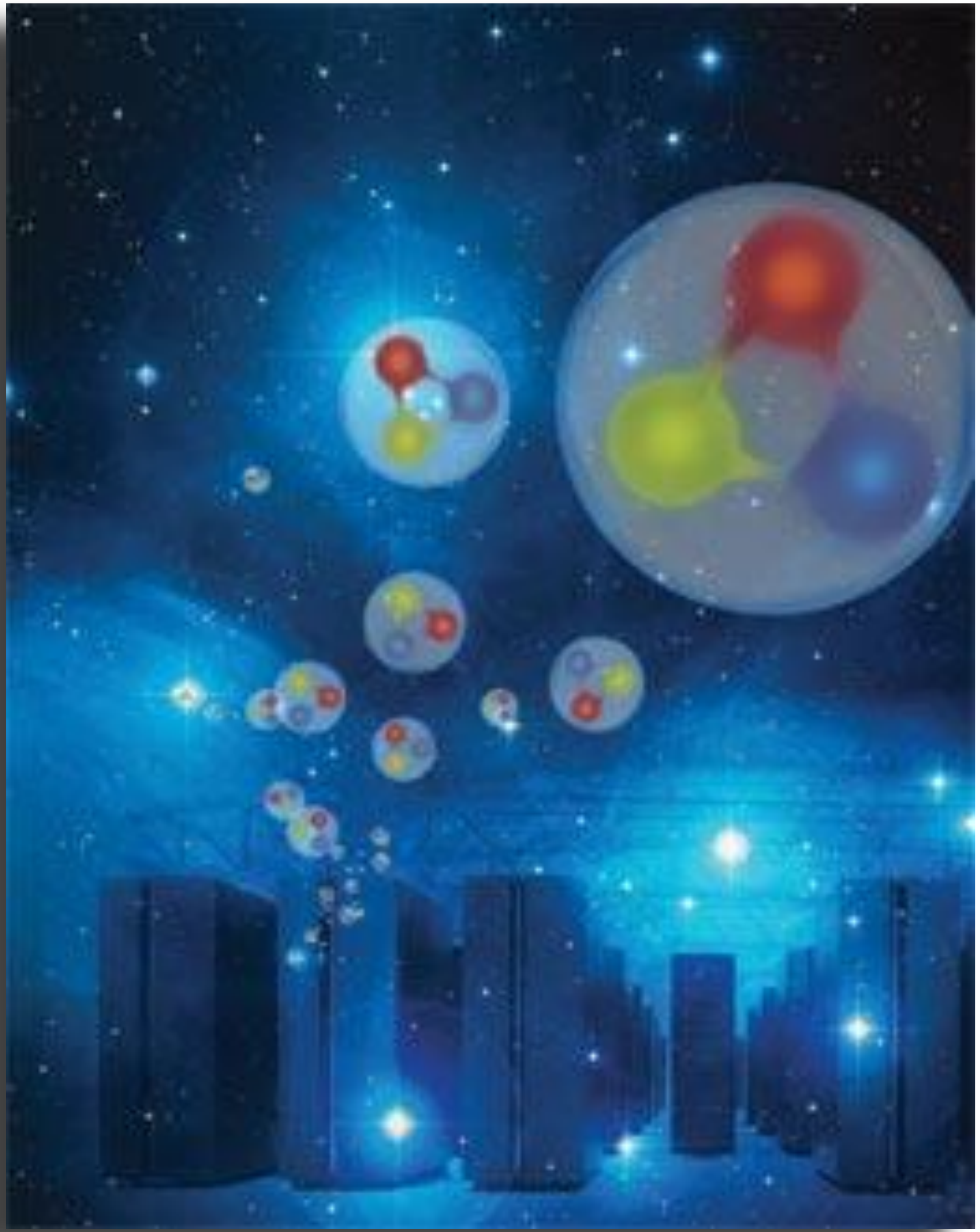


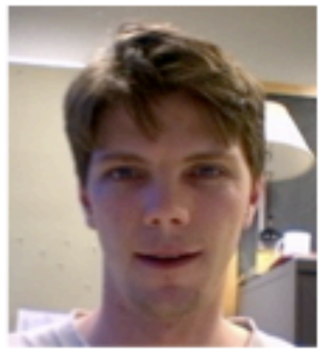
S. Durr *et al.*

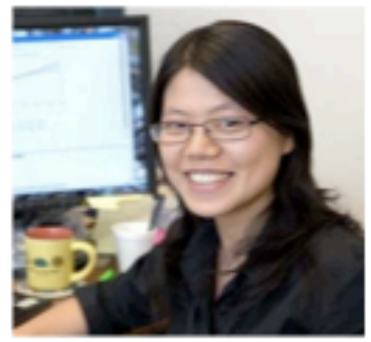
Science

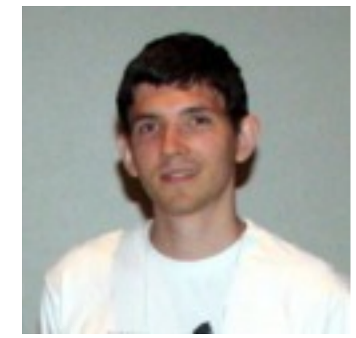
Bound States in Finite Volume

Martin J. Savage
October 2011
Barcelona

NPLQCD







Silas Beane
New Hampshire

Emmanuel Chang
Barcelona

William Detmold
Willam+Mary

Huey-Wen Lin
U. of Washington

Tom Luu
LLNL

Saul Cohen
U. of Washington

+

Kostas Orginos
William+Mary

Assumpta Parreno
Barcelona

Marton Savage
U. of Washington

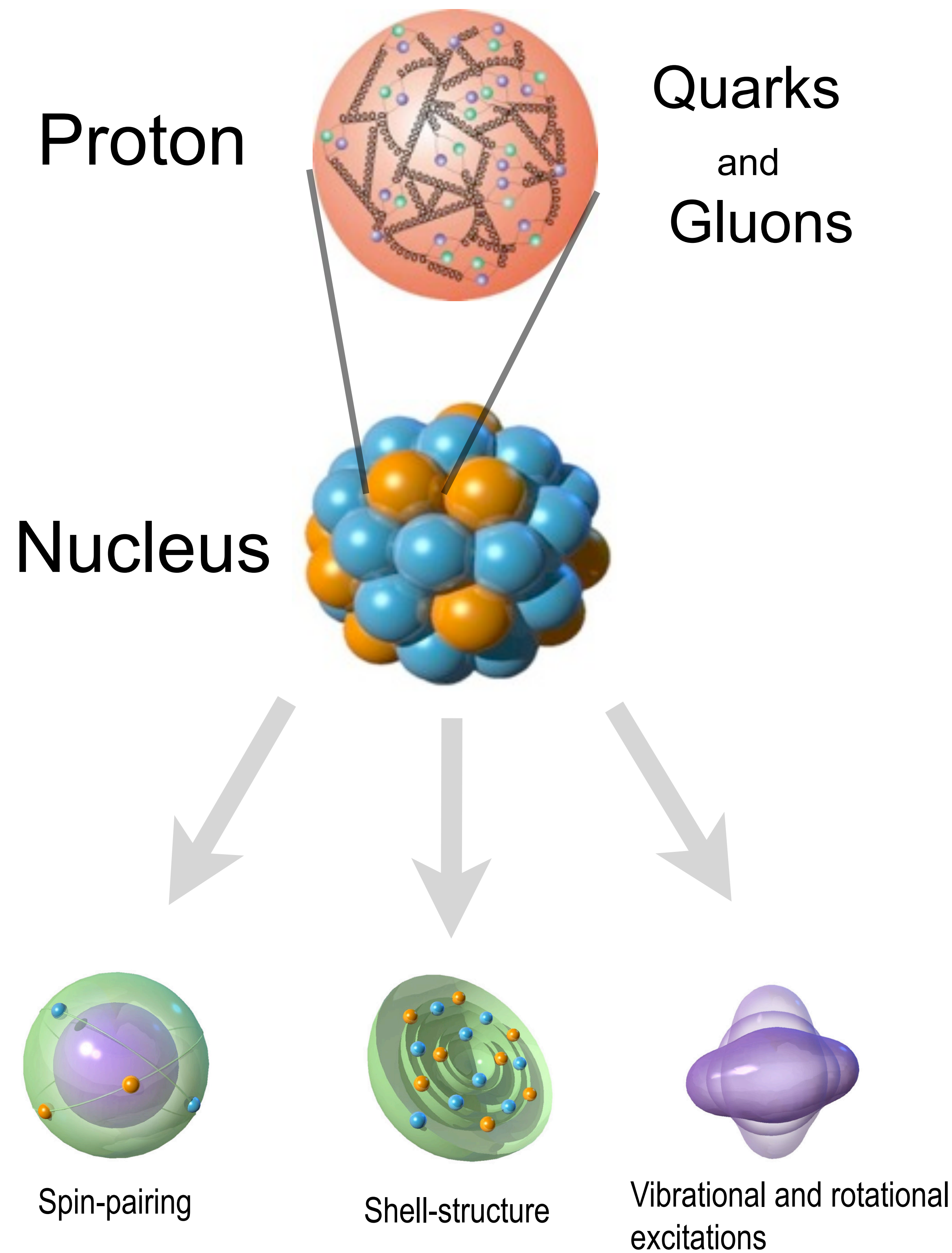
Aaron Torok
Indiana

Andre Walker-Loud
LBNL

... to make predictions for the structure and interactions of nuclei using lattice QCD.

USQCD US Lattice Quantum Chromodynamics

The Structure and Interactions of Matter from Quantum Chromodynamics

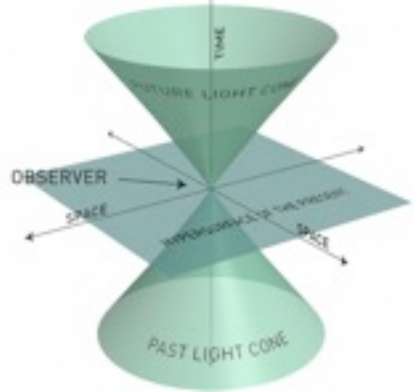


$$\Lambda_{\mathrm{QCD}}$$

$$\frac{m_u}{\Lambda_{\mathrm{QCD}}} \qquad \frac{m_d}{\Lambda_{\mathrm{QCD}}} \qquad \frac{m_s}{\Lambda_{\mathrm{QCD}}}$$

$$\alpha_e$$

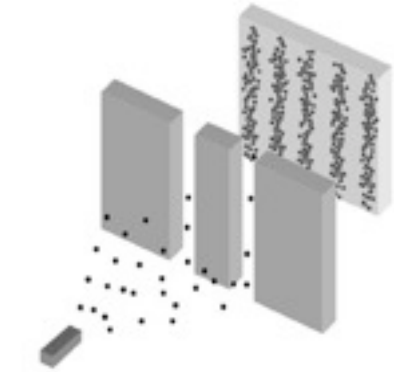
Small number of input parameters responsible for all of strongly interacting matter



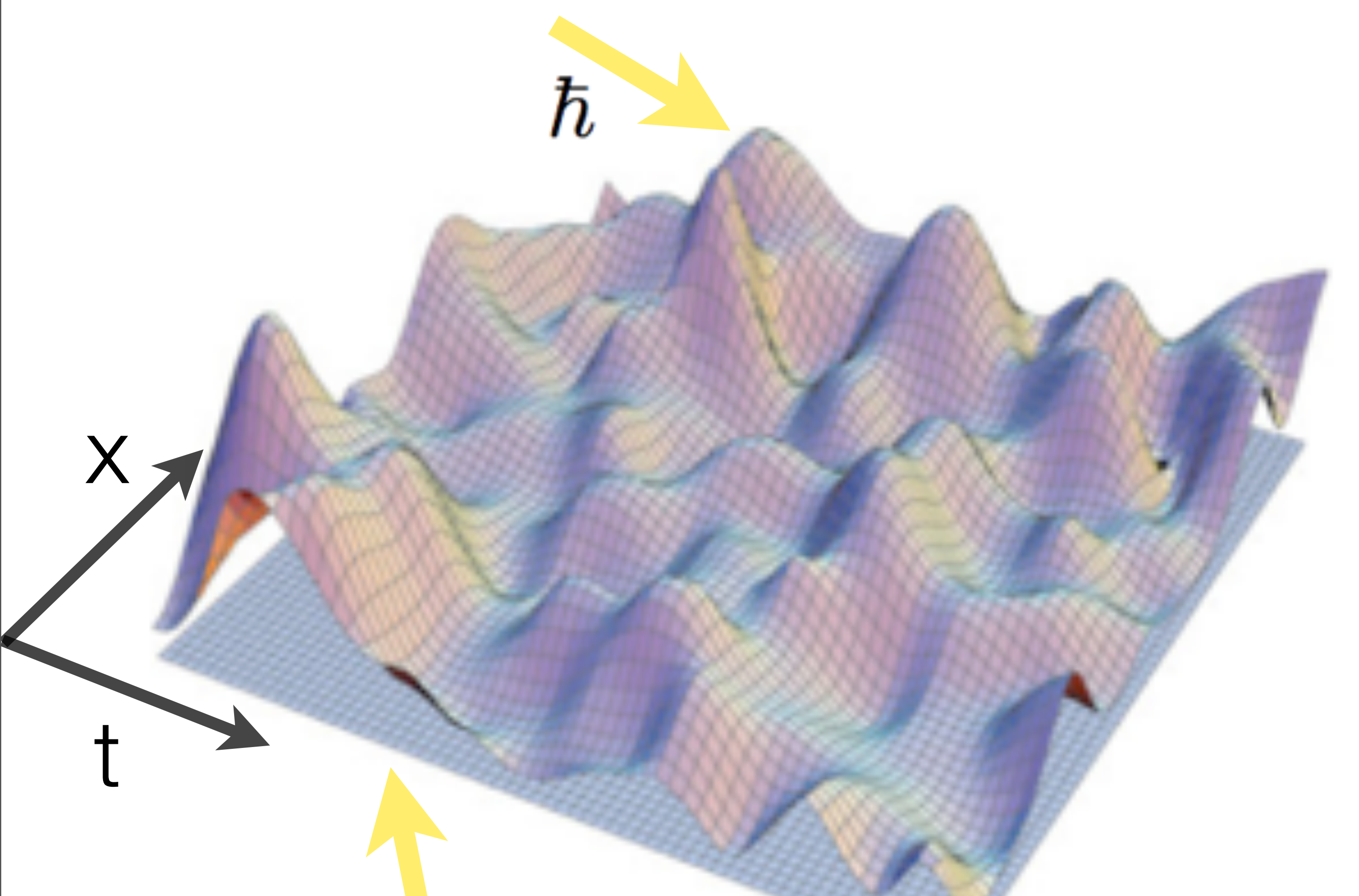
Quantum Field Theory

Scalar Field

a number at each point in space-time

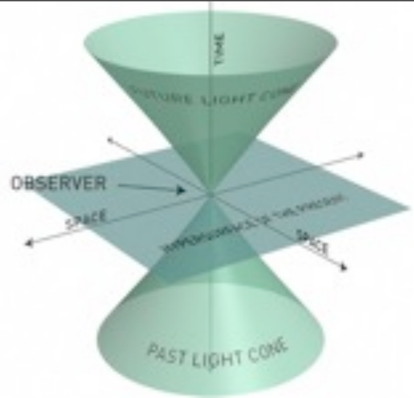


Quantum Vacuum



Classical Vacuum

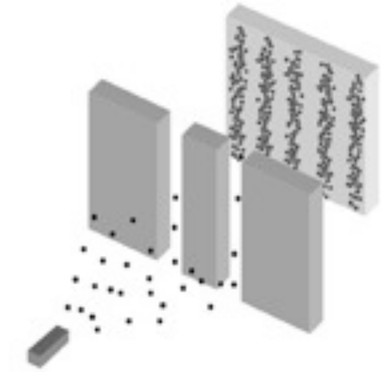
$$e^{\frac{i}{\hbar}S[\phi]}$$



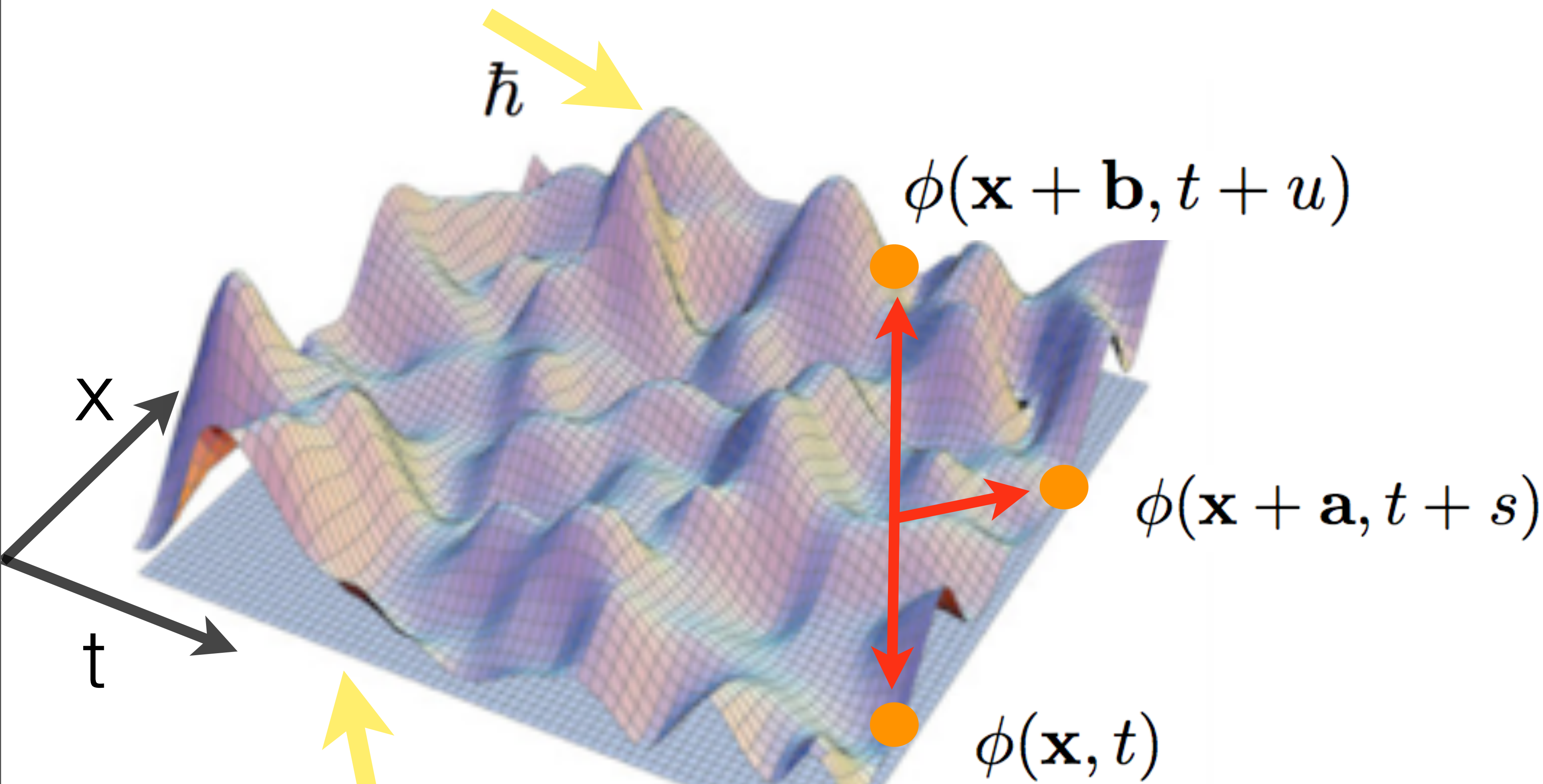
Quantum Field Theory

Scalar Field

a number at each point in space-time



Quantum Vacuum



$$e^{\frac{i}{\hbar}S[\phi]}$$

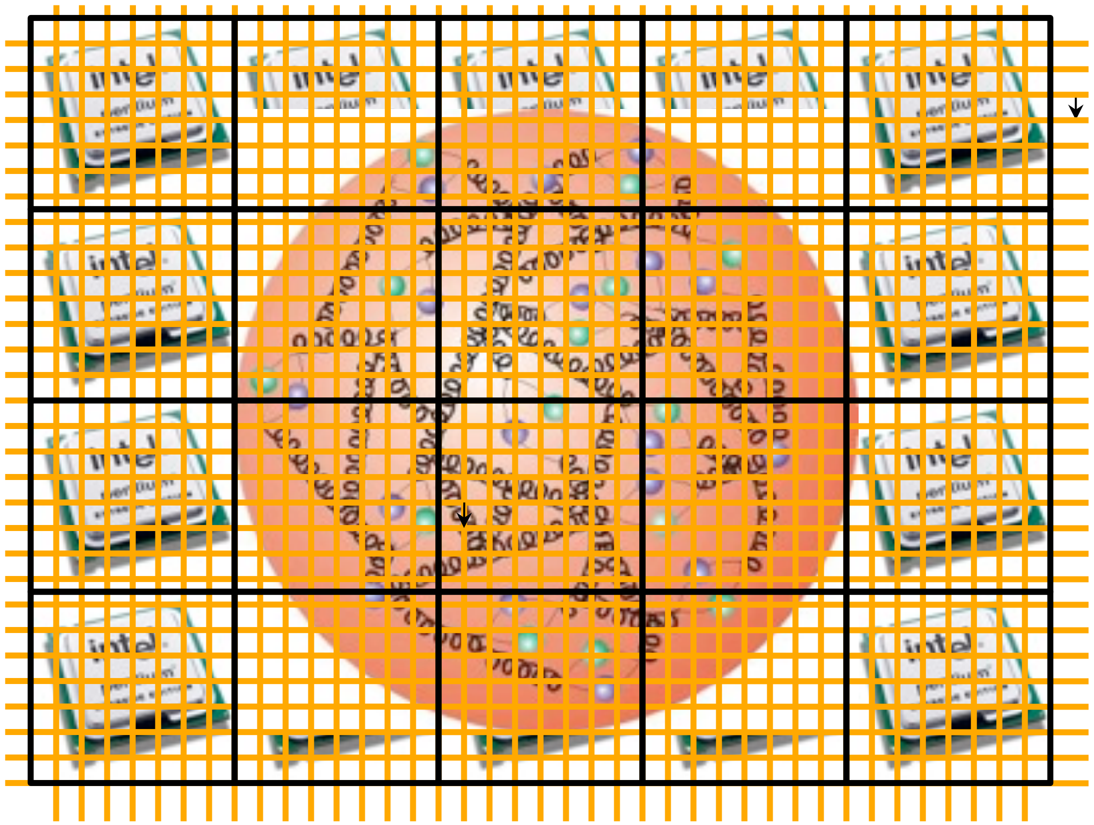
Classical Vacuum

e.g. $\langle\phi(\mathbf{x},t)\phi(\mathbf{x}+\mathbf{a},t+s)\phi(\mathbf{x}+\mathbf{b},t+u)\rangle$

