Status Update on $\pi^+\pi^+\pi^+$ with Elongated Boxes

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Scattering from the Lattice: Applications to Phenomenology and Beyond 2018

Outline

1. Lattice Methods & Ensembles
2. Operator Discussion
3. Computational Details
4. Preliminary Results

Lattice Methods & Ensembles

LQCD Methodology

- Quantum numbers of system
- Construct operators
- Compute finite volume energy levels
    - GEVP
- Physical Quantities

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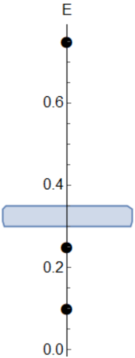
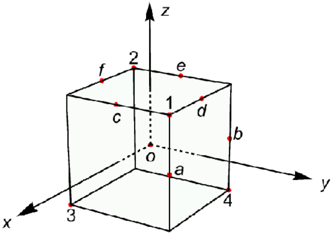
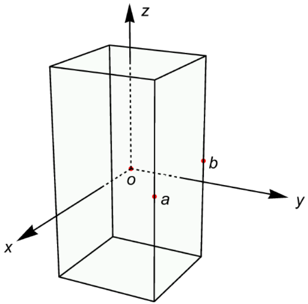


Ensembles





ensemble	$N_t \times N_{x,y}^2 \times N_z$	η	a[fm]	N_{cfg}	aM_π	am_N	$am_{u/d}^{pcac}$	af_π
$\mathcal{E}_1$	$48 \times 24^2 \times 24$	1.0	0.1210(2)(24)	300	0.1934(5)	0.644(6)	0.01237(9)	0.0648(8)
$\mathcal{E}_2$	$48 \times 24^2 \times 30$	1.25	–	–	–	–	–	–
$\mathcal{E}_3$	$48 \times 24^2 \times 48$	2.0	–	–	–	–	–	–
$\mathcal{E}_4$	$64 \times 24^2 \times 24$	1.0	0.1215(3)(24)	400	0.1390(5)	0.62(1)	0.00617(9)	0.060(1)
$\mathcal{E}_5$	$64 \times 24^2 \times 28$	1.17	–	–	–	–	–	–
$\mathcal{E}_6$	$64 \times 24^2 \times 32$	1.33	–	–	–	–	–	–

Operator Discussion

Method

- Select N lowest seed operators s.t.
- Variational method gives at $N-1$ energy levels

- Project operators onto irreps of lattice group

Single Pion Operator

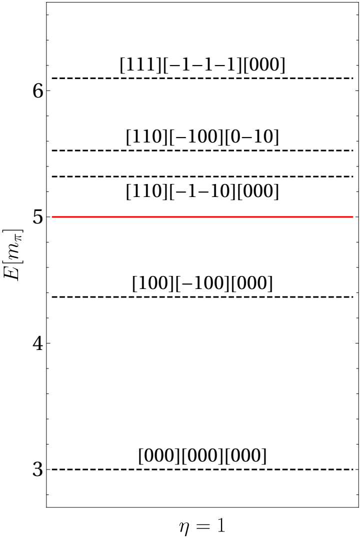
$\pi(p,t)^+ = \sum_x \bar{d}(x,t) e^{-ipx} \gamma_5 u(x,t) = \bar{d}(t)\Gamma(p)u(t)$

Three pion operator in irrep Γ of G

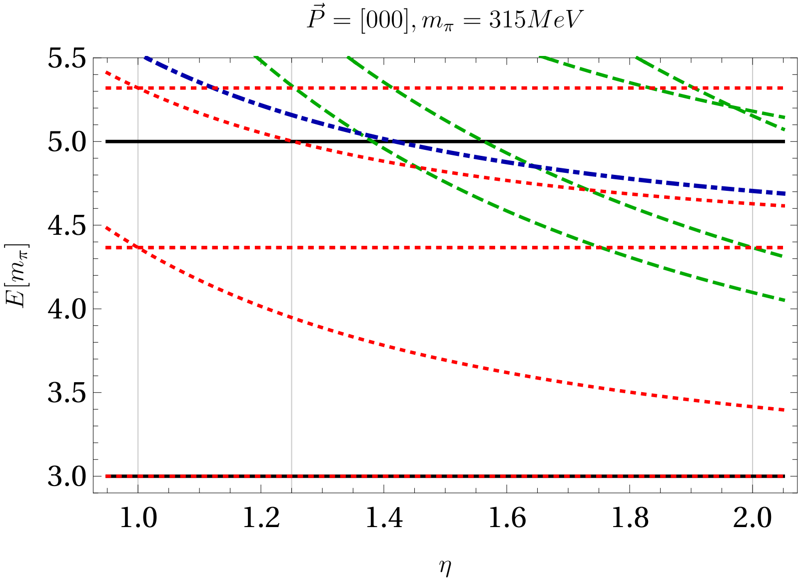
$\pi\pi\pi(p_1,p_2,p_3,t) = \frac{1}{|G|}\sum_{g\in G} \chi_\Gamma(g)\pi(R(g)p_1,t)\pi(R(g)p_2,t)\pi(R(g)p_3,t)$

