Effects of boundary conditions and gradient flow in 1+1 dimensional lattice $\phi^4$ theory

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In this work we study the effects of boundary condition and gradient flow in 1+1 dimensional lattice $\phi^4$ theory. Simulations are performed with periodic (PBC) and open (OPEN) boundary conditions in the temporal direction and the lattice fields are then smoothed by applying gradient flow. Our results with observables such as the $\langle |\phi| \rangle$ and the susceptibility indicate that at a given volume, the phase transition point is shifted towards a lower value of lattice coupling $\lambda_0$ for fixed $m_0^2$ in the case of OPEN as compared to the PBC, with this shift found to be diminishing as the volume increases. We have employed the finite size scaling (FSS) analysis to obtain the true critical behavior, mainly to emphasize the necessity of an FSS formalism incorporating the surface effect in the case of the open boundary. Above features have been found to be illuminated more clearly by the application of gradient flow. Finally we compare and contrast the extraction of the boson mass from the two point function (PBC) and the one point function (OPEN) as the coupling, starting from moderate values, approaches the critical value corresponding to the vanishing of the mass gap. In the critical region, finite volume effects become dominant in the latter. The surface effect seems to be resulted in a less sharper phase transition for OPEN compared to the PBC for all observables studied here.

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I. INTRODUCTION AND MOTIVATION

The quantum field theory of 1+1 dimensional $\phi^4$ interaction, in spite of its apparent simplicity, has a very rich structure and hence has been the testing ground for various new non-perturbative approaches towards the field theory. It also provides ample opportunity to study newly proposed algorithms and calculational techniques. Extensive numerical results have been presented in this theory in an earlier work [1]. In this work we present numerical studies in this theory in the context of comparison between periodic (PBC) and open boundary conditions (OPEN) in the temporal direction and the effects of gradient flow (also known as Wilson flow).

In addition to the periodic boundary conditions in both the temporal and spatial directions, one can have other types of boundary conditions. For the scalar field, for example, one can have anti-periodic boundary condition in the spatial direction (APBC). In the latter case one can study quantum kinks [2]. Lattice Quantum ChromoDynamics (LQCD) conventionally uses PBC in both the temporal and spatial directions for the gauge field. However, in this case, the spanning of gauge configurations over different topological sectors becomes more and more difficult as the continuum limit is approached. As a remedy, open boundary condition in the temporal direction has been proposed [3–5]. Numerical studies in pure Yang-Mills theory [6–10] and QCD [11] have yielded encouraging results.

In order for OPEN to be effective, boundary artifacts should be negligible so that one has a bulk region of considerable extent. This is possible as long the system is not gap less (critical) [12]. The success of OPEN in pure Yang-Mills theory and QCD hinges on the existence of a mass gap in these systems, namely glueball and pion respectively. On the other hand, 1+1 dimensional lattice $\phi^4$ theory offers an opportunity to investigate in detail the artifacts induced by the open boundary condition as the system approaches criticality.

For extracting various observables in lattice field theories, smoothing of lattice fields is essential, in order to overcome lattice artifacts. The gradient (Wilson) flow [13–15] provides a very convenient tool for smoothing, with a rigorous mathematical underpinning. For some recent studies of gradient flow in the context of scalar theory, see Refs. [16–19]. In our previous work on Yang-Mills theory, we have demonstrated the effectiveness of gradient flow in the extraction of the topological susceptibility and glueball masses. Thus it will be very interesting to study the effect of gradient flow on various observables, independent of the boundary condition, in 1+1 dimensional lattice $\phi^4$ theory.

II. BOUNDARY CONDITIONS AND GRADIENT FLOW

In the continuum, the Euclidean Lagrangian (density) for $\phi^4$ theory is given by

$$\mathcal{L} = \frac{1}{2} \partial_\mu \phi \partial^\mu \phi + \frac{1}{2} m^2 \phi^2 + \frac{\lambda}{4!} \phi^4. \quad (1)$$

On a periodic (on all space-time directions) lattice, the Euclidean action in ‘d’ space-time dimension is conventionally written as [11]

$$S = -\sum_x \sum_\mu \tilde{\phi}_x \tilde{\phi}_{x+\mu} + \left(d + \frac{m_0^2}{2}\right) \sum_x \tilde{\phi}_x^2 + \frac{\lambda_0}{4!} \sum_x \tilde{\phi}_x^4 \quad (2)$$

where all the parameters and fields have been made dimensionless by multiplying them with appropriate powers of lattice spacing ‘$a$’.