Quantum Fluctuations in the Vacuum Dictate Observables

Lattice QCD

Monte-Carlo Evaluation of QCD Path Integral



Lattice Spacing :
$a << 1/\Lambda\chi$
(Nearly Continuum)

Lattice Volume :
$m_\pi L >> 2\pi$
(Nearly Infinite Volume)

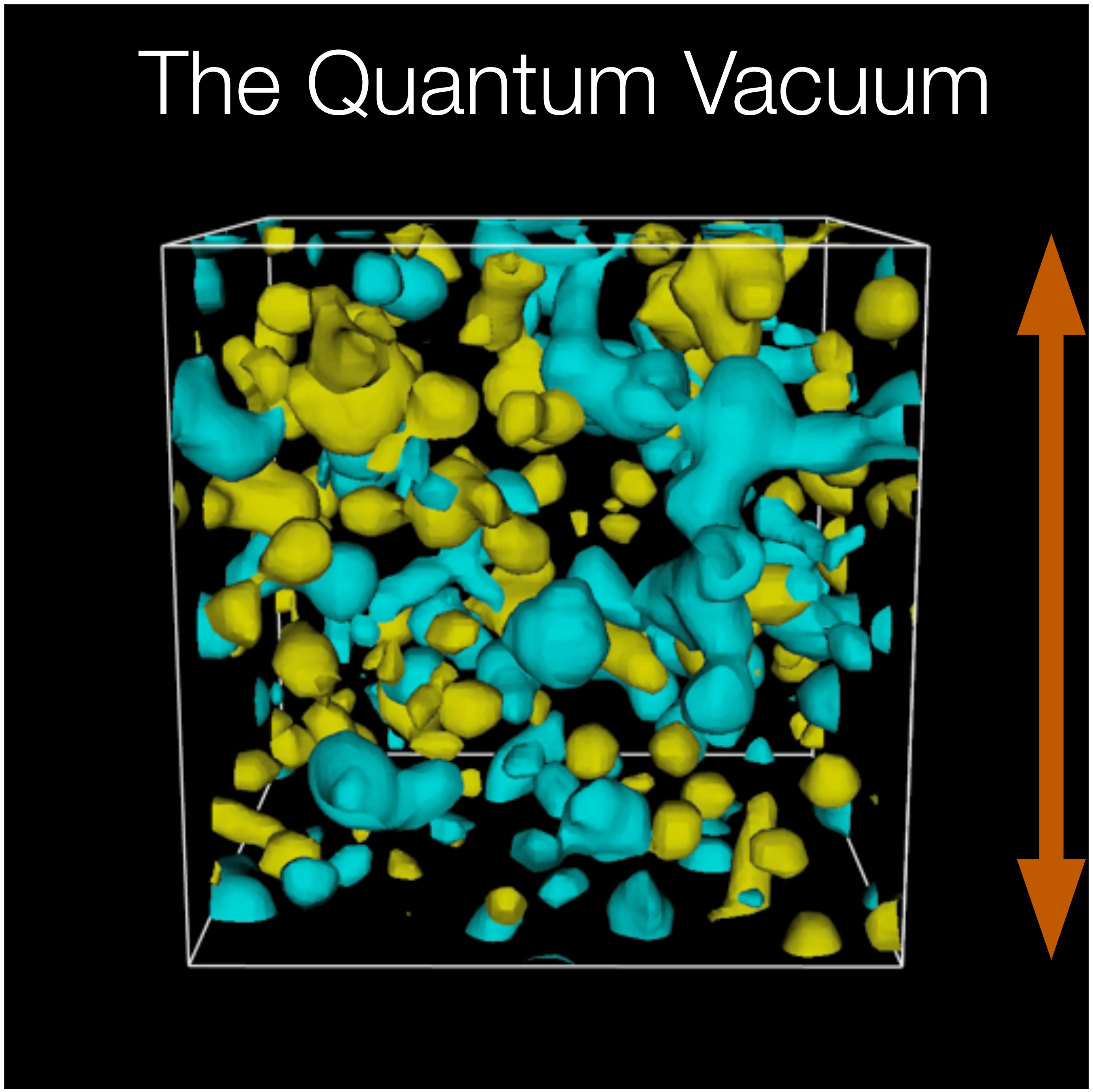
Effective Field Theory gives form of extrapolation $a = 0$ and $L = \infty$

Propagators Gauge Configurations

$$\langle \hat{\theta} \rangle \sim \int \mathcal{D}\mathcal{U}_\mu \; \hat{\theta}[\mathcal{U}_\mu] \; \mathrm{det}[\kappa[\mathcal{U}_\mu]] \; e^{-S_{YM}} \quad \rightarrow \frac{1}{N} \sum_{\mathrm{gluon\ \ cfgs}}^{N} \hat{\theta}\,[\mathcal{U}_\mu]$$

At the Heart of Visible Matter

The Vacuum is Complex

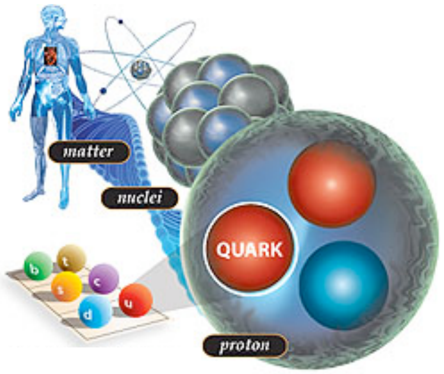


$$L \sim 4 \ \mathrm{fm}$$

$$\Delta t \sim 6 \times 10^{-24} \ s$$

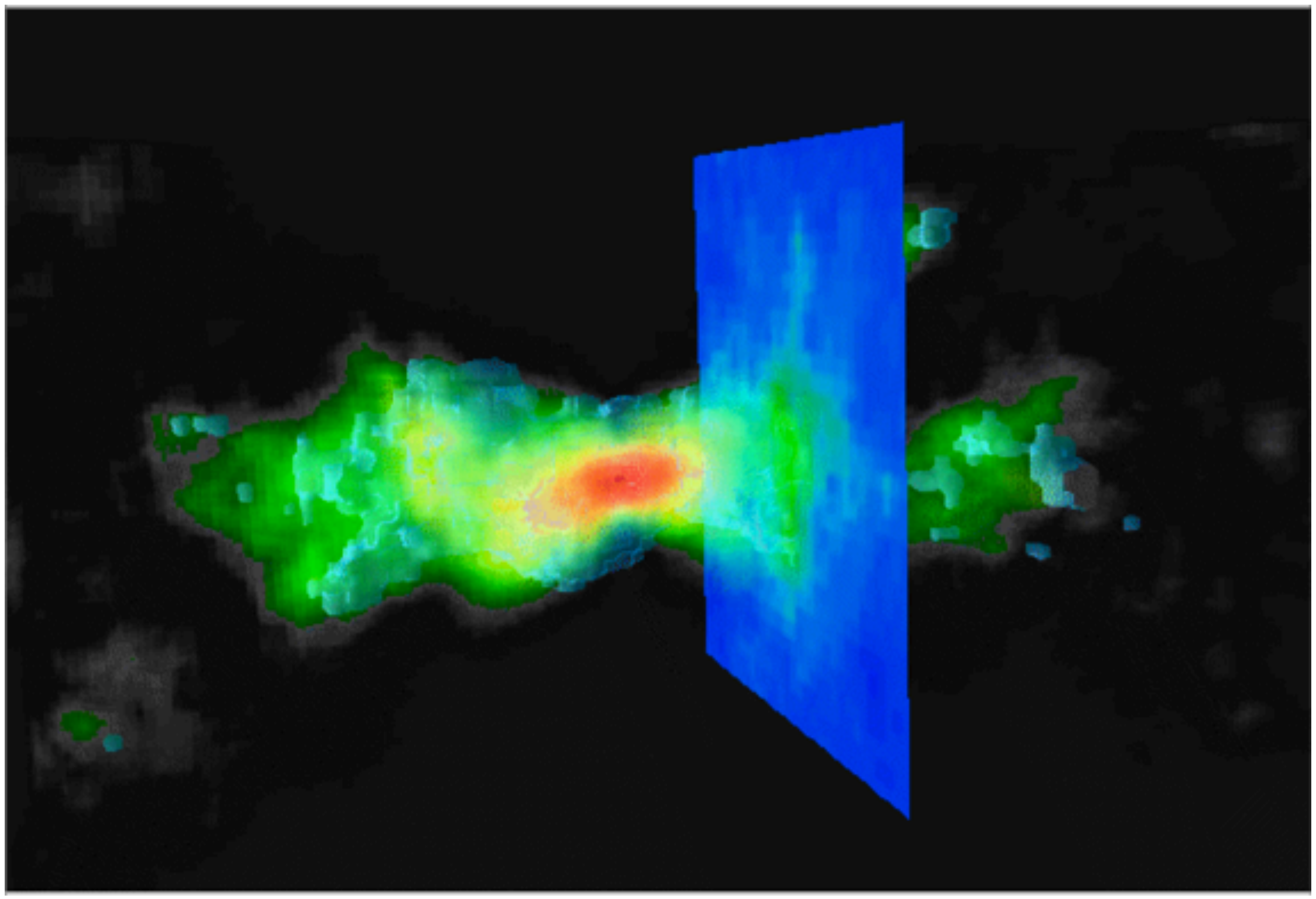
“Pixelation” ~ $(0.12 \times 10^{-15}\ \mathrm{m})^3$

Topological Charge Density
Massimo DiPierro



At the Heart of Visible Matter

Quarks and Gluons are Confined (T=0)



Rajan Gupta *et al*

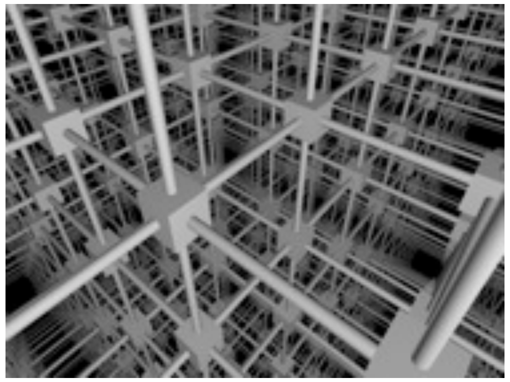
Quark Propagator on One Gauge Configuration

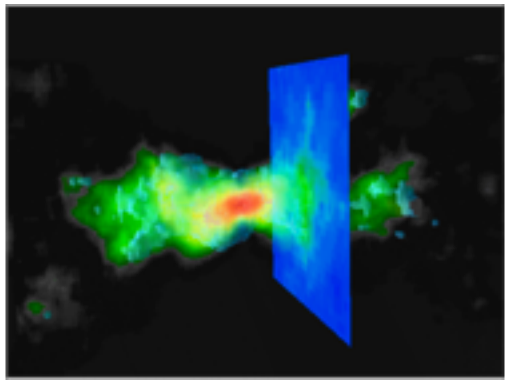
No isolated (free) quarks

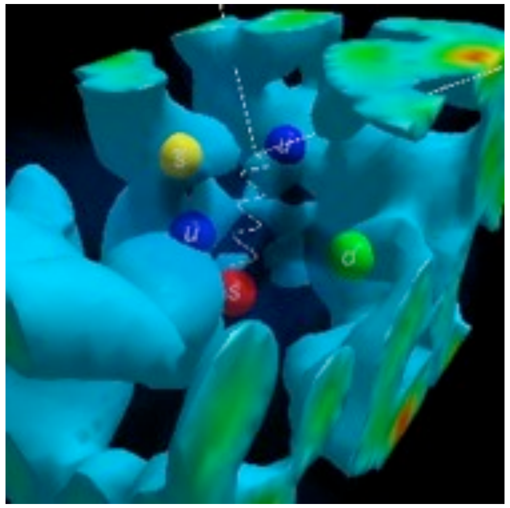
Cancellation of Probability Amplitudes

Pion, Nucleon from same propagators

LQCD Calculations Today





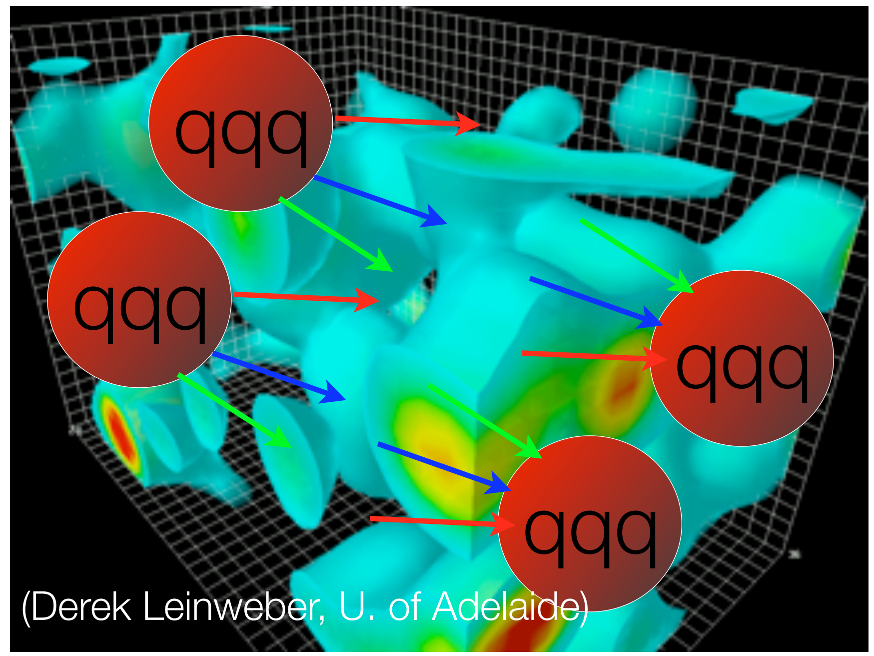


- Configurations
  - HMC, 2+1 (+1) flavors , isotropic or anisotropic
  - Domain-Wall, Clover, Staggered : det of matrix >> 10^8 x 10^8
  - >= physical quark masses
  - L from ~2.5 fm to > 12 fm , a from ~0.1 fm to < 0.05 fm
  - No EM and degenerate light quarks
  - <~ 128K cpu cores , ~10K trajectories, ~ 1K cfgs , < 10 GB/cfg
  - generated once, saved for use by many (USQCD)

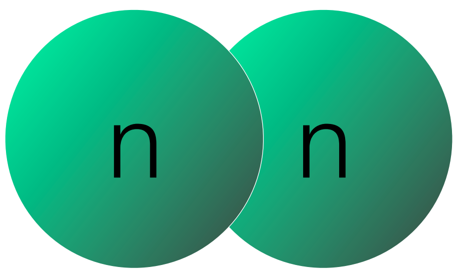
- Propagators
  - <~64K cpu and ~256 gpu (parallel code)
  - generated, used for correlation functions, deleted
  - < 100 GB
  - 1 (HEP) to 500 (NP) propagators per cfg
  - invert Dirac operator : deflation, multi-grid, ...

- Contractions
  - Hundreds of different correlation functions per propagator
  - permutations - recursion - needs algorithmic development, arprec
  - one xml file saved for subsequent analysis

Multi-Hadron Systems



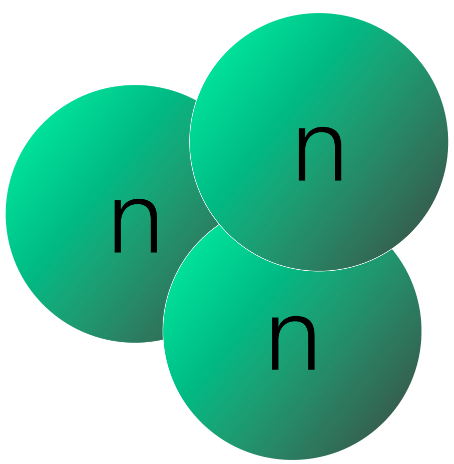
NN-interaction
verification

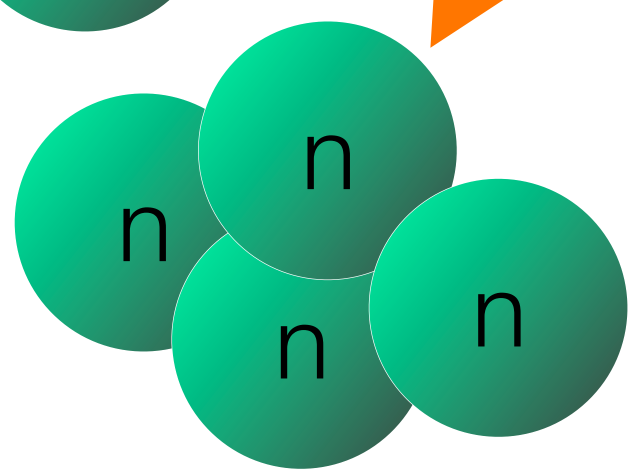


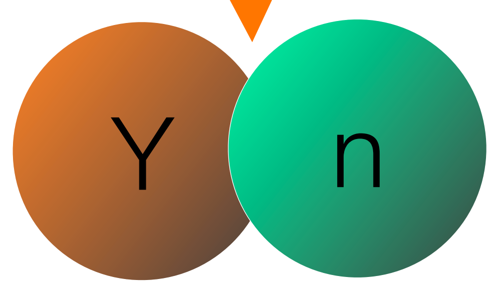
Hadron-Hadron

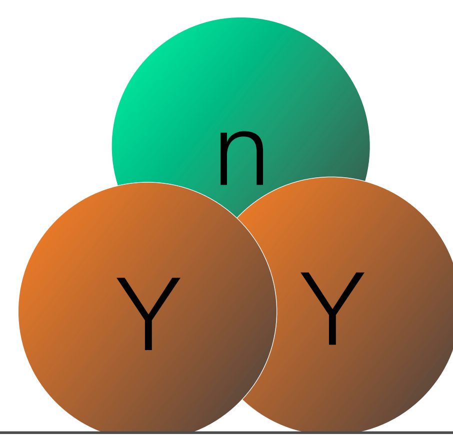
1) T-Matrix (E) ala Luscher
NPLQCD

2) $U(E, \mathbf{r}, \mathbf{r}', \mathrm{sink})$
HALQCD







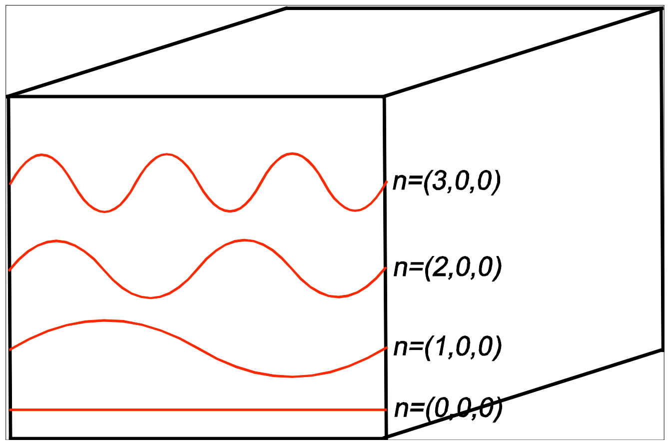


Two-Particle Energy Levels (Luscher)

Below Inelastic Thresholds :

Measure on lattice $\Rightarrow$ $$\delta E = 2\sqrt{p^2 + m^2} - 2m$$

UV regulator



Gives the scattering amplitude at δE

Two-Particle Energy Levels (Luscher)

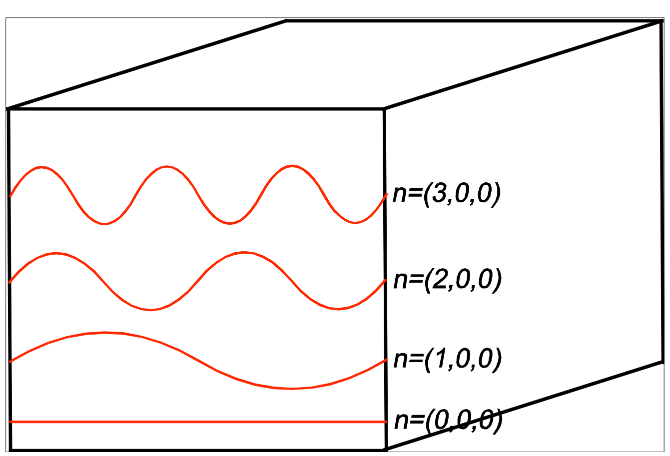
Below Inelastic Thresholds :

Measure on lattice $\Rightarrow$ $$\delta E = 2\sqrt{p^2+m^2} - 2m$$

$$\boxed{p\cot\delta(p) = \frac{1}{\pi L}\,\mathbf{S}\left(\left(\frac{Lp}{2\pi}\right)^2\right)}$$

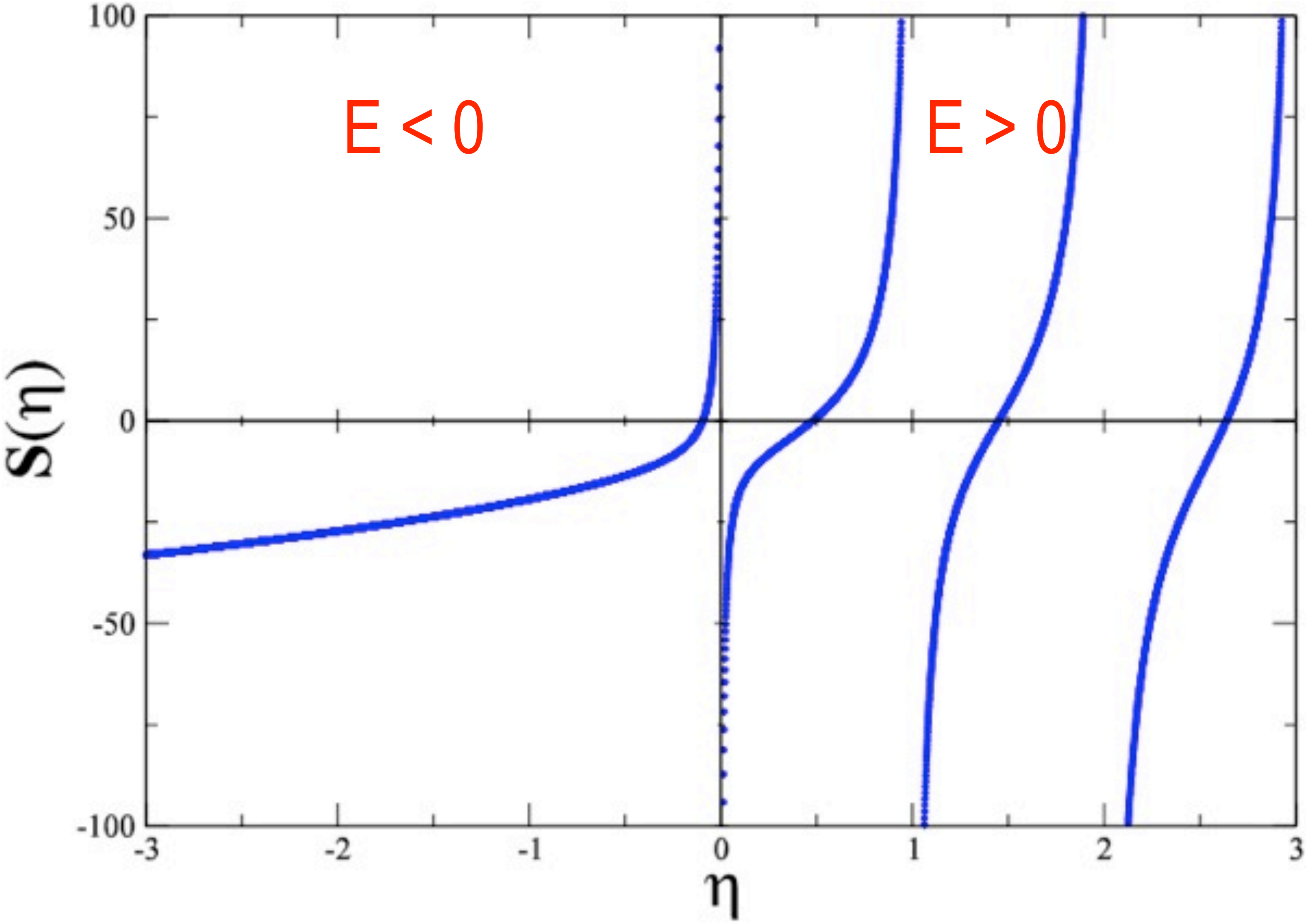
UV regulator

$$\mathbf{S}(\eta) \equiv \sum_{\mathbf{j}}^{\Lambda_j} \frac{1}{|\mathbf{j}|^2 - \eta} - 4\pi\Lambda_j$$



Gives the scattering amplitude at δE

Luscher Relation



A_1^+

Bound-state or Scattering state ?

