Exploring the spectrum of SU(3) Yang-Mills theory using Wilson flow and open boundary

Jyotirmoy Maiti

Barasat Govt. College

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Motivation

Extraction of glueball masses

- Computations need to be done at smaller lattice spacings to reduce cut-off effects as low lying glueball masses are much higher than masses of hadronic ground states
- Large vacuum fluctuations present in the correlators of gluonic observables makes it much more difficult compared to hadronic mass extractions.

Long history of calculations:
Bali *et al*, '93
Vaccarino and Weingarten, '99
Morningstar and Peardon, '97 and '99
Chen *et al*, '06
A recent one: Majumdar, Mathur and Mondal, '14

- So far a^{-1} have been pushed upto 3.73 GeV. Calculations at even higher lattice scale face the difficulty of efficient spanning of the space of gauge configurations.

Motivation contd.

- To preserve translational invariance, lattice theories usually employ periodic boundary conditions in all space-time direction
  $\Rightarrow$ topological sectors become disconnected in continuum limit
- On lattice, statistical weight of gauge fields "between the sectors" diminishes with high power of lattice spacing
  $\Rightarrow$ transitions between sectors suppressed in simulations
  $\Rightarrow$ autocorrelation times of physical quantities grow rapidly
- A possible way out: open boundary condition in time direction
  Lüscher and Schaefer, '11 and '13
  $\Rightarrow$ no barriers between different topological sectors.
- Two fold task:
  - reproduction of results obtained from periodic lattices
  - extention to even smaller lattice spacings.

Gradient flow

- Consider free scalar field theory in Euclidean space

$$S_E[\phi] = \int d^4x \; [\frac{1}{2} \; \partial_\mu \phi \; \partial_\mu \phi + \frac{1}{2} m^2 \phi^2] \text{ with } x = (\vec{x}, x_0)$$

- For field variation $\phi \rightarrow \phi + \delta\phi$

$$\delta S_E = S_E[\phi + \delta\phi] - S_E[\phi] = \int d^4x \; (\delta\phi) \; [-\partial_\mu \partial_\mu \phi + m^2 \phi]$$

- Field can be varied through gradient flow in some 'fictitious time' t

$$\frac{\partial \xi(x,t)}{\partial t} = \nabla^2 \xi(x,t) - m^2 \xi(x,t) \text{ with } \xi(x, t=0) = \phi(x)$$

S. K. Donaldson and P. B. Kronheimer, *The Geometry of Four-Manifolds*, Oxford University Press, USA (1997).

- Solution:

$$\xi(x,t) = \int d^4y \; K_t(x-y)\phi(y) \text{ where } K_t(z) = \frac{e^{(-z^2/4t)}}{(4\pi t)^2} e^{-m^2 t}$$

- So, the flow is a continuous smoothing operation with r.m.s. radius of smoothing to be $\sqrt{8t}$

Gradient flow contd.

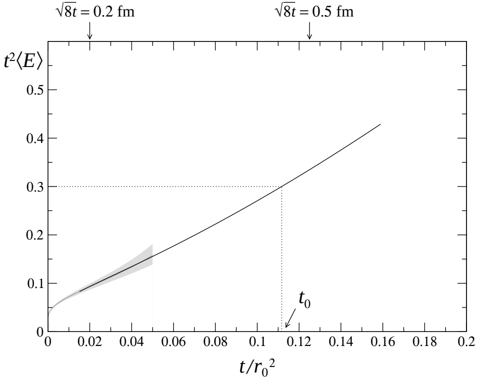
- Flow of SU(N) gauge fields

$$\begin{aligned} \dot{B}_\mu(x,t) &= D_\nu G_{\nu\mu}(x,t) \quad \sim -\frac{\delta S_{YM}[B]}{\delta B_\mu} \\ G_{\mu\nu} &= \partial_\mu B_\nu - \partial_\nu B_\mu + [B_\mu, B_\nu], \qquad D_\mu = \partial_\mu + [B_\mu, \cdot] \\ B_\mu(t,x)|_{t=0} &= A_\mu(x) \quad : \text{initial condition} \end{aligned}$$

