Simulating Quantum Chromodynamics coupled with Quantum Electromagnetics on the lattice

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The 36th Annual International Symposium on Lattice Field Theory

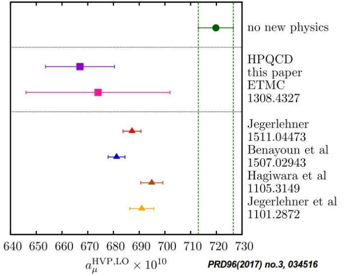
East Lansing, MI, USA

July 22-28, 2018

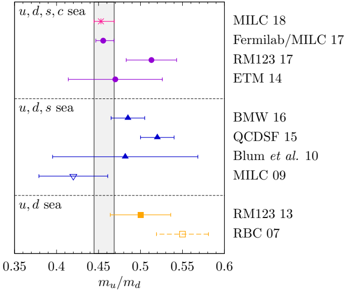
Motivation

- Many lattice-QCD calculations are now reaching a precision for which electromagnetic (EM) and isospin-breaking effects may enter near the level of current lattice uncertainties.

- Current dominant errors for the calculation of the hadronic contributions to the muon anomalous magnetic moment (g - 2) are from omission of EM and isospin breaking, and from quark-disconnected contributions. (HPQCD, PRD 96(2017) no.3, 034516)



- The calculation of EM and isospin-violating effects in the kaon and pion systems is a long-standing problem and is crucial for determining the light up- and down-quark masses. (MILC, arXiv:1807.05556, and Fermilab Lattice, MILC, and TUMQCD Collaborations arXiv:1802.04248)



QCD + QED action

In the continuum, the QCD Lagrangian density (in Minkowski space) for one spin-1/2 field without interacting with the EM field is

$$\mathcal{L}_{\mathrm{QCD}} = \mathcal{L}_{\mathrm{QCD}_F} + \mathcal{L}_{\mathrm{QCD}_G} = \sum_f \bar{\psi}_i^f (i\gamma_\mu D_{ij}^{f\mu} - M^f)\psi_j^f - \frac{1}{4g^2} G_{\mu\nu}^a G_a^{\mu\nu}. \qquad (1)$$

The Euclidean QCD + QED Lagrangian density is

$$\mathcal{L} = \sum_f \bar{\psi}_i^f (\gamma_\mu D_{ij}^{f\mu} + M^f)\psi_j^f + \frac{1}{4g^2} G_{\mu\nu}^a G_a^{\mu\nu} + \frac{1}{4e^2} F_{\mu\nu} F^{\mu\nu}, \qquad (2)$$

with

$$D_\mu^f = \partial_\mu + iA_\mu(x) + iq^f A'_\mu(x), \qquad (3)$$

$$q^f = 2/3 \quad \text{for u quark,} \quad e \approx \sqrt{4\pi/137}, \qquad (4)$$

$$G_{\mu\nu}^a = \partial_\mu A_\nu^a(x) - \partial_\nu A_\mu^a(x) + f_{abc} A_\mu^b(x) A_\nu^c(x), \qquad (5)$$

$$F_{\mu\nu} = \partial_\mu A'_\nu(x) - \partial_\nu A'_\mu(x). \qquad (6)$$

The QCD + QED action becomes

$$S = \int dx^4 \mathcal{L} = S_F + S_{G_{QCD}} + S_{G_{QED}}. \qquad (7)$$

QCD + QED action

- The lattice QCD ($SU(3)$) gauge action $S_{G_{QCD}}$ is a function of
  - the link variable $U_\mu(n) = e^{iA_\mu(n)}$ and the QCD coupling g.
- The lattice QED ($U(1)$) gauge action $S_{G_{QED}}$ is a function of
  - the link variable $U'^{q}_\mu(n) = e^{iqA'_\mu(n)}$ for compact QED;

  or

  - the real valued vector potential of an EM field $A'_\mu(x)$ for non-compact QED.

  and

  - the QED coupling e.
- The lattice fermion action S_F is a function of
  - the link variables $U_\mu(n)$ and $U'^{q}_\mu(n)$ (i. e., S_F has both SU(3) and U(1) components).

QCD + QED action

- The naive QCD+QED lattice fermion action is

$$S_F^{naive} = \sum_{x,y} \bar{\psi}(x)[M(U^{eff})]_{xy}\psi(y), \tag{8}$$

where $\psi(x)$ is the charged spin 1/2 particle field.