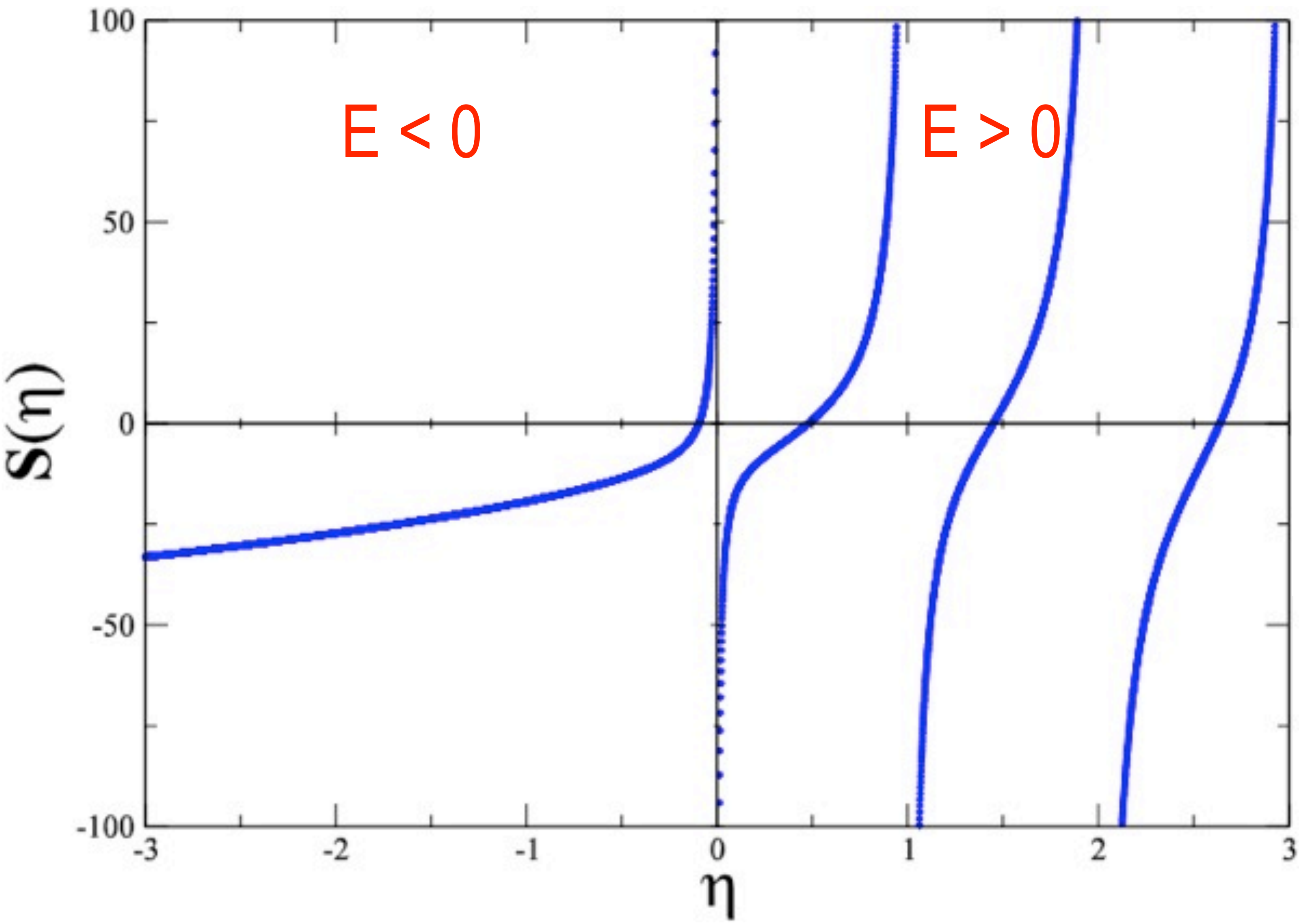
$$k = \frac{2\pi}{L} n$$

$$n = (nx, ny, nz)$$

Non-interacting particles

$$V = 0 \quad \rightarrow \quad a = r = 0$$
$$S = \infty$$

Luscher Relation



A_1^+

Bound-state or
Scattering state ?

$$p \cot \delta(p) = \frac{1}{\pi L} \mathbf{S}\left(\left(\frac{Lp}{2\pi} \right)^2 \right)$$

$$k = \frac{2\pi}{L} n$$

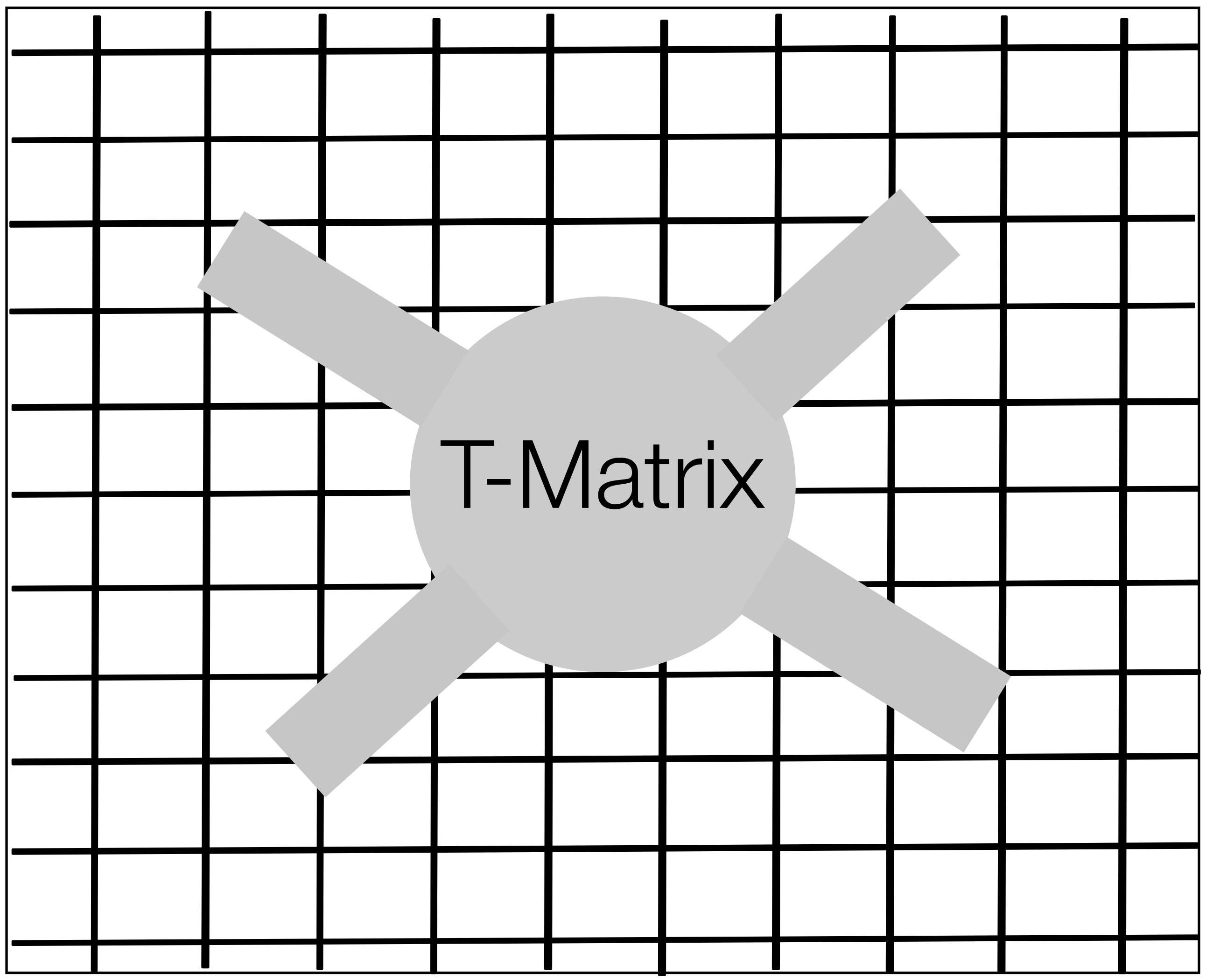
$$n = (nx, ny, nz)$$

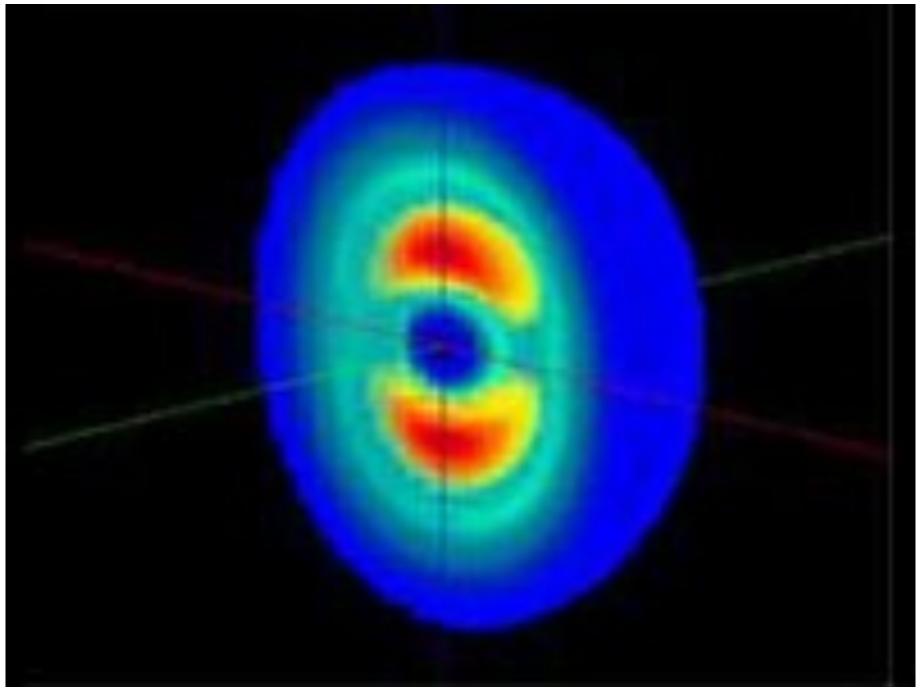
Non-interacting particles

$$V = 0 \quad \rightarrow \quad a = r = 0$$

$$S = \infty$$

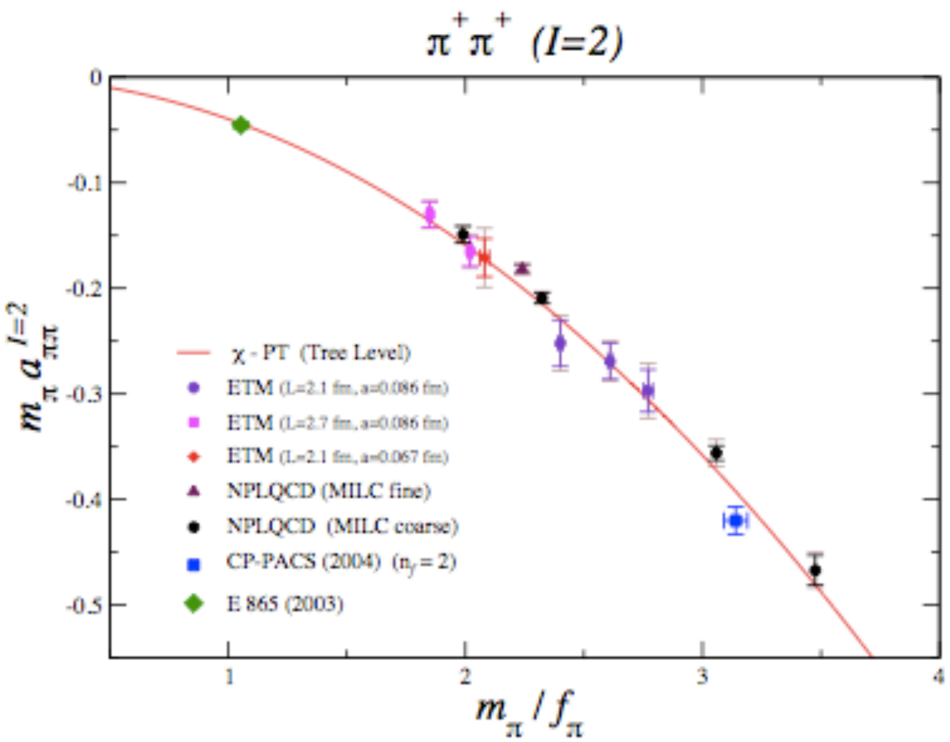
Large Scattering Lengths are OK !

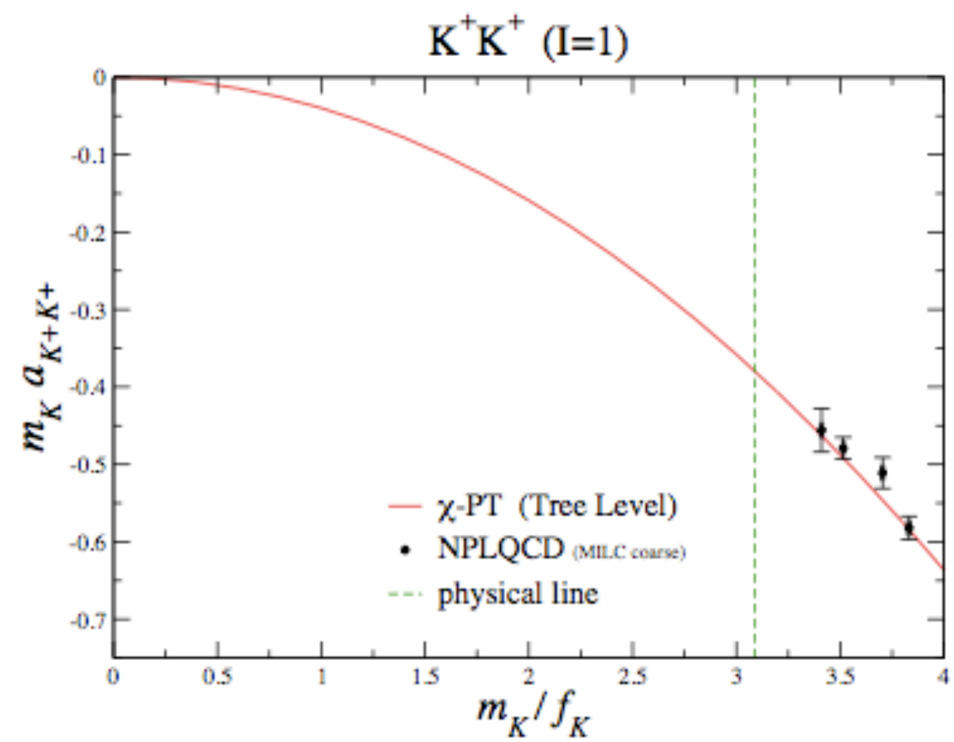


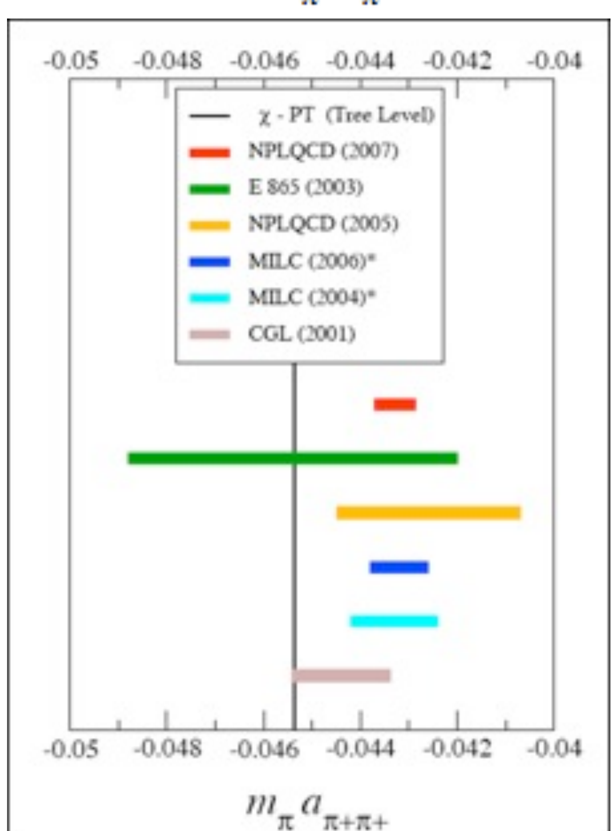


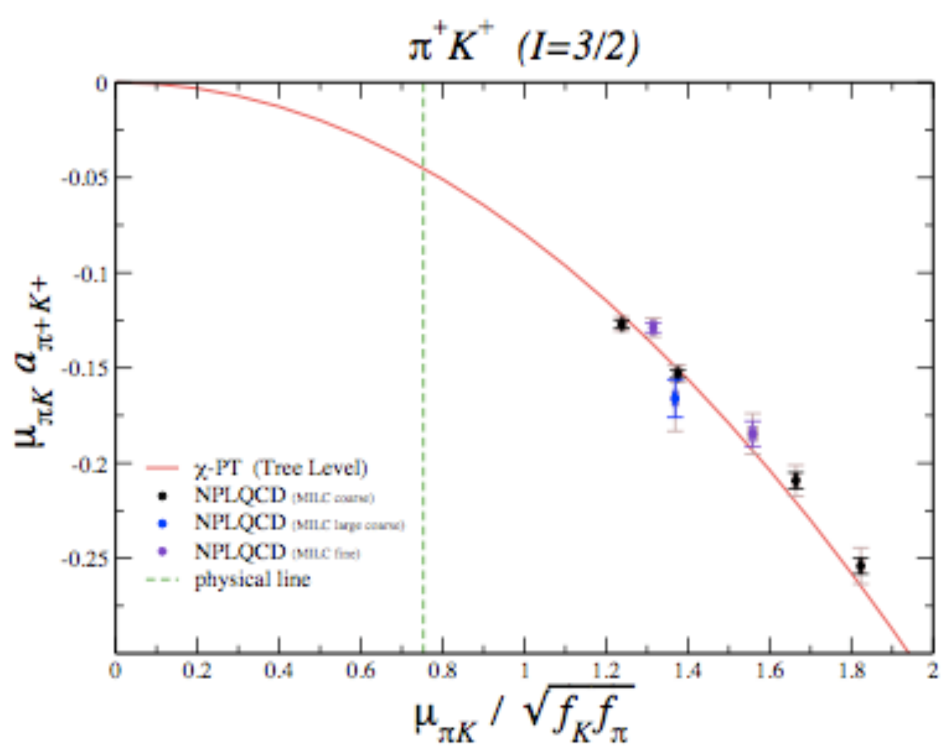
Require : $L >> r_0$ but ANY a

Lattice QCD and the Simplest Hadronic Interactions



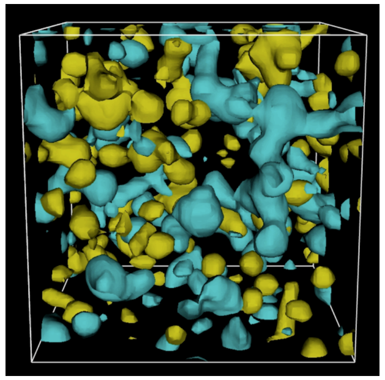




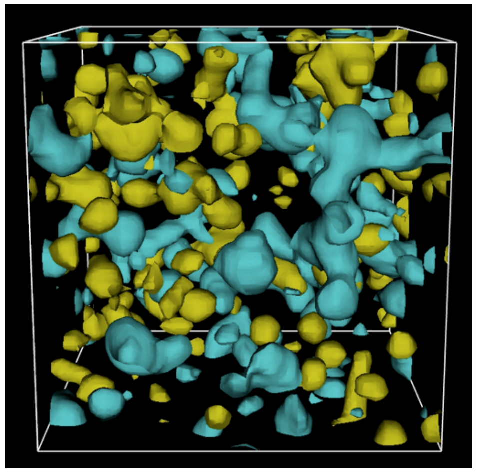


Multi-Volume Study by NPLQCD : 2009 - 2011

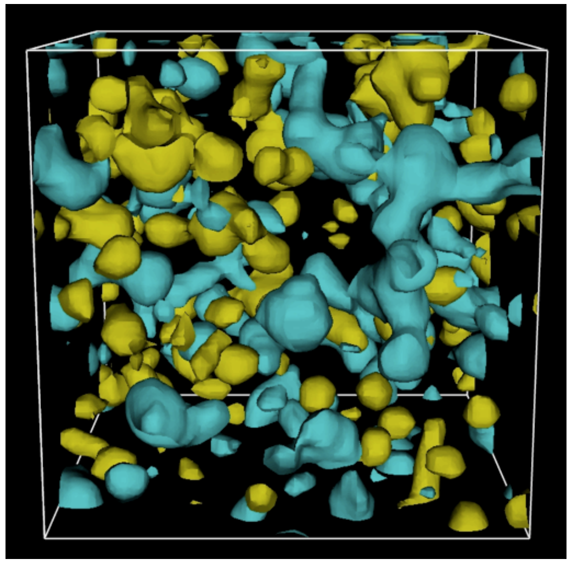
lattice spacing : $b \sim 0.123$ fm
pion mass : $m_\pi \sim 390$ MeV
fermion action : Clover
anisotropy : $\xi_t \sim 3.5$