- Properties:
  - Gauge invariant operators remain UV finite for $t > 0$, proven to all orders in perturbation theory for YM theory Lüscher and Weisz, '11
    $\Rightarrow$ quantities get renormalized at scale $\mu = 1/\sqrt{8t}$ in continuum limit
    $\Rightarrow$ continuum limit to be taken at fixed t
  - excellent numerical precision
- Example: Energy density in 1-loop

$$\langle E(t)\rangle \equiv \frac{1}{4}\langle G^c_{\mu\nu}(t) G^c_{\mu\nu}(t)\rangle = \frac{3\left(N^2-1\right)}{128\pi^2 t^2}\bar{g}^2(\mu)\left[1 + c_1\bar{g}^2 + \mathcal{O}\left(\bar{g}^4\right)\right]$$

$\Rightarrow$ automatically renormalized at $t > 0$ at scale $\mu = 1/\sqrt{8t}$



- $t^2 \langle E \rangle$ dimensionless
- Numerical observation: $t^2 \langle E \rangle \approx kt$ for $t = \mathcal{O}\left(r_0^2\right)$
  $\Rightarrow$ to be exploited to set scale
- Ideal candidate: t_0 defined through $t_0^2 \langle E(t_0) \rangle = 0.3$ Lüscher, '10
  Alternative quantity: w_0 Borsanyi, Dürr *et al*, '12

Simulation details:

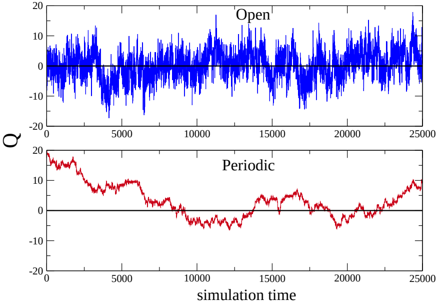
- Worked with Wilson gauge action (Gradient flow to be called Wilson flow)
- publicly available openQCD code used

Lattice size	β	a[fm]
$24^3 \times 48$	6.21	0.0667(5)
$32^3 \times 64$	6.42	0.0500(4)
$48^3 \times 96$	6.59	0.0402(3)
$24^3 \times 48$	6.21	0.0667(5)
$32^3 \times 64$	6.42	0.0500(4)
$48^3 \times 96$	6.59	0.0402(3)
$64^3 \times 128$	6.71	0.0345(4)

Numerics contd.

- Probe to study topology of gauge fields: Topological charge
- We employ clover leaf construction for field tensor $G_{\mu\nu}$ to define the topological charge density $q(x)$ to compute $Q = \int q(x)dx$
- Expected to give result same as that from geometrical construction in continuum limit
  Reason: fields generated by Wilson flow are smooth at scale of lattice spacing Lüscher, '10
  $\rightarrow$ numerically shown to give result agreeing with that from geometrical ones for periodic lattices Lüscher and Palombi, '10

Trajectory history of topological charge

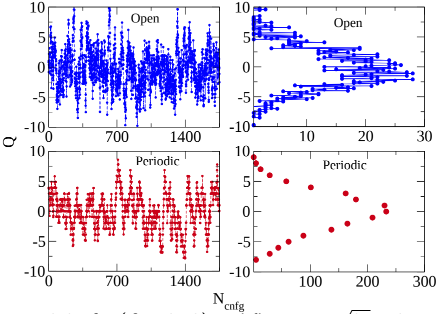


$a = 0.04$ fm ($\beta = 6.59$) with flow time $\sqrt{8t} = 0.16$ fm.

Observations:

- It is evident that with open boundary condition, thermalization is reached very fast compared to periodic boundary condition.
- Also after thermalization, successive configurations are much more correlated for the later than the former.
- We have checked that for larger lattice spacings difference is not so marked.

Distribution of Q

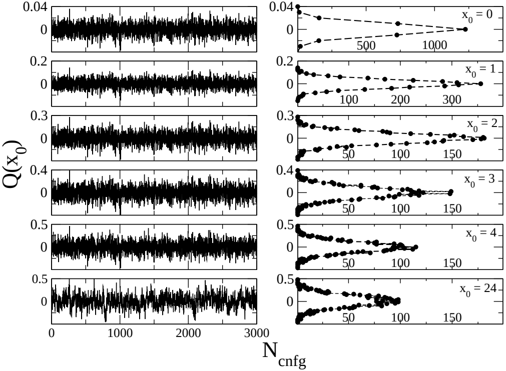


$a = 0.05$ fm ($\beta = 6.42$) and flow time $\sqrt{8t} = 0.47$ fm

Observations:

- As expected, Q-values are not general integers for open boundary whereas they are closed to integers for periodic lattices
- Even at this not so small lattice spacing open boundary gives much better spanning over Q than periodic for same number of configurations.