- The staggered fermion classical Hamiltonian is obtained by changing the $\psi(x)$ field to the staggered field $\chi(x)$, introducing the pseudo-fermion filed Φ(on even sites only) and the canonical momentum h and h' conjugate to A_μ and A'_μ,

$$\mathcal{H}[\Phi_e^q; A'; U; U'^q; g; e] = \sum_i \frac{1}{2} h_i^2 + \sum_i \frac{1}{2} {h'}_i^2 + S_{PF} + S_{G_{QCD}} + S_{G_{QED}}. \tag{9}$$

- The staggered pseudo-fermion action with n_f degenerate fermion flavors is

$$S_{PF} = \left\langle \Phi \middle| \left[M^\dagger [U^{eff}] M[U^{eff}] \right]^{-n_f/4} \middle| \Phi \right\rangle, \tag{10}$$

$$M_{x,y}\left[U^{eff}\right] = 2m\delta_{x,y} + D_{x,y}\left[U^{eff}\right] = 2m\delta_{x,y} + \sum_\mu \eta_{x,\mu}\left(U^{eff}_{x,\mu}\delta_{x,y-\mu} - U^{eff\dagger}_{x-\mu,\mu}\delta_{x,y+\mu}\right). \tag{11}$$

Non-compact QED

- The non-compact U(1) lattice gauge action is defined as

$$S^{NC}_{G_{QED}}(A'_\mu(n)) = \frac{1}{4e^2}\sum_{n,\mu,\nu} F^2_{\mu\nu}(n), \quad (12)$$

$$= \frac{1}{2e^2}\sum_{n,\mu<\nu} F^2_{\mu\nu}(n) = \frac{\beta_{u1}}{2}\sum_{n,\mu<\nu} F^2_{\mu\nu}(n), \quad (13)$$

with

$$F_{\mu\nu}(n) = [A'_\mu(n) + A'_\nu(n+\hat{\mu}) - A'_\mu(n+\hat{\nu}) - A'_\nu(n)]. \quad (14)$$

- The U(1) momentum is defined via

$$\frac{dU'^q_\mu(n)}{d\tau} = i\dot{A}'_\mu(n) q^f\, U'^q_\mu(n) \equiv iH'^q_\mu(n)\, U'^q_\mu(n), \quad (15)$$

with

$$U'^q_\mu(n) = e^{iqA'_\mu(n)}, \quad (16)$$

$$H'^q{}_\mu(n) = h'_\mu(n)\, q^f. \quad (17)$$

Since $\dot{A}'_\mu(n) = h'_\mu(n)$, $h'_\mu(n)$ is a conjugate field to $A'_\mu(n)$, we can consider $A'_\mu(n)$ as coordinate and $h'_\mu(n)$ as momentum conjugate to the corresponding coordinate.

- The kinetic part of the Hamiltonian can then be written as

$$\sum_{n,\mu}\frac{1}{2}h'^2_\mu(n) = \frac{1}{2q^{f2}}\sum_{n,\mu}[H'^q{}_\mu(n)^2]. \quad (18)$$

Non-compact QED: gauge force

- U(1) gauge field update:
  Since $\dot{A'}_\mu(n) = h'_\mu(n)$, the A' should be updated according to
$$A' \to A' + h' d\tau. \tag{19}$$

- U(1) momentum update:
  The U(1) gauge force contributing to the U(1) momentum change is
$$\frac{dh'}{d\tau} = -\frac{dS^{NC}_{G_{QED}}}{dA'}, \tag{20}$$
  with
$$dS^{NC}_{G_{QED}}/dA'_\mu(n) = \frac{1}{e^2}\sum_\nu \left[[A'_\mu(n) + A'_\nu(n+\mu) - A'_\mu(n+\nu) - A'_\nu(n)] - [A'_\mu(n-\nu) + A'_\nu(n-\nu+\mu) - A'_\mu(n) - A'_\nu(n-\nu)]\right], \tag{21}$$
$$= \beta_{u1}\sum_\nu [F_{\mu\nu}(n) - F_{\mu\nu}(n-\nu)]. \tag{22}$$