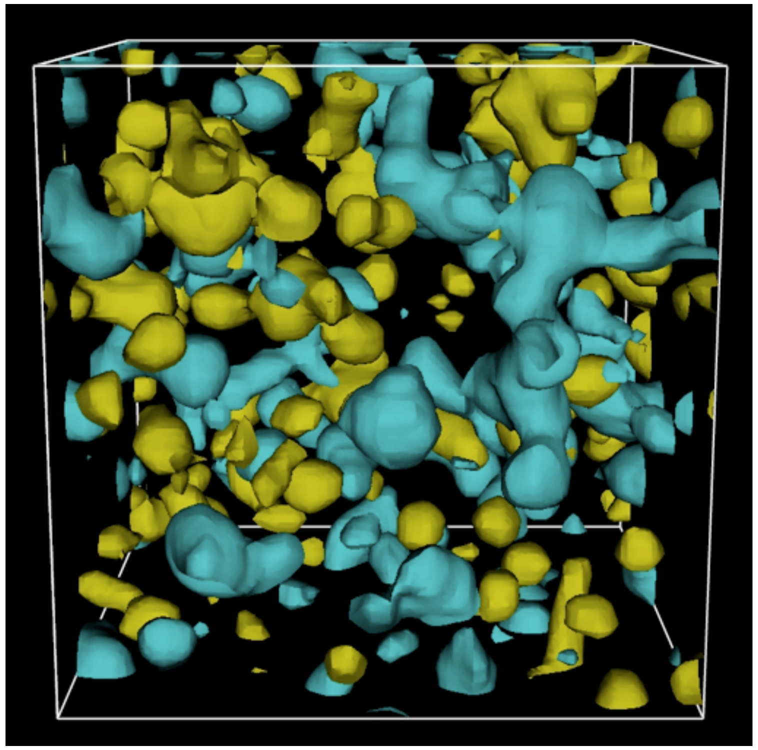
$L \sim 2$ fm



$L \sim 2.5$ fm



$L \sim 3$ fm



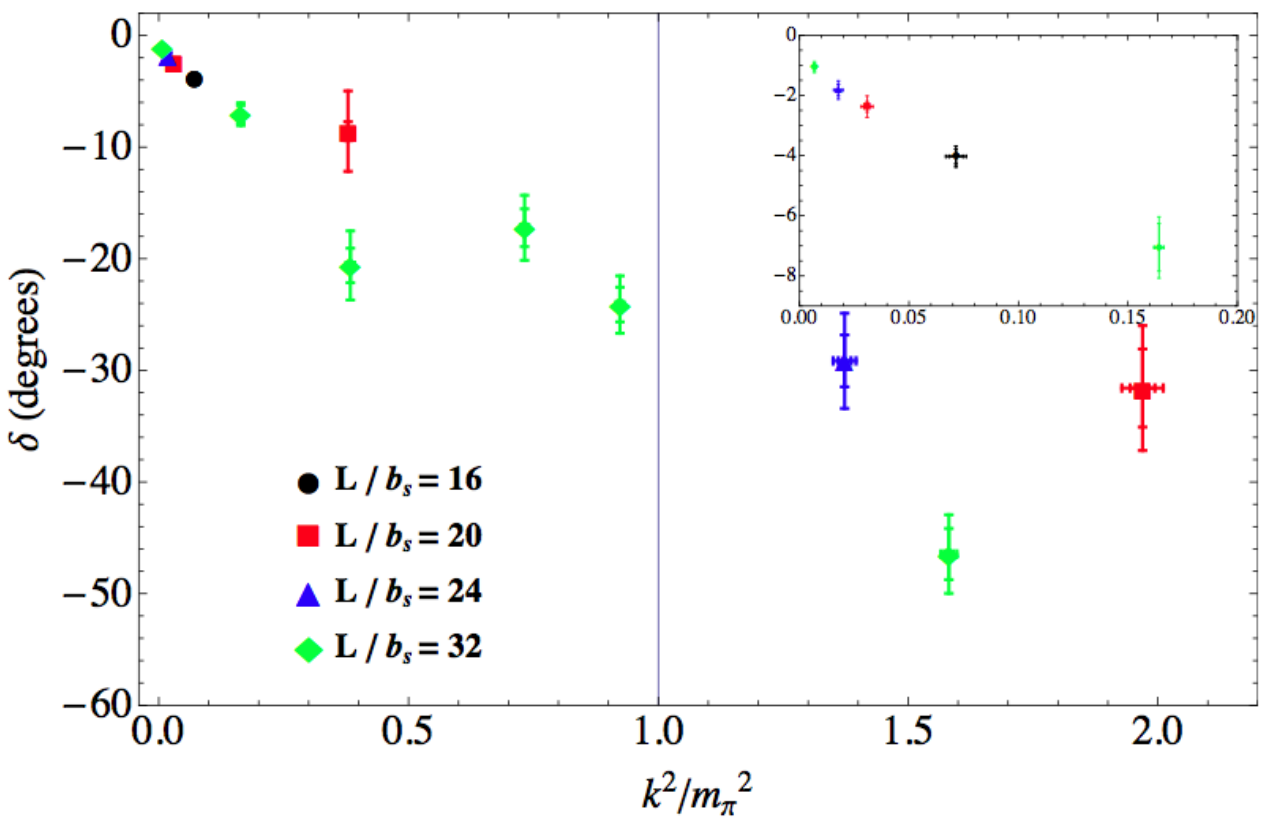
$L \sim 4$ fm

resources $:\sim 80 \times 10^6$ core hrs

$m_\pi L \sim 4\ ,\ 5\ ,\ 6\ ,\ 8 \qquad m_\pi T \sim 9\ ,\ 9\ ,\ 9\ ,\ 18$

$\mathrm{I} = 2 \;\; \pi\pi$ Scattering Phase-Shift

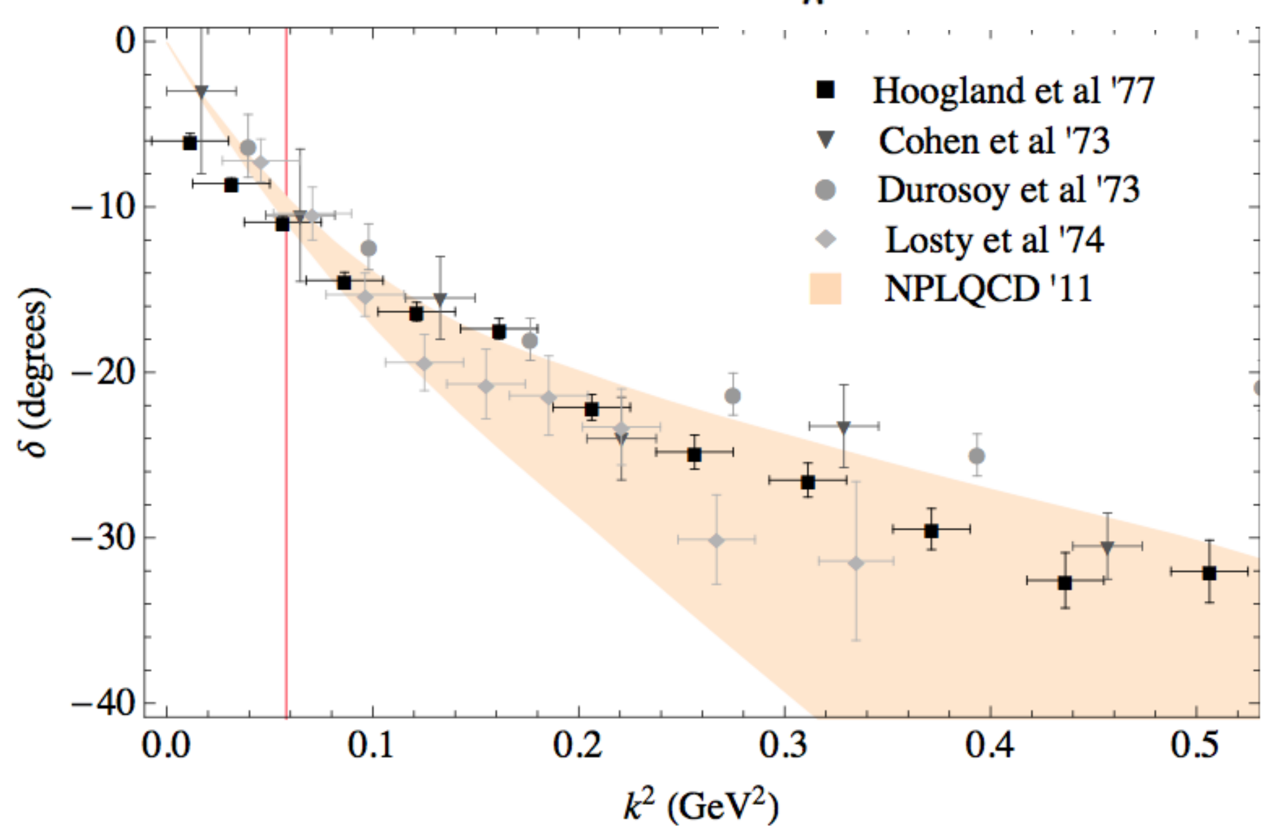
(Emmanuel Chang)



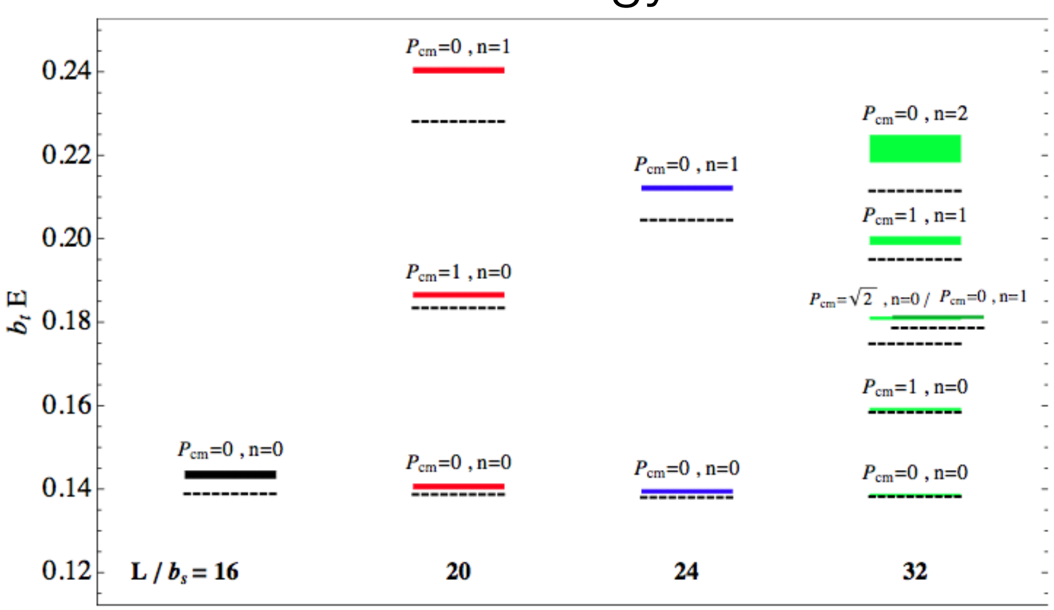
$m_\pi \sim 390$ MeV

χPT

$m_\pi \sim 139$ MeV



lattice energy-levels

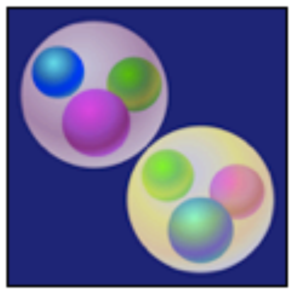


H-Dibaryon
An Exotic Nucleus

Jefferson Lab

sics » Synopses » Binding baryons on the lattice

Binding baryons on the lattice



Credit: Alan Stonebraker

Evidence for a Bound *H* Dibaryon from Lattice QCD

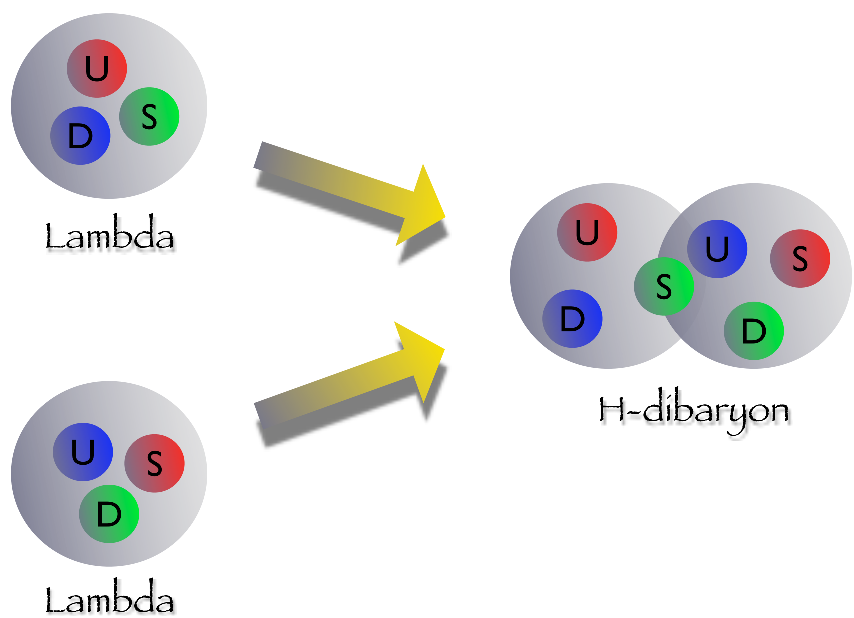
S. R. Beane, E. Chang, W. Detmold, B. Joo, H. W. Lin, T. C. Luu, K. Orginos, A. Parreño, M. J. Savage, A. Torok, and A. Walker-Loud (NPLQCD Collaboration)

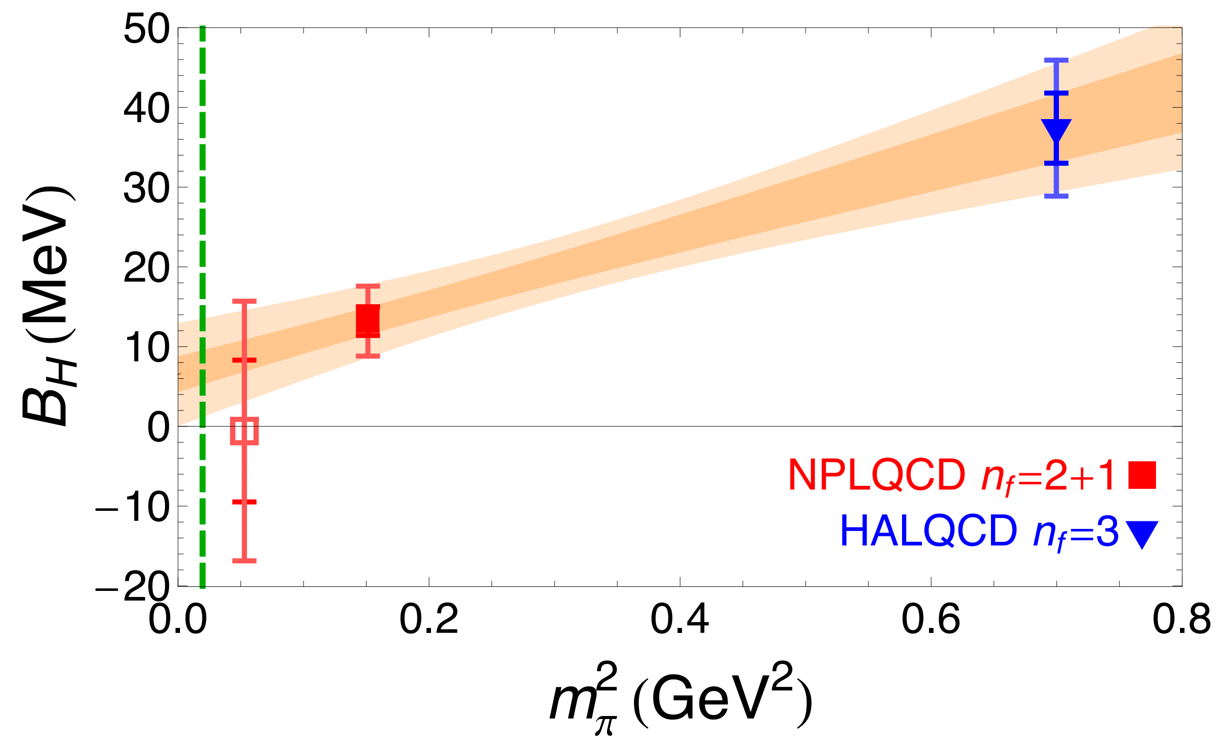
Phys. Rev. Lett. **106**, 162001 (Published April 20, 2011)

Bound *H* Dibaryon in Flavor SU(3) Limit of Lattice QCD

Takashi Inoue, Noriyoshi Ishii, Sinya Aoki, Takumi Doi, Tetsuo Hatsuda, Yoichi Ikeda, Keiko Murano, Hidekatsu Nemura, and Kenji Sasaki (HAL QCD Collaboration)

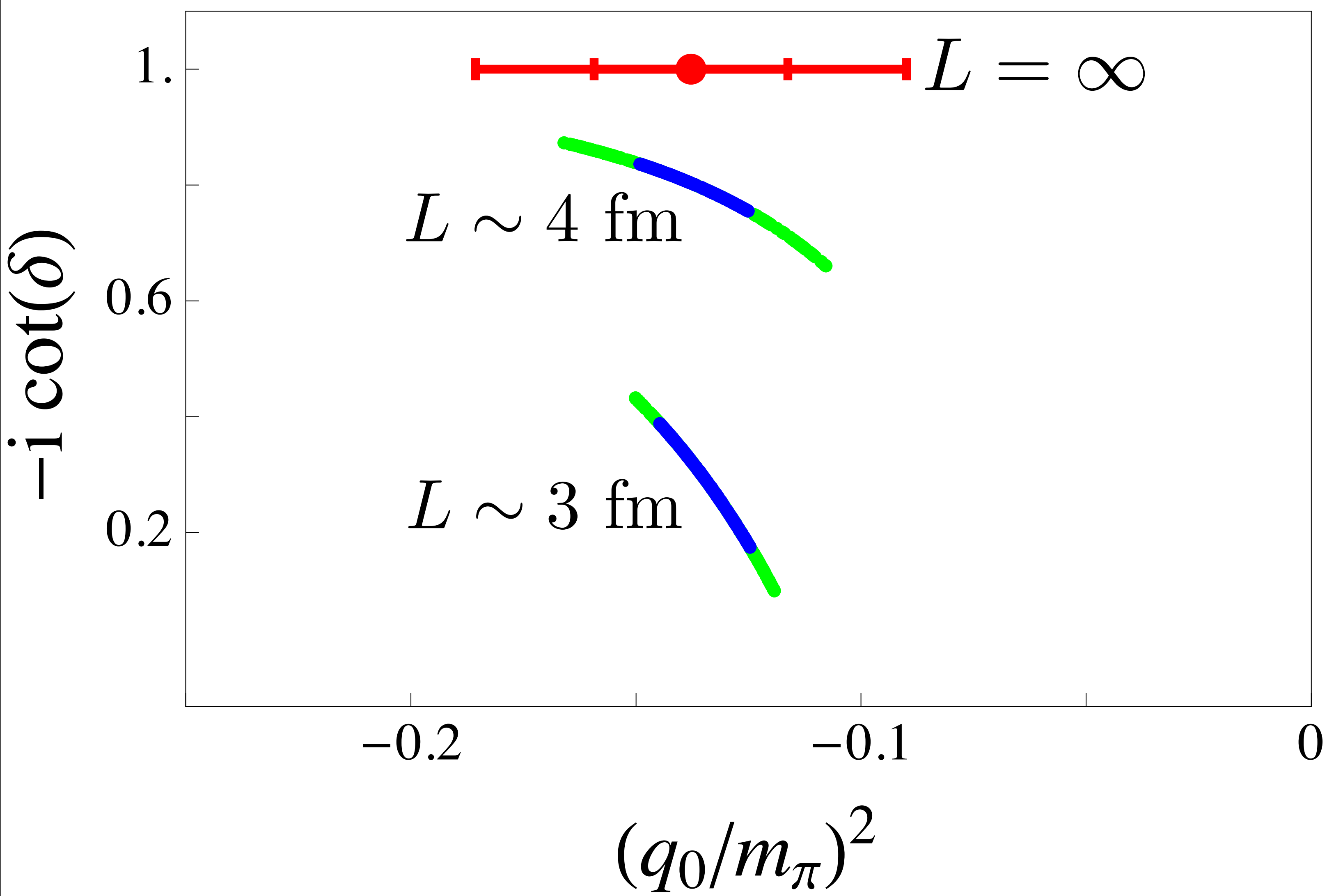
Phys. Rev. Lett. **106**, 162002 (Published April 20, 2011)

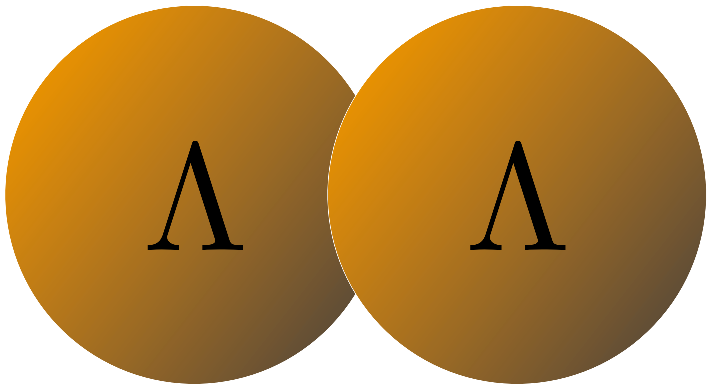




NSAC Milestone 2014 HP10: Carry out *ab initio* microscopic studies of the structure and dynamics of light nuclei based on two-nucleon and many-nucleon forces and lattice QCD calculations of hadron interaction mechanisms relevant to the origins of the nucleon-nucleon interaction

