambda \to \infty} \sum_{\mathbf{j}}^{|\mathbf{j}|<\Lambda} \frac{1}{|\mathbf{j}|^2 - q^2 \left(\frac{L}{2\pi}\right)^2} - 4\pi\Lambda$$

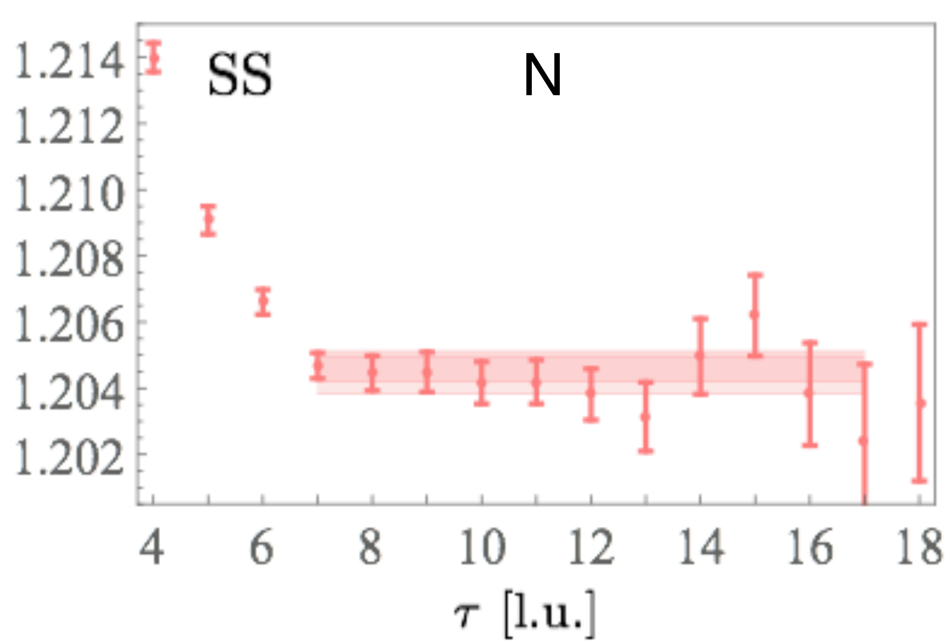

p2
p1
Continuum limit
but finite volume
p2
p1
L
Infinite volume
L → ∞
p2
p1

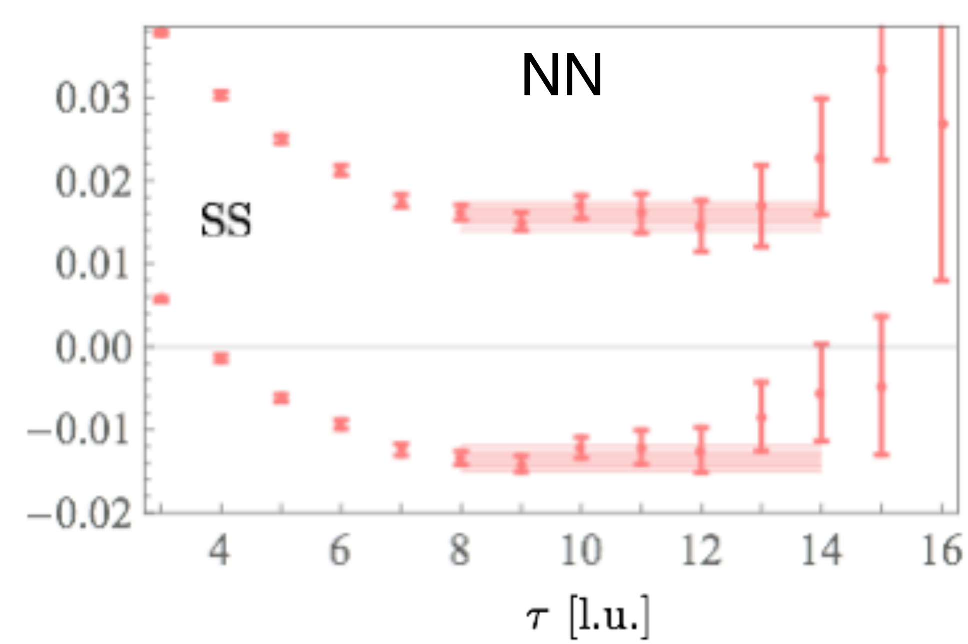

E_L
$\sim \frac{1}{mL^2}$
B_L
poles


E_∞
Resonance pole
B_∞
bound state
cut

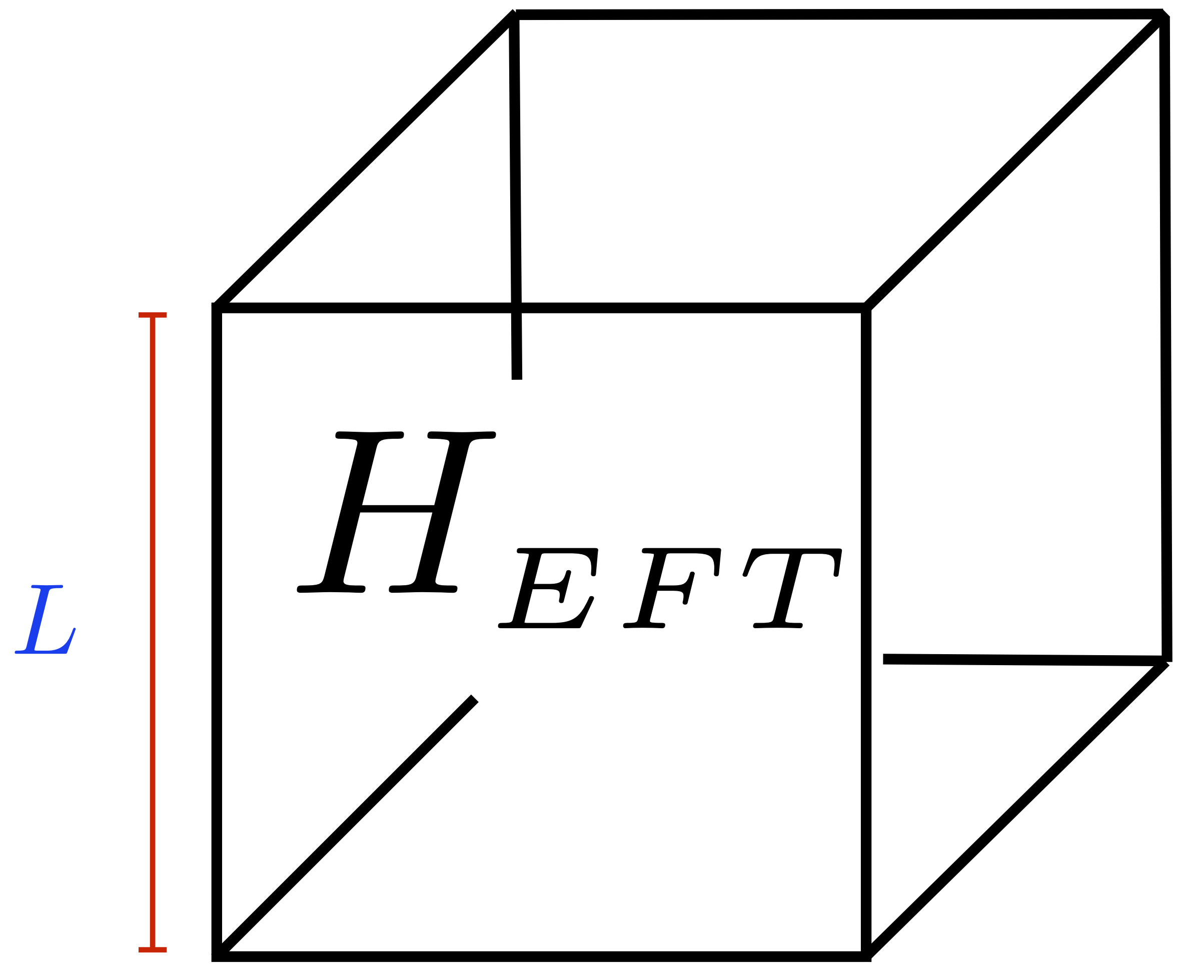
Baryon-Baryon S-wave phase shifts







Alternate method: match to the potential



Effective field theory Hamiltonian in a finite volume with periodic BCs

$$V(\mathbf{r}) = V(\mathbf{r} + \mathbf{m}L)$$

$$\psi(\mathbf{r}) = \psi(\mathbf{r} + \mathbf{m}L)$$

$$V(\mathbf{r}) = \int \frac{d^3\mathbf{k}}{(2\pi)^3}\, e^{i\mathbf{k}\cdot\mathbf{r}}\, \tilde{V}(\mathbf{k}) \;\rightarrow\; V_L(\mathbf{r}) = \frac{1}{L^3} \sum_{\mathbf{n}} e^{i2\pi\mathbf{n}\cdot\mathbf{r}/L}\, \tilde{V}(\frac{2\pi}{L}\mathbf{n})$$

$$\psi(\mathbf{r}) = \int \frac{d^3\mathbf{k}}{(2\pi)^3}\, e^{i\mathbf{k}\cdot\mathbf{r}}\, \tilde{\psi}(\mathbf{k}) \;\rightarrow\; \psi_L(\mathbf{r}) = \frac{1}{L^3} \sum_{\mathbf{n}} e^{i2\pi\mathbf{n}\cdot\mathbf{r}/L}\, \tilde{\psi}_L(\frac{2\pi}{L}\mathbf{n})$$

3-dimensional Schrödinger equation in finite volume

$$\frac{-\hbar^2}{2\mu}\boldsymbol{\nabla}^2\psi_L(\mathbf{r}) \; + \; V_L(\mathbf{r})\psi_L(\mathbf{r}) \; = \; E\;\psi_L(\mathbf{r})$$

3-dimensional Schrödinger equation in finite volume

$$\frac{-\hbar^2}{2\mu}\boldsymbol{\nabla}^2\psi_L(\mathbf{r}) \;+\; V_L(\mathbf{r})\psi_L(\mathbf{r}) \;=\; E\;\psi_L(\mathbf{r})$$

$$\Downarrow$$

$$\frac{\hbar^2}{2\mu}\left(\frac{2\pi}{L}\right)^2|\mathbf{n}|^2\;\tilde{\psi}_L(\frac{2\pi}{L}\mathbf{n}) \;+\; \sum_{\overline{\mathbf{n}}}\;\tilde{V}(\frac{2\pi}{L}\,(\mathbf{n}-\overline{\mathbf{n}}))\;\tilde{\psi}_L(\frac{2\pi}{L}\overline{\mathbf{n}}) \;=\; E_L\;\tilde{\psi}_L(\frac{2\pi}{L}\mathbf{n})$$

3-dimensional Schrödinger equation in finite volume

$$\frac{-\hbar^2}{2\mu}\nabla^2\psi_L(\mathbf{r}) \; + \; V_L(\mathbf{r})\psi_L(\mathbf{r}) \; = \; E \; \psi_L(\mathbf{r})$$