Fermion forces

- The fermion force has contributions from both SU(3) and U(1).
- Taking the MC simulation time τ derivative of the Hamiltonian and requring it to be zero, one gets the SU(3) and U(1) fermion forces.
- The SU(3) contribution (QCD force) is

$$\begin{aligned} i\dot{H}_\mu(n) &= \left[U_\mu(n)\frac{\partial S}{\partial U_\mu(n)} - \frac{\partial S}{\partial {U_\mu}^\dagger(n)}U_\mu^\dagger(n)\right] \\ &\quad -\frac{1}{N_c}\mathrm{Tr}\left[U_\mu(n)\frac{\partial S}{\partial U_\mu(n)} - \frac{\partial S}{\partial {U_\mu}^\dagger(n)}U_\mu^\dagger(n)\right], \qquad (23) \\ &= 2\left[U_\mu(n)\frac{\partial S}{\partial U_\mu(n)}\right]_{AT}, \qquad (24) \end{aligned}$$

where the operation *AT* stands for taking the anti-Hermitian and traceless part of the matrix

$$M_{AT} = \frac{1}{2}(M - M^\dagger) - \frac{1}{2N_c}\mathrm{Tr}(M - M^\dagger). \qquad (25)$$

Fermion forces

- The fermion force has contributions from both SU(3) and U(1).

- Taking the MC simulation time τ derivative of the Hamiltonian and requring it to be zero, one gets the SU(3) and U(1) fermion forces.

- The U(1) contribution (QED force) is

$$i\dot{h'}_{\mu}(n) = \sum_{q} q^{f}\,\mathrm{Tr}\left[U_{\mu}(n)\frac{\partial S}{\partial U_{\mu}(n)} - \frac{\partial S}{\partial U^{\dagger}_{\mu}(n)}U^{\dagger}_{\mu}(n)\right], \tag{26}$$

or

$$\dot{h'}_{\mu}(n) = 2\sum_{q^f} q^{f}\,\mathrm{ImTr}\left[\mathrm{U}_{\mu}(\mathrm{n})\frac{\partial \mathrm{S}}{\partial \mathrm{U}_{\mu}(\mathrm{n})}\right]. \tag{27}$$

- In Eqs. (23, 24, 26, and 27), $U_{\mu}(n)$ is the product of SU(3) $U_{\mu}(n)$ and U(1) $U'^{q}_{\mu}(n)$.

Pure gauge U(1) test

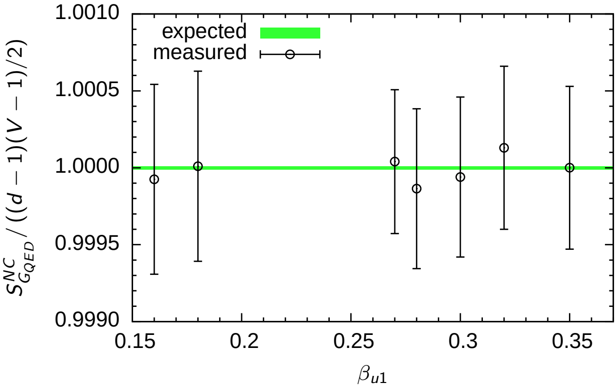
- The pure gauge U(1) Hamiltonian is

$$\mathcal{H}[A'; e] = \sum_i \frac{1}{2} {h'}_i^2 + S^{NC}_{G_{QED}}. \tag{28}$$

- The non-compact U(1) gauge action $S^{NC}_{G_{QED}}$ is only a function of the dimensionality d and lattice volume V on the finite periodic lattice

$$S^{NC}_{G_{QED}} = \frac{(d-1)(V-1)}{2}. \tag{29}$$

- One can use this to check the correctness of the pure gauge U(1) code.

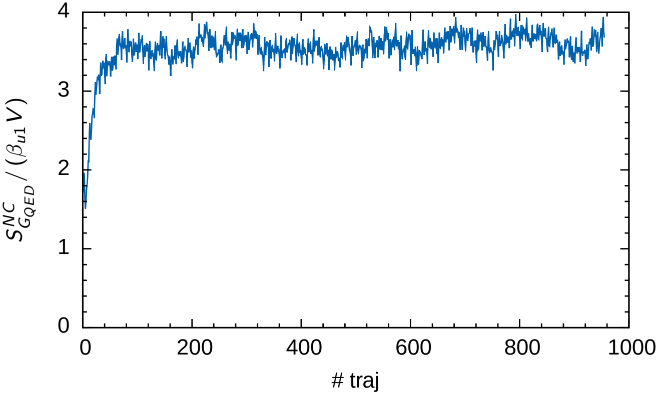


U(1) with fermions test

- The U(1) with fermion Hamiltonian is

$$\mathcal{H}[\Phi_e^q; A'; U'^q; e] = \sum_i \frac{1}{2} {h'_i}^2 + S_{PF} + S^{NC}_{G_{QED}}. \tag{30}$$