- To investigate the effect of open boundary in the temporal direction on topological charge density $q(x)$, we study the distribution of $Q(x_0) = \sum_{\vec{x}} q(\vec{x}, x_0)$ at different time slices x_0.

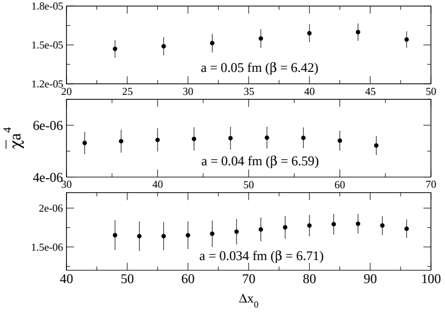


$\beta = 6.42$ and lattice volume $32^3 \times 64$

- Observations: As we move from the boundary towards deep inside the bulk, spanning of $Q(x_0)$ steadily improves before getting settled there.

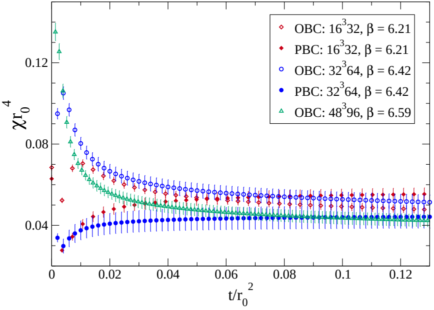
- To investigate the effect of open boundary on topological susceptibility $\chi = \langle Q^2 \rangle / V$ we study the behaviour of subvolume susceptibility $\overline{\chi}(\Delta x_0) = \frac{\langle \tilde{Q}^2 \rangle}{\tilde{V}}$ with temporal width Δx_0

where $\tilde{Q} = \sum_{x_0 = \frac{T}{2} - \frac{\Delta x_0}{2}}^{\frac{T}{2} + \frac{\Delta x_0}{2} - 1} Q(x_0)$ and subvolume $\tilde{V} = V_{\rm space}\ \Delta x_0$ de Forcrand *et al*, '99

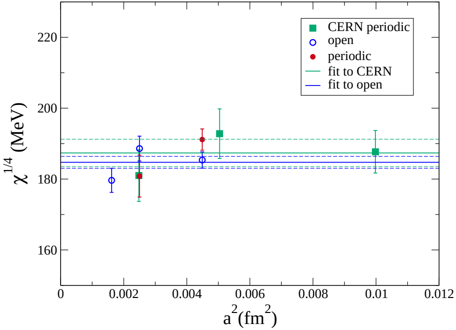


Observation: slight dip close to temporal boundary consistent with the behavior of $Q(x_0)$ but overall, the effect on $\overline{\chi}(\Delta x_0)$ is within statistical uncertainties.

Stability of χ with flow time

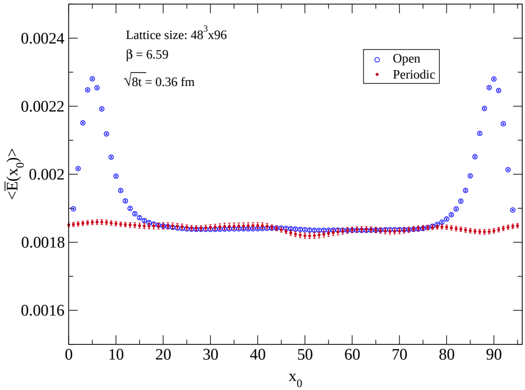


- Observations: non-monotonous behaviour for both open and periodic boundary at early flow times but converging later on



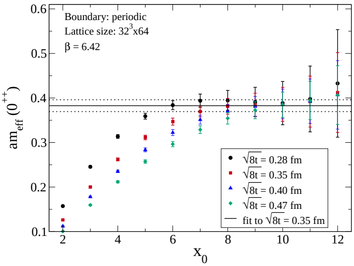
- Results for open and periodic lattices are very close to each other at a given physical volume.
- $\chi^{1/4} = 184.7(1.7)$ MeV from fit to data for open boundary.
  A. Chowdhury, A. Harindranath, JM, P. Majumdar, JHEP **02**,045 (2014)
- This compares well with CERN result 187.4(3.9) MeV from periodic lattices.
  Lüscher, Palombi, '10