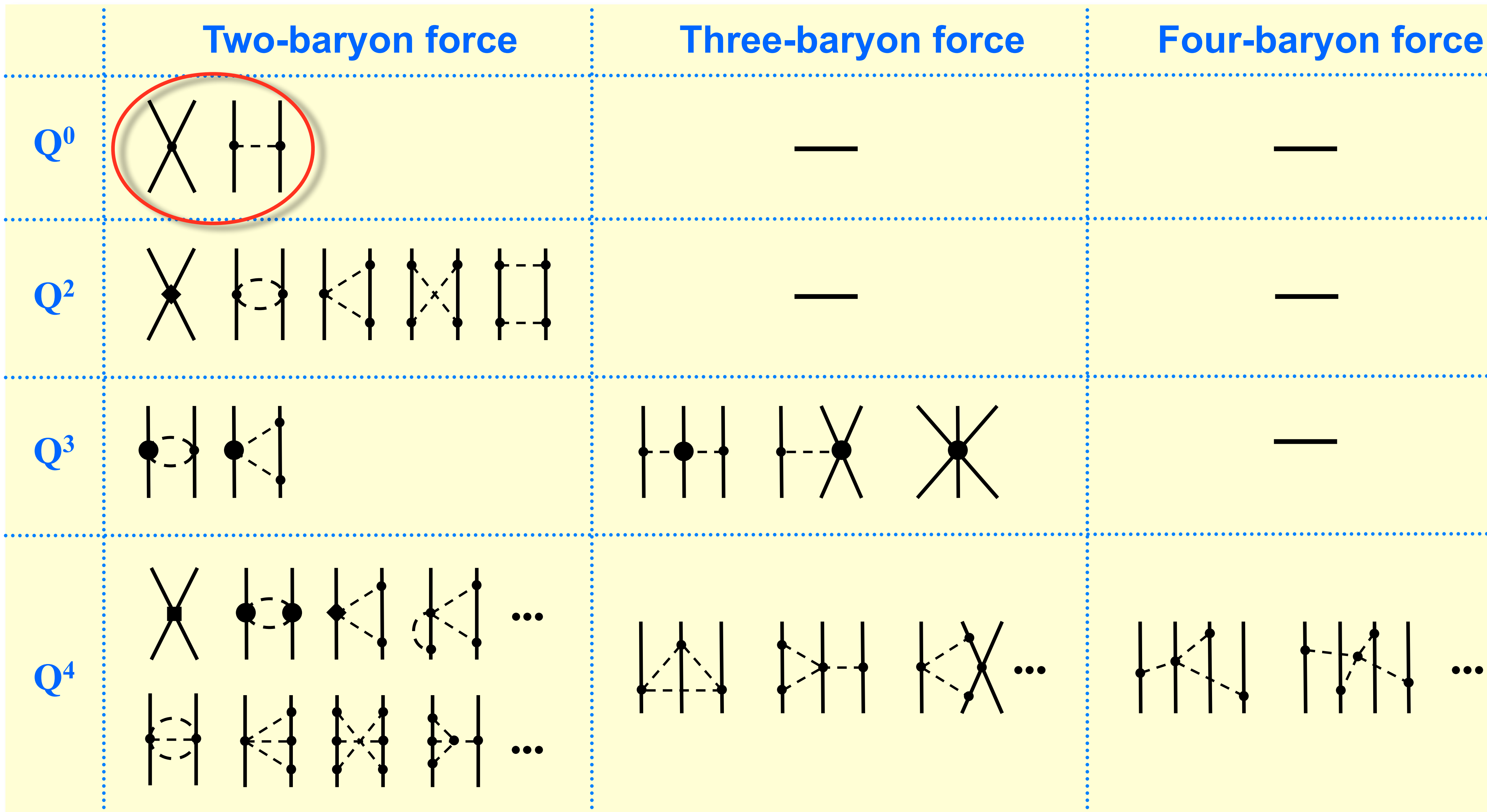
↓

$$\frac{\hbar^2}{2\mu}\left(\frac{2\pi}{L}\right)^2 |\mathbf{n}|^2 \; \tilde{\psi}_L(\frac{2\pi}{L}\mathbf{n}) \; + \; \sum_{\overline{\mathbf{n}}} \tilde{V}(\frac{2\pi}{L}(\mathbf{n}-\overline{\mathbf{n}})) \; \tilde{\psi}_L(\frac{2\pi}{L}\overline{\mathbf{n}}) \; = \; E_L \; \tilde{\psi}_L(\frac{2\pi}{L}\mathbf{n})$$

$$\hat{H}_{\mathbf{n},\mathbf{n}'} \; = \; \frac{2\pi^2\hbar^2}{\mu L^2} \; |\mathbf{n}|^2 \; \delta_{\mathbf{n},\mathbf{n}'} \; + \; \tilde{V}(\frac{2\pi}{L}(\mathbf{n}-\mathbf{n}'))$$

Diagonalize large symmetric matrix

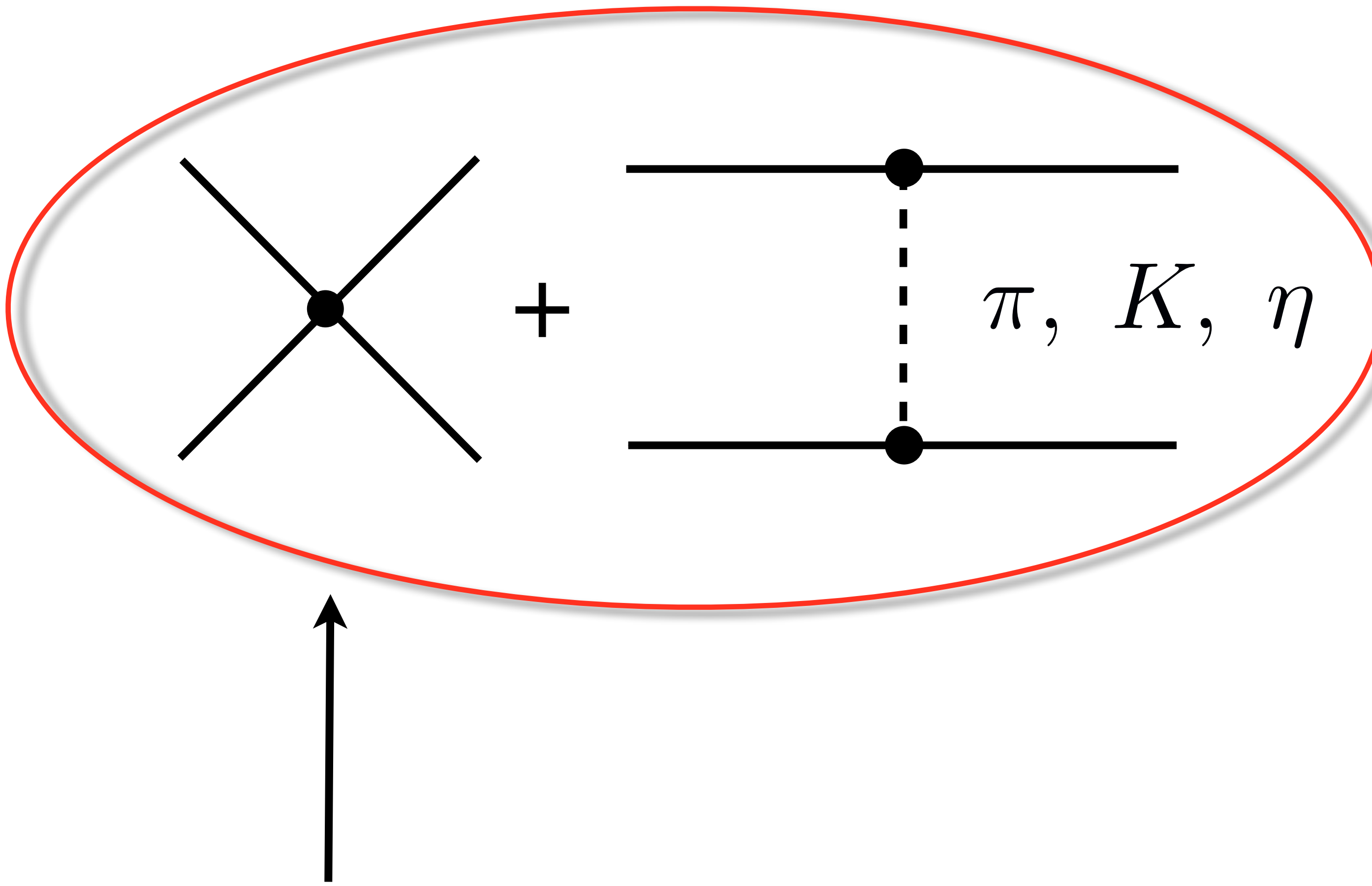
Nuclear Effective Field Theory



2 baryon force ≫ 3 baryon force ≫ 4 baryon force . . .

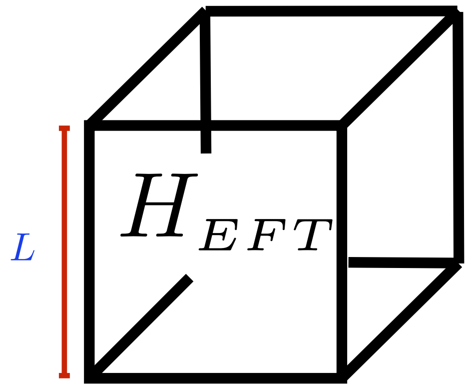
Match to Effective Field Theory!