However, in order to impose open boundary condition in the temporal direction we follow the construction of the transfer matrix. For this purpose the lattice action is written in terms of time slice action density $E(t)$ as $S = \sum_i E(t)$ and the kinetic term in the temporal direction is distributed symmetrically around the time slice ‘$t$’. The details are given below.

First, with the aid of forward and backward lattice derivatives

$$\partial^f_\mu \phi = \frac{1}{a} \left(\phi_{x+\mu} - \phi_x\right) \quad \text{and} \quad \partial^b_\mu \phi = \frac{1}{a} \left(\phi_x - \phi_{x-\mu}\right), \quad (3)$$

we write the symmetrized expression for kinetic term as

$$\frac{1}{2} \partial_\mu \phi \partial^\mu \phi = \frac{1}{4} \left(\partial^f_\mu \phi \partial^f_\mu \phi + \partial^b_\mu \phi \partial^b_\mu \phi\right)$$

$$= \frac{1}{4a^2} \left(2 \sum_\mu \phi^2_x + \phi^2_{x+\mu} + \phi^2_{x-\mu} - 2\phi_x \phi_{x+\mu} - 2\phi_x \phi_{x-\mu}\right). \quad (4)$$
This enables one to write down the time slice action density for periodic lattice as

\[ E_{\text{PBC}}(t) = T_t + V_t + \frac{1}{2} T_{t,t+1} + \frac{1}{2} T_{t-1,t} \]  

(5)

where

\[ V_t = \sum_{\vec{x}} \left( \frac{1}{2} a^2 m^2 \phi_{\vec{x},t}^2 + \frac{a^2 \lambda}{4!} \phi_{\vec{x},t}^4 \right), \]

\[ T_t = \frac{1}{4} \sum_{\vec{x},k} \left( 2 \phi_{\vec{x},t}^2 + \phi_{\vec{x}+k,t}^2 + \phi_{\vec{x}-k,t}^2 - 2 \phi_{\vec{x},t} \phi_{\vec{x}+k,t} - 2 \phi_{\vec{x},t} \phi_{\vec{x}-k,t} \right), \]

\[ T_{t,t+1} = \frac{1}{2} \sum_{\vec{x}} \left( \phi_{\vec{x},t}^2 + \phi_{\vec{x},t+1}^2 - 2 \phi_{\vec{x},t} \phi_{\vec{x},t+1} \right), \]

\[ T_{t-1,t} = \frac{1}{2} \sum_{\vec{x}} \left( \phi_{\vec{x},t}^2 + \phi_{\vec{x},t-1}^2 - 2 \phi_{\vec{x},t} \phi_{\vec{x},t-1} \right) \]

with \( \hat{k} \) being the unit vector in an arbitrary spatial direction.

Following this definition, we denote \( e^{-H_{m}(t,t+1)} \) as the general transfer matrix element between the time slices \( t \) and \( t + 1 \) where

\[ H_m(t, t + 1) = \frac{1}{2} (T_t + V_t) + \frac{1}{2} (T_{t+1} + V_{t+1}) + T_{t,t+1}. \]  

(6)

Particularly for a lattice of temporal extent \( T \), the transfer matrix element between the boundary time slices \( t = T - 1 \) and \( t = 0 \) is determined by

\[ H_m(T - 1, 0) = \frac{1}{2} (T_{T-1} + V_{T-1}) + \frac{1}{2} (T_0 + V_0) + T_{T-1,0}. \]

Now, if the temporal boundary becomes open, the corresponding term drops out from the partition function. This leads us to relate the actions for lattices with two different boundary conditions in the temporal direction (periodic and open) as \( S_{\text{PBC}} = S_{\text{OPEN}} + \Delta S \) where \( \Delta S = H_m(T - 1, 0) \).