$\pi\pi\pi((1,0,-1),(-1,0,1),(0,0,0)) = [10-1][-101][000]$

Selecting Seeds



Advantages of Elongating?



Cubic Box Operators

- O_1 – $[000][000][000] \xrightarrow{A_1^+} [000][000][000]$
- O_2 –
  $[100][-100][000] \xrightarrow{A_1^+} [100][-100][000] + [-100][100][000] + \text{“}y\text{”} + \text{“}z\text{”}$

$$\begin{pmatrix} \langle O_1 O_1^\dagger \rangle & \langle O_1 O_2^\dagger \rangle \\ \langle O_2 O_1^\dagger \rangle & \langle O_2 O_2^\dagger \rangle \end{pmatrix}$$

- Correlation matrix has $1 + 6 \times 2 + 36 = 49$ terms

Elongated Box Operators

- $\mathcal{O}_1$ – $[000][000][000] \xrightarrow{A_1^+} [000][000][000]$
- $\mathcal{O}_2 - [100][-100][000] \xrightarrow{A_1^+} [100][-100][000] + [-100][100][000] +$ "y"
- $\mathcal{O}_3$ – $[001][00-1][000] \xrightarrow{A_1^+} [001][00-1][000] + [00-1][001][000]$

$$\begin{pmatrix} \langle O_1 O_1^\dagger \rangle & \langle O_1 O_2^\dagger \rangle & \langle O_1 O_3^\dagger \rangle \\ \langle O_2 O_1^\dagger \rangle & \langle O_2 O_2^\dagger \rangle & \langle O_2 O_3^\dagger \rangle \\ \langle O_3 O_1^\dagger \rangle & \langle O_3 O_2^\dagger \rangle & \langle O_3 O_3^\dagger \rangle \end{pmatrix}$$

- Correlation matrix has $1 + 4 \times 2 + 16 + 2 \times 2 + 8 \times 2 + 4 = 49$ terms
- Same computational cost for an extra energy level.
- $\mathcal{O}_3$ has a lower non-interacting energy.

Computational Details

Quark Lines

Quark Lines

$\mathcal{Q}(t, t_f, p) = \tilde{M}^{-1}(t, t_f)\Gamma(p)$

- $\tilde{M}^{-1}$ is the Laph smeared propagator
- Operators have their own quark lines
- Precompute them, correlation matrix has operators repeated
- Better to include all operators at beginning

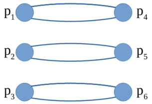
$$\begin{pmatrix} \langle O_0 O_0^\dagger \rangle & \langle O_0 O_1^\dagger \rangle & \cdots & \langle O_0 O_N^\dagger \rangle \\ \langle O_1 O_0^\dagger \rangle & \langle O_1 O_1^\dagger \rangle & & \\ \vdots & & \ddots & \\ \langle O_N O_0^\dagger \rangle & & & \langle O_N O_N^\dagger \rangle \end{pmatrix}$$

Wick Contractions

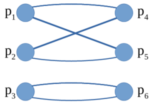
Generic Contraction

$$\langle \bar{d}(t)\Gamma(p_1)u(t)\bar{d}(t)\Gamma(p_2)u(t)\bar{d}(t)\Gamma(p_3)u(t) \\ \times \bar{u}(0)\Gamma(p_4)d(0)\bar{u}(0)\Gamma(p_5)d(0)\bar{u}(0)\Gamma(p_6)d(0)\rangle \quad (1)$$

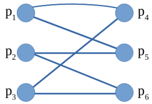
- For an arbitrary 6 momenta there are 36 diagrams

6: 

