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Comment on the subtlety of defining a real-time path integral in lattice gauge theories

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Recently, Hoshina, Fujii, and Kikukawa pointed out that the naive lattice gauge theory action in the Minkowski signature does not result in a unitary theory in the continuum limit, and Kanwar and Wagman proposed alternative lattice actions to the Wilson action without divergences. We show here that the subtlety can be understood from the asymptotic expansion of the modified Bessel function, which has been discussed for the path integral of compact variables in nonrelativistic quantum mechanics. The essential ingredient for defining the appropriate continuum theory is the $i\varepsilon$ prescription, and with the proper implementation of this we show that the Wilson action can be used for real-time path integrals. It is important that $i\varepsilon$ should be implemented for both timelike and spacelike plaquettes. We also suggest why $i\varepsilon$ is required for the Wilson action from the Hamiltonian formalism: it is needed to manifestly suppress the contributions from singular paths, for which the Wilson action can give different values from those of the actual continuum action.

Subject Index B01, B38, B64

1. Introduction

The real-time path integral [1] has recently been revisited both analytically [2–4] and numerically [5–12] for the study of real-time dynamics in quantum theories. On the numerical side in particular, many developments have been made to tame the infamous sign problem (e.g., complex Langevin [5,6,13–16], contour deformation techniques including Lefschetz thimble methods [2,3,7–9,11,17–30], and the tensor renormalization group [10,31–40]), which can enable us to investigate real-time quantum systems via numerical calculation. It is thus becoming not only of theoretical interest but also of practical importance to establish an appropriate way to calculate real-time path integrals. Recently, Hoshina, Fujii, and Kikukawa [41] pointed out that the naive lattice gauge theory action in the Minkowski signature does not result in a unitary theory in the continuum limit, and Kanwar and Wagman [30] proposed alternative lattice actions to the Wilson action removing divergences to give a well-defined continuum limit.[1] In this paper we point out that the subtlety can be understood from the asymptotic expansion of the modified Bessel function, which has been discussed in nonrelativistic quantum mechanics

[1]See also Ref. [42] for a discussion on the unitarity of the time evolution operator and the role of imaginary time in theories with compact variables.

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of compact variables [43,44]. To get rid of the unwanted part of the asymptotic expansion, we need to incorporate the $i\varepsilon$ prescription, i.e., an infinitesimal Wick rotation [45]. The first point of this paper is that we can use the Wilson action for numerical studies, but with $i\varepsilon$ implemented. It is also possible to expand the Boltzmann weight with the characters to define the real-time action, in which case we express the characters not with the modified Bessel functions themselves but with their asymptotic expansion in $\varepsilon \to +0$. In the latter case, $i\varepsilon$ is already built into the action, and thus, safely setting $\varepsilon = 0$, the theory has an appropriate continuum limit.

In the above two actions, the key ingredient is the $i\varepsilon$ prescription, which we know is essential in the continuum theory to obtain the causal structure of the Green functions. However, it may seem uncertain why such an $i\varepsilon$ is required without knowing the actual continuum quantum theory. As the second point of this paper, starting from the Hamiltonian formalism, we suggest why $i\varepsilon$ becomes required for the Wilson action. Note that the Wilson action is only guaranteed to reproduce the action values of the continuum action for smooth field configurations. Here, $i\varepsilon$ is needed to manifestly suppress the contributions from these singular paths in the path integral.[2]

As an illustrative example, we begin with a simple one-dimensional quantum mechanical system in a periodic box [30]. We define the lattice action by discretizing time direction resulting in a $U(1)$ theory, and review the subtlety in defining the continuum limit of the real-time path integral for this model [30,43,44]. We explain in particular how the correct continuum limit emerges with $i\varepsilon$ by analyzing the asymptotic expansion of the modified Bessel function [43]. We then consider the meaning of $i\varepsilon$ by deriving the path integral from the Hamiltonian formalism. This model gives the essential structure for the necessity for $i\varepsilon$.

With the detailed picture in quantum mechanics, the lattice gauge field theory can be seen in a straightforward manner. We first describe the subtlety of real-time path integrals in gauge theories [30] with the modified Bessel function. The expansion of the Boltzmann weight with characters shows that we need to incorporate $i\varepsilon$ for both timelike and spacelike plaquettes. Next, we show that the Wilson action can be used with $i\varepsilon$ by using the two-dimensional $SU(2)$ and $SU(3)$ theories. Lastly, we suggest the meaning of $i\varepsilon$ from the Hamiltonian formalism, in particular considering the $SU(2)$ Wilson theory [46].

The remainder of this paper is organized as follows. In Sect. 2 we first review the subtlety of the real-time path integral in the quantum mechanics on S^1. We then suggest the meaning of $i\varepsilon$ by deriving the path integral expression from the Hamiltonian formalism. In Sect. 3, we move to the lattice gauge theory case. After describing the subtlety of the real-time path integral similarly to Sect. 2, we demonstrate that the Wilson action can be used with $i\varepsilon$. Lastly, we clarify the meaning of $i\varepsilon$ in gauge theory from the Hamiltonian formalism. Section 4 is devoted to the conclusion and outlook.

2. Quantum mechanics example

In this section we describe the subtlety in defining the real-time path integral of the quantum mechanics on S^1. The subtlety in this case is similar to lattice gauge theories [30].

[2]The author is sincerely grateful to Yoshio Kikukawa and the referee of *Progress in Theoretical and Experimental Physics* for pointing out the misstatements in the first version of the manuscript that resulted from not recognizing the well-defined distributional meaning of the Feynman kernel. Major parts of Sect. 2.2 have been revised accordingly from the first version.

2.1 *Subtlety of real-time path integral in quantum mechanics on S^1*

We consider a one-dimensional quantum system with the action:

$$S[\phi] \equiv \frac{\beta}{2}\int_0^T dt\,(\partial_t\phi)^2, \tag{1}$$

where $\phi(t)$ is the angular variable on S^1. This model is equivalent to the ordinary one-dimensional quantum mechanics in a periodic box (see, e.g., Refs. [47–53]) by the identification

$$x(t) \equiv \frac{L}{2\pi}\phi(t), \tag{2}$$

where L is the spatial extent of the system and β gives the particle mass, $(2\pi)^2\beta/L^2$. We concentrate here on the free case for simplicity. The corresponding Hamiltonian of the system is

$$H \equiv \frac{1}{2\beta}p_\phi^2, \tag{3}$$

where p_ϕ is the conjugate momentum of ϕ. In quantum mechanics, the plane waves $\{\exp(in\phi)\}_{n\in\mathbb{Z}}$ are the eigenfunctions of the momentum operator, which in this case diagonalize the Hamiltonian with the energy levels:

$$E_n \equiv \frac{1}{2\beta}n^2. \tag{4}$$

To define the path integral, we discretize the time $T = Na$ and introduce the $U(1)$ variables $U_\ell \equiv e^{i\phi_\ell}$, where $\phi_\ell = \phi(a\ell)$ ($\ell = 0, \ldots, N$). The transition amplitude from level n_i to n_f,

$$A_{n_f,n_i}(T) \equiv \langle n_f|e^{-i\hat{H}T}|n_i\rangle, \tag{5}$$

may be expressed on the lattice naively as

$$A^{(\mathrm{lat})}_{n_f,n_i}(T) \equiv \mathcal{N}\int (dU)\, e^{iS(U)}(U_N^*)^{n_f}U_0^{n_i}, \tag{6}$$

where

$$(dU) \equiv \prod_{\ell=0}^{N} dU_\ell \equiv \prod_{\ell=0}^{N}\frac{d\phi_\ell}{2\pi}, \tag{7}$$

$$S(U) \equiv \frac{\beta}{2a}\sum_{\ell=0}^{N-1}|U_{\ell+1} - U_\ell|^2 = -\frac{\beta}{a}\sum_{\ell=0}^{N-1}\mathrm{Re}(U_{\ell+1}U_\ell^*) + \mathrm{const.} \tag{8}$$