LO potential:



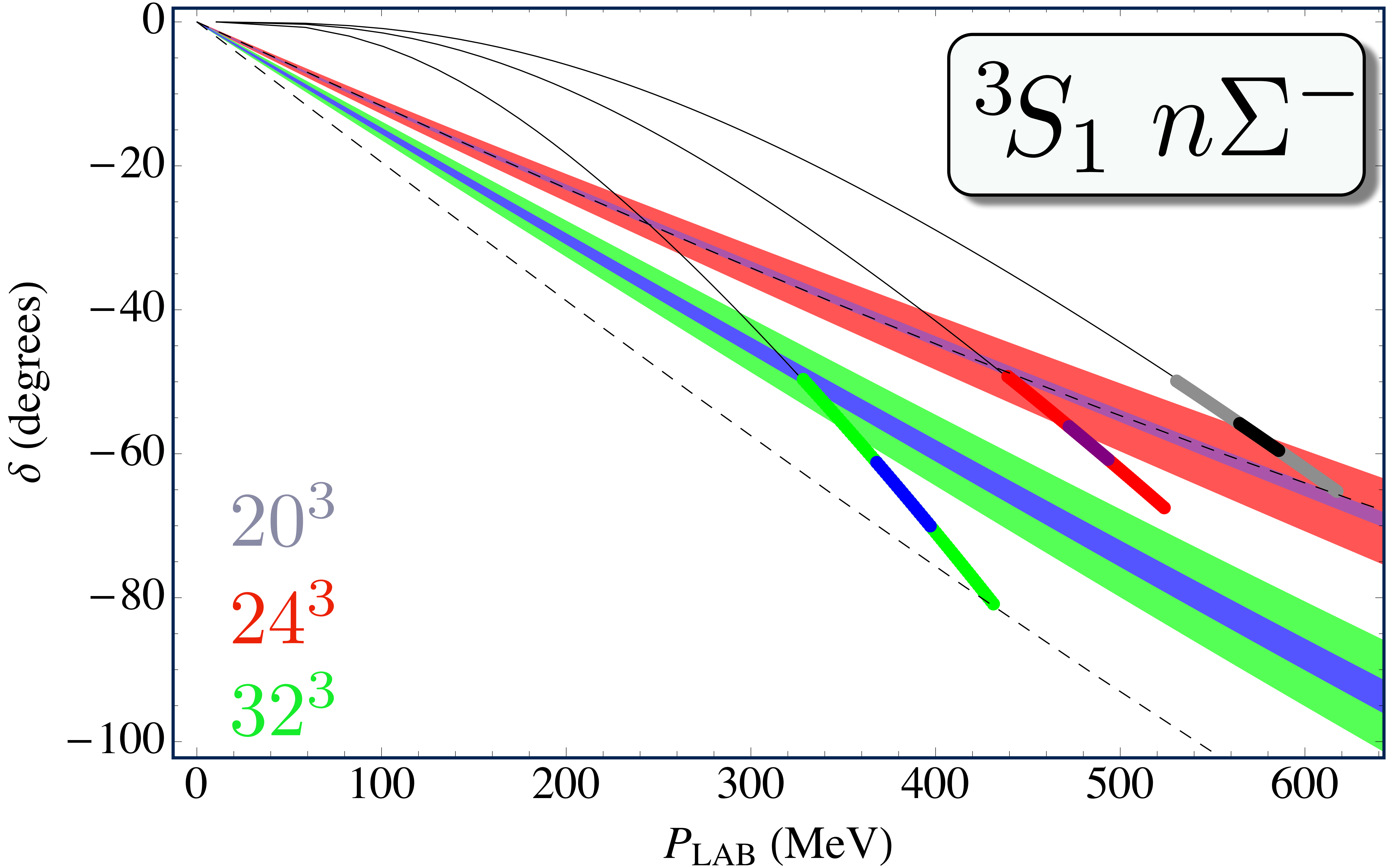
Fit coupling to match energy levels

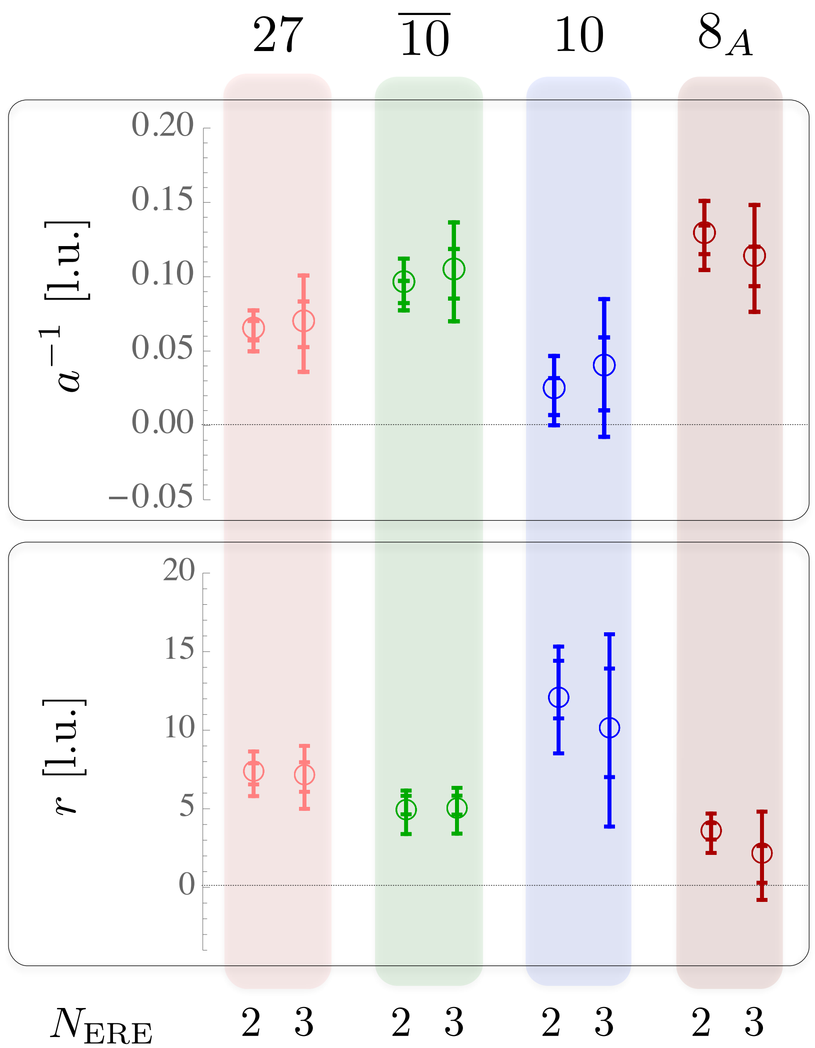
Now we have LO potential at ALL pion masses!

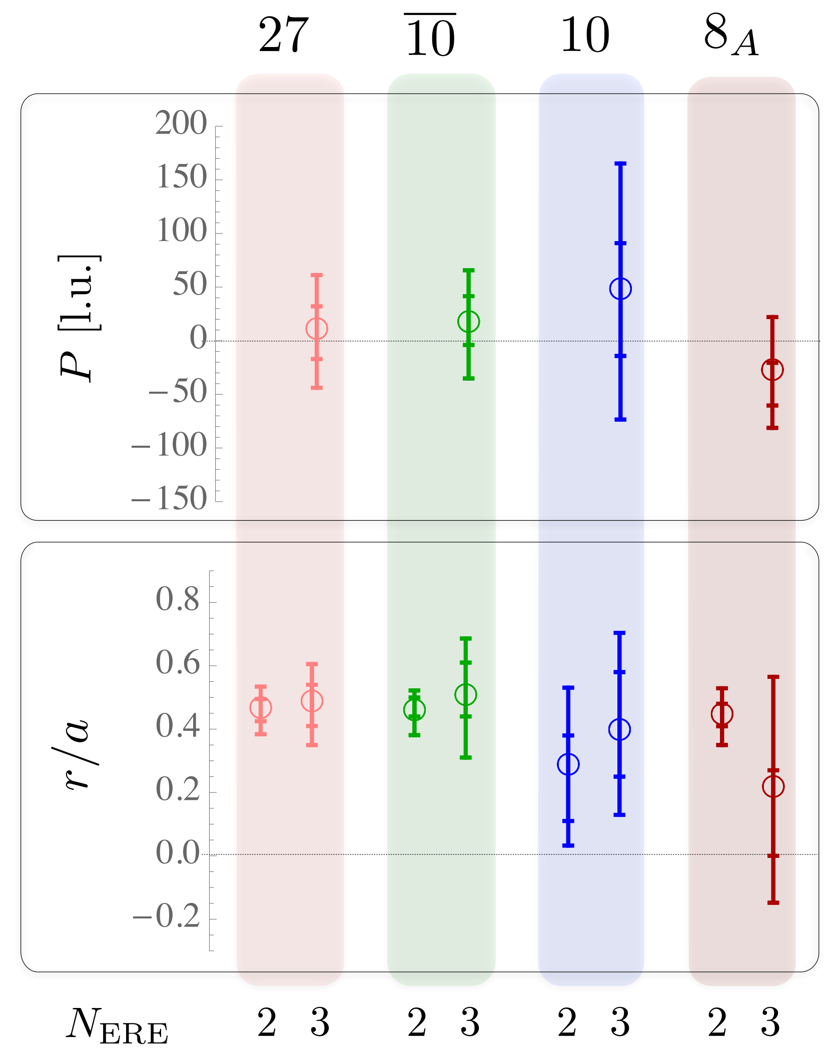


vs.

$$p \cot \delta \;=\; \frac{1}{\pi L}\mathcal{S}(\tilde{p})$$







$SU(6)$ from large-N_c

$$\left[-\frac{1}{a^{(27)}}+\mu\right]^{-1}=\frac{M_B}{2\pi}(a-\frac{b}{27})+\mathcal{O}\left(\frac{1}{N_c^2}\right),\qquad \left[-\frac{1}{a^{(\overline{10})}}+\mu\right]^{-1}=\frac{M_B}{2\pi}(a-\frac{b}{27})+\mathcal{O}\left(\frac{1}{N_c^2}\right),$$