$= \mathrm{tr}\left[\mathcal{Q}(p_1)\mathcal{Q}(p_4)\right] \times \mathrm{tr}\left[\mathcal{Q}(p_2)\mathcal{Q}(p_5)\right] \times \mathrm{tr}\left[\mathcal{Q}(p_3)\mathcal{Q}(p_6)\right]$

18: 

$= \mathrm{tr}\left[\mathcal{Q}(p_1)\mathcal{Q}(p_4)\mathcal{Q}(p_2)\mathcal{Q}(p_5)\right] \times \mathrm{tr}\left[\mathcal{Q}(p_3)\mathcal{Q}(p_6)\right]$

12: 

$= \mathrm{tr}\left[\mathcal{Q}(p_1)\mathcal{Q}(p_4)\mathcal{Q}(p_2)\mathcal{Q}(p_5)\mathcal{Q}(p_3)\mathcal{Q}(p_6)\right]$

Numbers of Sub Diagrams

- In example with ops [000][000][000], [100][-100][000]
- Naively there are 3234 sub diagrams
  - $N_2 = 1764$ two-point
  - $N_4 = 882$ four-point
  - $N_6 = 588$ six-point
- After cyclic rotation of trace - 351 diagrams
  - $N_2 = 49$ two-point
  - $N_4 = 181$ four-point
  - $N_6 = 121$ six-point

- $\eta = 1.0$ ensemble has 2,883 diagrams
- $\eta = 2.0$ ensemble has 22,875 diagrams

GPU Matrix Multiplication

Batched matrix multiply

$$\begin{bmatrix} A_1 \\ A_2 \\ \vdots \\ A_N \end{bmatrix} \times \begin{bmatrix} B_1 \\ B_2 \\ \vdots \\ B_N \end{bmatrix} = \begin{bmatrix} A_1 \times B_1 \\ A_2 \times B_2 \\ \vdots \\ A_N \times B_N \end{bmatrix} = \begin{bmatrix} C_1 \\ C_2 \\ \vdots \\ C_N \end{bmatrix}$$

Procedure

Copy all quark lines to device
Allocate 3 arrays of size $N_2 \times$mat_size
cublasZgemmStridedBatched(A,B,C)
Copy to Host & Free A,B
Allocate 3 arrays of size $N_4 \times$mat_size
cublasZgemmStridedBatched(C_{4A}, C_{4B}, C_{4R})
Copy to Host & Free all C_{4x}