The normalization factor $\mathcal{N}$ can be determined by demanding $A^{(\mathrm{lat})}_{n_f,n_i}(0) = \delta_{n_f,n_i}$.

To obtain an analytic expression for $A^{(\mathrm{lat})}_{n_f,n_i}(T)$, we expand the exponential in terms of characters:

$$e^{-i(\beta/a)\mathrm{Re}\,U} = \sum_{n\in\mathbb{Z}} I_n\left(\frac{-i\beta}{a}\right)U^n, \tag{9}$$

where $I_n(\beta)$ is the modified Bessel function of the first kind. The integration in Eq. (6) can be performed analytically to give

$$A^{(\mathrm{lat})}_{n_f,n_i}(T) = \mathcal{N}\delta_{n_f,n_i}I^N_{n_f}\left(\frac{-i\beta}{a}\right). \tag{10}$$

$A^{(\mathrm{lat})}_{n_f,n_i}(T)$ is an analytic function of the coupling β for finite a; however, it is not in the limit $a \to 0$. This can be seen in the asymptotic expansion of $I_n(z)$ for $|z| \to \infty$ [43]:

$$I_n(z) \sim \frac{e^z}{\sqrt{2\pi z}} \sum_{k\geq 0} \frac{\Gamma(n+k+1/2)}{k!\,\Gamma(n-k+1/2)} \left(\frac{-1}{2z}\right)^k \\ \pm ie^{\pm in\pi} \frac{e^{-z}}{\sqrt{2\pi z}} \sum_{k\geq 0} \frac{\Gamma(n+k+1/2)}{k!\,\Gamma(n-k+1/2)} \left(\frac{1}{2z}\right)^k . \tag{11}$$

The plus signature applies for $-\pi/2 < \arg z < 3\pi/2$, and the negative signature for $-3\pi/2 < \arg z < \pi/2$. For $|\arg z| < \pi/2$, including the imaginary-time case ($\arg z = 0$), the second term will be completely irrelevant because of the exponential factor. However, at $\arg z = -\pi/2$, which is the case for Eq. (10), the second term also contributes equally to the first term. Therefore, the result will be different depending on how we approach the real-time continuum limit. To get the correct continuum limit, one can modify the kinetic term [43,44] by introducing a slight imaginary part,

$$\beta \to e^{i\varepsilon}\beta \qquad (\varepsilon > 0). \tag{12}$$

We first take the $a \to 0$ limit, keeping ε finite, and then take the $\varepsilon \to +0$ limit. In fact, for $|\arg z| < \pi/2$,

$$I_n(z)/I_0(z) \sim 1 - \frac{n^2}{2}\frac{1}{z} + \cdots , \tag{13}$$

which in our case gives

$$\left[I_n\left(\frac{-ie^{i\varepsilon}\beta}{a}\right)/I_0\left(\frac{-ie^{i\varepsilon}\beta}{a}\right)\right]^N \sim \left[1 - ie^{-i\varepsilon}\frac{n^2}{2}\frac{a}{\beta} + \cdots\right]^N \xrightarrow{a\to 0} \exp\left[-ie^{-i\varepsilon}\frac{n^2 t}{2\beta}\right]. \tag{14}$$

Therefore,

$$A^{(\mathrm{lat})}_{n_f,n_i}(T) \xrightarrow{a\to 0} \delta_{n_f,n_i} \exp\left[-ie^{-i\varepsilon}E_{n_f}T\right] \xrightarrow{\varepsilon\to +0} \delta_{n_f,n_i} \exp\left[-iE_{n_f}T\right], \tag{15}$$

which is the desired real-time amplitude.

Note that we will not obtain the correct continuum amplitude if we take $a \to 0$ exactly on $\varepsilon = 0$ [30]. In this case, the amplitude $A^{(\mathrm{lat})}_{n_f,n_i}(T)$ becomes a singular function with a highly oscillatory behavior because of the second term in Eq. (11).

2.2 *iε in the derivation of the path integral*

Although the argument in Sect. 2.1 is mathematically correct, it is uncertain why such an $i\varepsilon$ becomes required to obtain the correct continuum theory for the discretized action in Eq. (8). In this subsection we argue that, starting from the Hamiltonian formalism, we can understand the role of $i\varepsilon$ as manifestly suppressing the contributions from singular paths, for which the discretized action can give different values from those of the actual continuum action.[3]

We consider the Feynman kernel for an infinitesimal time increment a ,

$$\langle U'|e^{-ia\hat{H}}|U\rangle, \tag{16}$$

where $|U\rangle$ is the eigenstate of the unitary operator $\hat{U}$, $\hat{U}|U\rangle = U|U\rangle$, that satisfies the commutation relation

$$[\hat{U}, \hat{p}_\phi] = \hat{U}. \tag{17}$$

[3]The relation between the path integral and the Hamiltonian formalism for a compact variable was considered in Ref. [43], but was not used to explain the meaning of the $i\varepsilon$.

By inserting the momentum eigenstates $|n\rangle$,

$$\langle U|n\rangle \equiv U^n \qquad (n \in \mathbb{Z}), \tag{18}$$

we have

$$\begin{aligned}\langle U'|e^{-ia\hat{H}}|U\rangle &= \sum_{n\in\mathbb{Z}} \exp\left[\frac{-ia}{2\beta}n^2 + in(\phi' - \phi)\right] \\ &= e^{i\pi/4}\sqrt{\frac{2\pi\beta}{-a}} \sum_{w\in\mathbb{Z}} \exp\left[i\frac{\beta(\phi' - \phi + 2\pi w)^2}{2a}\right],\end{aligned} \tag{19}$$

where we write $U = \exp(i\phi)$, $U' = \exp(i\phi')$ with $\phi, \phi' \in [-\pi, \pi)$, and we have used the Poisson summation formula to obtain the second line. Although the kernel in Eq. (19) is not well defined as an ordinary function because the theta function

$$\vartheta(v, \tau) \equiv \sum_{n\in\mathbb{Z}} e^{\pi i n^2 \tau} e^{2\pi i n v} \tag{20}$$

is only analytic for $\mathrm{Im}\,\tau > 0$, the kernel has a definite meaning as a distribution. To see this, it should be sufficient to check the Fourier integral in which the kernel is multiplied by the plane waves because all the state vectors can be expressed as a linear combination of these basis vectors. For the kernel in Eq. (19), we trivially obtain

$$\int dU'\,(U'^*)^n \langle U'|e^{-ia\hat{H}}|U\rangle = (U^*)^n e^{-\frac{ia}{2\beta}n^2}, \tag{21}$$

which is a well-defined number for given n and U, and thus establishes the definite meaning of the kernel as a distribution.