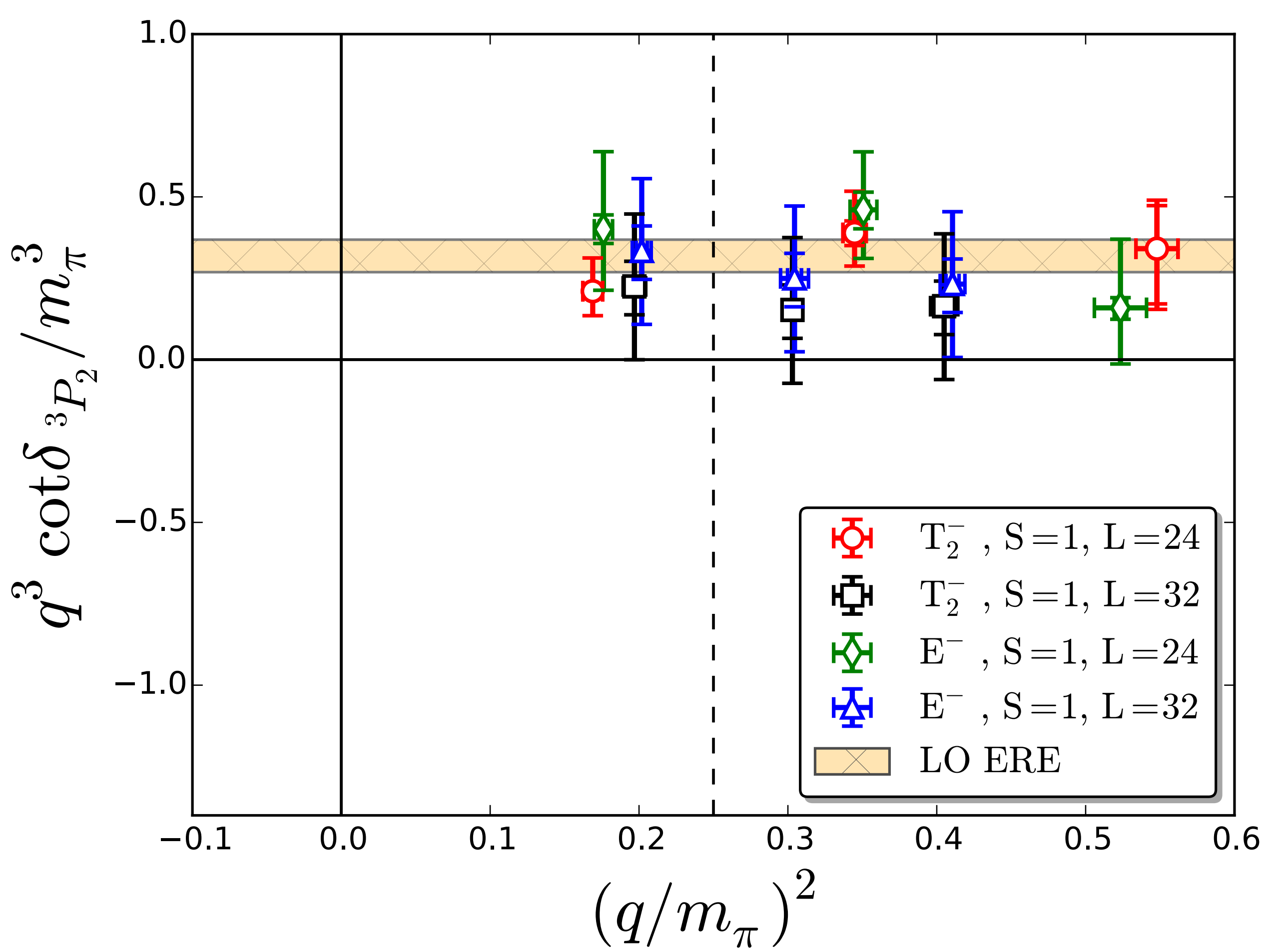
$$\left[-\frac{1}{a^{(10)}}+\mu\right]^{-1}=\frac{M_B}{2\pi}(a+\frac{7b}{27})+\mathcal{O}\left(\frac{1}{N_c}\right),\qquad \left[-\frac{1}{a^{(8_A)}}+\mu\right]^{-1}=\frac{M_B}{2\pi}(a+\frac{b}{27})+\mathcal{O}\left(\frac{1}{N_c}\right),$$

$$\left[-\frac{1}{a^{(8_S)}}+\mu\right]^{-1}=\frac{M_B}{2\pi}(a+\frac{b}{3})+\mathcal{O}\left(\frac{1}{N_c}\right),\qquad \left[-\frac{1}{a^{(1)}}+\mu\right]^{-1}=\frac{M_B}{2\pi}(a-\frac{b}{3})+\mathcal{O}\left(\frac{1}{N_c}\right),$$

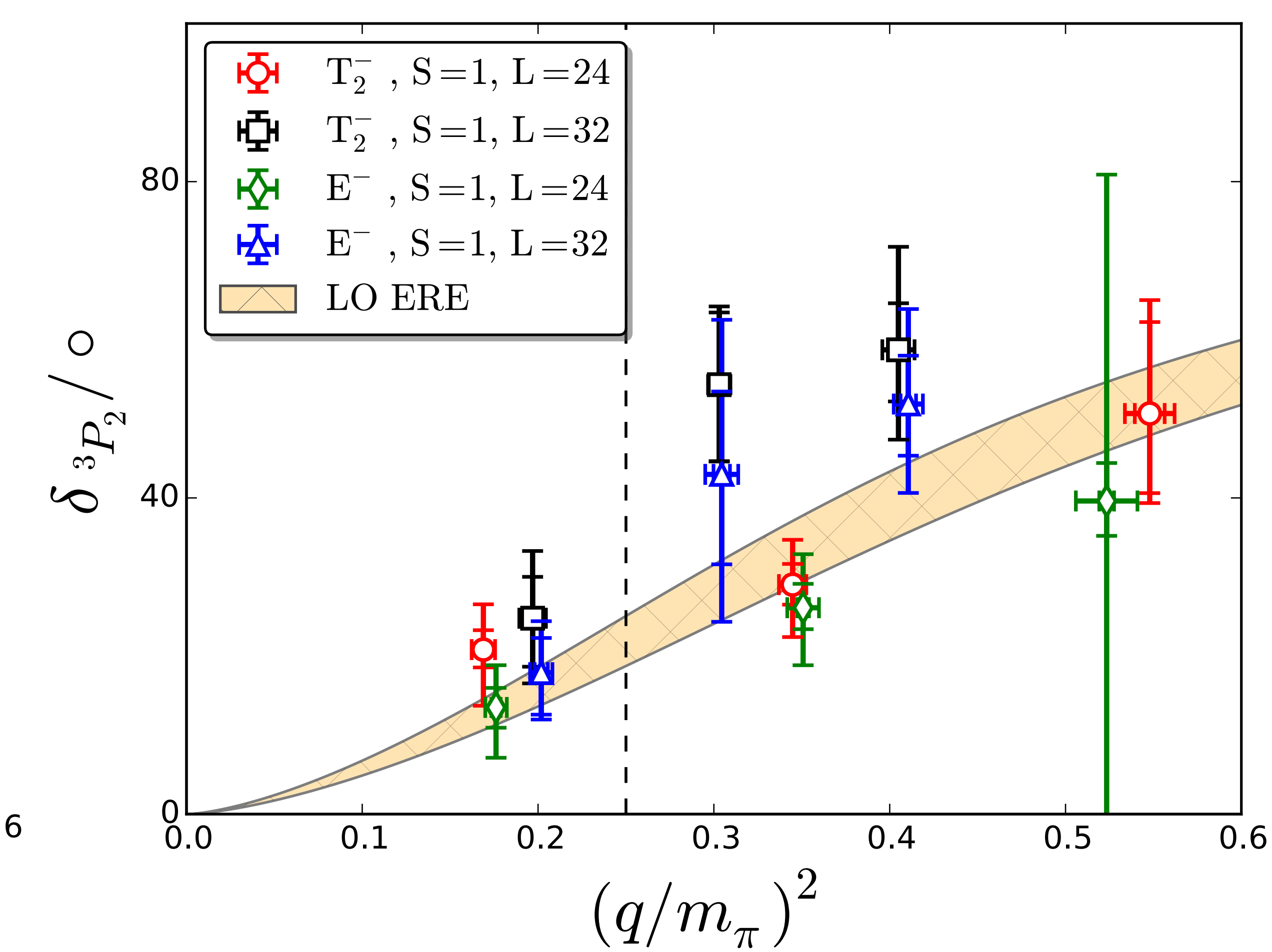
NN P-wave phase shifts

CalLat Collaboration (using NPLQCD resources)

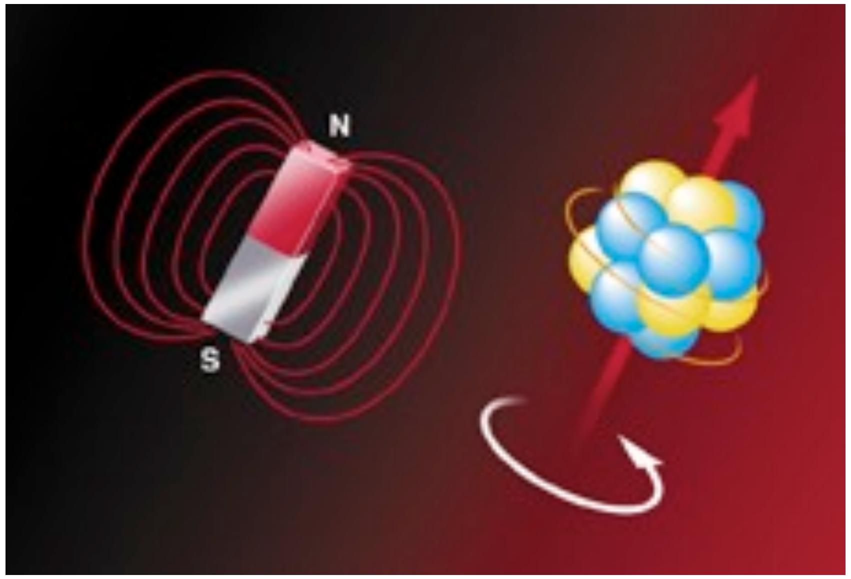
$m_\pi \sim 800$ MeV



Amy Nicholson *et al* (CallLatt)



Nuclear structure: magnetic moments



$U_Q(1)$ phase

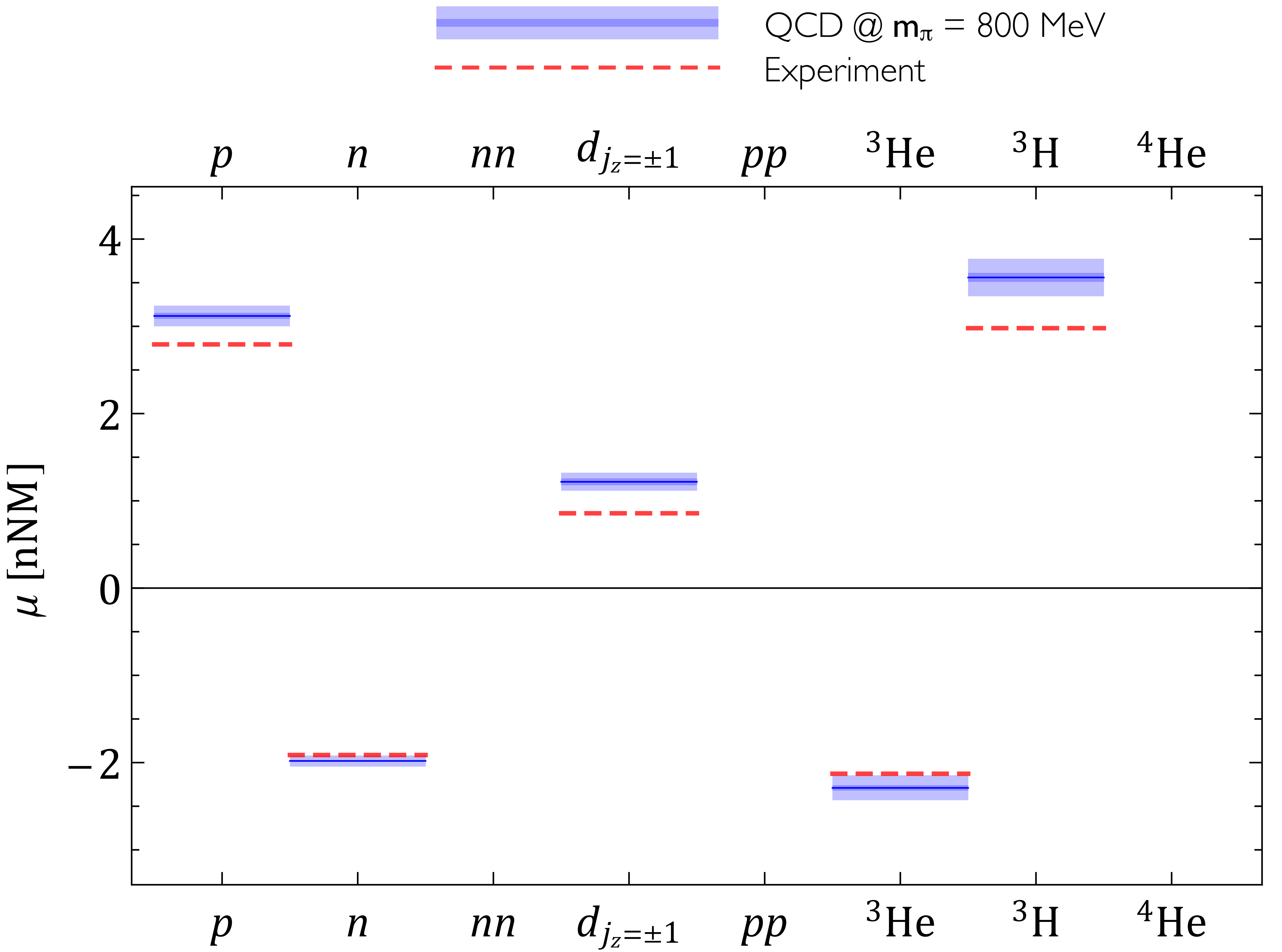
$$U_\mu(x) = e^{i\frac{6\pi Q_q \tilde{n}}{L^2} x_1 \delta_{\mu,2}} \times e^{-i\frac{6\pi Q_q \tilde{n}}{L} x_2 \delta_{\mu,1} \delta_{x_1,L-1}}$$