The absence of the term \( \Delta S \) from the action for a lattice with open boundary (temporal direction), in turn, also modifies the expressions for action densities at the temporal boundaries. They are given by

\[ E_{\text{OPEN}}(t = 0) = \frac{1}{2} (T_0 + V_0) + \frac{1}{2} T_{0,1} \]  

(7)

and

\[ E_{\text{OPEN}}(t = T - 1) = \frac{1}{2} (T_{T-1} + V_{T-1}) + \frac{1}{2} T_{T-2,T-1}. \]  

(8)

Within the bulk \( (0 < t < T - 1) \), \( E_{\text{OPEN}}(t) = E_{\text{PBC}}(t) \).

In order to smooth the lattice \( \phi \) field, gradient flow is used. For \( \phi^4 \) theory it is known that, in four dimensions, there are potential divergences in the correlation functions for flow time greater than zero and for this reason in Refs. [16] and [18] simple flow equation corresponding to free field theory has been used. Fujikawa [17] has proposed a modification of the flow equation to tackle this problem. However, the \( \phi^4 \) in 1+1 dimensions which we study here is free from such divergences. Here we follow the choice made in our previous works for Yang-Mills theory, namely, picking the gradient of the action to drive the flow. Thus for \( \phi^4 \) theory in the Euclidean space in 1+1 dimensions, in the continuum, the flow equation is chosen to be

\[ \frac{\partial \psi(x, \tau)}{\partial \tau} = - \frac{\delta S[\psi]}{\delta \psi(x, \tau)} \]

\[ = \partial_\mu \partial_\mu \psi(x, \tau) - m^2 \psi(x, \tau) - \frac{\lambda}{6} \psi^3(x, \tau) \]  

(9)

where \( \psi(x, \tau = 0) = \phi(x) \) with \( \tau \) being the flow time.

We numerically solve this equation on the lattice using the 2nd order Runge-Kutta method.
III. EXTRACTION OF BOSON MASS FROM LATTICES WITH DIFFERENT BOUNDARIES

For the extraction of boson mass we have used the simplest and the most familiar scalar operator - the time sliced field $\phi(t) = \frac{1}{V} \sum_{\vec{x}} \phi(\vec{x}, t)$ where $V$ is the spatial volume of the lattice. The mass can be easily extracted from the two point correlation function for this scalar operator which, in the case of periodic boundary in the temporal direction, behaves as

$$G(t) = \langle \phi(t) \phi(t=0) \rangle_{\text{PBC}} \approx C_0 + C_1 \left[ e^{-mt} + e^{-m(T-t)} \right]$$

$$= C_0 + 2C_1 e^{-mT/2} \cosh m \left( \frac{T}{2} - t \right) \quad (10)$$

where

$$C_1 = \frac{|\langle 0 | \phi(0) | B \rangle|^2}{2m} \quad (11)$$

with $|B\rangle$ being the one boson state. To improve statistics, one can average over the source time as well. The effective mass can be evaluated by solving the equation $F(m) = 0$

where

$$F(m) = (r_1 - 1) \left[ \cosh m(\Delta t - 1) - \cosh m\Delta t \right] + (1 - r_2) \left[ \cosh m(\Delta t + 1) - \cosh m\Delta t \right] \quad (12)$$

with

$$r_1 = \frac{G(t-1)}{G(t)}, \quad r_2 = \frac{G(t+1)}{G(t)} \quad \text{and} \quad \Delta t = T/2 - t \quad (13)$$

Note that the boson mass extracted from the propagator using Eq. (10) is the pole mass and hence is the physical mass [20], independent of the lattice spacing.

In the case of open boundary in the time direction, to avoid the boundary effects one needs to be well within the bulk while computing the two point correlation function. However, the second exponential will be absent from the expression of the two point function due to the loss of periodicity. On the other hand, as the time translational invariance is also lost in this case, one cannot average over the source time as well. However, within the bulk, well away from the boundary region translational invariance is recovered. So one can take average over few time slices to regain statistics.

However, this effort breaks down as one approaches the critical region. It will be shown later on in this study that, the effect of open boundary starts to engulf the whole bulk region as we move towards the critical point. Mass extraction from two point function becomes almost impossible.