We can now understand the need for $i\varepsilon$ discussed in Sect. 2.1 with distributional terms. In fact, the naive real-time path integral in Sect. 2.1 amounts to replacing the kernel in Eq. (19) by the expression

$$\langle U'|e^{-ia\hat{H}}|U\rangle \to e^{i\pi/4}\sqrt{\frac{2\pi\beta}{-a}} \exp\left[\frac{i\beta}{a}\left[1 - \mathrm{Re}\,(UU'^*)\right]\right]. \tag{22}$$

This replacement cannot be justified as a distributional relation because, as in Sect. 2.1, the Fourier integral gives

$$\begin{aligned}&\int dU'\,(U'^*)^n e^{i\pi/4}\sqrt{\frac{2\pi\beta}{-a}} \exp\left[\frac{i\beta}{a}\left[1 - \mathrm{Re}\,(UU'^*)\right]\right] \\ &= e^{i\pi/4}\sqrt{\frac{2\pi\beta}{-a}} e^{-in\phi} e^{i\beta/a} I_n\left(\frac{-i\beta}{a}\right) \\ &\sim e^{-in\phi}\left[e^{\frac{-ia}{2\beta}(n^2 - \frac{1}{4})} - i(-1)^n e^{\frac{2i\beta}{a}} e^{\frac{ia}{2\beta}(n^2 - \frac{1}{4})}\right],\end{aligned} \tag{23}$$

where the second term is dependent on n and ϕ. However, the first term has the correct n and ϕ dependence, and the second term can be removed by the $i\varepsilon$. We thus have the distributional identity after correcting the shift of the zero-point energy:[4]

$$\langle U'|e^{-ia\hat{H}}|U\rangle = \lim_{\varepsilon\to+0} e^{\frac{-ia}{8e^{i\varepsilon}\beta}} e^{i\pi/4}\sqrt{\frac{2\pi e^{i\varepsilon}\beta}{-a}} \exp\left[\frac{ie^{i\varepsilon}\beta}{a}\left[1 - \mathrm{Re}\,(UU'^*)\right]\right]. \tag{24}$$

This justifies the use of the discretized action in Eq. (8) under the $i\varepsilon$. The rest of this section is devoted to systematically deriving this distributional equality.

[4]The zero-point energy was absorbed in the normalization factor $\mathcal{N}$ in Sect. 2.1.

We begin with introducing the $i\varepsilon$ and regarding the original kernel in Eq. (19) as the $\varepsilon \to +0$ limit:

$$\langle U'|e^{-ia\hat{H}}|U\rangle = \lim_{\varepsilon\to+0} \langle U'|e^{-ia\hat{H}}|U\rangle\big|_{\beta\to e^{i\varepsilon}\beta}. \tag{25}$$

The expression inside the limit now becomes a well-defined function, and has a sharp peak around $U = U'$ for an infinitesimal a. This allows us to rewrite the expression as

$$\langle U'|e^{-ia\hat{H}}|U\rangle|_{\beta\to e^{i\varepsilon}\beta} \approx e^{i\pi/4}\sqrt{\frac{2\pi\, e^{i\varepsilon}\beta}{-a}} \exp\left(\frac{ie^{i\varepsilon}\beta}{2a}\lfloor\phi' - \phi\rfloor^2\right), \tag{26}$$

where the function $\lfloor\cdot\rfloor$ returns the value in $[-\pi, \pi)$ modulo 2π. The relation in Eq. (26) becomes a distributional equality for an infinitesimal a because the contributions with nontrivial winding are exponentially suppressed thanks to $\varepsilon > 0$.

On the other hand, the kernel

$$\exp\left[\frac{ie^{i\varepsilon}\beta}{a}\left[1 - \mathrm{Re}\,(UU'^*)\right]\right] = \exp\left[\frac{ie^{i\varepsilon}\beta}{a}\left[1 - \cos(\phi - \phi')\right]\right] \tag{27}$$

has a similar functional dependence to Eq. (26); the function in Eq. (27) has a sharp peak around $U = U'$ for an infinitesimal a, which allows us to expand the cosine in powers of $\lfloor\phi - \phi'\rfloor$ and convert the Fourier integral to a Gaussian integral:

$$\begin{aligned}
&\int_{-\pi}^{\pi}\frac{d\phi'}{2\pi}\, e^{-in\phi'}\exp\left[\frac{ie^{i\varepsilon}\beta}{a}\left[1 - \cos(\phi - \phi')\right]\right]\\
&= \int_{-\pi}^{\pi}\frac{d\phi'}{2\pi}\, e^{-in\phi'}\exp\left[\frac{ie^{i\varepsilon}\beta}{2a}\lfloor\phi - \phi'\rfloor^2 - \frac{ie^{i\varepsilon}\beta}{24a}\lfloor\phi - \phi'\rfloor^4 + \cdots\right]\\
&\approx e^{-in\phi}e^{-\frac{ia}{2\beta}n^2}\int_{-\infty}^{\infty}\frac{d\phi''}{2\pi}\exp\left[\frac{ie^{i\varepsilon}\beta}{2a}\phi''^2\right]\left(1 - \frac{ie^{i\varepsilon}\beta}{24a}\phi''^4 + \cdots\right).
\end{aligned} \tag{28}$$

We see the desired n and ϕ dependence in front of the Gaussian integral. The remaining integral only gives an overall constant that includes the shift of the zero-point energy:

$$\begin{aligned}
\int_{-\infty}^{\infty}\frac{d\phi''}{2\pi}\exp\left[\frac{ie^{i\varepsilon}\beta}{2a}\phi''^2\right]\left(1 - \frac{ie^{i\varepsilon}\beta}{24a}\phi''^4 + \cdots\right) &= \left(1 + \frac{ia}{8e^{i\varepsilon}\beta} + \cdots\right)\sqrt{\frac{-a}{2\pi\, ie^{i\varepsilon}\beta}}\\
&\sim \exp\left(\frac{ia}{8e^{i\varepsilon}\beta}\right)\sqrt{\frac{-a}{2\pi\, ie^{i\varepsilon}\beta}}.
\end{aligned} \tag{29}$$

Correcting this constant gives the distributional relation in Eq. (24).