- Hadronic and nuclear correlation functions are modified in the presence of a background magnetic field:

$$E_{h;j_z}(\mathbf{B}) = \sqrt{M_h^2 + P_\parallel^2 + (2n_L+1)|Q_h e\mathbf{B}|} - \boldsymbol{\mu}_h \cdot \mathbf{B} - 2\pi\beta_h^{(M0)}|\mathbf{B}|^2 - 2\pi\beta_h^{(M2)}\langle \hat{T}_{ij} B_i B_j \rangle + \ldots$$

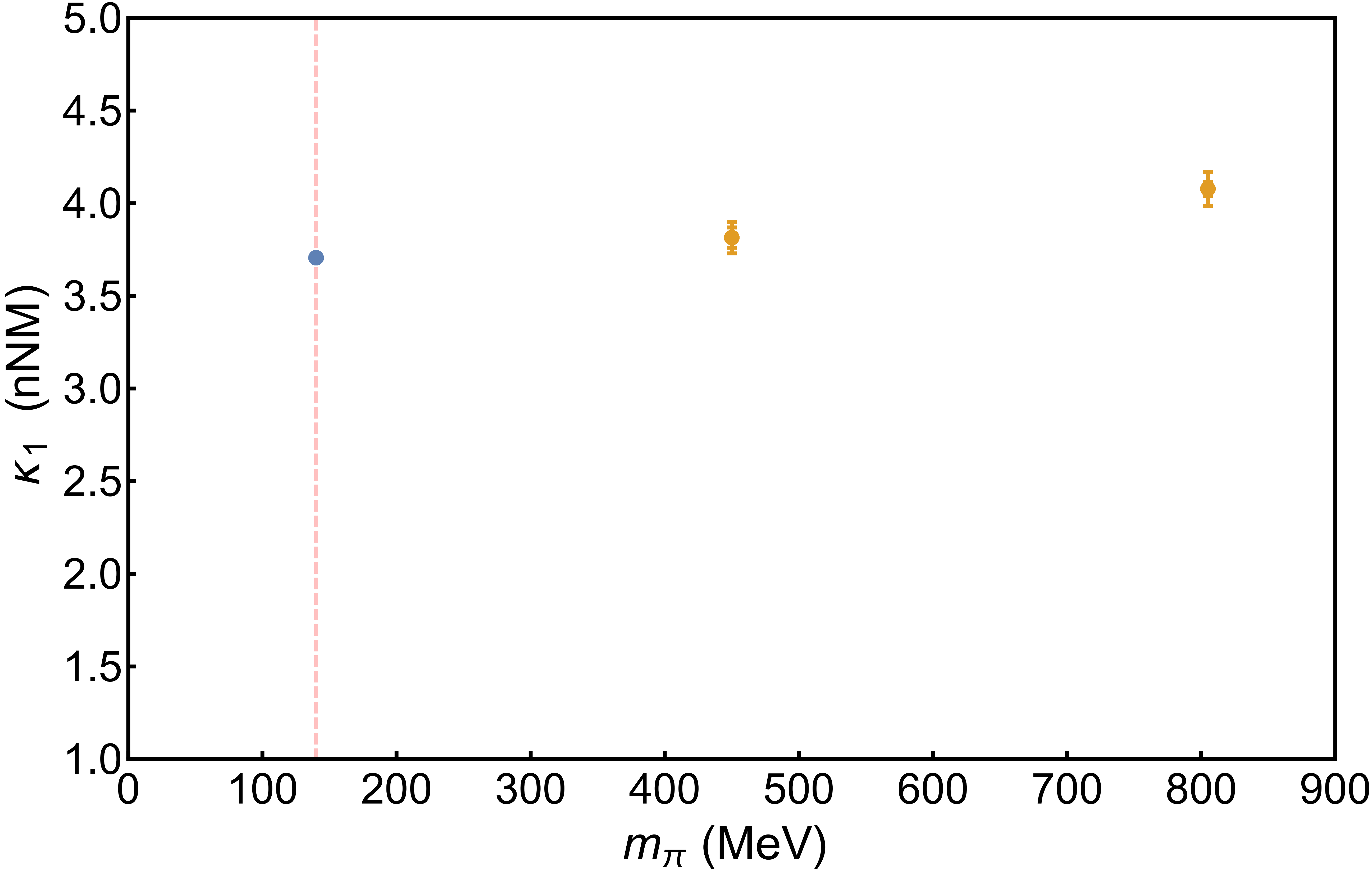
Landau level

- Can extract magnetic moments, polarizabilities, …
- Extendable to external electric fields, etc.