Surprisingly, the open boundary itself opens up new pathways to extract the mass. Following Ref. [9], in this section we review how the boson mass can be extracted from a one-point function in the case of open boundary using a generic time sliced scalar operator $O(t)$.

We start from

$$\langle O(t) \rangle_{\text{OPEN}} = \frac{\int D\phi \ O(t) \ e^{-S_{\text{OPEN}}}}{\int D\phi \ e^{-S_{\text{OPEN}}}} = \frac{\int D\phi \ O(t) \ e^{-S_{\text{PBC}} + \Delta S}}{\int D\phi \ e^{-S_{\text{PBC}} + \Delta S}} = \langle O(t) \rangle_{\text{PBC}} + \frac{\langle O(t) e^{\Delta S} \rangle_{\text{PBC}}^{\text{connected}}}{\langle e^{\Delta S} \rangle_{\text{PBC}}} \quad (14)$$

$$= \langle O(t) \rangle_{\text{PBC}} + \frac{1}{r} \langle O(t) e^{H_m(T-1,0)} \rangle_{\text{PBC}}^{\text{connected}} \quad (15)$$

where $r = \langle e^{\Delta S} \rangle_{\text{PBC}} = \langle e^{H_m(T-1,0)} \rangle_{\text{PBC}}$. As $e^{H_m(t,t+1)}$ is also a scalar operator, from Eq. (15) we have

$$\langle O(t) \rangle_{\text{OPEN}} \approx \langle O(t) \rangle_{\text{PBC}} + 2C_1' e^{-mT/2} \cosh m \left( \frac{T}{2} - t \right) \quad (16)$$

where $m$ is the scalar boson mass.

Thus we find that one can extract certain two-point correlators computed with periodic boundary condition in the temporal direction by analyzing the data for the functional average of a scalar operator (one-point function) computed
with open boundary (in the temporal direction) in the region of $t$ where it differs, due to the breaking of translational invariance, from the same computed with periodic boundary. Now due to time translational invariance in the case of PBC, we can assume $\langle O(t) \rangle_{\text{PBC}}$ to be constant and the evaluation of effective mass can then be done again following the Eqs. (12) and (13).

IV. SIMULATION DETAILS

As we have restricted ourselves to 1+1 dimensions within this study, the fields are dimensionless here. The notations for the bare parameters of the theory on the lattice are chosen to be $m_0^2 = a^2 m^2$ and $\lambda_0 = a^2 \lambda$. As we know, for the stability of the theory one must have $\lambda_0 \geq 0$ and the phase transition associated with the spontaneous breaking (or restoration) of $Z(2)$ symmetry takes place only for $m_0^2 < 0$.

For the study with periodic boundary in both directions, following the method of Brower and Tamaya [21], we have used Wolff’s single cluster algorithm [22, 23] blended with the standard metropolis algorithm in 1:1 ratio for the generation of field configurations. For the details of the whole procedure, see [1]. However, in the study with open boundary in the temporal direction (periodic in spatial direction), we resort only to the standard metropolis algorithm for configuration generation.

Following the discussions in [1], we have used $\langle |\phi| \rangle$ as the order parameter to investigate the phase structure. Here, $\phi = \sum \phi(x)/\text{lattice volume}$. The absolute value is taken to avoid the effect of tunnelling enforced by the algorithm of configuration generation. For the phase diagram we mainly resorted to the former study [1]. Here, we will study the effects of gradient flow and boundary conditions on the phase diagram in due course.

In this work, we explored the phase structure and the spectrum of the theory for two different sets of bare parameters given by $m_0^2 = -0.5$ and $m_0^2 = -1.0$. For each set of parameters (i.e., $m_0^2$ and $\lambda_0$), we have first discarded $10^8$ configurations for thermalization and then generated another $10^8$ configurations for the measurement purpose. Measurements are done on one in every thousand configurations. In order to study the finite size effects on the results, whole investigations have been done with four different lattice volumes such as $48^2$, $64^2$, $96^2$ and $128^2$.

Configurations chosen for measurements are placed under gradient flow which is run for one hundred steps, to be called as flow level, with a stepsize of $\delta t = 0.02$. Measurements are done after every ten flow levels in addition to the measurement done before the flow is started.