Note the ordering of the limit. The distributional relation in Eq. (24) is for an infinitesimal a and for $\varepsilon > 0$, and thus we first take the $a \to 0$ limit keeping $\varepsilon > 0$. Correspondingly, we take $\varepsilon \to +0$ outside the path integral once we adopt the discretized action in Eq. (8):

$$A_{n_f,n_i}(T) = \mathcal{N}\lim_{\varepsilon\to+0}\lim_{a\to+0}\int (dU)\, e^{-i(e^{i\varepsilon}\beta/a)\sum_{\ell=0}^{N-1}\mathrm{Re}(U_{\ell+1}U_\ell^*)}(U_N^*)^{n_f}(U_0)^{n_0}. \tag{30}$$

This establishes the necessity of $i\varepsilon$ in the real-time path integral discussed in Sect. 2.1.

From the above derivation, we can understand the role of $i\varepsilon$ for the discretized action in Eq. (19) as follows. Firstly, as expected, large fluctuations basically do not contribute to the amplitude in the original theory, which can be seen from the facts that the kernel in Eq. (19) becomes the periodic delta function at $a = 0$ and that we are able to safely introduce $i\varepsilon$ in Eq. (25). On the other hand, the discretized action in Eq. (8) is designed in such a way that it reproduces the continuum action for smooth fields but not necessarily for these large fluctuations. As we have discussed, this difference in fact changes the distributional property of the kernel, and we thus need to suppress the contributions from singular paths in advance with $i\varepsilon$ when using the action in Eq. (8). As shown in Eq. (28), the nonlinearity of the cosine function only affects the overall constant.

3. Gauge theory case

In this section we consider the gauge theory. The structure is basically the same as in the quantum mechanical system discussed in Sect. 2.

3.1 *Necessity of iε in lattice gauge theories*

The lattice Yang–Mills action for the $SU(N_c)$ gauge group in four-dimensional Minkowski spacetime can be given by [5,54]:

$$S(U) \equiv \beta_t \sum_x \sum_i \left[1 - \frac{1}{N_c} \mathrm{Re}\,\mathrm{tr}\,[U_{x,i} U_{x+i,t} U^\dagger_{x+t,i} U^\dagger_{x,t}]\right]$$
$$- \beta_s \sum_x \sum_{i<j} \left[1 - \frac{1}{N_c} \mathrm{Re}\,\mathrm{tr}\,[U_{x,i} U_{x+i,j} U^\dagger_{x+j,i} U^\dagger_{x,j}]\right], \tag{31}$$

where

$$\beta_t \equiv \frac{a}{a_0} \frac{2N_c}{g^2}, \tag{32}$$

$$\beta_s \equiv \frac{a_0}{a} \frac{2N_c}{g^2}, \tag{33}$$

with the spatial lattice spacing a and the time increment a_0. We take the normalization of the generators as $\mathrm{tr}\, T^a T^b = (1/2)\delta^{ab}$. The local Boltzmann factor can be expanded with the characters χ_R as

$$e^{i(-1)^r (\beta_r/N_c) \mathrm{Re}\,\mathrm{tr}\, U} = \sum_{R:\mathrm{irrep}} d_R\, c_R(i(-1)^r \beta_r) \chi_R(U), \tag{34}$$

where $r = t, s$ labels the timelike and spacelike directions, $(-1)^t = -1$, $(-1)^s = +1$, and d_R is the dimension of the irreducible representation R. The functions c_R are given by [55,56]

$$c_R(i(-1)^r \beta_r) = \frac{1}{d_R} \sum_{n\in\mathbb{Z}} \det_{1\le j,k\le N_c} I_{\ell_k - k + j + n}(i(-1)^r \beta_r / N_c), \tag{35}$$

where ℓ_k ($\ell_1 \ge \ell_2 \ge \cdots \ge \ell_{N_c-1} \ge \ell_{N_c} \equiv 0$) is the number of boxes in the kth row of the Young diagram representing the irreducible representation R of $SU(N_c)$. Since $\beta_r \to \infty$ in the continuum limit of asymptotically free theories, we again confront the subtlety coming from the asymptotic expansion of the modified Bessel function. To obtain the continuum limit, we introduce slight imaginary parts:

$$\beta_t \to e^{i\varepsilon} \beta_t, \tag{36}$$

$$\beta_s \to e^{-i\varepsilon} \beta_s. \tag{37}$$

It is noteworthy that we should also give the infinitesimal imaginary part for the spacelike plaquettes.[5] The sign of the imaginary part for the timelike plaquettes can be justified by the argument in Sect. 3.3. To explain the sign for the spacelike plaquettes, one can use the symmetry argument that, since the continuum theory should be Lorentz invariant, the asymptotic formula should be the same for the timelike and spatial plaquettes. The signs agree with those given by the ordinary $i\varepsilon$ in the continuum theory.

[5] This point was not mentioned in Ref. [30].

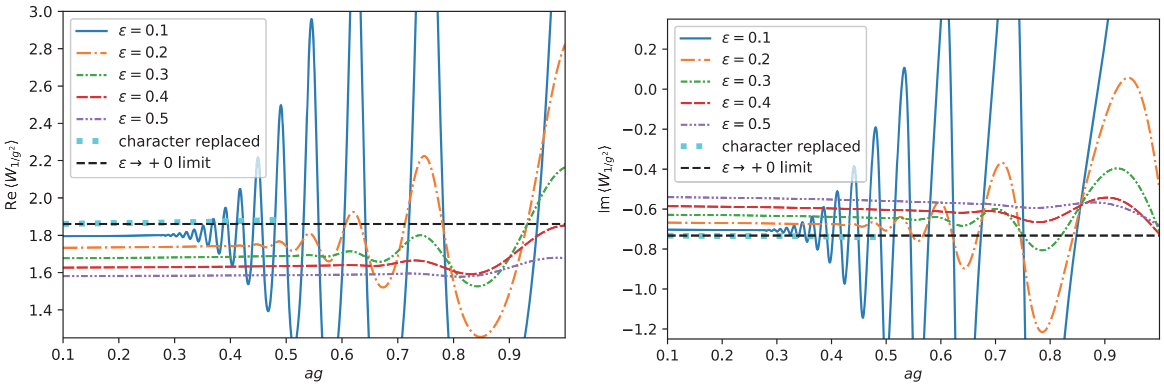

Fig. 1. The expectation value of the Wilson loop $\langle W_A \rangle$ with the area $A = 1/g^2$ evaluated with the analytic formula in Eq. (39) for $SU(2)$. The values of ε are $\varepsilon = 0.1, \ldots, 0.5$. The cyan dotted line shows the $\varepsilon = 0$ values with the modified Bessel function replaced by the asymptotic expansion, dropping the unwanted part, which is drawn in the region where the asymptotic expansion gives sufficient convergence up to the machine precision. The black dashed line shows the $a \to 0$, $\varepsilon \to +0$ value, Eq. (40).

3.2 *Convergence properties of the Wilson action*

To confirm the convergence properties related to $i\varepsilon$, we consider the $SU(N_c)$ Wilson theory in two-dimensional spacetime with $N_c = 2, 3$. We only have the timelike plaquettes in this case, and we set

$$\beta_t = \frac{2N_c}{(ag)^2}, \tag{38}$$

treating spacetime uniformly.