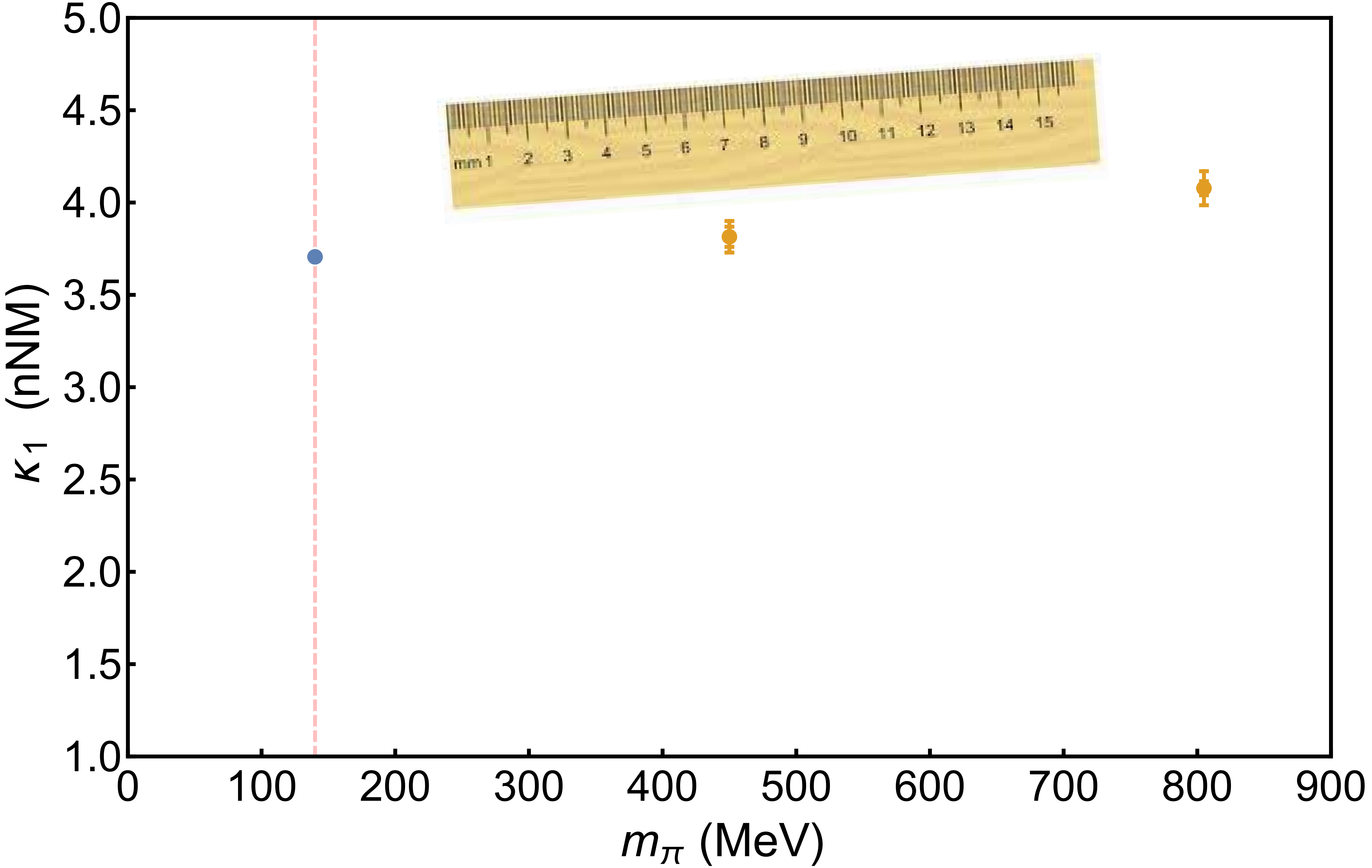


- Almost no quark mass dependence in units of $\dfrac{e}{2M(m_\pi)}$

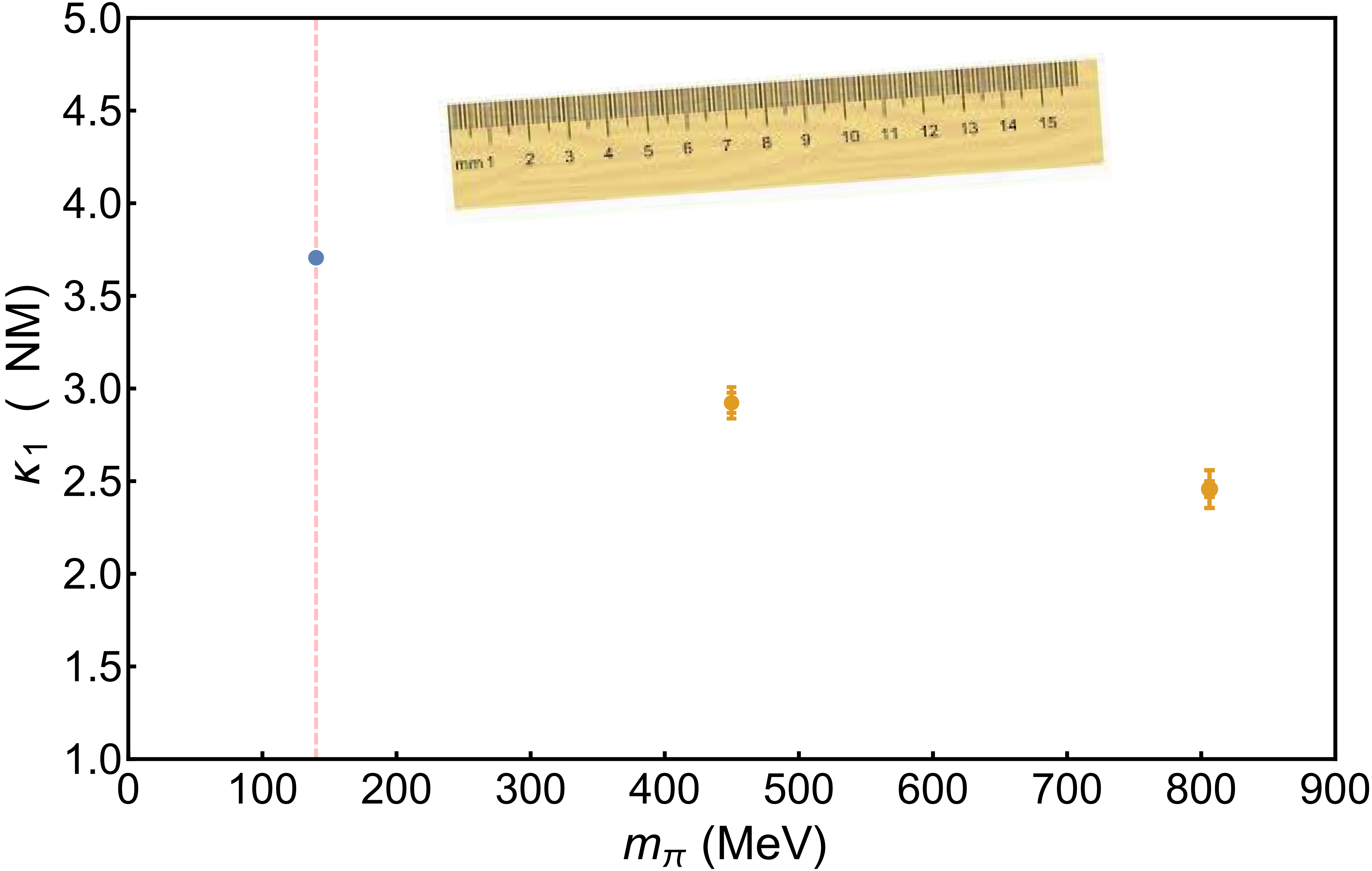
Nucleon isovector magnetic moment



Nucleon isovector magnetic moment

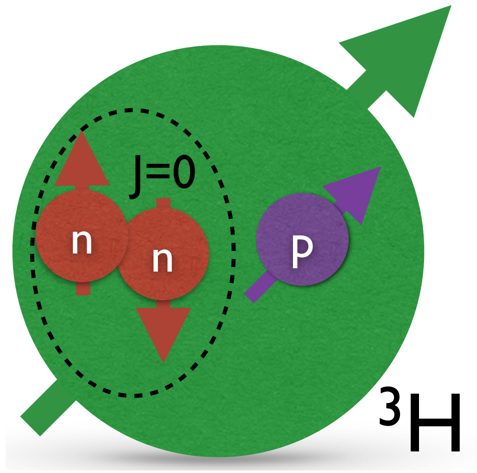


Nucleon isovector magnetic moment

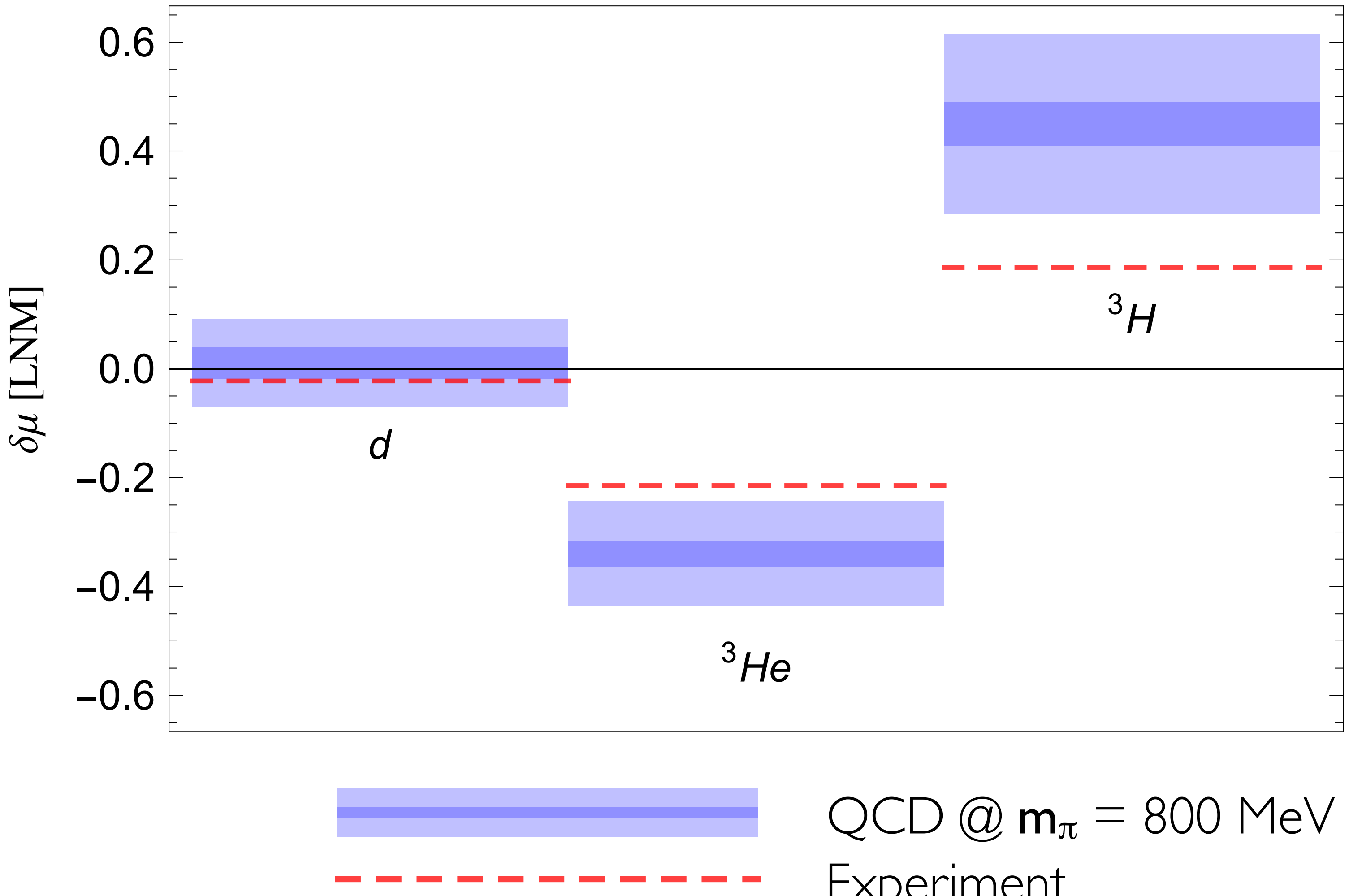


Nuclei as groupings of nucleons: shell model!

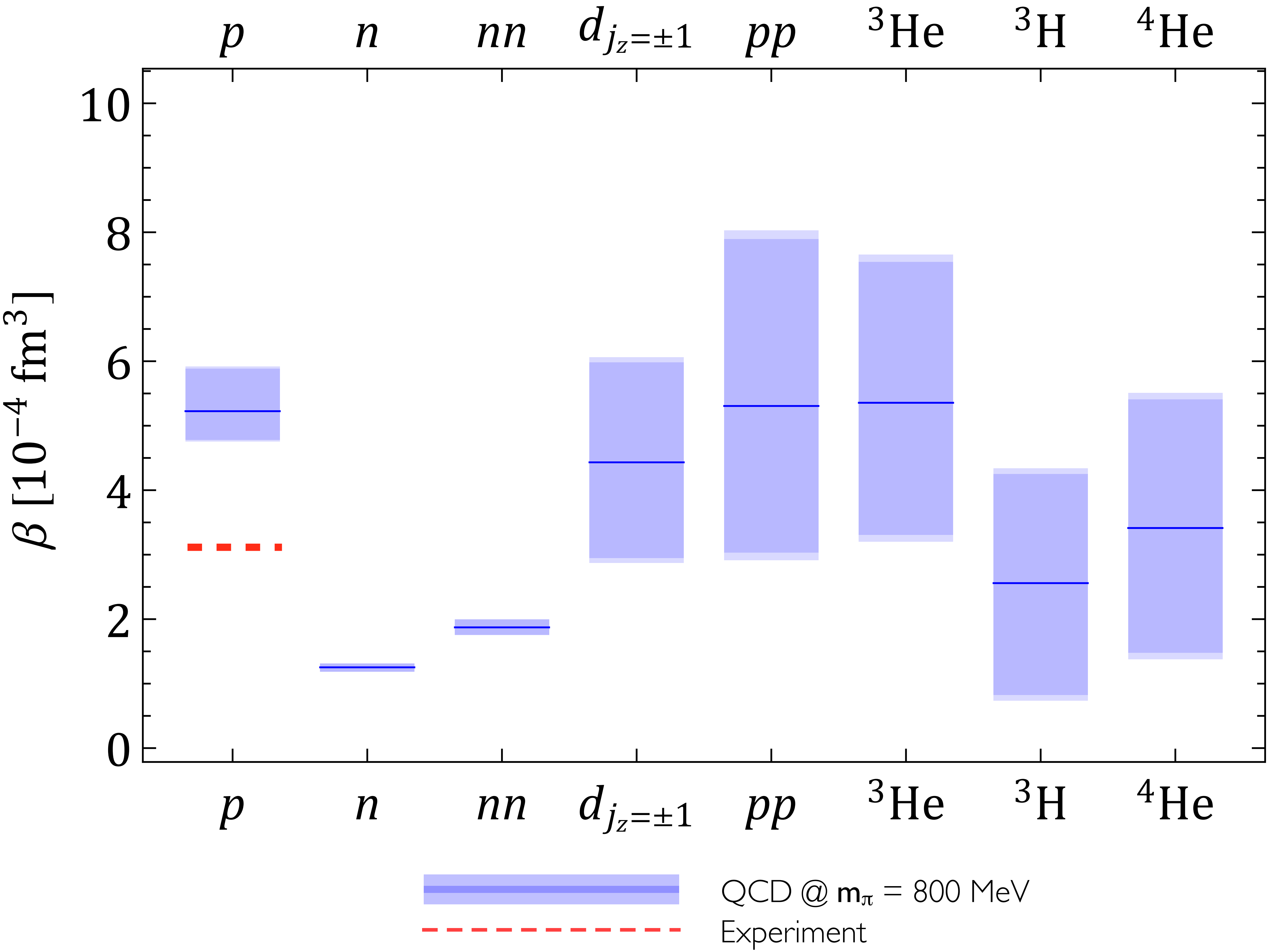
$$\mu_{^3\mathrm{H}} = \mu_p$$
$$\mu_{^3\mathrm{He}} = \mu_n$$
$$\mu_d = \mu_p + \mu_n$$