- Time history of the U(1) gauge action

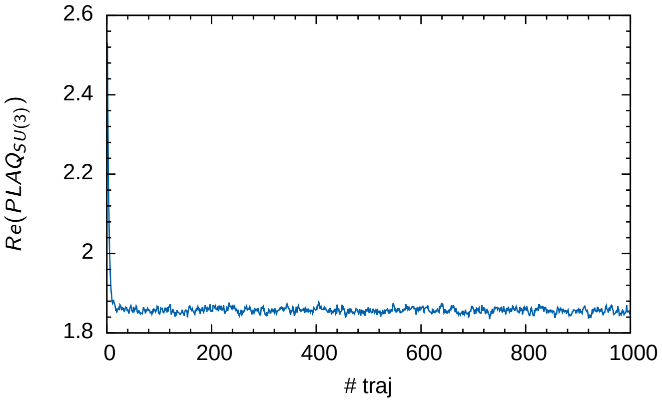


SU(3) with fermions test

- The SU(3) with fermion Hamiltonian is

$$\mathcal{H}[\Phi_e^q; A'; U'^q; e] = \sum_i \frac{1}{2} h_i^2 + S_{PF} + S_{G_{QCD}}. \tag{31}$$

- Time history of the SU(3) Plaquette

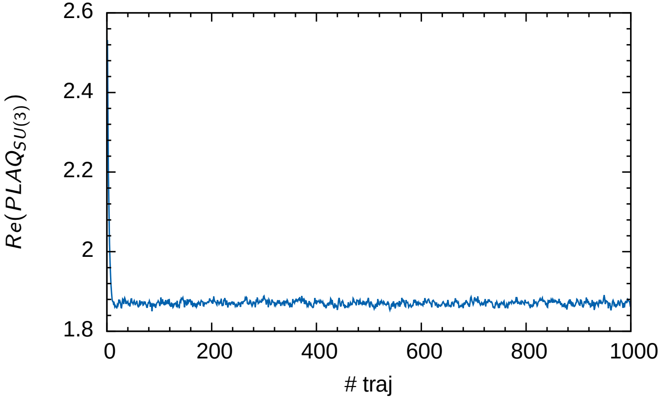


SU(3) + U(1) with fermions test

- The SU(3) + U(1) with fermion Hamiltonian is

$$\mathcal{H}[\Phi_e^q; A'; U'^q; e] = \sum_i \frac{1}{2} h_i^2 + \sum_i \frac{1}{2} {h'}_i^2 + S_{PF} + S_{G_{QCD}}. + S_{G_{QED}}^{NC}. \qquad (32)$$

- Time history of the SU(3) Plaquette



Integration algorithms

- The integration algorithm is based on decomposing the Hamiltonian in exactly integrable pieces
$$H(\phi, h) = H_1(\phi) + H_2(h), \tag{33}$$
with $H_1(\phi) = S(\phi)$ and $H_2(h) = \sum_i h_i^2/2$ for example.
The algorithm consists of repeated applying the following two elementary steps
$$I_1(\epsilon) : (h, \phi) \to (h, \phi + \epsilon \nabla_h H_2(h)), \tag{34}$$
$$I_2(\epsilon) : (h, \phi) \to (h - \epsilon \nabla_\phi S(\phi), \phi). \tag{35}$$

- The leap-frog algorithm corresponds to the following updates
$$I_\epsilon(\tau) = [I_1(\epsilon/2) I_2(\epsilon) I_1(\epsilon/2)]^{N_s}, \tag{36}$$
with $\tau = N_s \epsilon$ the length of the trajectory. The leading violation due to the finite step-size ϵ is $\mathcal{O}(\epsilon^2)$.

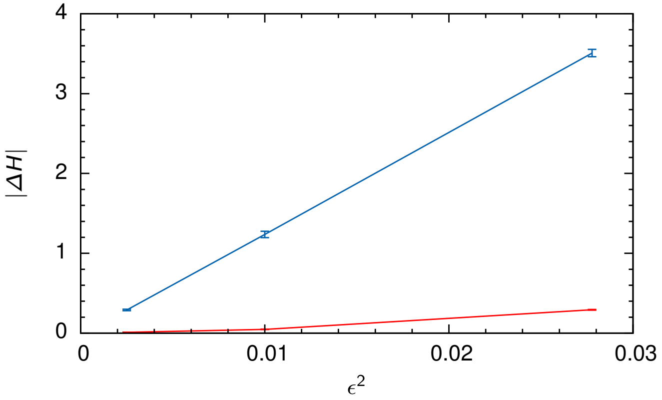
- The Omelyan integrator
$$[I_1(\xi\epsilon) I_2(\epsilon/2) I_1((1 - 2\xi)\epsilon) I_2(\epsilon/2) I_1(\xi\epsilon)]^{N_s}, \tag{37}$$
reduces the coefficient of the ϵ^2 term and improves the scaling behavior.