The expectation value of the $\ell \times \tau$ Wilson loop with the physical area $A \equiv \ell\tau a^2$, W_A, can be expressed by the characters of the trivial and fundamental representations [56,57],

$$\langle W_A \rangle = N_c \left(\frac{c_{\text{fund}}(-ie^{i\varepsilon}\beta_t)}{c_{\text{triv}}(-ie^{i\varepsilon}\beta_t)} \right)^{\ell\tau}, \tag{39}$$

for which the continuum limit is known from the analysis of the heat-kernel action [30,58]:

$$\lim_{\varepsilon \to +0} \lim_{a \to 0} \langle W_A \rangle = N_c e^{-i(N/4)(1-1/N^2)g^2 A}. \tag{40}$$

Since g is dimensionful, we fix $g = 1$ in the following.

We begin with $SU(2)$. The character expansion coefficients in Eq. (35) have the well-known form for the spin-j representation ($d_j = 2j + 1$),

$$c_j(-ie^{i\varepsilon}\beta_t) = \frac{2I_{2j+1}(-ie^{i\varepsilon}\beta_t)}{-ie^{i\varepsilon}\beta_t}, \tag{41}$$

with which we can confirm the $a \to 0$, $\varepsilon \to +0$ limit in Eq. (40) from Eq. (39):

$$\langle W_A \rangle \sim 2\left(1 - \frac{3}{2}\frac{ie^{-i\varepsilon}a^2 g^2}{4}\right)^{A/a^2} \xrightarrow{a \to 0, \varepsilon \to +0} 2e^{-i(3/8)g^2 A}. \tag{42}$$

Figure 1 shows the expectation value $\langle W_A \rangle$ with the area $A = 1$, where the results are calculated directly using the modified Bessel function for various ε. We see that, for relatively large a, the unwanted part of the asymptotic expansion in Eq. (11) contributes to give oscillatory behavior. This shows that in practice, for a given a, we need to prepare ε large enough that the unwanted part can be neglected. On the other hand, instead of implementing $i\varepsilon$, we can expand the action in terms of the characters and replace the modified Bessel function with its asymptotic expansion, dropping the unwanted part in advance. The corresponding result with $\varepsilon = 0$ is shown

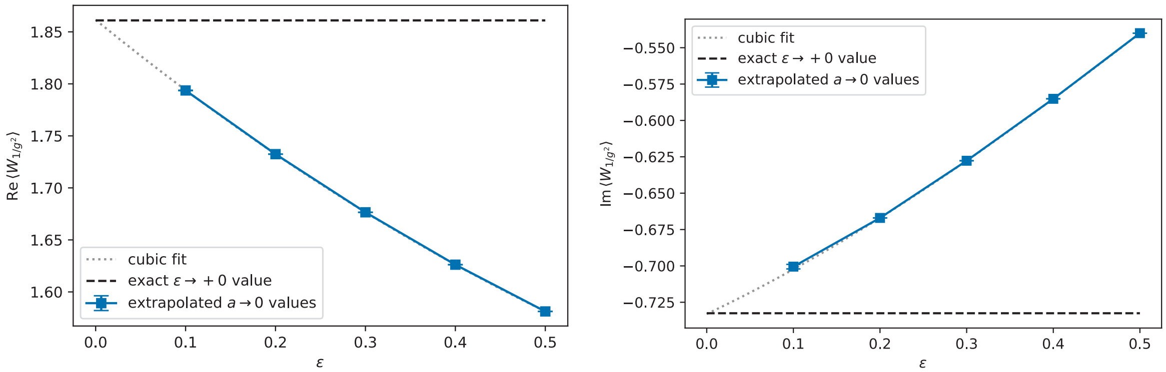

Fig. 2. The extrapolated $a \to 0$ values of $\langle W_{1/g^2} \rangle$ with various ε for $SU(2)$. The $a \to 0$ values are then fitted to obtain the final $\varepsilon \to +0$ result. The exact $\varepsilon \to +0$ value in Eq. (40) is shown with the black dashed line for comparison.

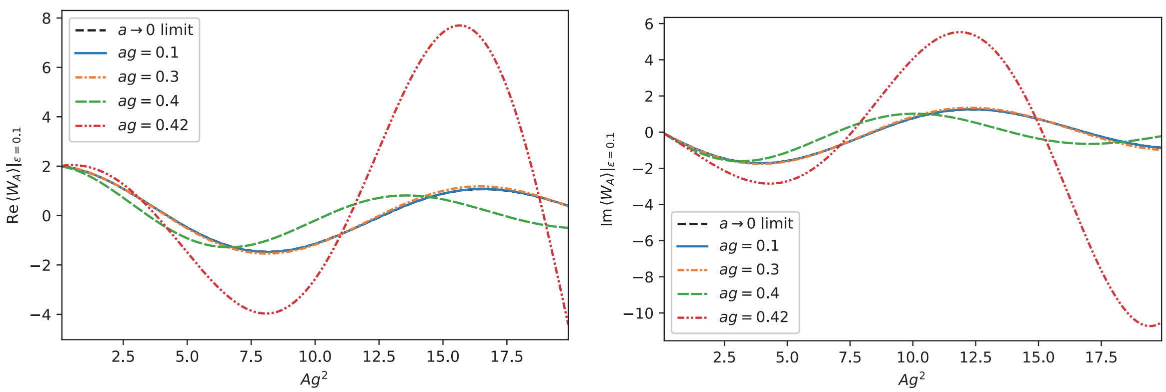

Fig. 3. The area A dependence of $\langle W_A \rangle$ evaluated with various a keeping $\varepsilon = 0.1$ fixed ($N_c = 2$).

with the cyan dotted line in Fig. 1 for the region where the asymptotic expansion gives sufficient convergence up to the machine precision. The continuum value in Eq. (40) is shown with the black dashed line for comparison. For completeness, we perform the $\varepsilon \to +0$ extrapolation of the $a \to 0$ limits. To obtain the $a \to 0$ values for each ε, we fit five points $a = 0.1, 0.15, \ldots, 0.3$ with the linear function of a^2. The systematic error is calculated from the estimated variance of the fitting parameter. The obtained values for the $A = 1$ case are shown in Fig. 2. We fit these values with quadratic and cubic functions of ε to give the final $\varepsilon \to +0$ value. We use the cubic result for the central value, and take the difference from the quadratic value as the estimate of the systematic error. The chi-squared for the cubic fits are $\chi^2/\mathrm{DOF} = 3.3$ and 1.4, respectively, for the real and imaginary parts. The obtained estimate $\lim_{a \to 0,\, \varepsilon \to +0} \langle W_{A=1} \rangle \approx 1.86146(93) - 0.7331(36)i$ agrees with the analytical value $\lim_{a \to 0,\, \varepsilon \to +0} \langle W_{A=1} \rangle = 1.8610 - 0.7325i$ within the estimated systematic error. To see how the finite a or ε effect depends on A, we also plot $\langle W_A \rangle$ with various a for $\varepsilon = 0.1$ (Fig. 3) and the $a \to 0$ values with various ε (Fig. 4). We see that the effect of finite a or ε becomes larger as we increase A.