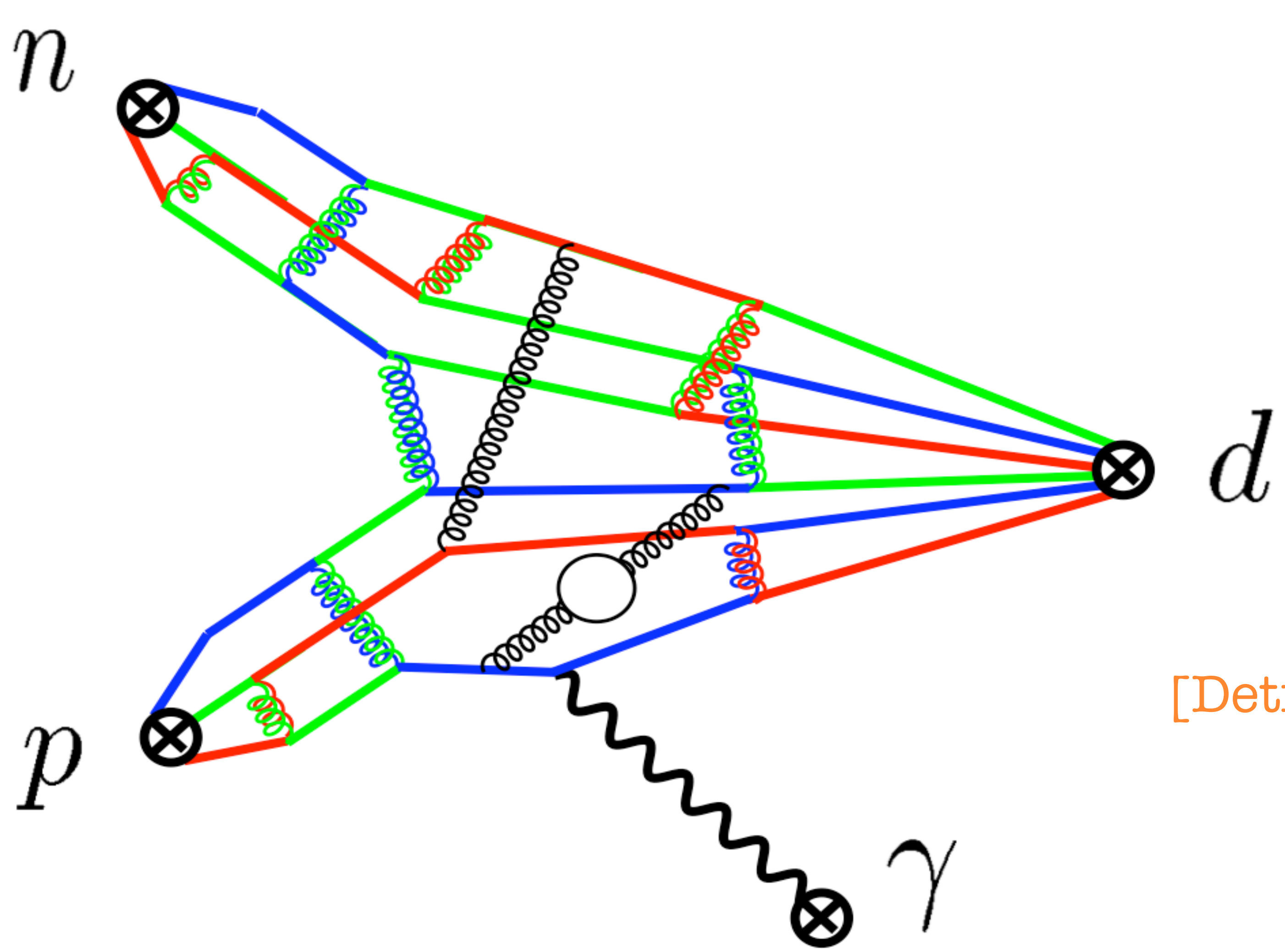
Difference between nuclear magnetic moments and shell model predictions



Nuclear structure: polarizabilities



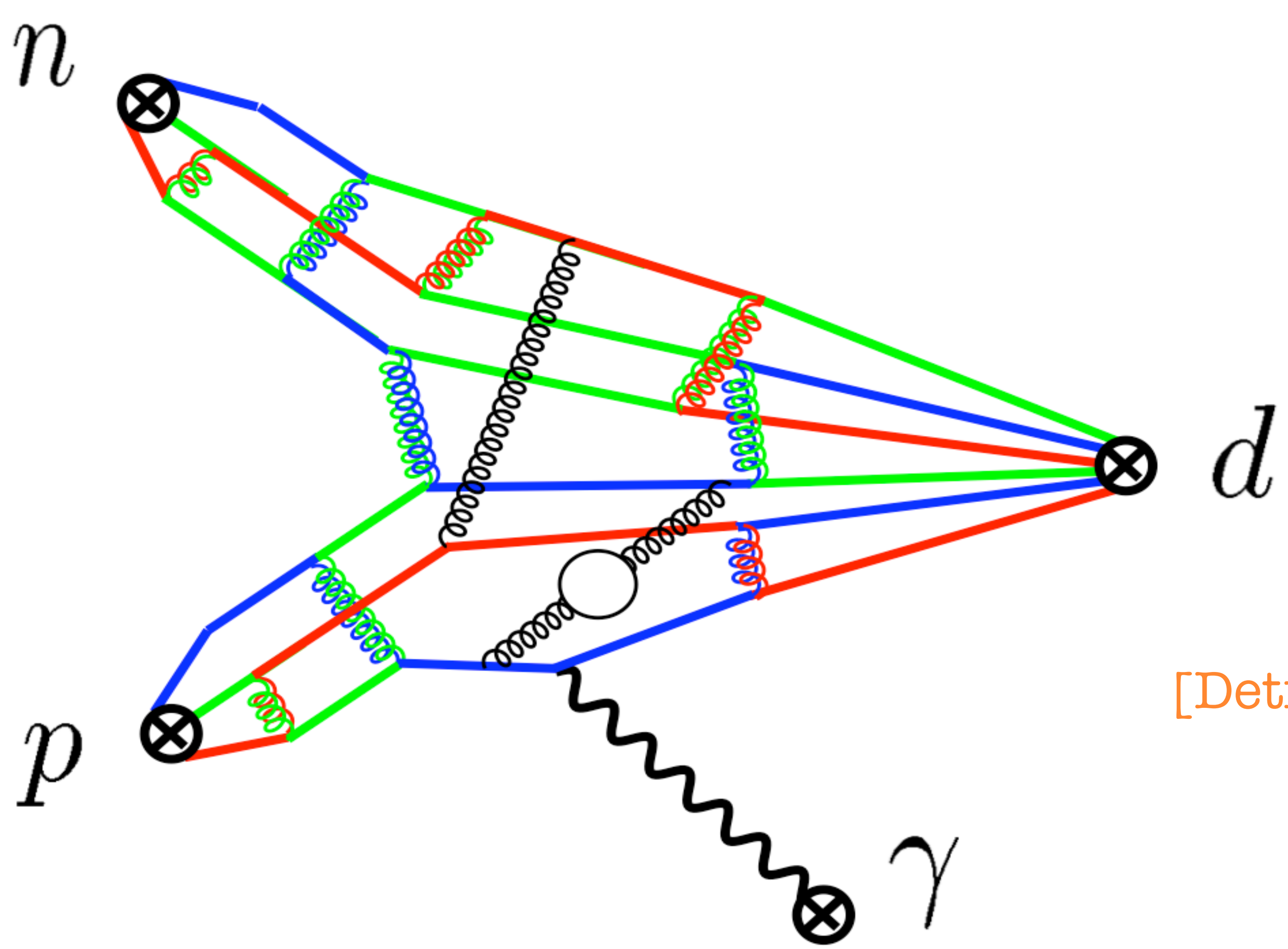
Nuclear reaction: $np \to d\gamma$



[Detmold and Savage (2004)]

$$\Delta E_{^3S_1,^1S_0} = \mp Z_d^2 \left(\kappa_1 + \gamma_0 l_1\right) \frac{|e\mathbf{B}|}{M} + \ldots = \mp \left(\kappa_1 + \overline{L}_1\right) \frac{|e\mathbf{B}|}{M} + \ldots$$