H-Dibaryon
Infinite Volume Extrapolation





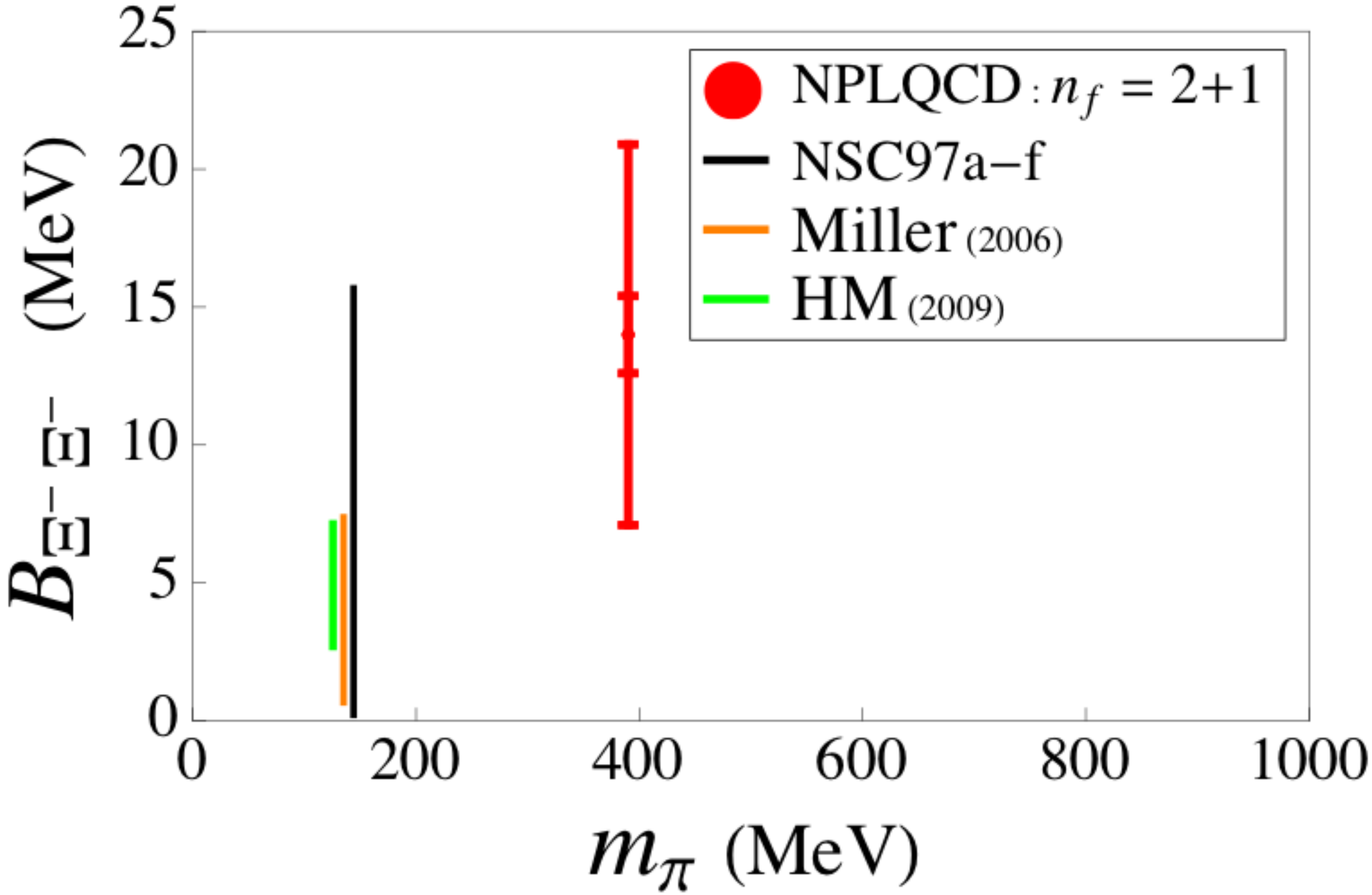
$$\mathcal{A} \sim \frac{1}{\cot\delta - i}$$

$$E \sim -B \; + \; c_1 \, \frac{e^{-\gamma L}}{L} \; + \; \ldots.$$

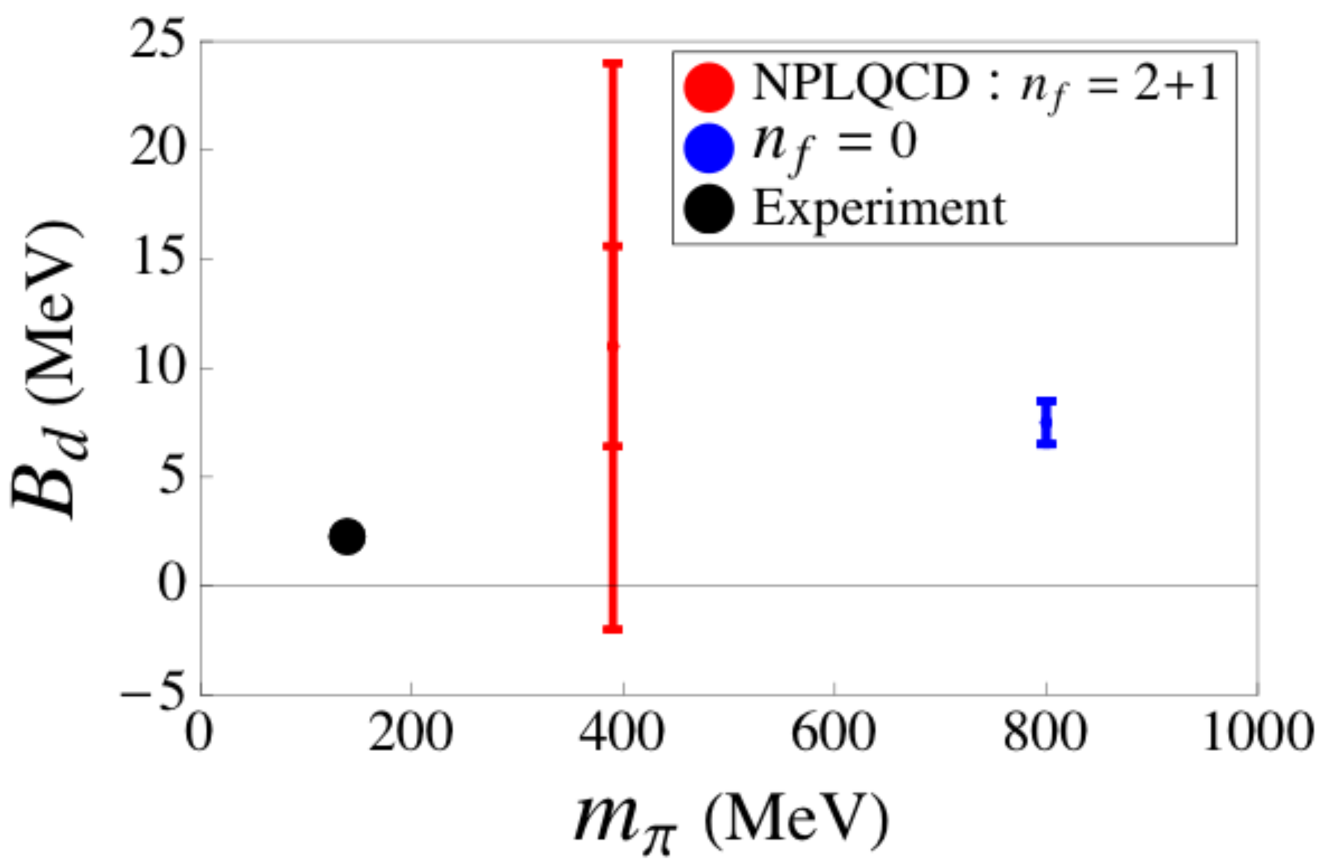
$$\boxed{B = 13.2 \text{ +- } 1.8 \text{ +- } 4.0 \text{ MeV}}$$

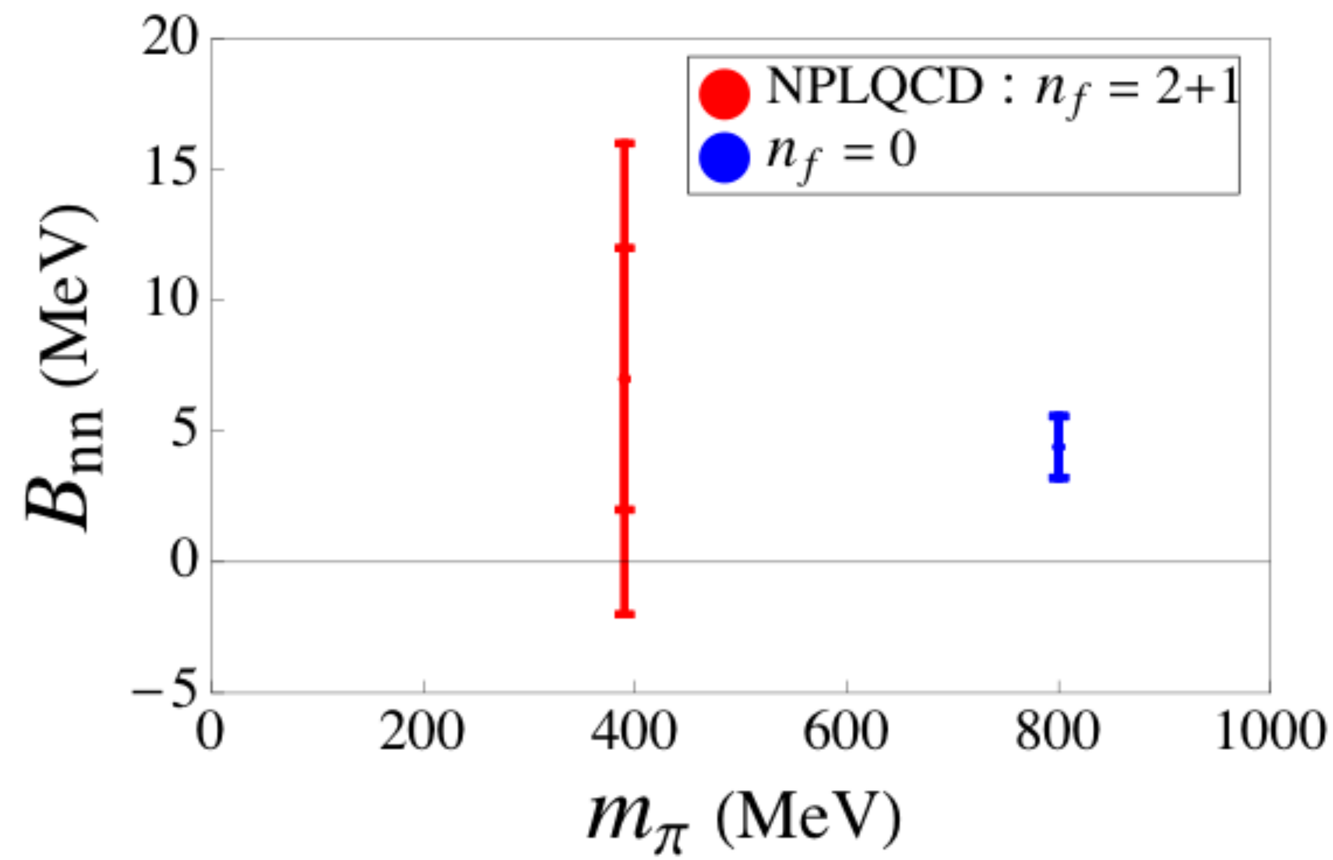
pion mass = 390 MeV

$\Xi^-\Xi^-$ Bound State

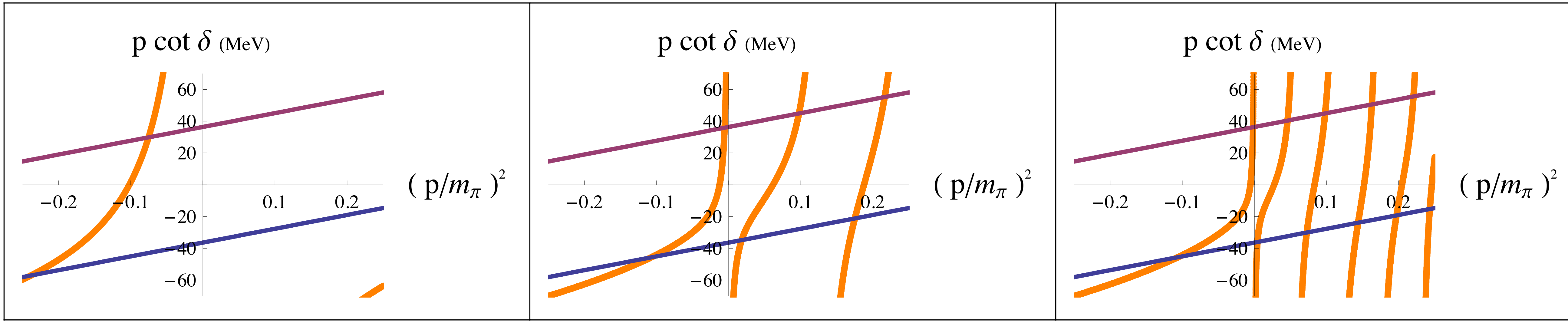


NN Bound States

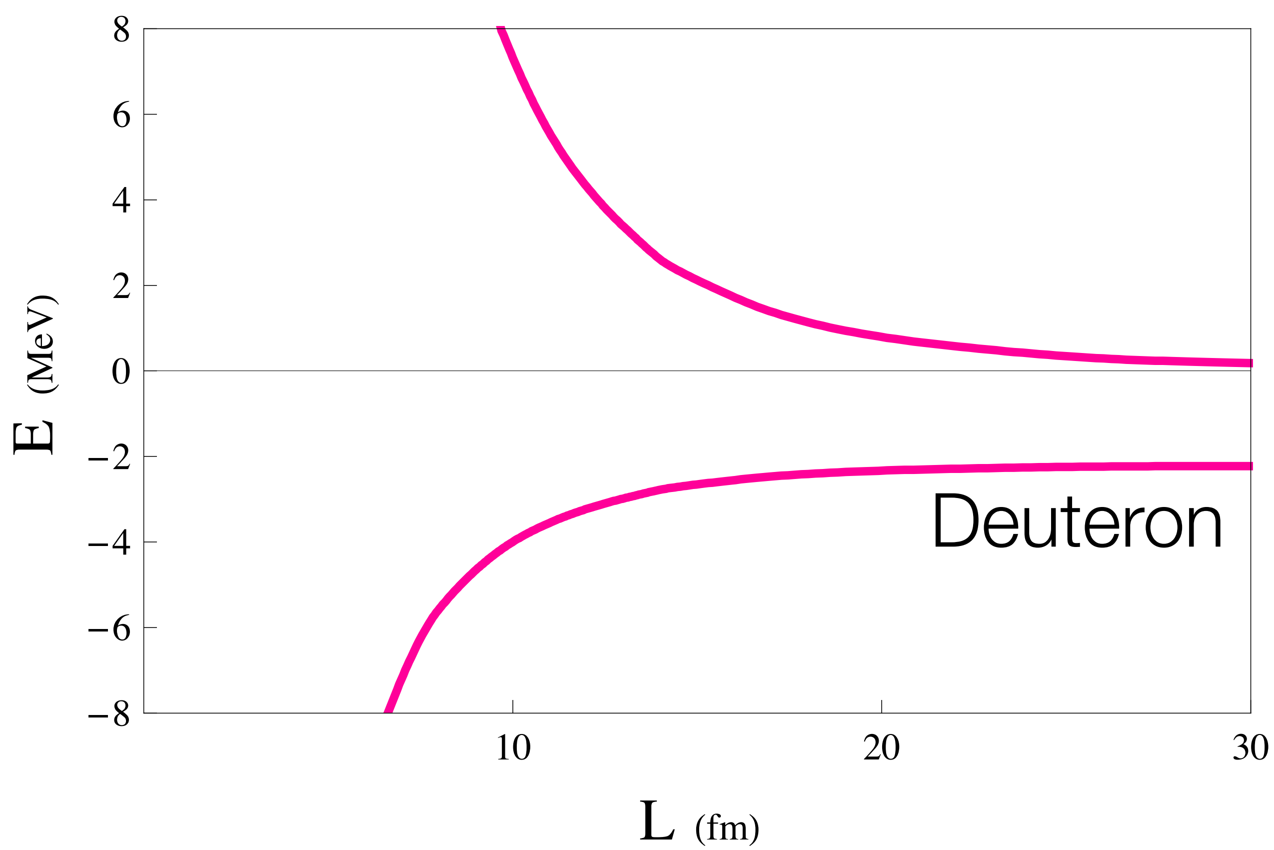




Expectations at Physical Quark Masses : $^3S_1$ - $^3D_1$



L=8.5 fm L=24.5 fm L=36.8 fm



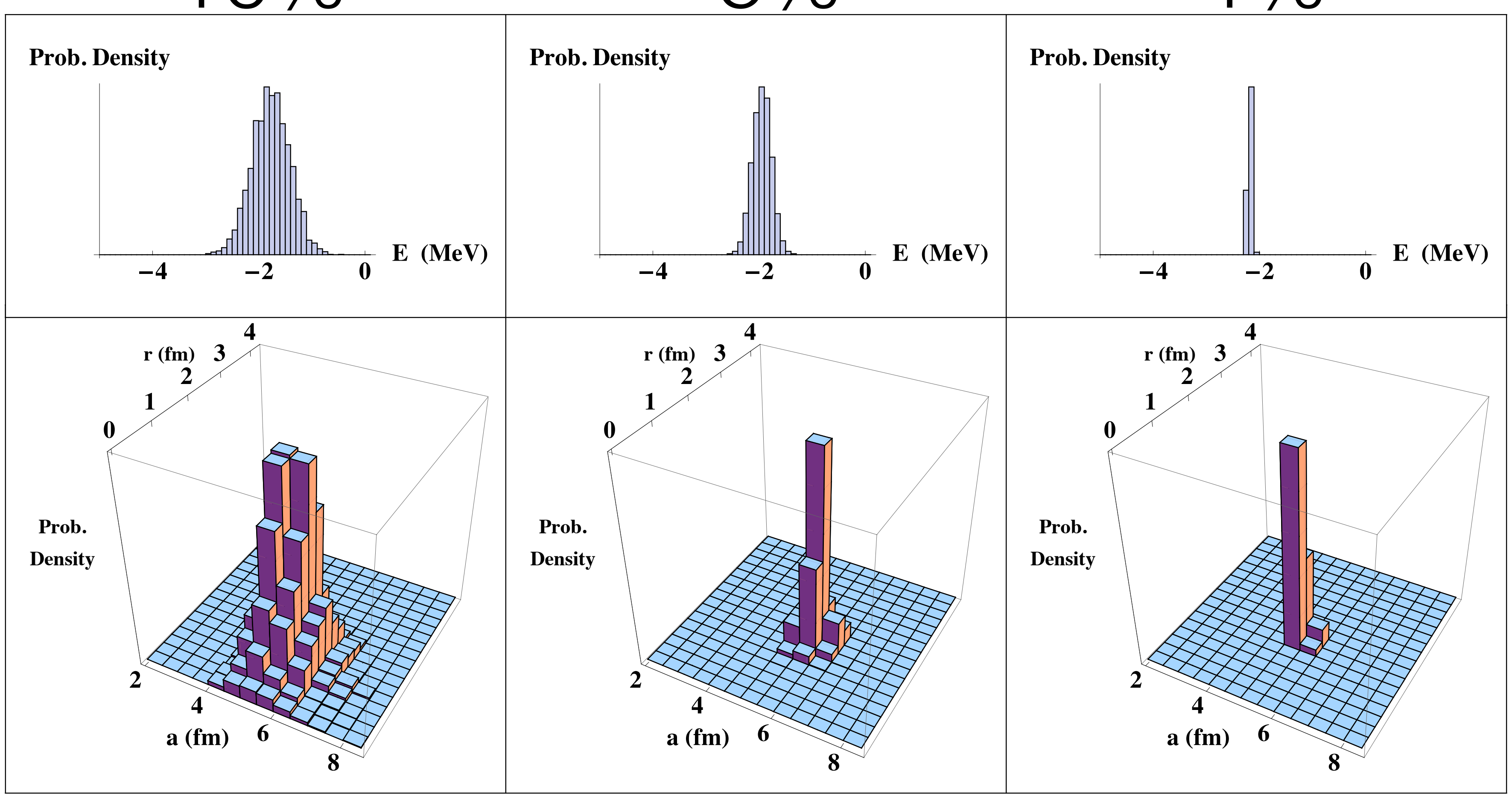
Simulated Calculations of the Deuteron

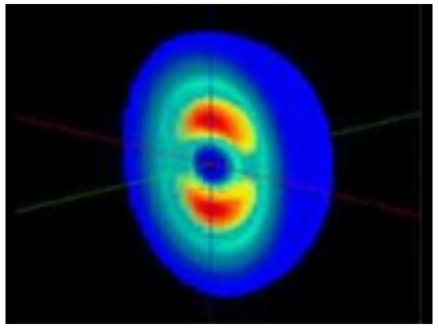
(NOT actual calculations)

Precision Level of Energy Shift	Bound State Energy (MeV)	1st ContinuumLevel (MeV)
0%	-3.147	4.005
1%	-3.111 ± 0.031	4.015 ± 0.040
5%	-2.95 ± 0.16	4.24 ± 0.20
10%	-2.66 ± 0.31	3.65 ± 0.40

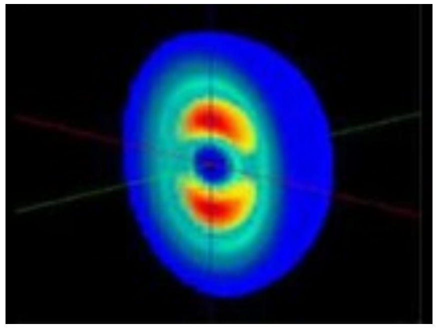
$$E_D \sim 2\ \mathrm{GeV}$$
$$\Delta E_D \sim 2\ \mathrm{MeV}$$