V. NUMERICAL RESULTS

In this section we present and discuss our numerical results showing the effects of the boundary conditions and the gradient flow on various observables of interest. In principle, one could divide this into two separate studies altogether as the gradient flow and the boundary condition are two completely disjoint categories. Neither of them has anything to do with the other. However, on one hand, we wanted to study the smoothening utility of the gradient flow irrespective of the choice of the boundary condition and on the other hand we have a different aim to study the effect of boundary condition as well. Thus they have come together in the same discussion here. Nevertheless they are independent of each other.

A. The field variable

As the translational invariance is lost in the temporal direction when open boundary condition is imposed in that direction, time sliced scalar field $\phi(t)$ could serve as an important observable to study the effect of open boundary as compared to periodic boundary. For the reasons stated earlier, here too, we take absolute value before evaluating the configuration average.

In Figs. 1 and 2 respectively for periodic and open boundary conditions in temporal directions, we present the expectation value of $|\phi(t)|$ in three different subdiagrams - one without any gradient flow and two others with two different levels of gradient flow all for a particular set of lattice parameters $m_0^2 = 0.5$, $\lambda_0 = 1.65$ and $128^2$ lattice. The figures clearly show the smoothening effect with the increase of flow level. Note that, values of $\langle |\phi(t)| \rangle$ are gradually rising up with increasing flow level. The widths of windows for the values of $\langle |\phi(t)| \rangle$ are taken to be same in all the three subdiagrams instead of taking them to be proportional to the respective average values. This actually has reduced the manifestation of smoothening effect to some extent.

To make exhibition of boundary effect clearer, in Fig. 3 we compare the behaviour of $|\phi(t)|$ for $m_0^2 = -0.5$ and $L = 128$ for periodic and open boundary conditions without any gradient flow for three different values of $\lambda_0$ all in
the broken symmetric phase. For the smallest value of the coupling which is far away from the critical point, effects of open boundary are found to be only at the edges leaving a long bulk region matching with the counterpart in PBC. As the coupling increases one gets closer to the region of phase transition and effect of open boundary extends on both side squeezing the bulk. For $\lambda_0 = 1.86$, we are already in the critical region and we observe that the bulk region has almost vanished. The same is presented in Fig. 4 for gradient flow level 50. We notice that it only smoothens the data (which is, although, hardly visible here because of the wide scale of values for $\langle |\phi(t)| \rangle$ covered in the figure) leaving the boundary effects unchanged.

In Fig. 5 we plot $\langle |\phi| \rangle$ versus $\lambda_0$ for different values of the gradient flow level for $128^2$ lattice at $m_0^2 = -0.5$. The monotonous rise in the value of $\langle |\phi| \rangle$ with increasing gradient flow level is consistent with the behaviour of $\langle |\phi(t)| \rangle$. Details of the behavior in the critical region are shown in the inset of the figure. The trend is seemed to be retained across the phase transition with an additional feature exhibiting a sharper fall of the observable across the transition point as the flow level is increased.

In Fig. 6, we present the comparison between $\langle |\phi| \rangle$ computed using PBC and the same obtained with OPEN for different lattice sizes at $m_0^2 = -0.5$ before applying the gradient flow on the fields. Deep in both the broken-symmetric
FIG. 3. Comparison of $\langle |\phi(t)| \rangle$ between PBC and OPEN for $m_0^2 = -0.5$, $L = 128$ and three different values of $\lambda_0$ without any gradient flow.

and the symmetric phases, for all the lattice volumes, the results for PBC and OPEN are found to be matching within our statistical error. However, inside the critical region a clear disagreement is observed. Phase transition appears to take place at smaller values of $\lambda_0$ in the case of OPEN compared to the PBC. However, the gap between the transition point in two different boundaries seems to be vanishing with the increase of lattice size. In addition, although not clearly prominent, it appears that the fall of $\langle |\phi| \rangle$ across the transition point is slightly sharper for PBC in comparison with OPEN. Both these behaviors are consistent with the expectation that the effect of boundary surface diminishes in infinite volume limit. The picture remains to be almost unaltered by the application of gradient flow other than raising the values universally little bit. This has been emphasized in Fig. 7.