- In the MILC code for the HISQ fermion related calculations, an Omelyan based "3G1F" integrator is used.

- The algorithm can be made exact by a Metropolis acceptance step: Hybrid Monte Carlo algorithm.

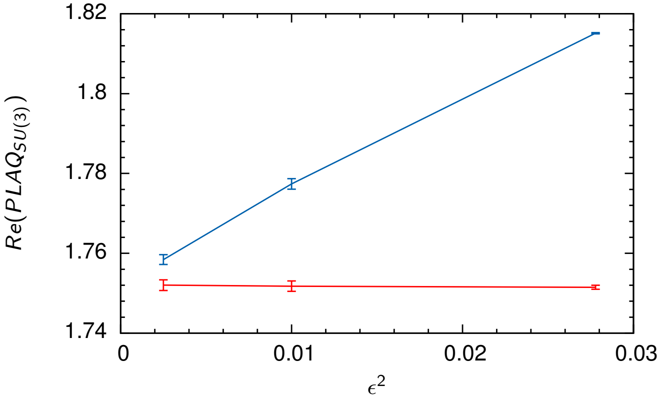
SU(3) + U(1) with fermions test

- The change of the Hamiltonian during the trajectory is expected to scale with ϵ^2 for the integrators used.
- Scaling of the the change of action $|\Delta H|$ with the step sizes ϵ. The upper blue points are from the leap-frog integrator and the lower red points are from the "3G1F" integrator.



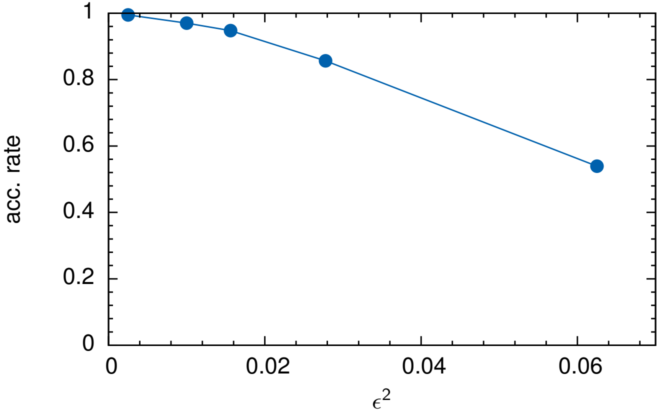
SU(3) + U(1) with fermions test

- The change of the Hamiltonian during the trajectory is expected to scale with ϵ^2 for the integrators used.
- Scaling of the SU(3) Plaquette with the step sizes ϵ. The upper blue points are from the leap-frog integrator and the lower red points are from the "3G1F" integrator.



SU(3) + U(1) with fermions test

- In principle, the Hybrid Monte Carlo algorithm can be run at any step size. The acceptance rate depends on the step sizes.
- Dependence of the acceptance rate as a function of the step-size ϵ



Summary

- Lattice QCD + QED code for staggered fermion HISQ action now exists.
- The code has been tested and compared with theoretical expectations.
- It is currently based on the MILC code and runs efficiently on conventional CPUs.
- Parts of the code can be run on GPUs and Intel Xeon Phi processors.
- Exascale MILC code projects are ongoing.

Thank You!

BACKUP

Appendix: Non-compact U(1) analytic results

- The partition function of the non-compact U(1) gauge action is

$$Z = \int [dA'_\mu(n)] e^{-S^{NC}_{G_{QED}}}. \tag{38}$$

- The density of state is

$$N(E) = \int [dA'_\mu(n)] \delta \left(\frac{1}{2} \sum_{n,\mu<\nu} F^2_{\mu\nu}(n) - \frac{d(d-1)}{2} VE \right), \tag{39}$$

where E is the average "energy" in a d-dimensional lattice. It is defined as

$$S^{NC}_{G_{QED}} = \frac{\beta_{u1}}{2} \sum_{n,\mu<\nu} F^2_{\mu\nu}(n) = \beta_{u1} \frac{d(d-1)}{2} V \langle E \rangle . \tag{40}$$