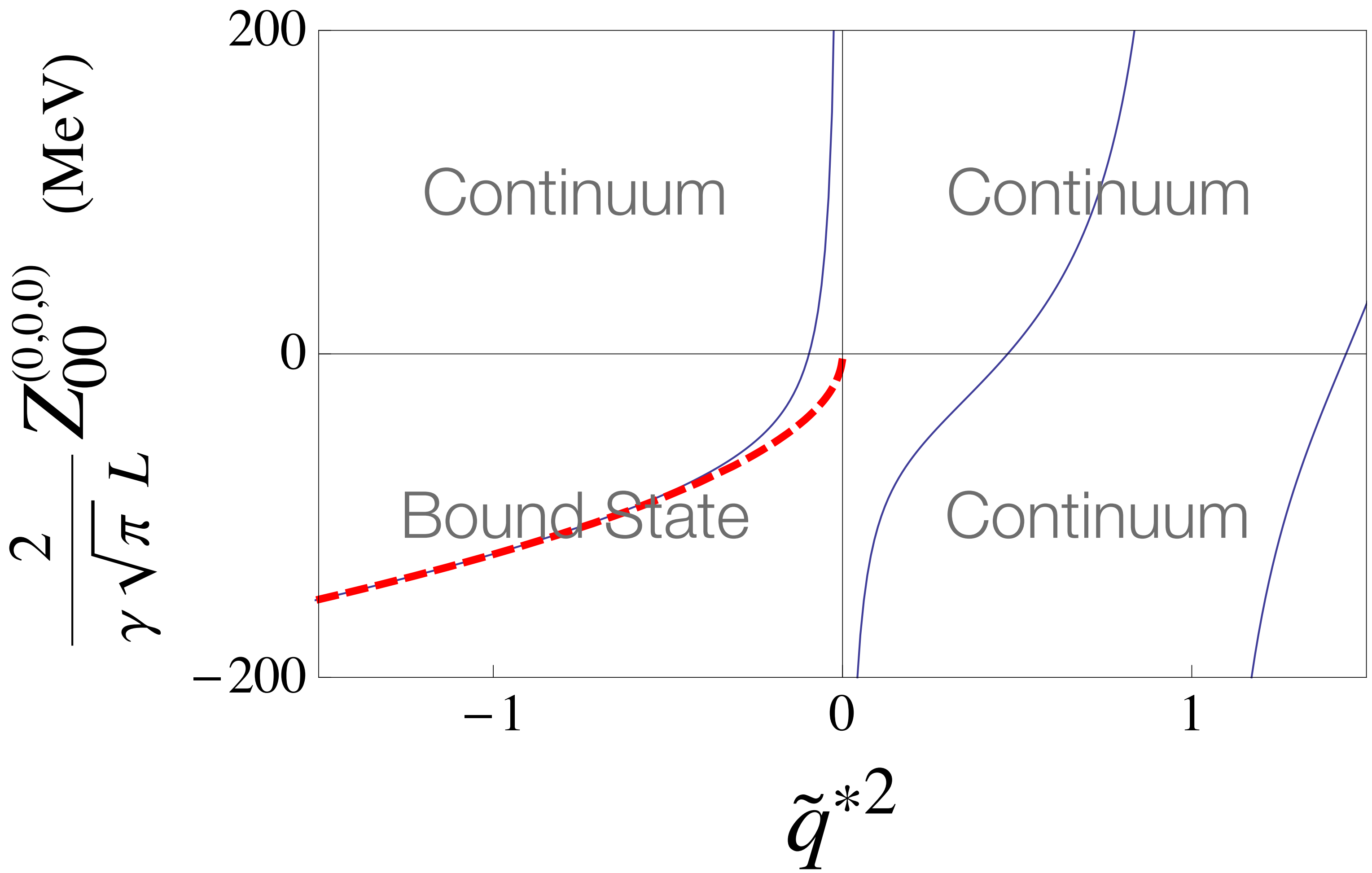
10% 5% 1%





Bound-States at Rest (I)



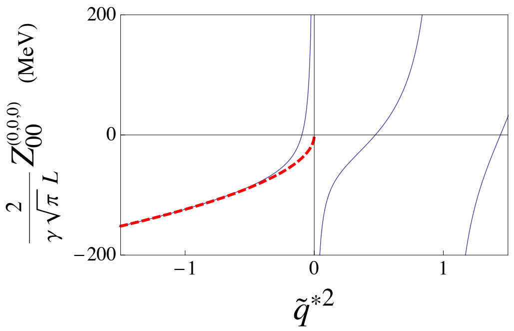


(Luscher)

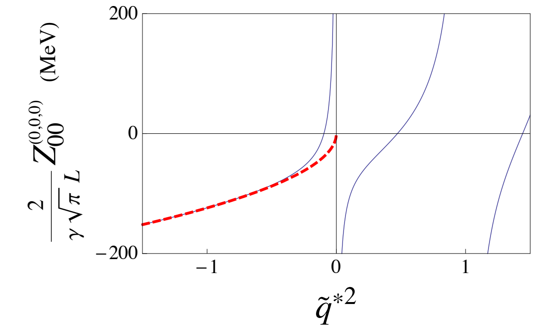
Difference between red and blue is FV effect

$$E = 2\sqrt{q^2+m^2} - 2m$$

$$Z_{00}^{(0)} = \sum_{\mathbf{n}} \frac{1}{|\mathbf{n}|^2 - \tilde{q}^2} \quad , \quad \tilde{q} = \frac{qL}{2\pi}$$



Bound-States at Rest (II)

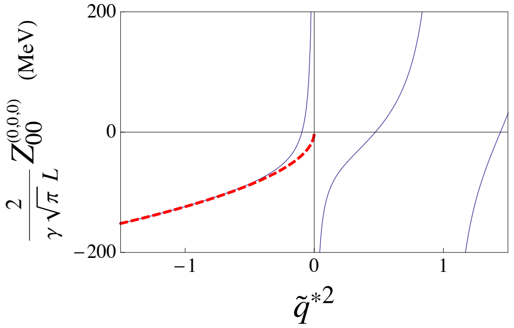


$$Z_{00}^{(0)} = \sum_{\mathbf{n}} \frac{1}{|\mathbf{n}|^2 - \tilde{q}^2} \quad , \quad \tilde{q} = \frac{qL}{2\pi}$$

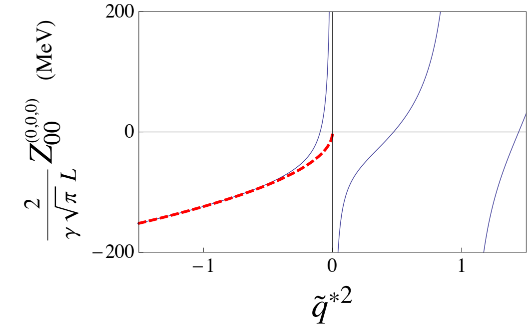
U.V. divergent

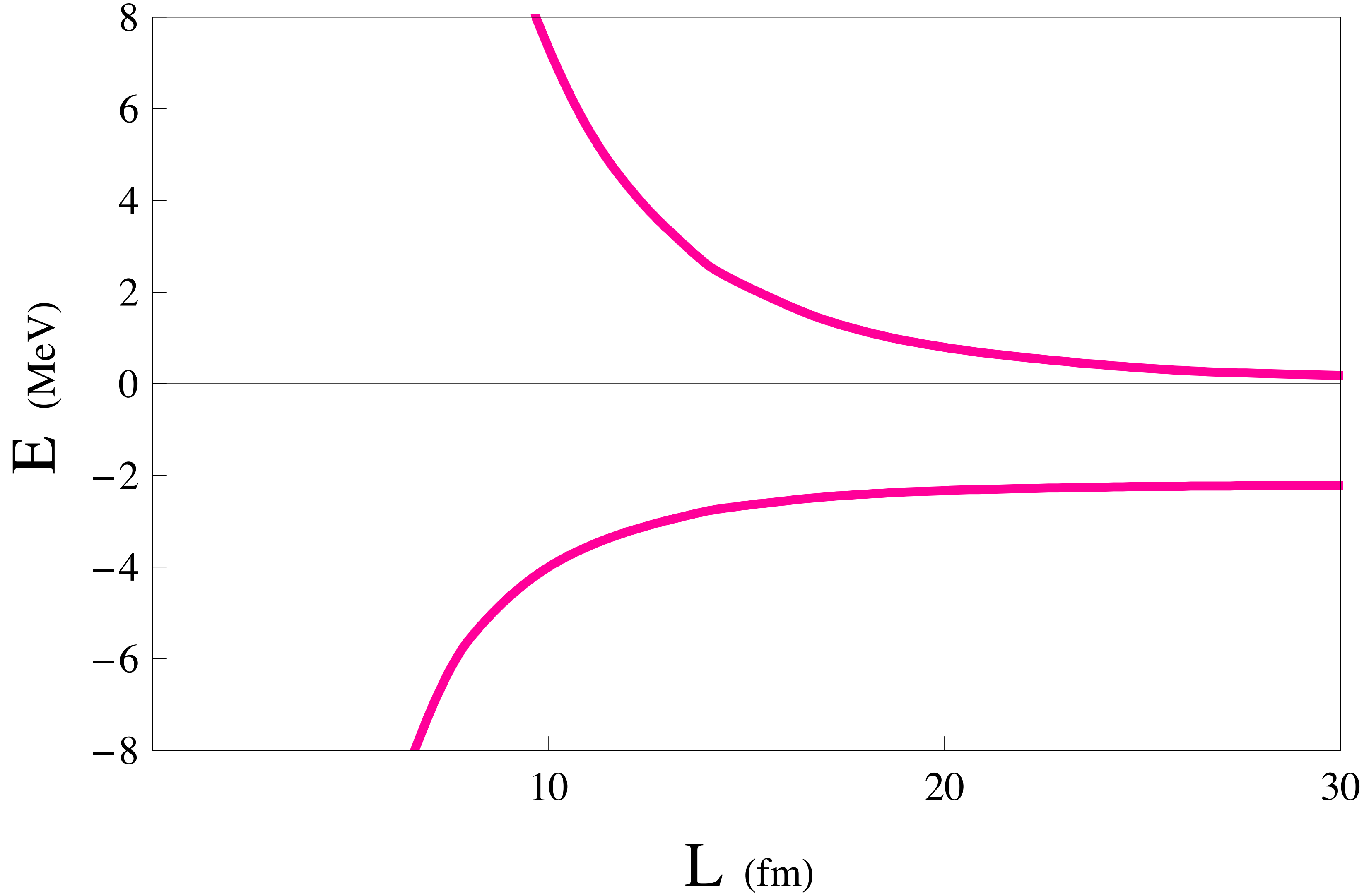
Analytic Continuation same as spherical cut-off

$$\begin{aligned} Z_{00}^{(\mathbf{0})} = & \frac{1}{2\sqrt{\pi}} \sum_{\mathbf{r}} \frac{e^{-\Lambda(|\mathbf{r}|^2 - \tilde{q}^2)}}{|\mathbf{r}|^2 - \tilde{q}^2} \\ & + \frac{\pi}{2} \left[2\tilde{q}^2 \int_0^\Lambda dt \frac{e^{t\tilde{q}^2}}{\sqrt{t}} - \frac{2}{\sqrt{\Lambda}} e^{\Lambda \tilde{q}^2} \right] \\ & + \frac{\pi}{2} \sum_{\mathbf{w} \neq \mathbf{0}} \int_0^\Lambda dt \frac{1}{t^{\frac{3}{2}}} e^{t\tilde{q}^2} e^{-\frac{\pi^2 |\mathbf{w}|^2}{t}} \end{aligned}$$

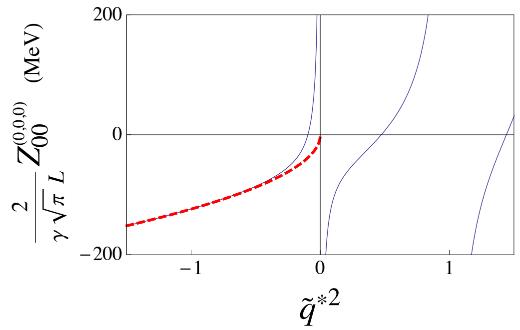


Bound-States at Rest (III)

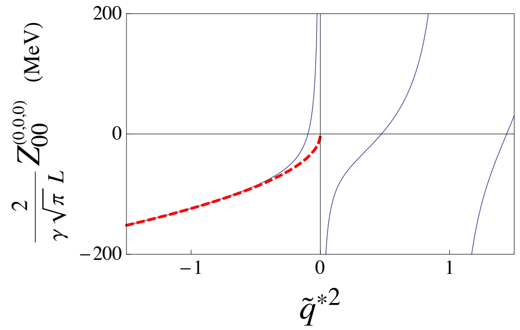


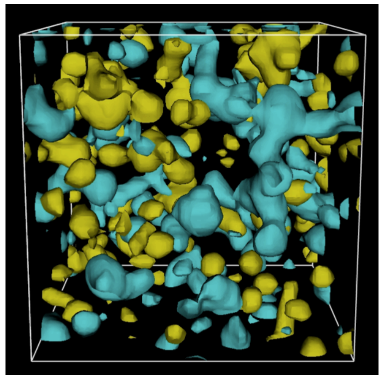


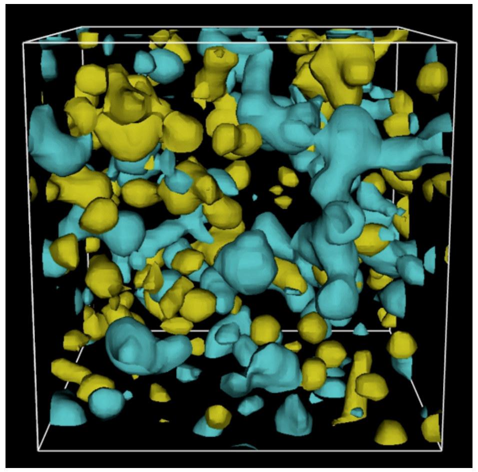
$$\kappa(L) \;=\; \kappa_0 + \frac{Z_\psi^2}{L}\left[\, 6e^{-\kappa_0 L} + 6\sqrt{2}e^{-\sqrt{2}\kappa_0 L} + \frac{8}{\sqrt{3}}e^{-\sqrt{3}\kappa_0 L}\right] + \ldots$$

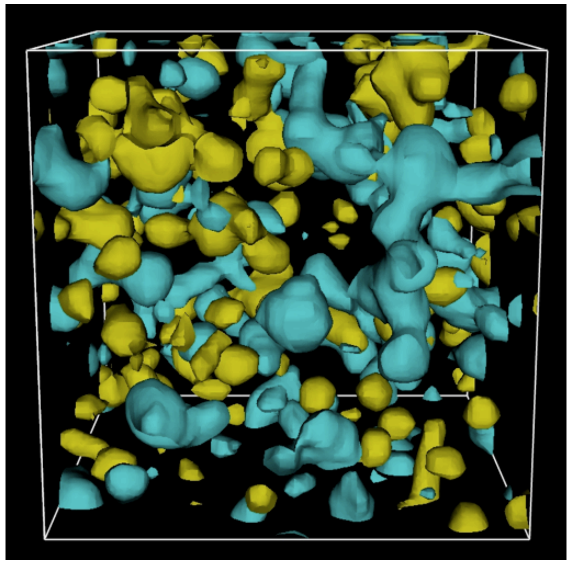


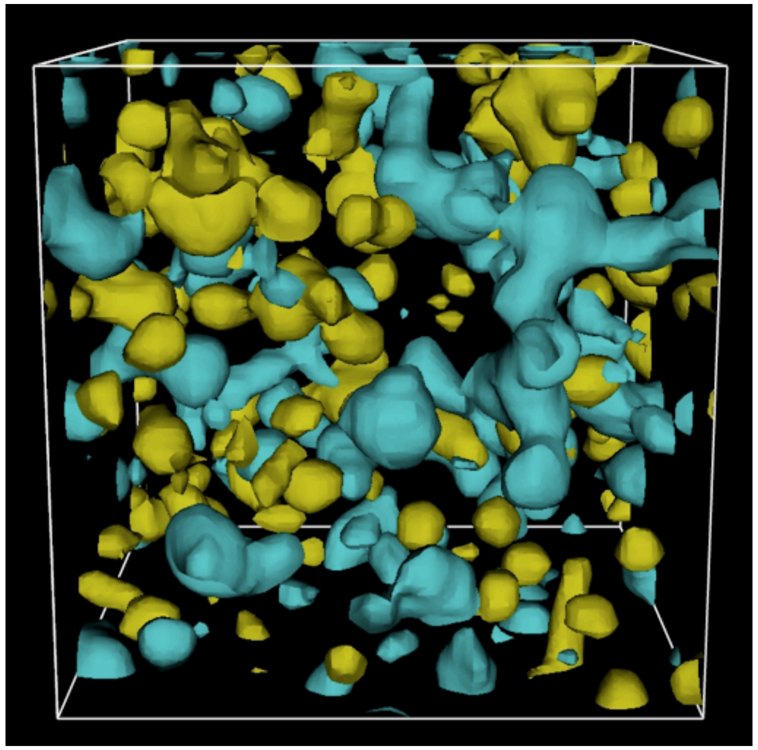
Bound-States at Rest (IV)



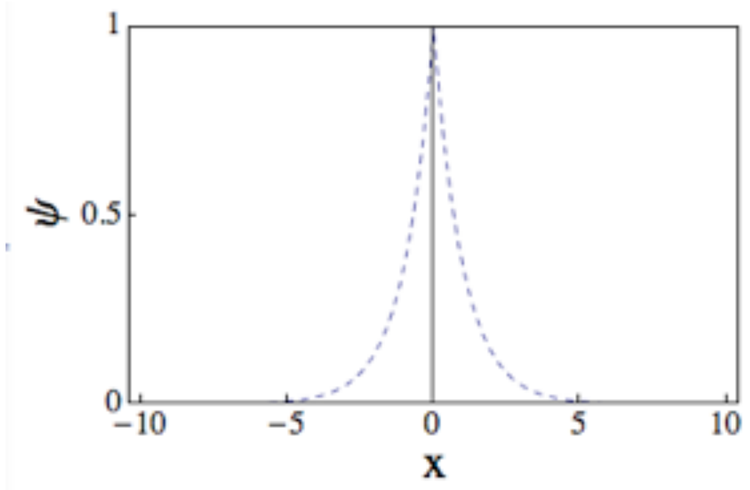


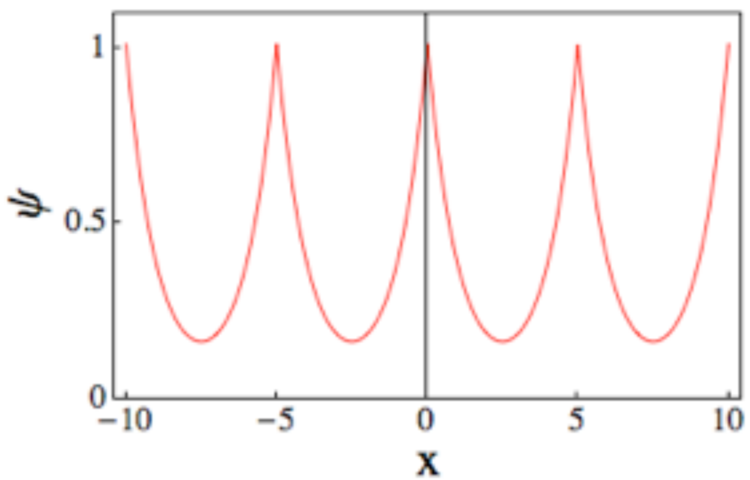




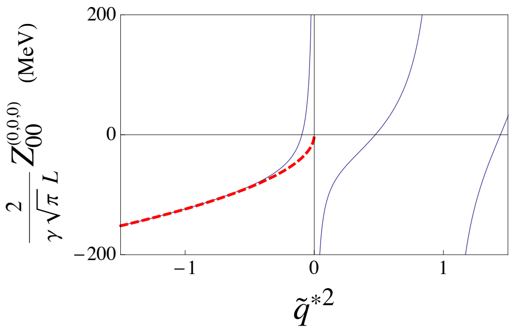


Ground-states only requires multiple ensembles of gauge fields

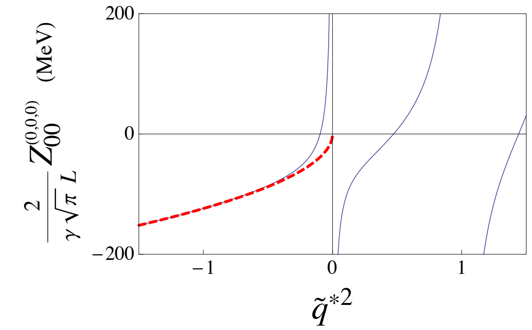


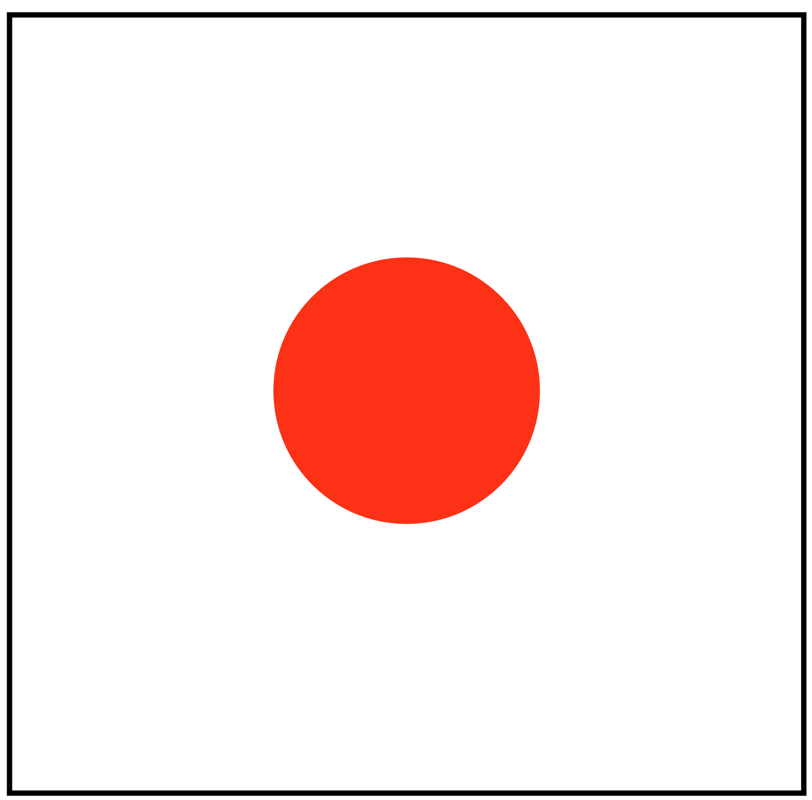


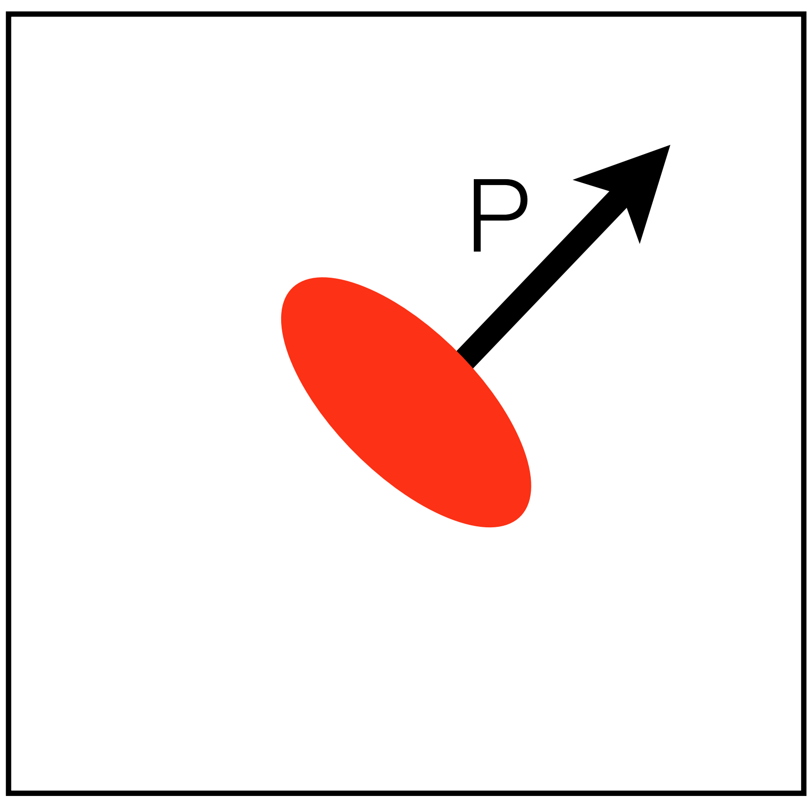
Volume-dependence from excluded momentum modes