For $SU(3)$, we show in Fig. 5 the expectation value $\langle W_A \rangle$ with the area $A = 1$, and in Fig. 6 the extrapolation of the $a \to 0$ values to the $\varepsilon \to +0$ limit. The extrapolations are performed similarly to the $SU(2)$ case, where we replace the range of a with $a = 0.1, 0.125, \ldots, 0.2$. The obtained estimate $\lim_{a \to 0,\, \varepsilon \to +0} \langle W_{A=1} \rangle \approx 2.359(22) - 1.854(19)i$ agrees with the analytical value $\lim_{a \to 0,\, \varepsilon \to +0} \langle W_{A=1} \rangle = 2.358 - 1.855i$ within the error. The chi-squared for the cubic

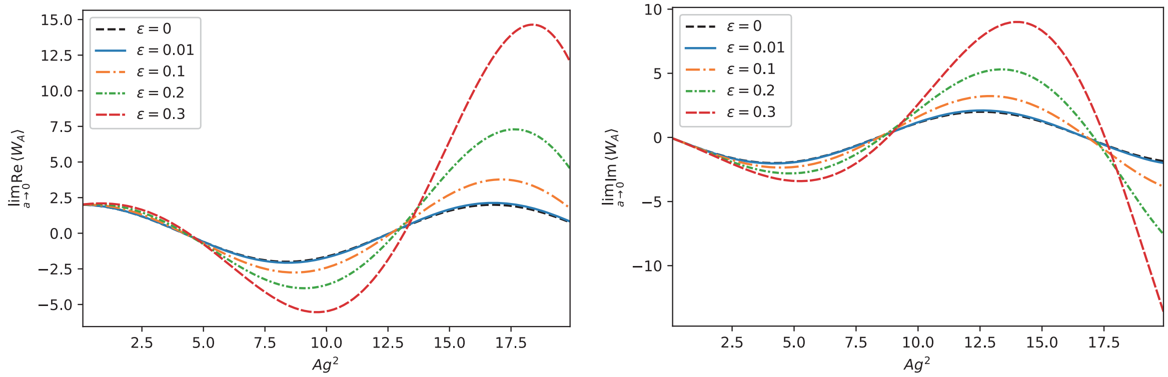

Fig. 4. The area A dependence of $\lim_{a\to 0}\langle W_A\rangle$ evaluated with various ε ($N_c = 2$).

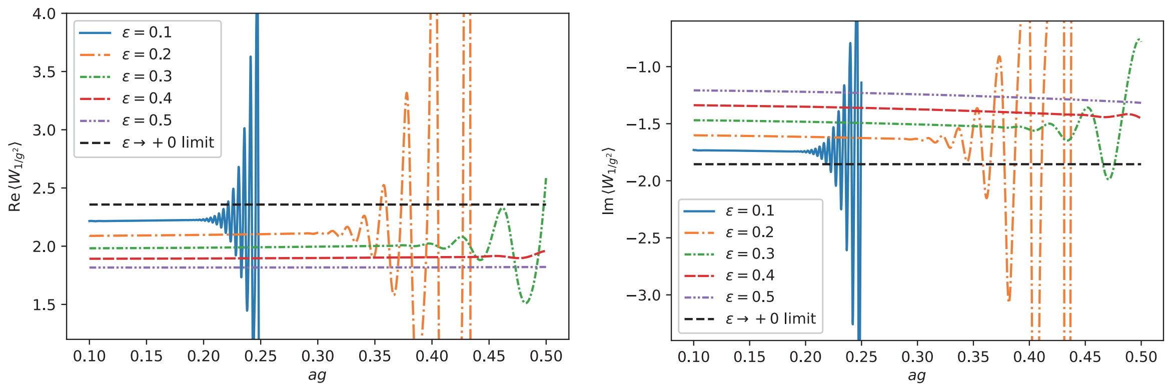

Fig. 5. The expectation value of the Wilson loop $\langle W_A\rangle$ with the area $A = 1/g^2$ evaluated with the analytic formula in Eq. (39) for $SU(3)$. The values of ε are $\varepsilon = 0.1, \ldots, 0.5$. The plots are truncated before the curves become highly oscillatory. The black dashed line shows the $a \to 0$, $\varepsilon \to +0$ value, Eq. (40).

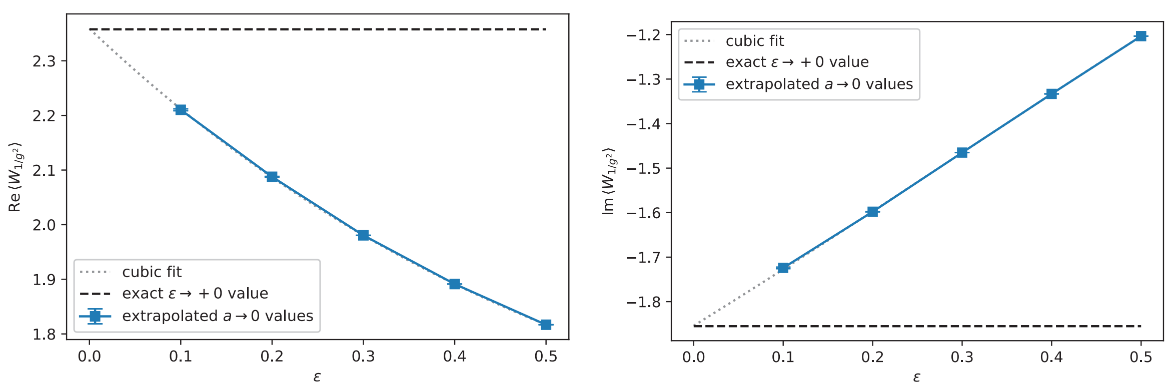

Fig. 6. The extrapolated $a \to 0$ values of $\langle W_{1/g^2}\rangle$ with various ε for $SU(3)$. The $a \to 0$ values are then fitted to obtain the final $\varepsilon \to +0$ result. The exact $\varepsilon \to +0$ value in Eq. (40) is shown with the black dashed line for comparison.

fits are $\chi^2/\mathrm{DOF} = 3.3$ and 6.7, respectively, for the real and imaginary parts. The above investigations show that the Wilson action with $i\varepsilon$ correctly reproduces the appropriate continuum limit.[6]

[6] For the range of β_t studied here, the asymptotic expansion does not converge up to machine precision in the calculation of the character coefficients in the $SU(3)$ case. The corresponding plot is therefore not shown in Fig. 5.