- Sine the gauge group is non-compact, the above density of state is divergent even on a finite lattice. One can factorize the divergent part by multiplying the integrand with a Gaussian factor (i.e., introducing a photon mass term)

$$N(E, M) = \int [dA'_\mu(n)] \delta \left[\frac{1}{2} \sum_{n,\mu<\nu} F^2_{\mu\nu}(n) - \frac{d(d-1)}{2} VE \right] e^{-M^2 \sum_{n,\mu} A'^2_{\mu(n)}}. \tag{41}$$

Appendix: Non-compact U(1) analytic results

- The gauge action is quadratic and can be diagonalized via a unitary transformation. The number of zero modes of the quadratic form is

$$z_0 = V + d - 1. \tag{42}$$

- The density of state can then be written as

$$N(E, M) = \int \prod_{n=1}^{dV - z_0} dB_n \delta\left[\frac{1}{2}\sum_n \lambda_n B_n^2 - \frac{d(d-1)}{2} VE\right] \tag{43a}$$

$$\times \prod_n e^{-M^2 B_n^2} \left(\int dB e^{-M^2 B}\right)^{z_0}. \tag{43b}$$

The integrations in Eq. (43b) are Gaussian: $\int_{\infty}^{-\infty} e^{-ax^2} = \sqrt{\pi/a}$ and contain all the divergence as $M \to 0$. The factor in Eq. (43a) is finite.

Appendix: Non-compact U(1) analytic results

- Using the hyper-spherical coordinates in $(dV - z_0)$-dimensional space, one can integrate over Eq. (43a) and get the density of state. Specifically, changing the variables B_n to $r\cos\theta_1, \cdots$

$$
\begin{aligned}
& \int \prod_{n=1}^{dV - z_0} dB_n \delta\left[\frac{1}{2}\sum_n \lambda_n B_n^2 - \frac{d(d-1)}{2} VE\right], && (44a)\\
= \quad & C_1 \int dr^{n-1} \delta\left[r^2 - R\right], && (44b)\\
= \quad & C_1 [\frac{1}{2} R^{\frac{n}{2}-1}(1 - e^{in\pi})], && (44c)
\end{aligned}
$$

with

$$
\begin{aligned}
n &= dV - z_0, && (45)\\
R &= \frac{d(d-1)}{2} VE. && (46)
\end{aligned}
$$

Note that when $n \equiv dV - z_0$ is even, the above integral is 0.

- The density of state is then

$$N(E) = CE^{\frac{dV - z_0}{2} - 1}. \quad (47)$$

Appendix: Non-compact U(1) analytic results

- Now we have the analytic functional form of the density of state Eq. (47). The partition function is now a one-dimensional integral

$$Z = \int_0^\infty dE N(E) e^{-\beta_{u1} \frac{d(d-1)}{2} VE} \tag{48}$$

$$= C \int_0^\infty dE E^{\frac{dV - z_0}{2} - 1} e^{-\beta_{u1} \frac{d(d-1)}{2} VE} \tag{49}$$

$$\equiv C \int_0^\infty dE E^a e^{-bE} \tag{50}$$

$$= C b^{-1-a} \Gamma(1+a). \tag{51}$$

with

$$a = \frac{dV - z_0}{2} - 1, \tag{52}$$

$$b = \beta_{u1} V \frac{d(d-1)}{2}. \tag{53}$$

Again the divergence of Z is contained in the constant C.

Appendix: Non-compact U(1) analytic results

- The average Plaquette energy E is then

$$
\begin{aligned}
< E > &= \frac{\int_0^\infty dEN(E)Ee^{-\beta_{u1}\frac{d(d-1)}{2}VE}}{\int_0^\infty dEN(E)e^{-\beta_{u1}\frac{d(d-1)}{2}VE}} && (54)\\
&\equiv \frac{C\int_0^\infty dEE^{a+1}e^{-bE}}{C\int_0^\infty dEE^{a}e^{-bE}} && (55)\\
&= \frac{1}{b}\frac{\Gamma(2+a)}{\Gamma(1+a)} && (56)\\
&= \frac{a+1}{b} && (57)\\
&= \frac{1}{\beta_{u1}}\frac{dV-z_0}{d(d-1)V} && (58)\\
&= \frac{1}{\beta_{u1}}\frac{(d-1)V-d+1}{d(d-1)V} && (59)\\
&= \frac{1}{\beta_{u1}}\frac{V-1}{dV}. && (60)
\end{aligned}
$$

From Eq. (60), we can see that $\beta_{u1}\langle E\rangle$ only depends on the dimensionality d and the volume V.