- To extract the mass of lowest scalar glueball (0^{++}) we compute the correlator of $\overline{E}(x_0) = \frac{a^3}{L^3} \sum_{\vec{x}} E(\vec{x}, x_0)$ using again clover leaf construction of field tensor



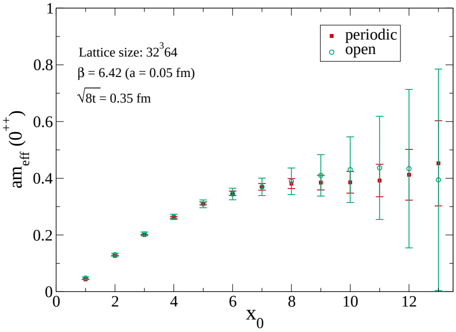
- Effect of breaking of translational invariance is clearly visible.
- Easy way to prevent boundary artifacts from affecting the correlator is to pick both sink and source points deep inside the bulk ⇒ need to work with large temporal extent.

- Averaging over source points done for periodic lattices ⇒ improved statistics compared to open boundary

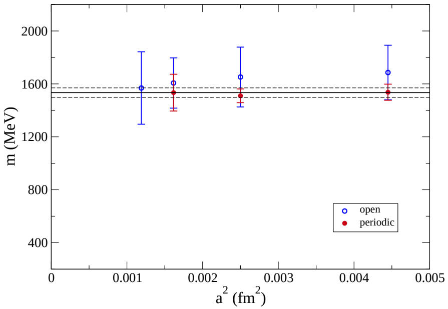


- Effective mass is sensitive to flow time for small temporal differences x_0 but becomes independent of flow times in plateau region within statistical error.

- Unlike for periodic lattices, we can not average over all source points to improve statistics due to lack of translational invariance
- Nevertheless, averaging over few source points chosen far away from boundary is done



- Effective masses agree for two choices of boundary conditions but as expected statistical error is larger for open boundary data.



- no significant scaling violation
  $\Rightarrow$ a constant fit to combined data gives continuum value of 0^{++} mass to be 1534(36) MeV.

A. Chowdhury, A. Harindranath and JM, JHEP **06**,067 (2014)

Scalar glueball mass from $\langle \overline{E}(x_0) \rangle$

- Open boundary acts like a wall source

$$\langle \overline{E}(x_0) \rangle \sim \cosh\, m x_0$$

private communication with Lüscher

- Behavior can be understood as follows

$$S_{\rm PBC} \;=\; S_{\rm OPEN} \;+\; L^3 \frac{1}{2} \Big(\overline{E}(x_0 = 0) \;+\; \overline{E}(x_0 = T-1) \Big)$$

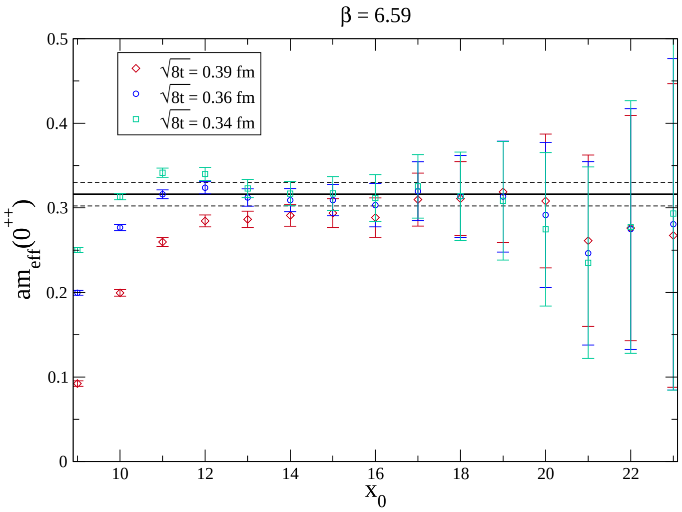
$$\text{where } \overline{E}(x_0) = \frac{1}{g^2} \frac{1}{L^3} \sum_{\mathbf{x}} \sum_{1 \le \mu,\nu \le 4} \mathrm{tr}\left[1 - \mathrm{Re}\; U(\mathbf{x}, x_0) \right] \; .$$