3.3 *iε in the derivation of the path integral*

In this subsection we suggest why we need $i\varepsilon$ for the Wilson action from the Hamiltonian formalism. For this, we use the $SU(2)$ Wilson action as an example, and follow the conventional Hamiltonian formalism of the Wilson action [46,59]. To get rid of the complication related to the gauge symmetry, we take the temporal gauge, $U_{x,t} = 1$. We keep the spatial lattice spacing a finite in this subsection. Then, at time slice t, the degrees of freedom of the system are the spatial link variables $U_{\mathbf{x},i}$. To describe fluctuations around $U_{\mathbf{x},i}$, we introduce the local coordinates $\theta^a_{\mathbf{x},i}$ by

$$e^{i\theta^a_{\mathbf{x},i}T^a}U_{\mathbf{x},i}. \tag{43}$$

In particular, we can track the infinitesimal time evolution in terms of $\theta^a_{\mathbf{x},i}$. With the conjugate momentum

$$p^a_{\mathbf{x},i} \equiv \frac{a}{g^2}\dot{\theta}^a_{\mathbf{x},i}, \tag{44}$$

we can write down the Hamiltonian [46],

$$H \equiv \frac{g^2}{2a}\sum_{\mathbf{x},i}(p^a_{\mathbf{x},i})^2 + V(U), \tag{45}$$

where we defined the potential

$$V(U) \equiv \frac{2N_c}{ag^2}\sum_{\mathbf{x},i<j}\left(1 - \frac{1}{N_c}\mathrm{Re}\,\mathrm{tr}\,[U_{\mathbf{x},i}U_{\mathbf{x}+i,j}U^\dagger_{\mathbf{x}+j,i}U^\dagger_{\mathbf{x},j}]\right). \tag{46}$$

We now derive the amplitude in path integral form for the $SU(2)$ Wilson theory. The canonical operators $\hat{U}_{\mathbf{x},i}$, $\hat{p}^a_{\mathbf{x},i}$ satisfy the commutation relation

$$[\hat{U}_{\mathbf{x},i}, \hat{p}^a_{\mathbf{x},i}] = T^a\hat{U}_{\mathbf{x},i}. \tag{47}$$

The configuration basis consists of the tensor product states

$$|U\rangle \equiv \prod_{\mathbf{x},i}|U_{\mathbf{x},i}\rangle, \tag{48}$$

where

$$\hat{U}_{\mathbf{x},i}|U_{\mathbf{x},i}\rangle = U_{\mathbf{x},i}|U_{\mathbf{x},i}\rangle. \tag{49}$$

It is convenient to introduce another basis [60],

$$|\{j_{\mathbf{x},i}, m_{\mathbf{x},i}, m'_{\mathbf{x},i}\}\rangle \equiv \prod_{\mathbf{x},i}|j_{\mathbf{x},i}, m_{\mathbf{x},i}, m'_{\mathbf{x},i}\rangle, \tag{50}$$

where

$$\langle U_{\mathbf{x},i}|j, m, m'\rangle \equiv D^j_{m,m'}(U_{\mathbf{x},i}), \tag{51}$$

with the matrix elements $D^j_{m,m'}(U)$ of the $SU(2)$ matrix U in the spin j representation. From the Peter–Weyl theorem, the basis $|\{j_{\mathbf{x},i}, m_{\mathbf{x},i}, m'_{\mathbf{x},i}\}\rangle$ satisfies the completeness relation,

$$1 = \sum_{\{j_{\mathbf{x},i},m_{\mathbf{x},i},m'_{\mathbf{x},i}\}}\left(\prod_{\mathbf{x},i}(2j_{\mathbf{x},i}+1)\right)|\{j_{\mathbf{x},i}, m_{\mathbf{x},i}, m'_{\mathbf{x},i}\}\rangle\langle\{j_{\mathbf{x},i}, m_{\mathbf{x},i}, m'_{\mathbf{x},i}\}|. \tag{52}$$

Furthermore, for finite $\eta^a_{\mathbf{x},i}$,

$$\begin{aligned}\langle U_{\mathbf{x},i}|e^{i\eta^a_{\mathbf{x},i}\hat{p}^a_{\mathbf{x},i}}|j, m, m'\rangle &= \left(Te^{i\int_0^1 ds\,\eta^a_{\mathbf{x},i}\mathcal{P}^a(s\eta_{\mathbf{x},i})}\langle U_{\mathbf{x},i}|\right)|j, m, m'\rangle \\ &= \left[Te^{i\int_0^1 ds\,\eta^a_{\mathbf{x},i}\mathcal{P}^a(s\eta_{\mathbf{x},i})}D^j(U_{\mathbf{x},i})\right]_{m,m'},\end{aligned} \tag{53}$$

where T denotes the ordered product of the matrices, and $\mathcal{P}^a(\theta)$ are the differential operators expressed in terms of the local coordinates on each link, θ^a [46,58–60]. In particular, $-(\mathcal{P}^a(\theta))^2$ is the Laplacian on S^3, and $(\mathcal{P}^a(0))^2 = (i^{-1}\partial_{\theta^a})^2$. Thus,

$$\langle U_{\mathbf{x},i}|(\hat{p}^a_{\mathbf{x},i})^2|j,m,m'\rangle = [(\mathcal{P}^a(0))^2 D^j(U_{\mathbf{x},i})]_{m,m'} = j(j+1)D^j_{m,m'}(U_{\mathbf{x},i}). \tag{54}$$

We now calculate the amplitude from state ψ_i to ψ_f:

$$A_{\psi_f,\psi_i}(T) \equiv \langle\psi_f|e^{-i\hat{H}T}|\psi_i\rangle. \tag{55}$$

We discretize $T \equiv Na_0$ and ignore higher-order terms of a_0. Note that

$$\begin{aligned}\langle U'|e^{-ia_0\hat{H}}|U\rangle &= \langle U'|e^{-i\frac{a_0g^2}{2a}\sum_{\mathbf{x},i}(\hat{p}^a_{\mathbf{x},i})^2}e^{-ia_0V(\hat{U})}|U\rangle \\ &= \prod_{\mathbf{x},i}\left[\sum_{j_{\mathbf{x},i}}(2j_{\mathbf{x},i}+1)\chi_{j_{\mathbf{x},i}}(U'_{\mathbf{x},i}U^\dagger_{\mathbf{x},i})e^{-i\frac{a_0g^2}{2a}j_{\mathbf{x},i}(j_{\mathbf{x},i}+1)}\right]e^{-ia_0V(U)}.\end{aligned} \tag{56}$$

By diagonalizing

$$U'_{\mathbf{x},i}U^\dagger_{\mathbf{x},i} \sim \mathrm{diag}(e^{i\delta\phi_{\mathbf{x},i}}, e^{-i\delta\phi_{\mathbf{x},i}}) \qquad (\delta\phi_{\mathbf{x},i} \in [-\pi,\pi)), \tag{57}$$

we can write the expression in the bracket appearing in Eq. (56) as (we drop the subscripts $\mathbf{x}$, i temporarily for notational simplicity)

$$\begin{aligned}&\sum_j(2j+1)\frac{\sin(2j+1)\delta\phi}{\sin\delta\phi}e^{-i\frac{a_0g^2}{2a}j(j+1)} \\ &\quad= -\frac{1}{2}\frac{1}{\sin\delta\phi}e^{i\frac{a_0g^2}{8a}}\frac{d}{d\delta\phi}\sum_{n\geq1}\left[e^{-i\frac{a_0g^2}{8a}n^2+in\delta\phi}+e^{-i\frac{a_0g^2}{8a}n^2-in\delta\phi}\right] \\ &\quad= -\frac{1}{2}\frac{1}{\sin\delta\phi}e^{i\frac{a_0g^2}{8a}}\frac{d}{d\delta\phi}\vartheta\left(\frac{\delta\phi}{2\pi},-\frac{a_0g^2}{8\pi a}\right),\end{aligned} \tag{58}$$

where we defined $n \equiv 2j+1$ in the second line. In order to further rewrite the expression, we introduce an infinitesimal imaginary part,

$$\vartheta\left(\frac{\delta\phi}{2\pi},-\frac{a_0g^2}{8\pi a}\right) \to \vartheta\left(\frac{\delta\phi}{2\pi},-e^{-i\varepsilon}\frac{a_0g^2}{8\pi a}\right). \tag{59}$$