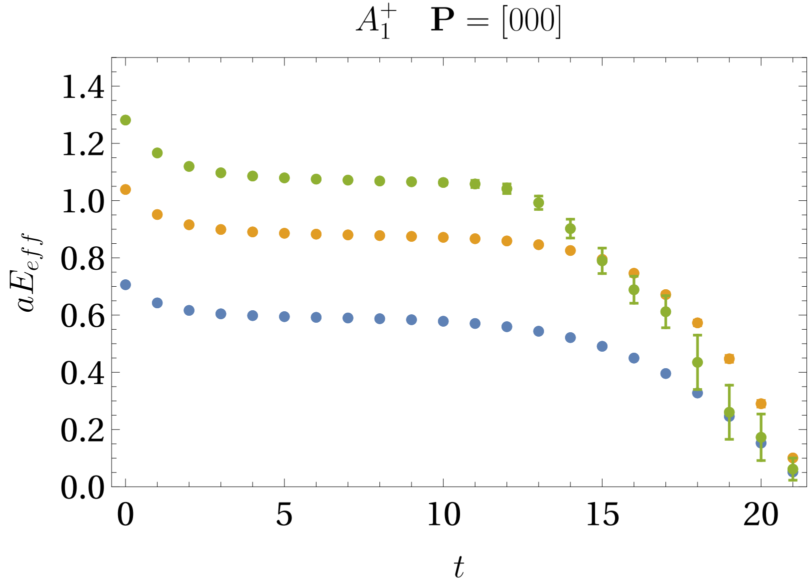
Current Runtime

- CPU Code - 12 Hours/cfg
- GPU Code - 3 Hours/cfg

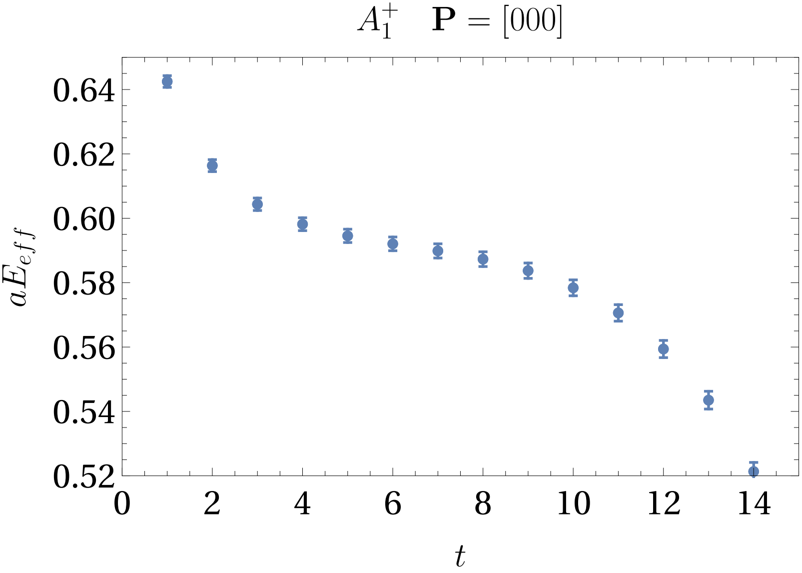
- CPU Code - Matrix multiplication unordered, only compiler can make good use of cache
- GPU Code - Unnecessary copying of QL to use cuBlas
- GPU Code - Multiple batches due to memory limitations of GPU

Preliminary Results

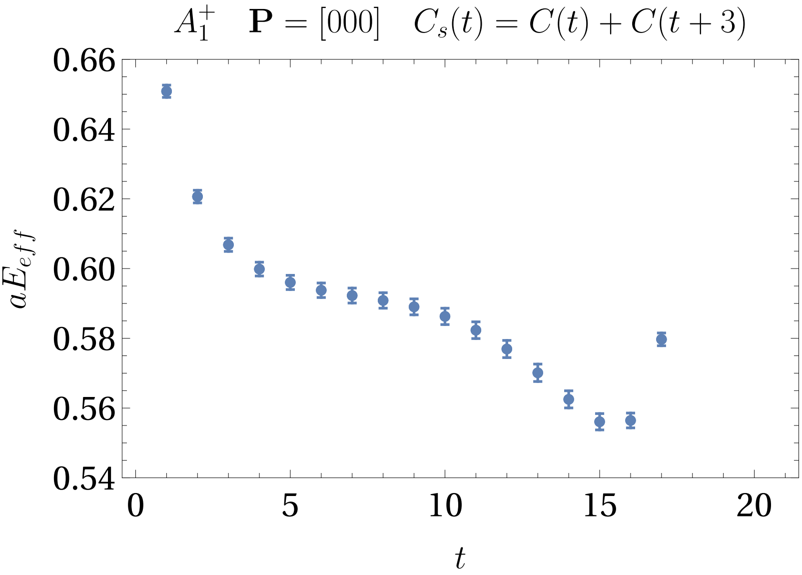
Correlators



Ground State



Shifted Correlator



Time Dependent Wrap Around Effects

Spectral Decomposition

$$C(t) = \sum_{n,m} \langle m \mid e^{-H(T-t)} O e^{-Ht} \mid n \rangle \langle n \mid O^\dagger \mid m \rangle$$

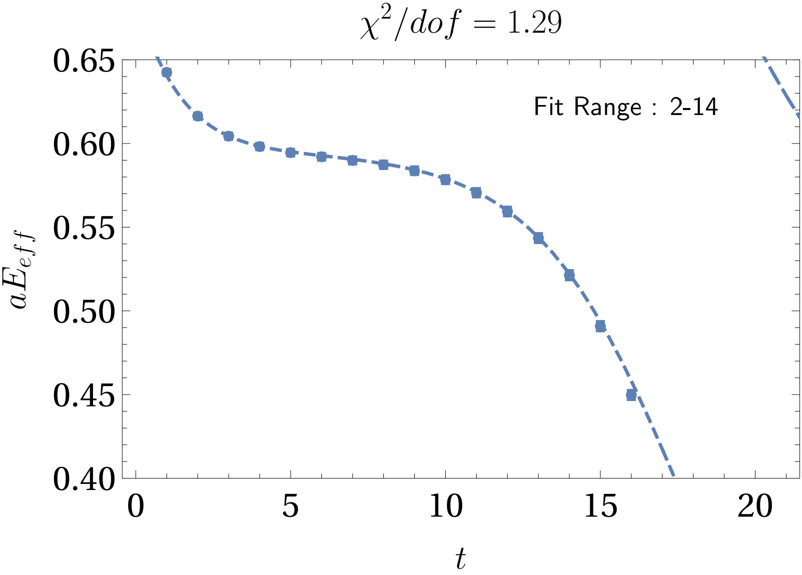
$$\mathbf{m} = \mathbf{0} : C(t) \propto e^{-E_{3\pi}^{(n)} t}$$