B. The susceptibility

In this subsection, we study the effects of gradient flow and the boundary conditions on the behaviour of another observable of interest, namely, the susceptibility defined as $\chi = \sum_x \langle \phi(x)\phi(0) \rangle$/lattice volume. In Fig. 8 we show the behaviour of susceptibility as a function of $\lambda_0$ for $m_0^2 = -0.5$ with PBC on $128^2$ lattice for different levels of gradient flow. Consistent with the trends as observed in the case of $\langle |\phi| \rangle$, the peak of susceptibility becomes higher and higher as the level of gradient flow increases leaving the peak position unchanged. This behavior is expected since the gradient flow serves to remove the lattice artifacts and brings the lattice theory closer to the continuum limit.

Analogous to the study done for $\langle |\phi| \rangle$, we compare the susceptibility between the periodic and open boundary conditions for different lattice sizes ($L$) at $m_0^2 = -0.5$ and gradient flow level 50 in Fig. 9. Here too, we observe that
FIG. 4. Comparison of $\langle |\phi(t)| \rangle$ between PBC and OPEN for $m_0^2 = -0.5$, $L = 128$ and three different values of $\lambda_0$ at gradient flow level 50.

FIG. 5. Plot of $\langle |\phi| \rangle$ versus $\lambda_0$ for different values of the gradient flow level for $m_0^2 = -0.5$ and $L = 128$ in the case of PBC.
FIG. 6. Plot of $\langle|\phi|\rangle$ versus $\lambda_0$ for PBC and OPEN without gradient flow for different $L$ at $m_0^2 = -0.5$.

FIG. 7. Plot of $\langle|\phi|\rangle$ versus $\lambda_0$ for PBC and OPEN at gradient flow level 50 for different $L$ at $m_0^2 = -0.5$.

compared to the case of PBC, the peak is shifted towards the smaller values of $\lambda_0$ in case of OPEN at a fixed $L$ and the magnitude of the shift decreases as $L$ increases.

This shift in the peak position of susceptibility between PBC and OPEN seems to be unaffected by gradient flow as per our expectation. This has been demonstrated in Figs. 10 and 11 for the smallest and largest lattice sizes $L = 48$ and $L = 128$ respectively both with $m_0^2 = -0.5$.

From all the figures here comparing susceptibility between PBC and OPEN, it appears that the peak is slightly sharper in the case of the former compared to the later consistent with the case of $\langle|\phi|\rangle$.

C. Finite size scaling analysis

The fact that the value of $\langle|\phi|\rangle$ changes with gradient flow even in the critical region raises an interesting question. Does the determination of critical coupling in a Finite Size Scaling (FSS) analysis gets affected by gradient flow? Here we study the possible effect of gradient flow in the FSS of the data for $\langle|\phi|\rangle$ to determine the critical coupling. We follow the discussion of the main aspects of finite size scaling [24–26] given in Ref. [1]. FSS assumes that, in a finite system, out of the three length scales involved, namely, the correlation length $\xi$, the size of the system $L$ and the
microscopic length $a$ (lattice spacing), the last one drops out near the critical region due to universality.

For any observable $P_L$, computed on a lattice of finite extent $L$, the nonanlicity near the critical point in the infinite volume limit can be expressed in the form of a scaling law $P_\infty(\tau) = A_\rho \tau^{-\rho}$ where $\tau = (\lambda_0 - \lambda_0)/\lambda_0^0$ and $\rho$ is the critical exponent associated with the observable. Following the arguments of FSS analysis, it can be shown that

$$L^{\rho/\nu} \frac{P_L(\tau)}{P_\infty(\tau)} = A_\rho^{-1} A_\xi^{-1/\nu} \left[ C_\rho + D_\rho A_\xi^{-1/\nu} \tau L^{1/\nu} + O(\tau^2) \right]$$

where $\nu$ is the critical exponent associated with the correlation length $\xi$. Eq. (17) implies that if we plot $L^{\rho/\nu} P_L(\tau)$ versus the coupling $\lambda_0$ for different values of $L$, all the curves will pass through the same point where $\tau = 0$ or equivalently $\lambda_0 = \lambda_0^0$ [26].