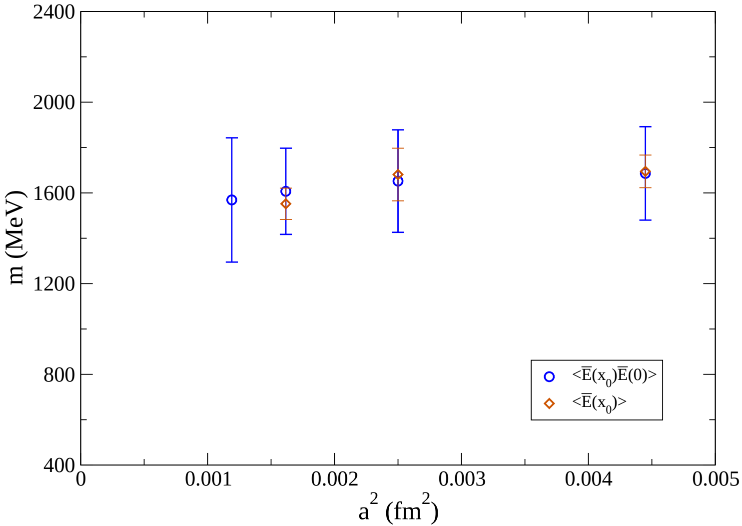
-

$$\Rightarrow \quad \Big\langle \overline{E}(x_0) \Big\rangle_{\rm OPEN} \;=\; \frac{\int \mathcal{D}U \; \overline{E}(x_0) \; e^{-S_{\rm OPEN}}}{\int \mathcal{D}U \; e^{-S_{\rm OPEN}}}$$

$$= \quad \Big\langle \overline{E}(x_0) \Big\rangle_{\rm PBC} + \frac{L^3}{4} \; \Big\langle \overline{E}(x_0) \Big(\overline{E}(x_0 = 0) \;+\; \overline{E}(x_0 = T-1) \Big) \Big\rangle_{\rm PBC}^{\rm cntd} \;+\; \ldots$$

$$= \quad \Big\langle \overline{E}(x_0) \Big\rangle_{\rm PBC} \;+\; \mathrm{Const.}\; \cosh m_G \left(\frac{T}{2} - x_0 \right) \;+\; \ldots$$


β = 6.59
√8t = 0.39 fm
√8t = 0.36 fm
√8t = 0.34 fm
0.5
0.4
0.3
0.2
0.1
0
10
12
14
16
18
20
22
x0
am_eff(0^++)



2400
2000
1600
1200
800
400
m (MeV)
0
0.001
0.002
0.003
0.004
0.005
a^2 (fm^2)
<Ē(x$_0$)Ē(0)>
<Ē(x$_0$)>

Lowest pseudoscalar glueball mass

- Tail of radial correlator of $q(x)$ can be approximated by negative of scalar propagator

$$\langle \phi(x)\phi(y)\rangle = \frac{m}{4\pi^2 r} K_1(mr)$$

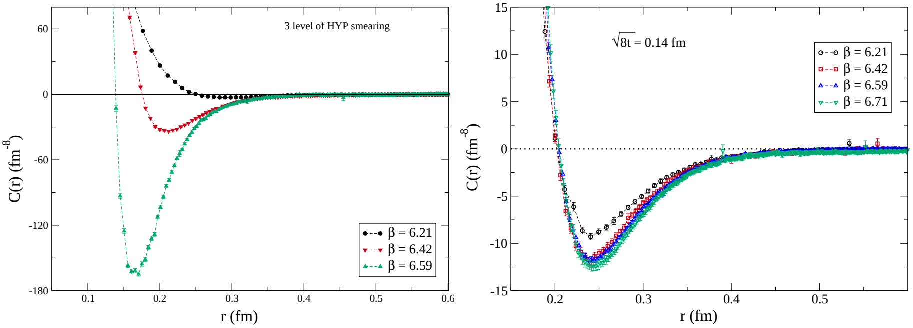
- Fit is done with asymptotic form of $K_1(z)$

$$K_1(z) \underset{\text{large } z}{\sim} e^{-z} \sqrt{\frac{\pi}{2z}} \left[1 + \frac{3}{8z}\right].$$