$$\mathbf{m} = \pi : C(t) \propto e^{E_\pi^{(m)}(T-t)} \sum_n \langle 0 \mid \pi\pi \, e^{-Ht} \mid n \rangle \langle n \mid O^\dagger \mid \pi \rangle$$

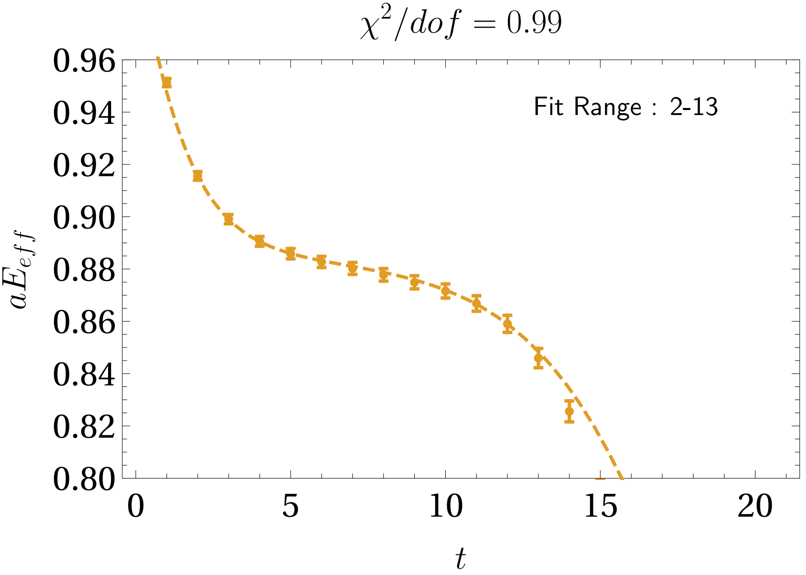
$$\propto e^{-E_\pi^{(m)}(T-t)} e^{-E_{\pi\pi}^{(n)} t}$$

Fit correlator with $A_1 e^{-m_1 t} + A_2 e^{-m_2 t} + A_3 e^{-\Delta E t}$

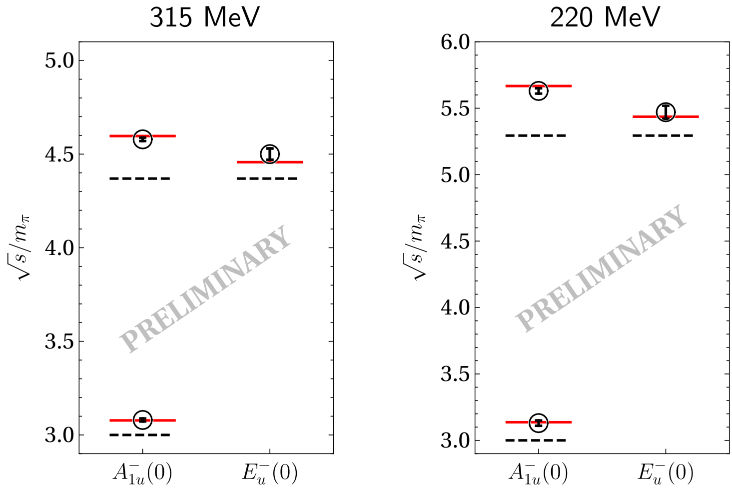
Ground State Fit



Excited State Fit



Current Spectra



Conclusion

- Running Ensembles
  - Additional operator for cubic boxes
  - Run all ensembles at $\mathbf{P} = [000]$
  - Add boosted operators for $m_\pi = 220$ MeV ensembles
- Fitting
  - Weight-Shifted Correlators
  - Ratio Correlators
- From $\mathbf{P} = [000]$, 22 at 315MeV, 7 at 220 MeV