The critical behavior of $\langle \phi \rangle$, the susceptibility $\chi$ and the mass gap $m = 1/\xi$ may be written as

$$\langle \phi \rangle = A_{\phi}^{-1} \tau^\beta, \quad \chi = A_{\chi} \tau^{-\gamma} \quad \text{and} \quad m = A_{\xi}^{-1} \tau^\nu.$$  

From the general expectation that in $1 + 1$ dimensions, $\phi^4$ theory and Ising model belong to the same universality class, we have used the Ising values for the corresponding exponents as inputs in our FSS analysis. Thus, $\beta = 0.125$, $\gamma = 1.75$ and $\nu = 1$. 

FIG. 8. Comparison of susceptibility for different levels of gradient flow with PBC at $m_0^2 = -0.5$ and $L = 128$.

FIG. 9. Comparison of susceptibility between PBC and OPEN for different $L$ at $m_0^2 = -0.5$ and gradient flow level 50.
The plot of $\langle |\phi| \rangle L^{0.125}$ versus $\lambda_0$ for different values of the gradient flow level at $m_0^2 = -0.5$ with periodic boundary in the temporal direction is presented in Fig. 12. In spite of the fact that $\langle |\phi| \rangle$ changes with gradient flow level, the critical coupling $\lambda^c_0$ is found to be unaffected by gradient flow. The critical coupling $\lambda^c_0$ is found to be little less than 1.94 for $m_0^2 = -0.5$. Similar FSS analysis has been done at $m_0^2 = -1.0$ leading to the same conclusion along with an estimated value of $\lambda^c_0 \approx 4.46$.

A similar FSS analysis of the susceptibility calculated at $m_0^2 = -0.5$ for various values of gradient flow level (for PBC) is presented in Fig. 13. Here, the smoothening effect of gradient flow has helped to pinpoint the location of critical coupling $\lambda^c_0$ which matches with the estimation done from the FSS analysis for $\langle |\phi| \rangle$. Similar FSS analysis done at $m_0^2 = -1.0$ also gives the corresponding value of $\lambda^c_0$ matching with the same obtained from FSS analysis for $\langle |\phi| \rangle$.

Using the same ansatz, we have tried an FSS analysis for both $\langle |\phi| \rangle$ and $\chi$ in the case of open boundary in the temporal direction. The results are respectively presented in Figs. 14 and 15. It is obvious from the figures that the critical point is not pinpointed that clearly compared to the case of PBC. A strange pattern is found for susceptibility for which the curves with different $L$, instead of passing through a point, appear to overlap within statistical errors at and between the values 1.92 and 1.94 of $\lambda_0$. Anyway, the effect of surface in the case of open boundary needs to be taken into the ansatz for finite size scaling analysis. For that purpose a more precise numerical study is necessary.
which is beyond the scope of this study.

D. The boson mass

Finally, in this subsection, we present the results for the mass spectrum of the theory. The boson mass has been extracted from the plateau along the time direction for effective mass which is computed from two point and one point correlation function of the time sliced scalar field $\phi(t)$ respectively for PBC and OPEN. For this purpose, we first find out the gradient flow level for which the plateau for effective mass is found to be the most stable one separately for each coupling (also for PBC and OPEN separately). The computation of mass has been done only for the two largest lattices namely for $L = 96$ and $L = 128$ since, for the smaller lattices, the temporal extent is not sufficiently long to get the fall of correlation function particularly within the critical region. Because of this, it is not meaningful to perform the formal FSS analysis. However, even with lattices of only two different sizes, we observe noticeable finite volume effect.

In Figs. 16 and 17 we compare the volume dependence of the boson mass versus $\lambda_0$ for periodic (top) and open (bottom) at $m_0^2 = -0.5$ and $m_0^2 = -1.0$ respectively. In the case of PBC, the effect of finite volume on the mass spectrum is clearly visible in the critical region. Although for OPEN, this effect is not that obvious from the respective figure. However, if we remember from the behaviors of $\langle |\phi| \rangle$ and $\chi$ that the phase transition point shifts towards the smaller values of $\lambda_0$ compared to PBC and that the shift is more for smaller volume, it appears that this leftward shift of transition point has overshadowed the finite volume effect.