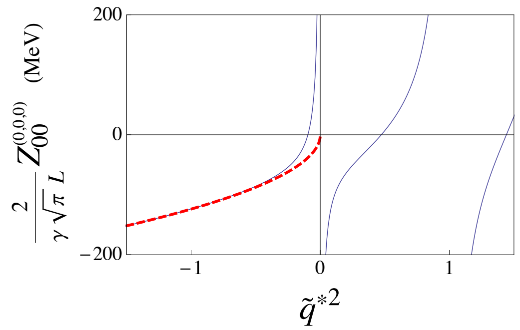


Bound-States in Motion

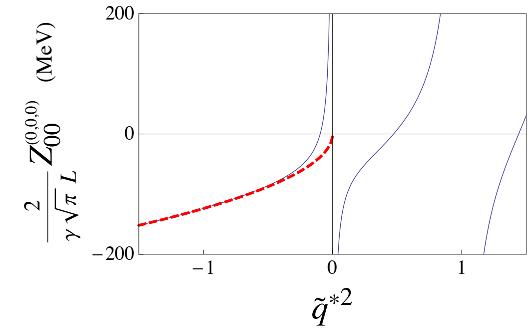








Bound-States in Motion
Equal Masses



$$\psi(\mathbf{x}_1, \mathbf{x}_2) = \psi(\mathbf{x}_1 + \mathbf{n}L, \mathbf{x}_2 + \mathbf{m}L) = e^{i\mathbf{P}\cdot(\mathbf{x}_1+\mathbf{x}_2)/2}\phi_L(\mathbf{x}_1 - \mathbf{x}_2)$$

$$\phi_L(\mathbf{x}) = (-)^{\mathbf{d}\cdot\mathbf{q}}\,\phi_L(\mathbf{x} + \mathbf{q}L) \quad , \quad \mathbf{P} = \frac{2\pi}{L}\mathbf{d}$$

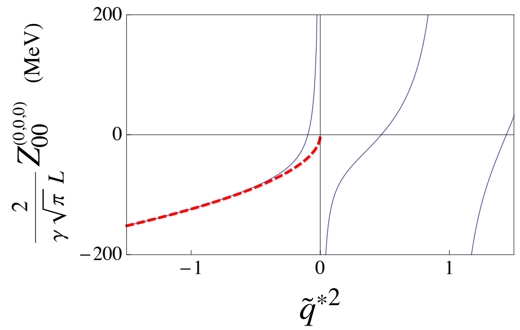
$\phi_L(x_0, \mathbf{x})$ but $x_0 = 0$ i.e. same time slice

$\phi_{CoM}(\mathbf{x}^*)$, i.e. indep. of time

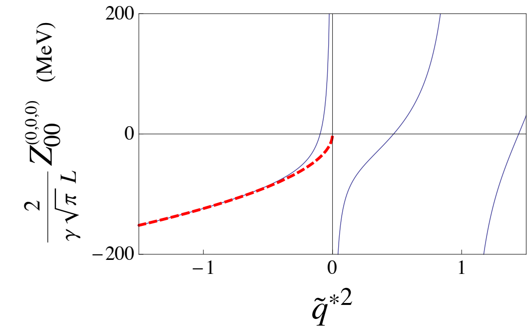
$$\Delta\mathbf{x}^* = \hat{\gamma}\,(\,\Delta\mathbf{x} + \mathbf{v}\Delta t) = \hat{\gamma}\Delta\mathbf{x}$$

$$\phi_{CoM}(\hat{\gamma}\mathbf{x})$$

$$\phi_{CoM}(\mathbf{x}^*) = \phi_{CoM}(\mathbf{x}^* + \hat{\gamma}\mathbf{n}L)$$



Bound-States in Motion (II)



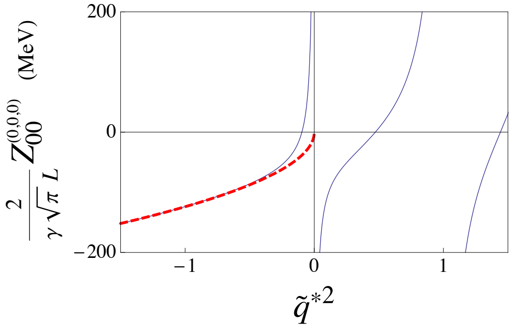
$$q^* \cot\delta(q^*) \ = \ \frac{2}{\gamma L \sqrt{\pi}}\, Z_{00}^{(\mathbf{d})}(1; \tilde{q}^{*2}, \tilde{\Delta} m_{12}^2)$$

(Gottlieb + Rummukainen
Kim, Sachrajda + Sharpe)

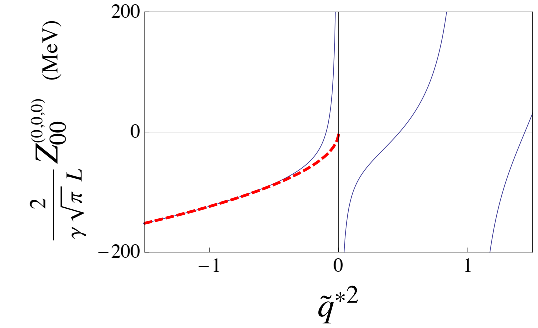
$$Z_{LM}^{(\mathbf{d})} \ = \ \sum_{\mathbf{r}} \frac{|\mathbf{r}|^L \, Y_{LM}(\Omega_{\mathbf{r}})}{|\mathbf{r}|^2 - \tilde{q}^{*2}} \quad , \quad \mathbf{r} \ = \ \frac{1}{\gamma}\left(\mathbf{n}_{\parallel} + \alpha \mathbf{d}\right) + \mathbf{n}_{\perp} \ = \ \hat{\gamma}^{-1}\left(\mathbf{n} + \alpha \mathbf{d}\right)$$

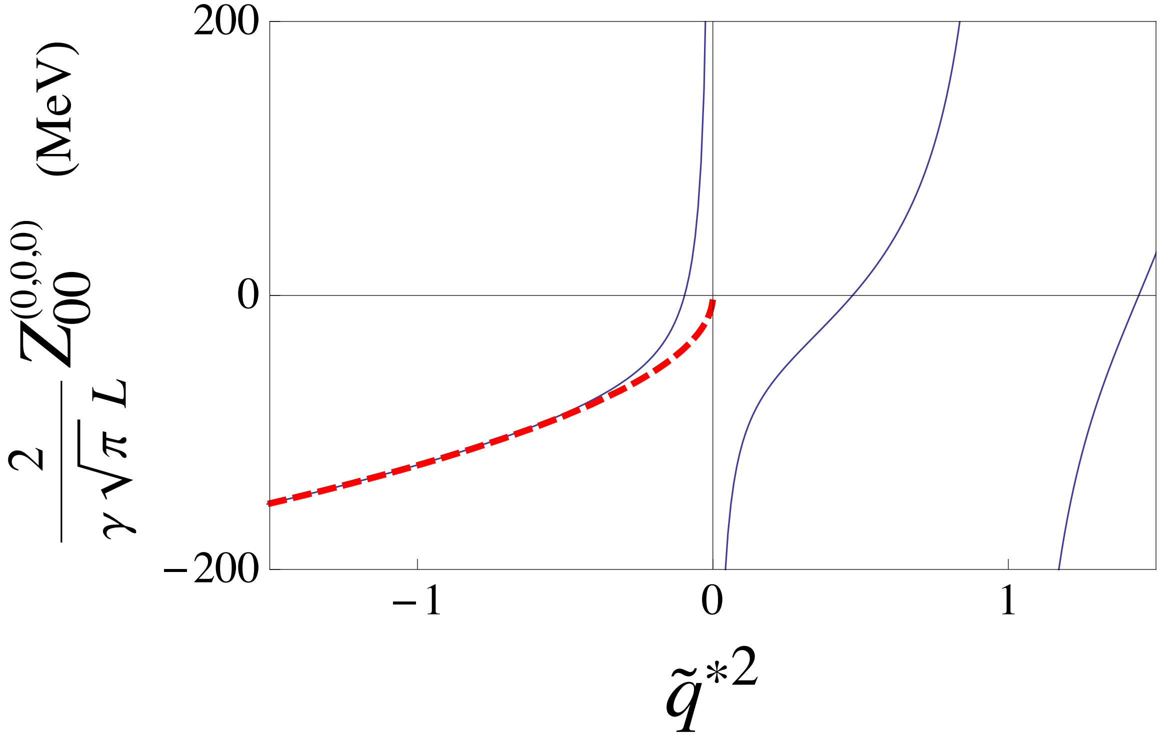
$$\alpha \ = \ \frac{1}{2}\left[1 \ + \ \frac{m_1^2 - m_2^2}{E^{*2}}\right]$$

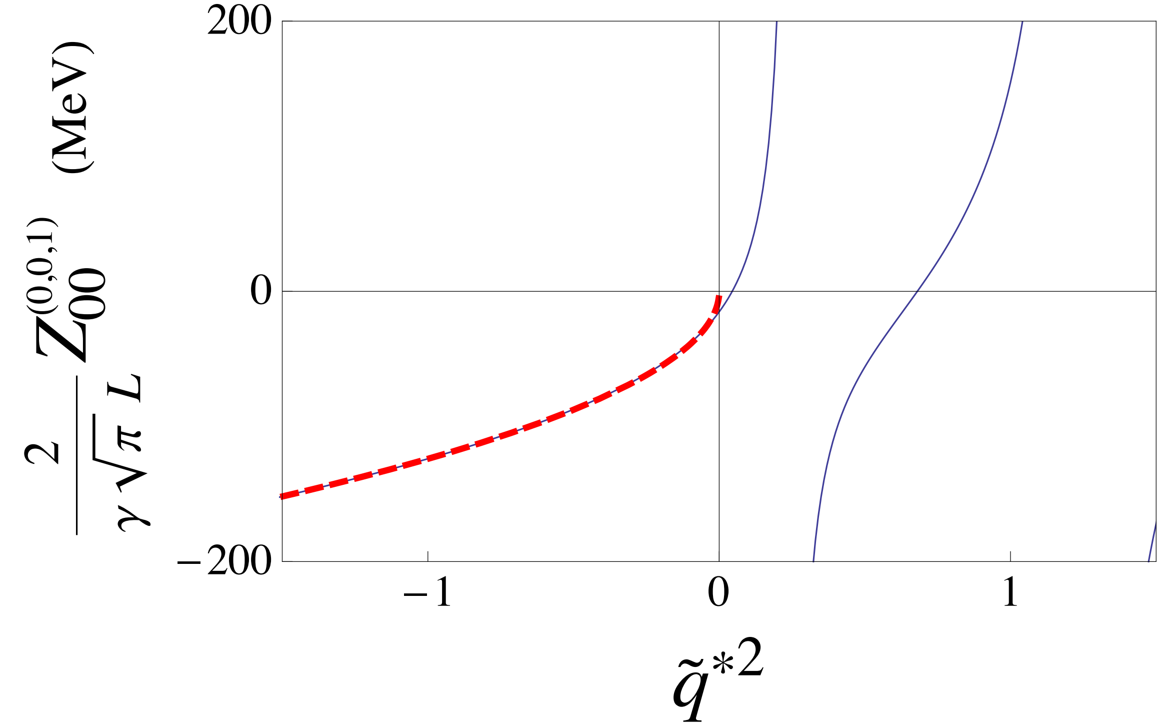
Bour + Konig + Lee + Hammer + Meissner - NRQM
and
Davoudi + MJS - QFT

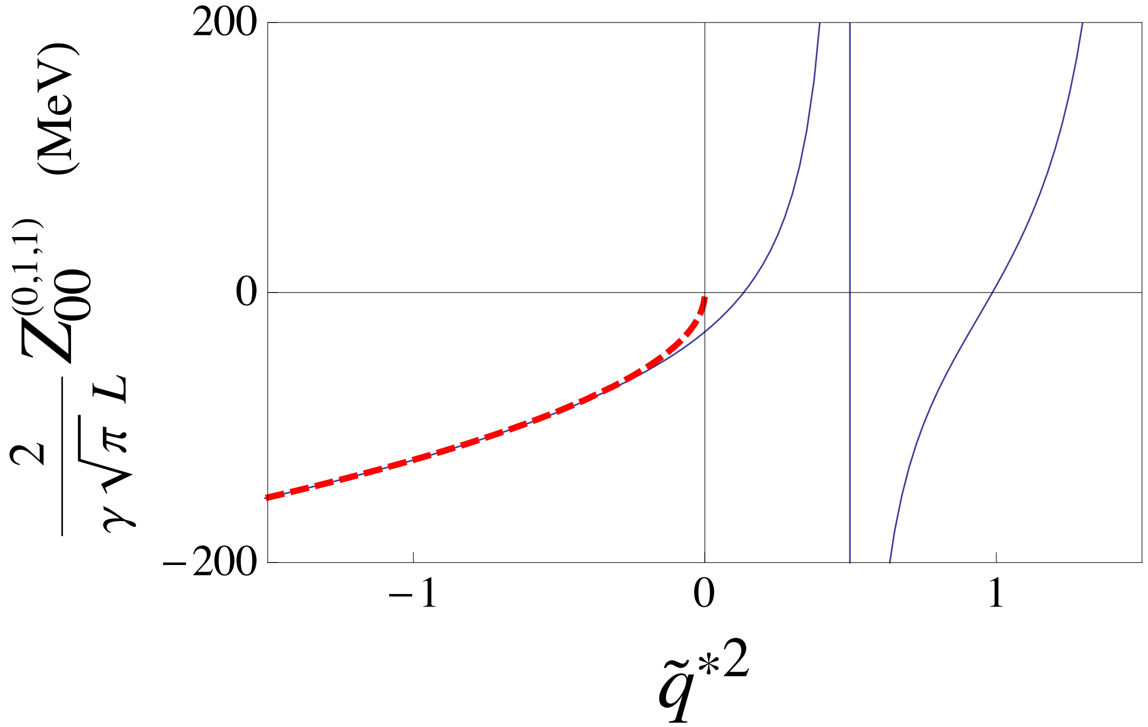


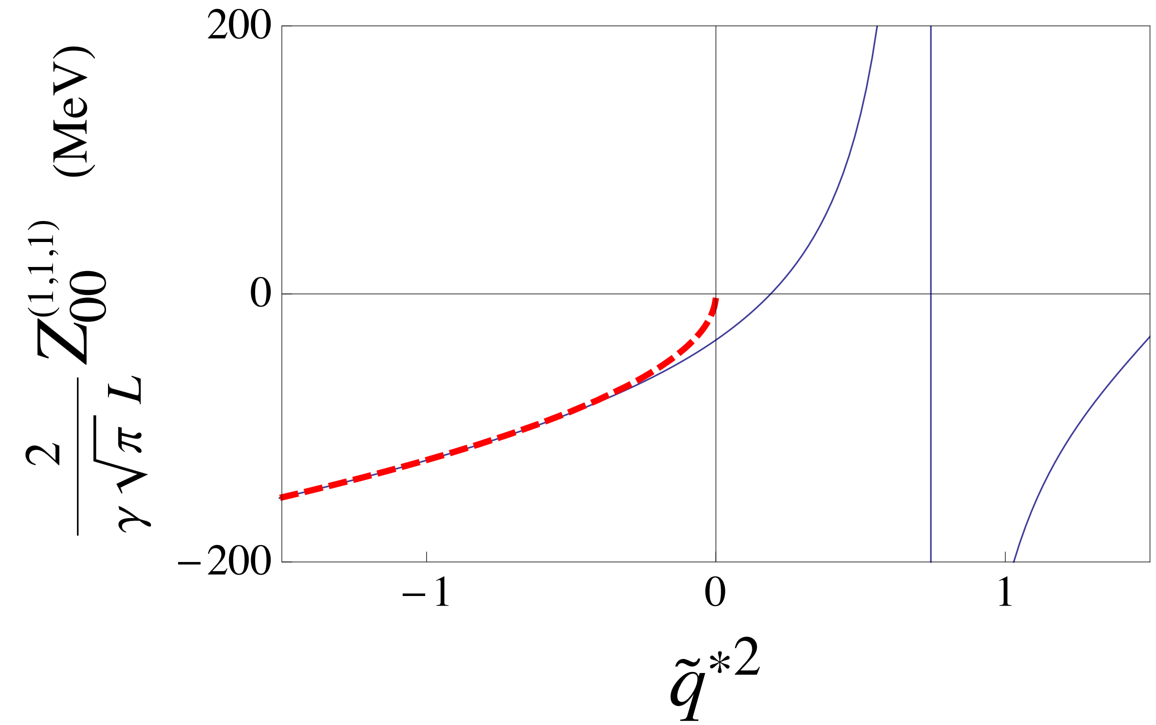
Bound-States in Motion (III) Equal Masses

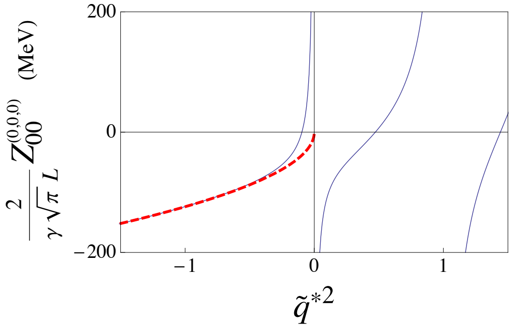




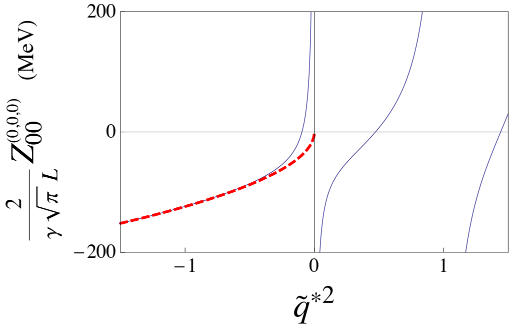


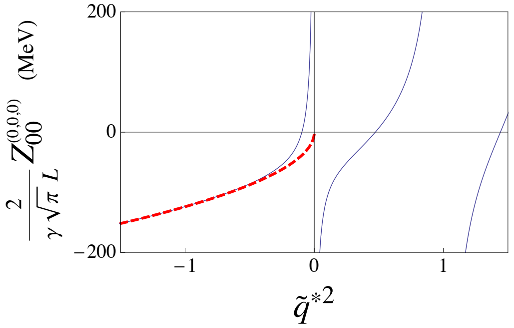




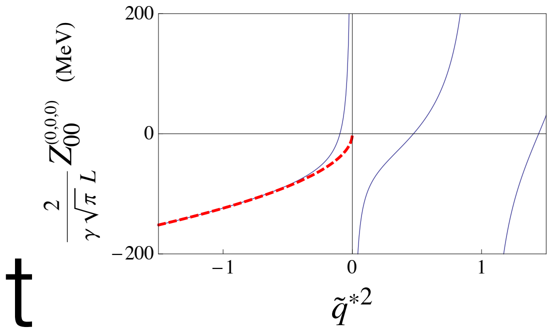


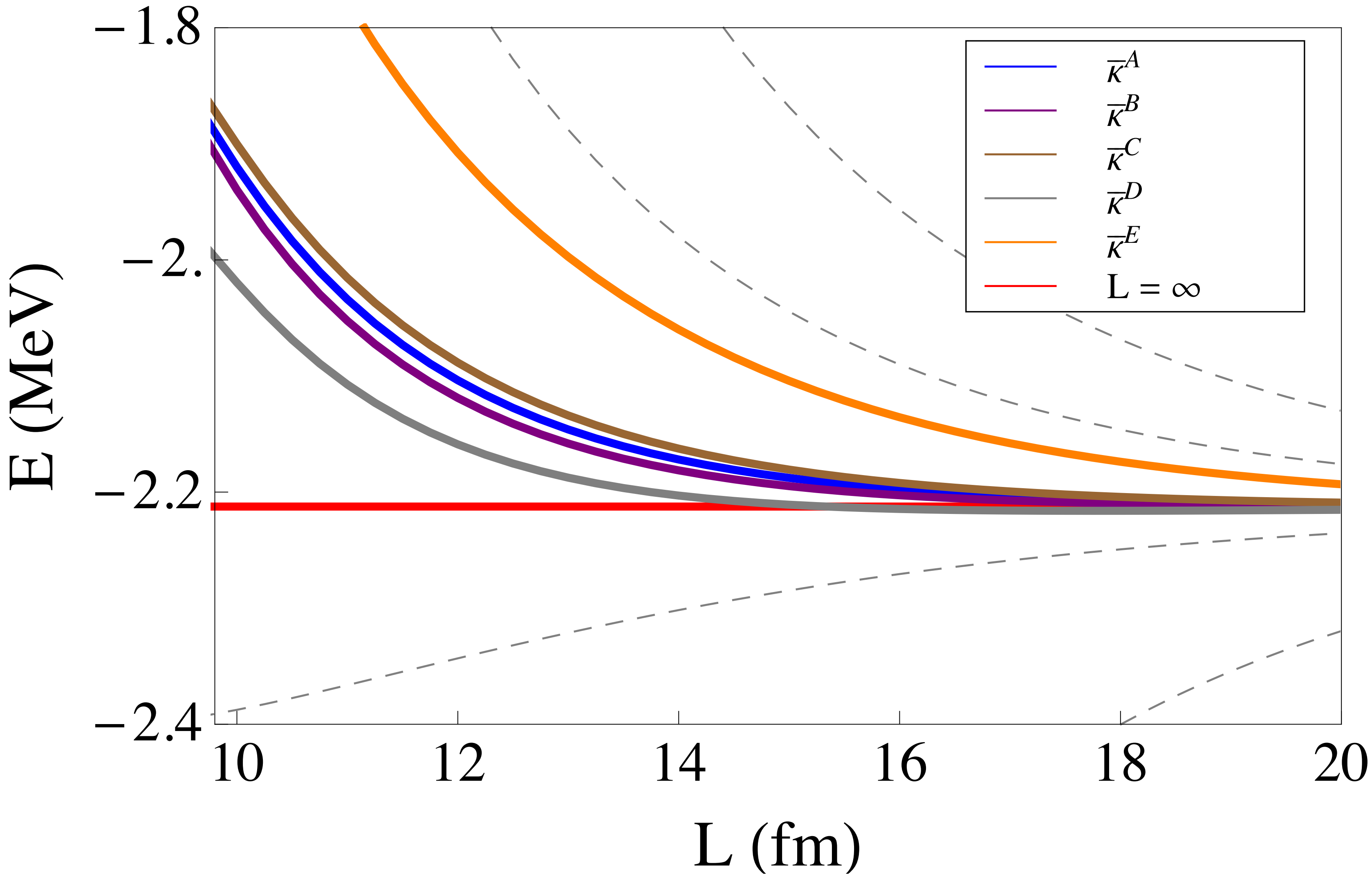
Bound-States in Motion (III)
Deuteron





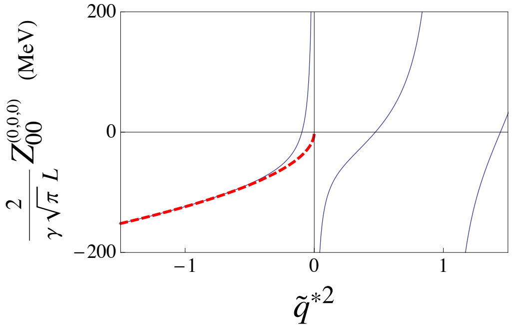
Bound-States in Motion (IV)
Deuteron - Exponential Improvement