The resulting function has a sharp peak around $\delta\phi = 0$, and thus

$$\begin{aligned}&-\frac{1}{2}\frac{1}{\sin\delta\phi}e^{i\frac{a_0g^2}{8a}}\frac{d}{d\delta\phi}\vartheta\left(\frac{\delta\phi}{2\pi},-e^{-i\varepsilon}\frac{a_0g^2}{8\pi a}\right) \\ &\quad\approx -\frac{1}{2}\frac{1}{\sin\delta\phi}e^{i\frac{a_0g^2}{8a}}\frac{d}{d\delta\phi}e^{i\pi/4}\sqrt{\frac{8\pi a}{-e^{-i\varepsilon}a_0g^2}}\exp\left[ie^{i\varepsilon}\frac{2a}{a_0g^2}(\delta\phi)^2\right] \\ &\quad= \mathrm{const}\cdot\frac{\delta\phi}{\sin\delta\phi}\exp\left[ie^{i\varepsilon}\frac{2a}{a_0g^2}(\delta\phi)^2\right],\end{aligned} \tag{60}$$

where in the second line we dropped the contributions with nontrivial winding that will be exponentially suppressed in the $a_0 \to 0$ limit. A finite contribution comes from the fluctuations of order $\delta\phi = O(a_0)$. With a similar argument as for Eq. (29), we can rewrite Eq. (60) up to an overall constant as

$$\mathrm{const}\cdot\frac{\delta\phi}{\sin\delta\phi}\exp\left[ie^{i\varepsilon}\frac{2a}{a_0g^2}(\delta\phi)^2\right] = \mathrm{const}'\cdot\exp\left[-ie^{i\varepsilon}\frac{2a}{a_0g^2}\mathrm{tr}\,[U'U^\dagger]\right]. \tag{61}$$

The amplitude is thus rewritten with the plaquette action in the desired path integral form with $i\varepsilon$:

$$A_{n_f,n_i}(T) \approx \mathcal{N}' \lim_{\varepsilon\to+0} \int \left(\prod_{\ell=0}^{N} dU_\ell\right) \exp\left[i \sum_{\ell=0}^{N-1} \left\{ -e^{i\varepsilon} \frac{2a}{a_0 g^2} \sum_{\mathbf{x},i} \mathrm{tr}[U_{\ell+1,\mathbf{x},i} U^\dagger_{\ell\mathbf{x},i}] \right.\right.$$
$$\left.\left. + \frac{2a_0}{ag^2} \sum_{\mathbf{x},i<j} \mathrm{tr}\left[U_{\ell,\mathbf{x},i} U_{\ell,\mathbf{x}+i,j} U^\dagger_{\ell,\mathbf{x}+j,i} U^\dagger_{\ell,\mathbf{x},j}\right] \right\} \right] \psi^*_f(U_N)\psi_i(U_0), \tag{62}$$

where $\mathcal{N}'$ is a normalization constant.

Despite the complications related to the field theory, the basic structure is the same as the quantum mechanical model in Sect. 2. The Wilson action is only guaranteed to reproduce the continuum action for smooth fields, and we need to suppress the contributions from singular paths in advance with $i\varepsilon$. The $i\varepsilon$ should thus be regarded as part of the definition of the real-time path integral when using the Wilson action.

Note also that, since we have only considered the formal $a_0 \to 0$ limit, the $i\varepsilon$ in the spatial plaquettes has not appeared in the discussion. In fact, in this treatment, the characters for the spatial plaquettes can be expressed in terms of the modified Bessel function of the form $I_n(2ia_0/(ag^2))$ [see Eq. (35)], for which we can apply the expansion of $I_n(z)$ around zero:

$$I_n(z) = \left(\frac{z}{2}\right)^n \sum_{k\geq 0} \frac{(z/2)^{2k}}{n!(n+k)!}. \tag{63}$$

The characters coming from the spatial plaquettes are thus analytic in the limit $a_0 \to 0$ for a fixed a, giving no complication. The subtlety for the spatial plaquettes arises when we take the continuum limit, taking $a_0 \to 0$ and $a \to 0$ at the same time, making g^2 run according to the renormalization group equation. In the latter treatment, which is required in extracting the continuum physics, we also need to incorporate $i\varepsilon$ for the spatial plaquettes as argued in Sect. 3.1.

4. Summary and outlook

We have discussed that $i\varepsilon$ is an essential ingredient in defining the real-time path integral for the Wilson action, and showed how its necessity can be explained from the Hamiltonian formalism. In numerical calculations, one needs to take $i\varepsilon$ into account for both timelike and spacelike plaquettes, and this can be done by calculating the continuum limit with several ε and taking the $\varepsilon \to +0$ limit, or rewriting the Boltzmann weight in terms of characters, dropping the unwanted part of the asymptotic expansion of the modified Bessel function for the character coefficients. We demonstrated in particular that, with $i\varepsilon$, the Wilson action gives the correct continuum limit using the two-dimensional theory as an example. We believe that this clarification of the subtlety will help us investigate more involved cases such as full quantum chromodynamics.

As we commented in Sect. 3.2, we need to choose ε large enough for a given lattice spacing to avoid the oscillation coming from the unwanted part of the asymptotic expansion. For the studied range of lattice spacings, this is satisfied numerically in two dimensions at $\beta_t \sin\varepsilon \gtrsim 4.5$ for $SU(2)$ and $\beta_t \sin\varepsilon \gtrsim 15$ for $SU(3)$. Since the characters are expressed with β_r in Eq. (35), these values should also give a rough estimate of the required ε in higher dimensions. The rather large bounds are, however, unpleasant for the four-dimensional application because of the existence of the critical slowing down at large β_r. A similar situation occurs for the action expressed with the characters in which the modified Bessel function is replaced by its asymptotic expansion, dropping the unwanted part. This is because the asymptotic expansion itself is divergent, and thus we need to choose the order to truncate the expansion. For large enough β_r, the summand becomes smaller than the machine precision at some order, and thus we can truncate the expansion there. However, a comparably large β_r is required for such convergence, especially in the $SU(3)$ case. Therefore, though our method gives a way to obtain the appropriate continuum prediction, it is desirable to circumvent the critical slowing down (see, e.g., Refs. [61–72]) or develop an action that is convergent at small β_r by, e.g., contour deformation [30]. Studies along these lines are in progress and will be reported elsewhere.

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