The effects of the boundary on the mass spectrum have been demonstrated in Figs. 18 and 19 respectively for two different values for the lattice mass parameters $m_0^2 = -0.5$ and $m_0^2 = -1.0$ respectively. The leftward shift of
the phase transition point is found to be almost diminishing for the larger lattice. The boundary effects are more prominent near the critical point as evident from the clearly sharper nature of transition in the case of PBC compared to that of OPEN.

VI. CONCLUSIONS

We have found the gradient flow to be very effective in reducing the unwanted lattice artifacts in the functional average of the time sliced field $\phi(t)$, the susceptibility and in the extraction of boson mass from both two-point (PBC) and one-point (OPEN) correlators. We have shown that, in spite of the fact that $\langle |\phi| \rangle$ changes with gradient flow (transition more prominent with increasing flow level), the transition point does not depend on the gradient flow level. In the case of susceptibility, it is found that the increase in the level of gradient flow raises the height of the peak but leaves the peak position (phase transition point for a given volume) practically unaltered. This behaviour is consistent with the expectation that the gradient flow helps to reduce the lattice artifacts and brings the lattice theory closer to the continuum physics where we expect the susceptibility to diverge as critical point is approached. Critical coupling $\lambda_0^c$ has been obtained for both $\langle |\phi| \rangle$ and $\chi$ from a detailed finite size scaling analysis of the data for various lattice sizes and gradient flow levels with results qualitatively unchanged with flow level but seem to be pin-pointed more clearly with nonzero value of flow level.

With all kinds of observables studied here, for a given volume, phase transition point has a left-ward shift in terms of $\lambda_0$ in the case of OPEN compared to the PBC for a fixed value of $m_0^2$ and this left-ward shift diminishes as volume increases. In addition, for a given volume, the phase transition curve is found to be more prominent or sharp in the case of PBC compared to the OPEN. Particularly, noticeable boundary effects are observed on the mass spectrum.
FIG. 14. Plot of $\langle |\phi| \rangle L^{0.125}$ versus $\lambda_0$ for different levels of gradient flow at $m^2_0 = -0.5$ with open boundary.

in the critical region where the effects of open boundary extend deeply into the bulk region (as emphasized by the behavior of $\langle |\phi(t)| \rangle$) and the finite volume artifacts become much more important compared to the case of the periodic boundary condition. An extensive analytical study of the boundary effects due to open boundary in the critical region, taking into consideration the finite size scaling will be very fruitful.

The main objective of the present study has been to investigate the effects of the gradient flow and the open boundary condition in the temporal direction in a theory with vanishing mass gap and without the complexities of renormalization. Since it is known that in 3+1 dimensional $\phi^4$ theory, the straight forward use of the gradient flow equation leads to new divergences in correlation functions at non-zero flow time, a detailed comparison of various proposals to overcome this problem needs to be investigated. Our current study has demonstrated that in the region of vanishing mass gap, open boundary introduces complexities when used in a lattice with finite volume. Our previous success with open boundary in pure Yang-Mills theory may be partly due to the reasonably large mass gap (glueball mass) in this theory. On the other hand the relevant mass gap of QCD (determined by the two pion state) is much lower and we expect open boundary to have non-trivial consequences in the scaling region. This requires a thorough investigation in the future.

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FIG. 15. Plot of $\chi L^{-1.75}$ versus $\lambda_0$ for different levels of gradient flow at $m_0^2 = -0.5$ with open boundary.

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FIG. 16. The volume dependence of the boson mass versus $\lambda_0$ for PBC (top) and OPEN (bottom) at $m_0^2 = -0.5$. 

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FIG. 17. The volume dependence of the boson mass versus $\lambda_0$ for PBC (top) and OPEN (bottom) at $m_0^2 = -1.0$. 

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FIG. 18. The effect of boundary condition on the boson mass versus $\lambda_0$ for $L=96$ (top) and $L=128$ (bottom) at $m_0^2 = -0.5$. 
FIG. 19. The effect of boundary condition on the boson mass versus $\lambda_0$ for $L=96$ (top) and $L=128$ (bottom) at $m_0^2 = -1.0$. 