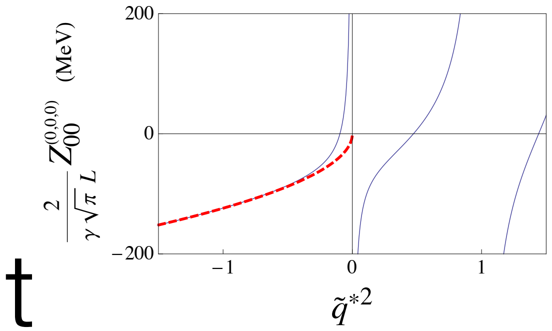


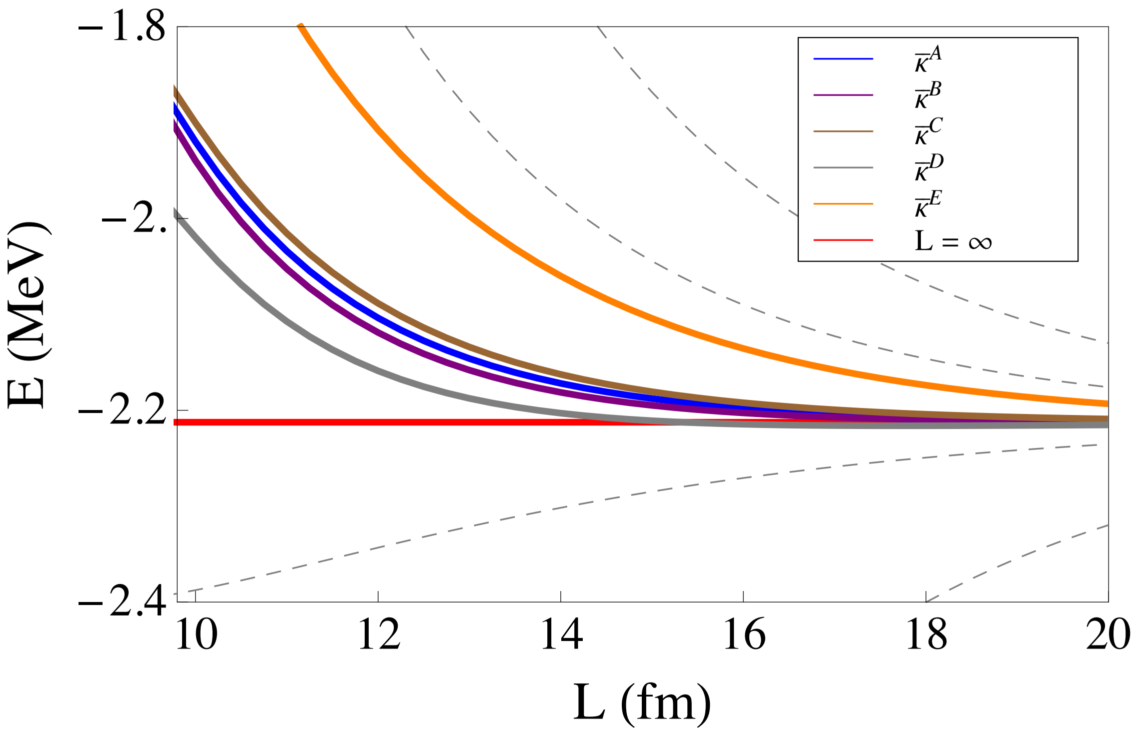
$$\overline{\kappa}^A = \frac{1}{8}\left(\kappa^{(0,0,0)} + 3\kappa^{(0,0,1)} + 3\kappa^{(0,1,1)} + \kappa^{(1,1,1)} \right)$$

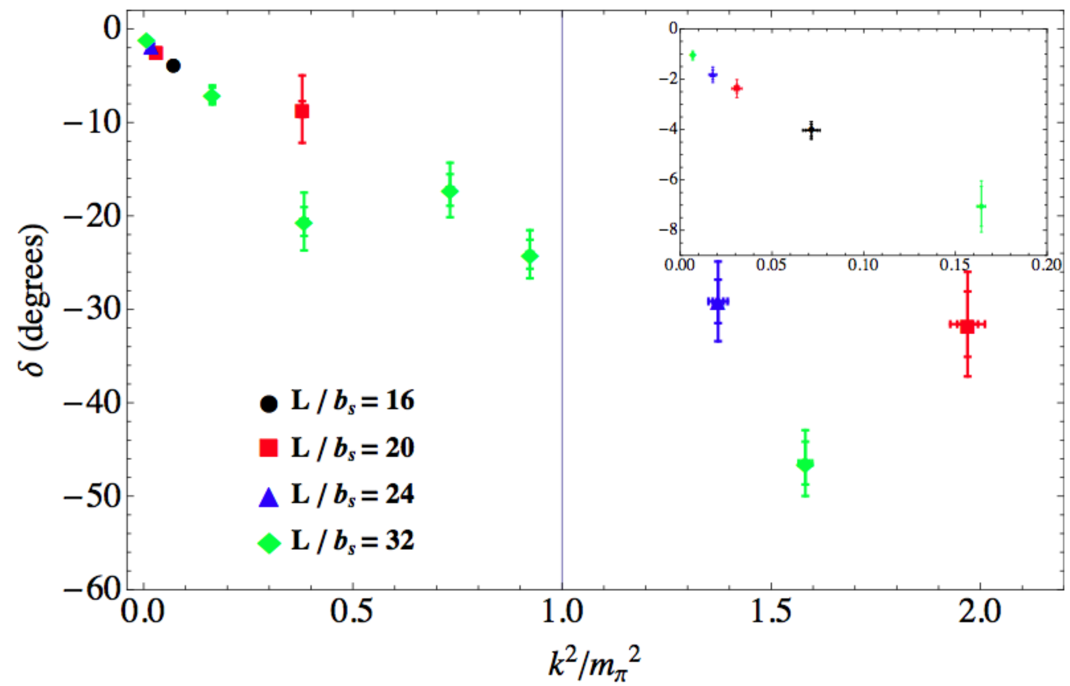
$$= \kappa_0 + \frac{3Z_\psi^2}{2L}\,\eta^2\,(1+\kappa_0 L)\,e^{-\kappa_0 L} + \mathcal{O}\left(\eta^4 e^{-\kappa_0 L} L, \frac{e^{-2\kappa_0 L}}{2L}\right) \qquad \eta = \frac{|\mathbf{P}|}{E^*}$$



Bound-States in Motion (V)
Deuteron - Exponential Improvement



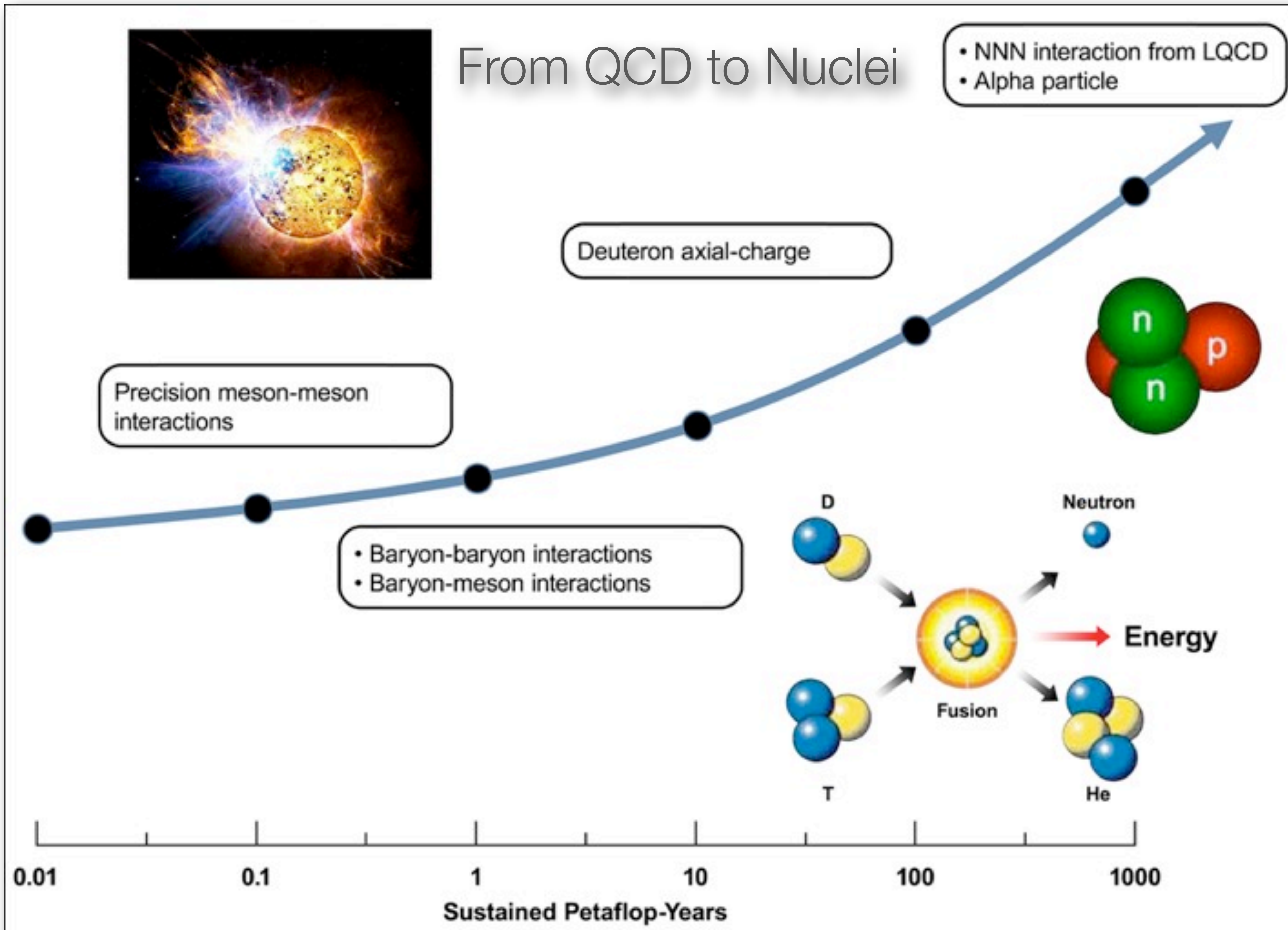


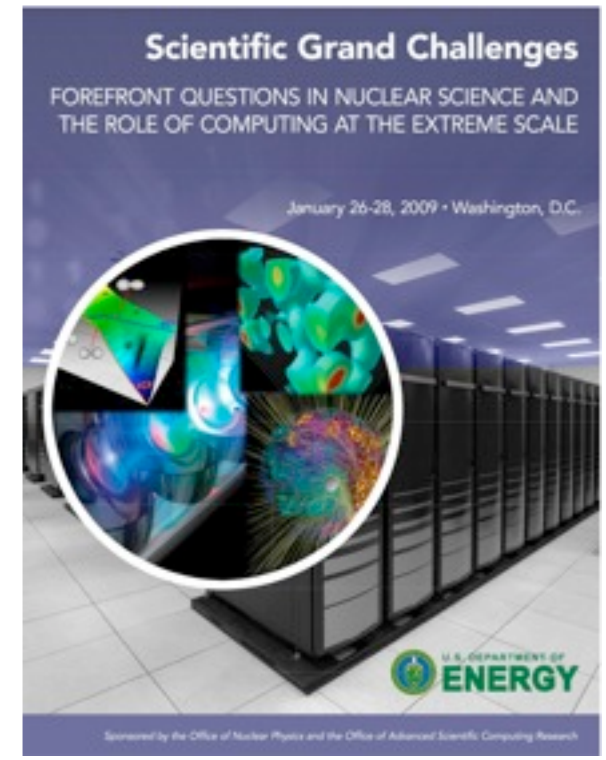


Lesson

- 1-enemble, multiple boosted systems
- much less computationally expensive
- exponentially improved volume dependence

Computational Requirements

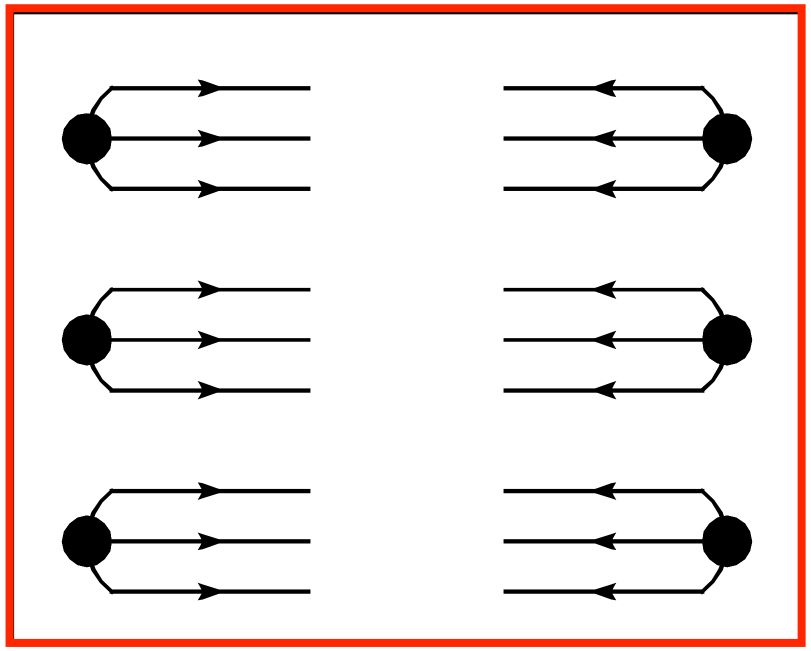




Electromagnetism
Isospin Breaking
The Real Deal !

Many Nucleons (Baryons)

Large number of Wick contractions



Proton : N $^{\text{cont}}$ = 2

^{235}U : N $^{\text{cont}}$ = 10^{1494}

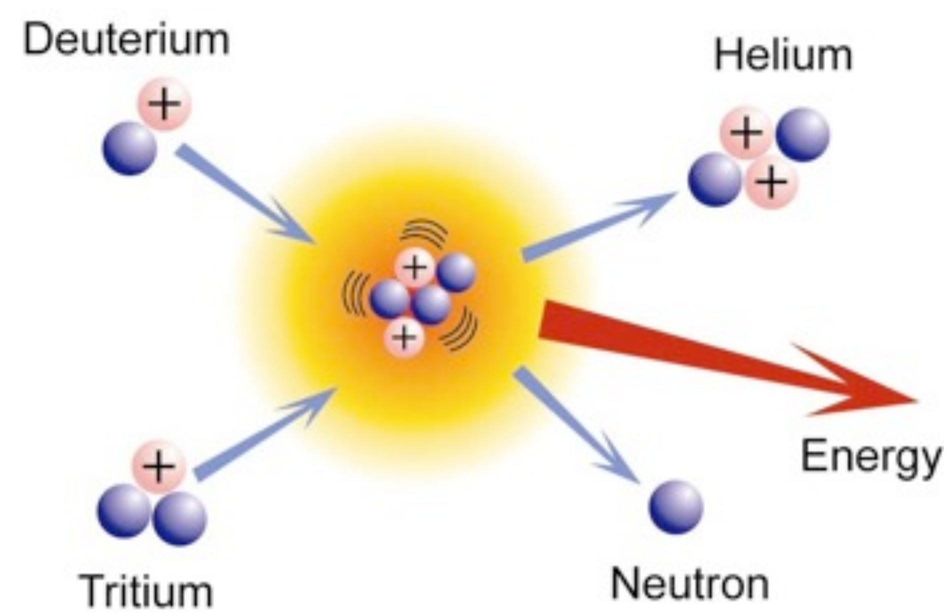
$$\begin{aligned} N_{\text{cont.}} &= u!d!s! \quad (\text{Naive}) \\ &= (A+Z)!(2A-Z)!s! \\ &\sim A^3 \ (\text{Kaplan}) \end{aligned}$$

Symmetries provide significant reduction

$$^3\text{He} \ : \ 2880 \rightarrow 93$$

Recursion Relations

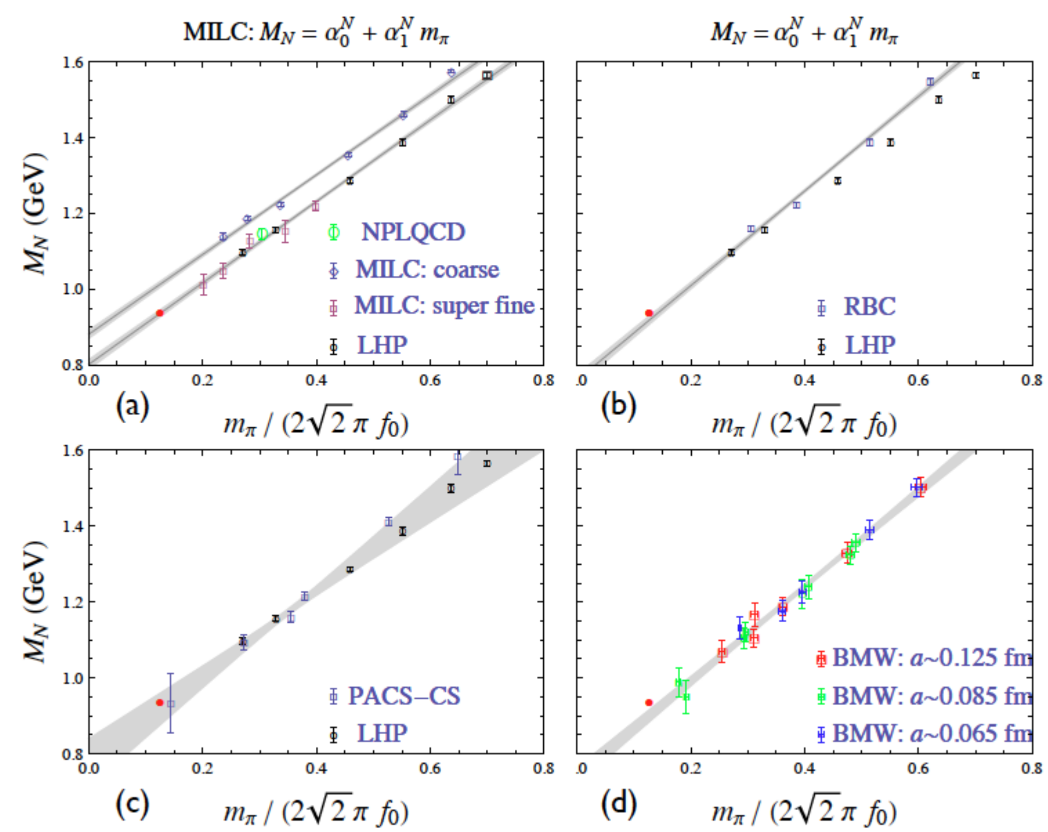
Beyond Computational Requirements: Formal Issues , e.g.



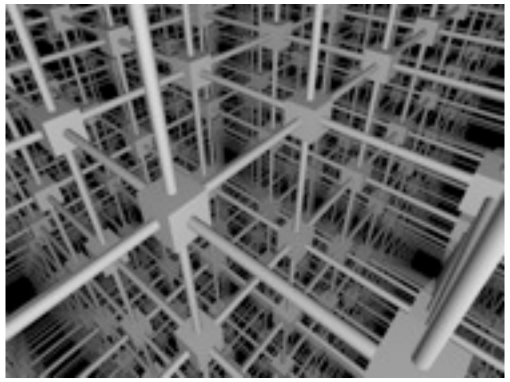
What Lattice QCD calculations are required to predict multi-body nuclear reactions ?

What length-scales determine the convergence of EFT expansions ?

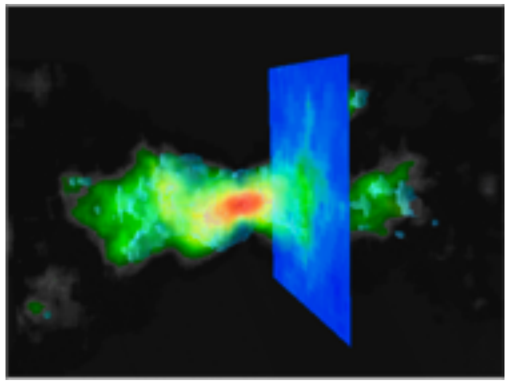
(to predict more complex systems than LQCD can access)
(quark masses, number of flavors?)

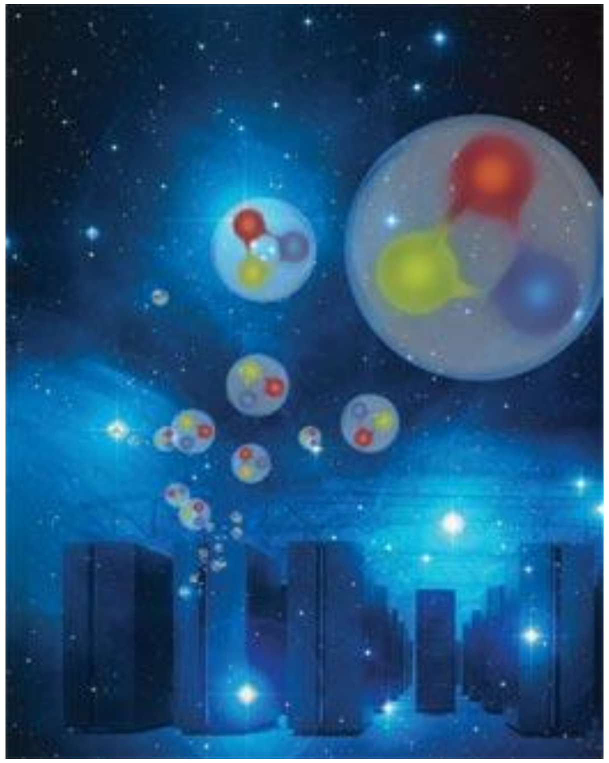


(A. Walker-Loud)



Remarks





Close to discovering how hadrons and nuclei emerge from quarks and gluons using Lattice QCD

Moving toward light nuclear systems with quantifiable and removable uncertainties

Lattice QCD is now able to calculate 2-body bound-states

Multiple ensembles of large-volume gauge-fields are expensive

Boosted states allow for better energy-sampling of scattering states and exponential improvement of bound-states

END