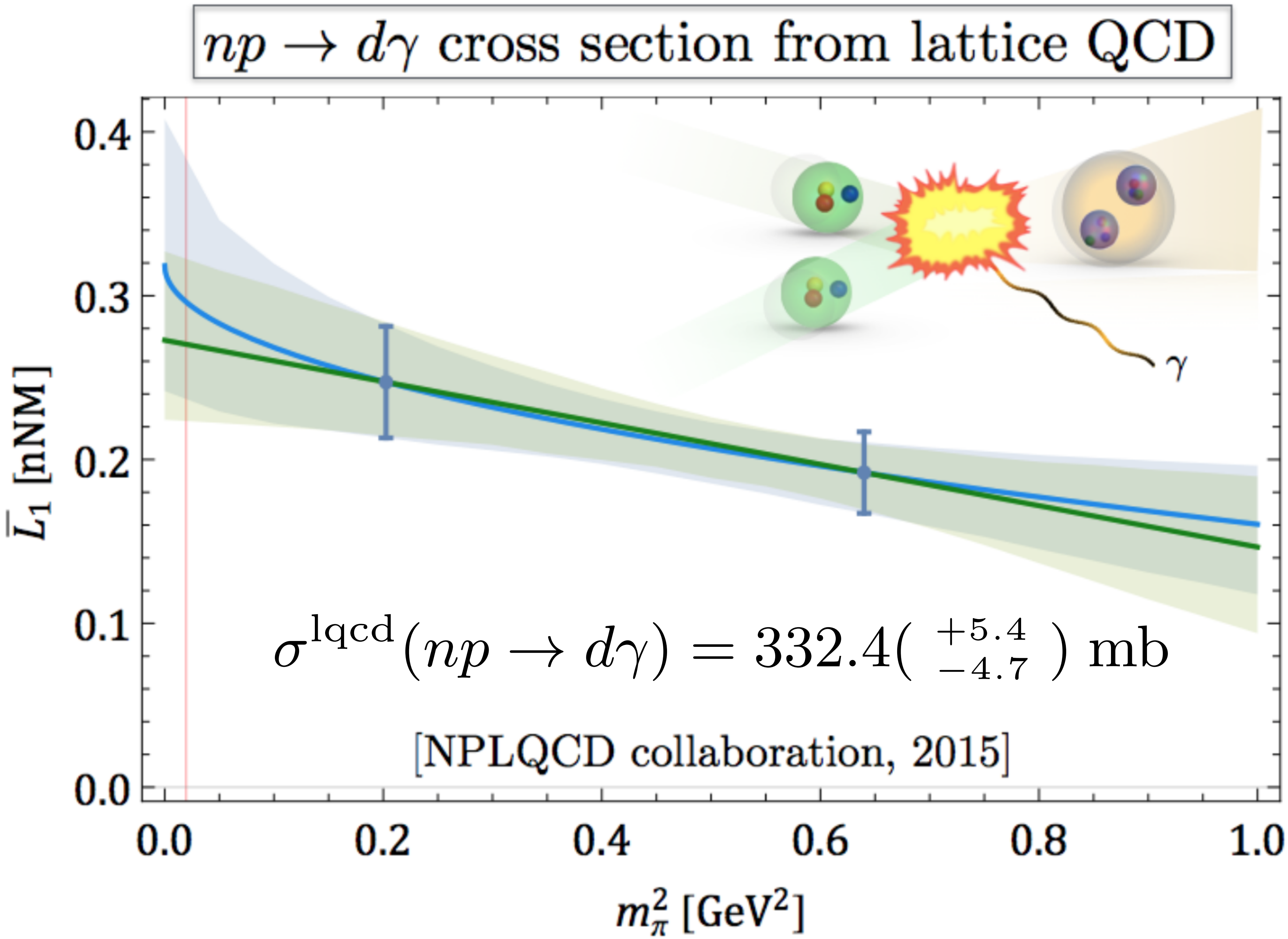
Nuclear reaction: $np \to d\gamma$



[Detmold and Savage (2004)]

$$\Delta E_{^3S_1,^1S_0} = \mp Z_d^2\,(\kappa_1 + \gamma_0 l_1)\,\frac{|e\mathbf{B}|}{M} + \ldots = \mp\left(\kappa_1 + \overline{L}_1\right)\frac{|e\mathbf{B}|}{M} + \ldots$$

$np \to d\gamma$

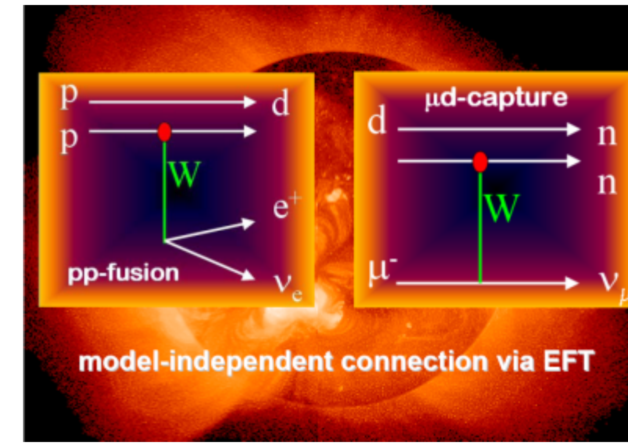


$$\sigma^{\rm expt}(np \to d\gamma) = 334.2(0.5)\ \text{mb}$$

Nuclear structure: axial transitions

- Axial coupling to the NN system
  - $\mu^- d \to nn\nu_\mu$: MuSun @ PSI
  - $\nu d \to e^+ nn$: SNO
  - *"calibrating the sun"* $pp \to de^+\nu_e$

MuSun



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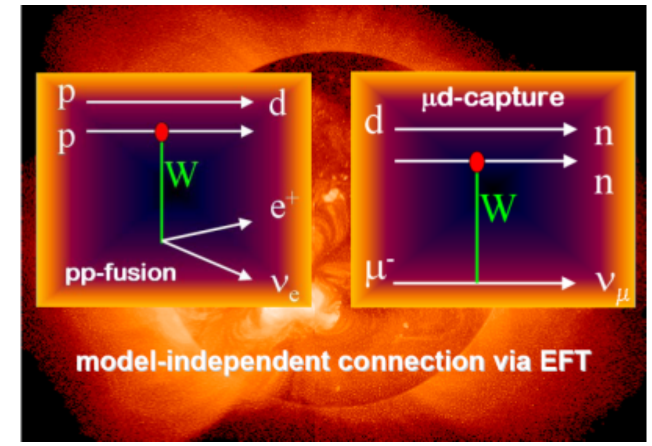
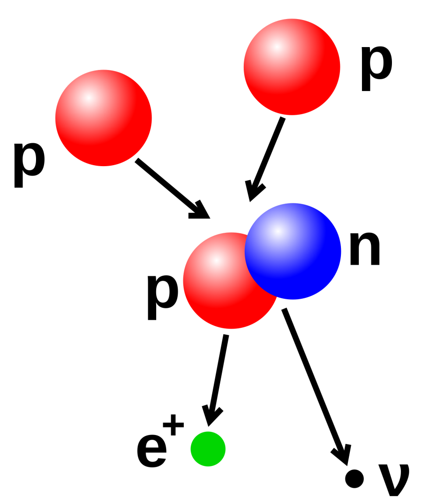
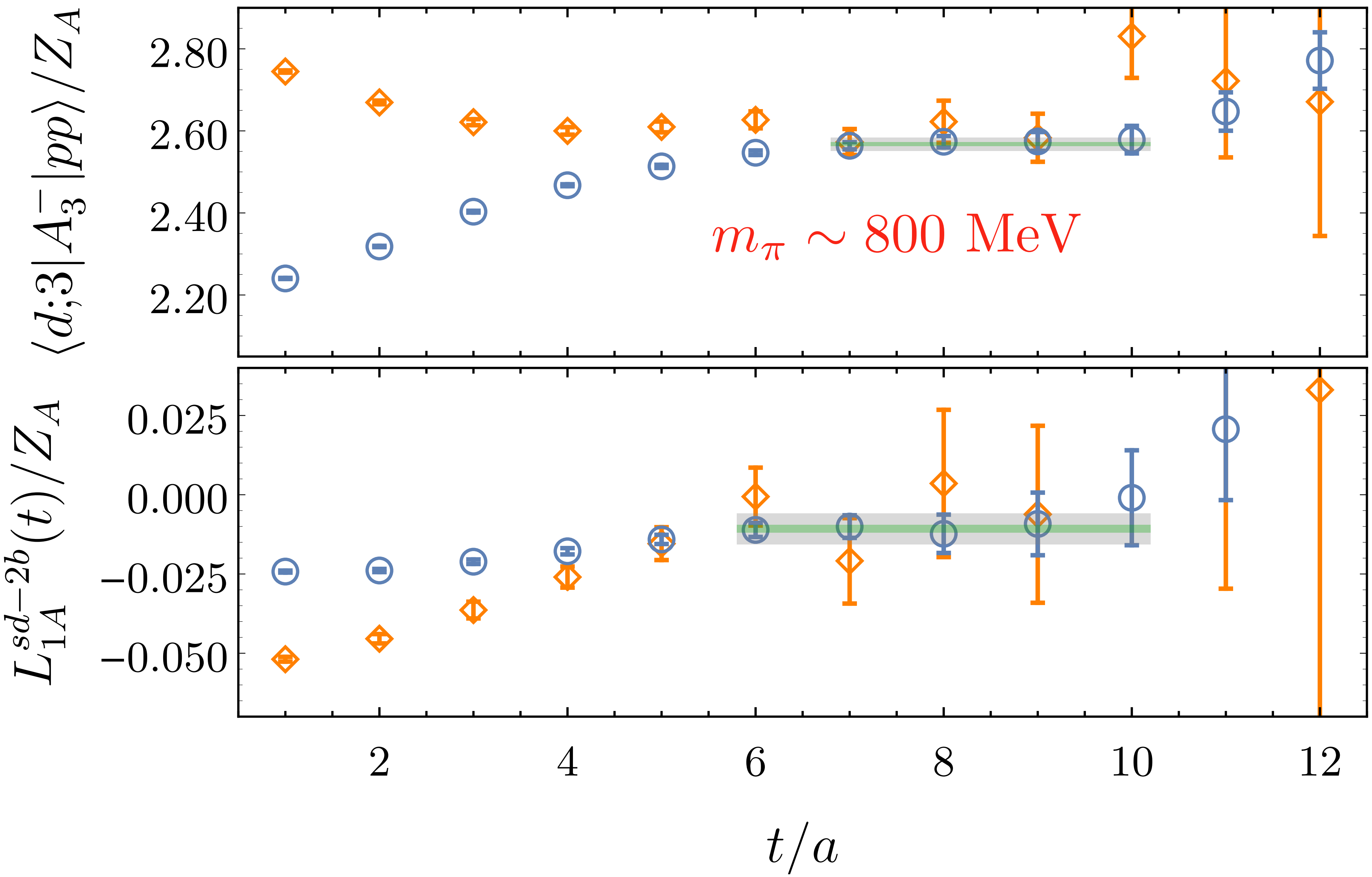


SNO

$$\left|\langle d; j \,|A_k^-|\, pp\rangle\right| \equiv g_A C_\eta \sqrt{\frac{32\pi}{\gamma^3}}\,\Lambda(p)\,\delta_{jk}$$



$$\Lambda(0) = \frac{1}{\sqrt{1-\gamma\rho}}\{e^\chi - \gamma a_{pp}[1 - \chi e^\chi E_1(\chi)] + \frac{1}{2}\gamma^2 a_{pp}\sqrt{r_1\rho}\} - \frac{1}{2g_A}\gamma a_{pp}\sqrt{1-\gamma\rho}\, L_{1,A}^{sd-2b}$$



$$\frac{L_{1,A}^{sd,2b}}{Z_A} = \frac{\left\langle {}^3S_1; J_z = 0 \left| A_3^3 \right| {}^1S_0; I_z = 0 \right\rangle - 2g_A}{2Z_A} = -0.0107(12)(48)$$

$\Lambda(0)_{lqcd} = 2.6585(6)(71)(25)$ $\Lambda(0)_{exp} = 2.652(2)$

- Progress has been made in benchmarking lattice QCD calculations of nucleon-nucleon interactions.
- The goal of lattice QCD is to calculate unknown observables with *fully-controlled* uncertainties.
- Background field method is proving remarkably successful. Scalar MEs have also been computed: large deviations in some cases from sum of single nucleon MEs.
- Prospect of a quantitative connection to QCD makes this an exciting time for nuclear physics.

USQCD US Lattice Quantum Chromodynamics

NSF Jefferson Lab Exploring the Nature of Matter OLCF Oak Ridge Leadership Computing Facility

NERSC National Energy Research Scientific Computing Center

Department of Energy United States of America