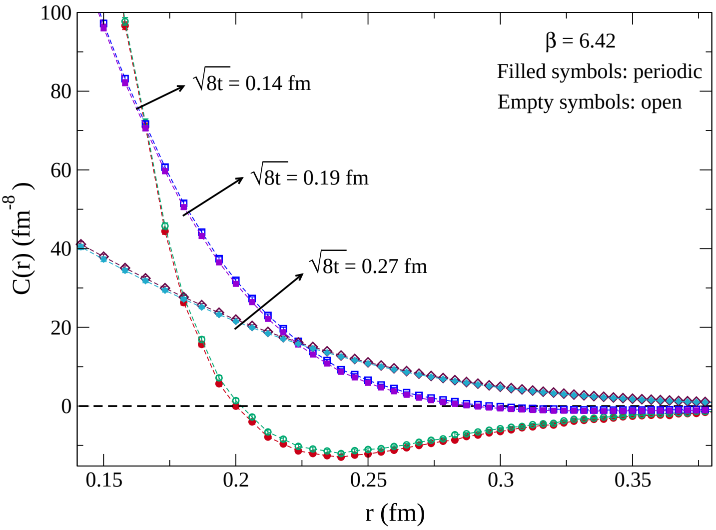
Chen *et al*, '06; Bazavov *et al*, '06

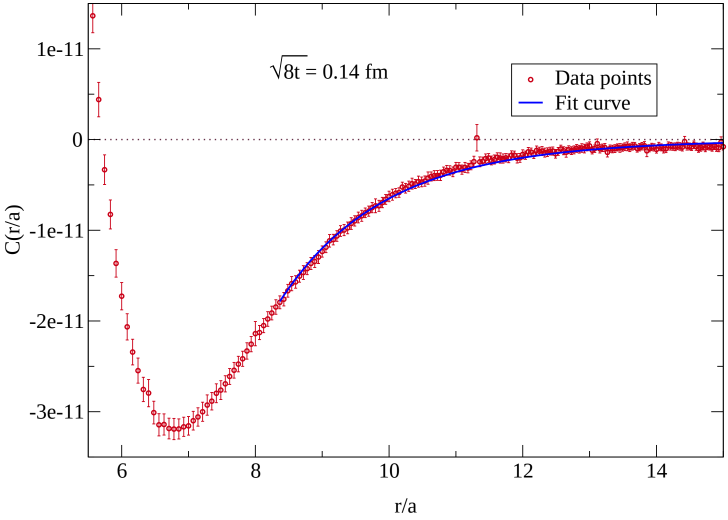
- Wilson flow helps to get proper scaling

Comparison with HYP smearing

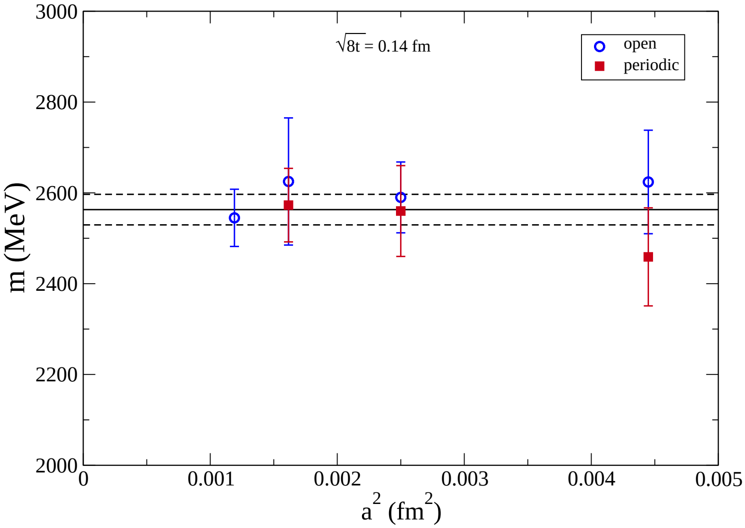


Comparison between periodic and open





$\sqrt{8t}$ = 0.14 fm
Data points
Fit curve
1e-11
0
-1e-11
-2e-11
-3e-11
C(r/a)
6
8
10
12
14
r/a



A. Chowdhury, A. Harindranath and JM, arXiv:1409.6459

Concluding remarks

- With open boundary in temporal direction, we are able to overcome, to a large extent, the problem of trapping during simulation. Simulation becomes cheaper.
- Usage of Wilson flow enables to calculate and compare quantities at fixed lattice scale with ease.
- Quantities studied: topological susceptibility, lowest scalar and pseudoscalar glueball masses
- Results agree with the same for periodic lattices.
- But with open boundary computations have been extended to lower lattice spacings

THANK YOU