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

Nobuyuki Matsumoto

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# Background (1/3)

#### Interest for the real-time path integral

Real-time dynamics of quantum theories, especially non-perturbative features:

- e.g., creation and evolution of jets in heavy-ion collisions
  - evolution of the universe in very early stage
  - non-equilibrium properties of quark-gluon plasma



taken from PHENIX website

Nonperturbative calculation of Euclidean path integrals has been successfully performed with Monte Carlo methods; e.g., Fukaya, Onogi, et al. [JLQCD] 08

however, there exists the notorious *sign problem* in its application to real-time path integrals:

Since integrands are highly oscillatory,

we need an exponentially large sample size,  $O(e^{DOF})$ , to a have meaningful estimation

makes the conventional way of calculation practically impossible.

The real-time path integral of QCD has hardly been explored.

Recently, many ideas have been developed to overcome the sign problem real-time path integrals becoming numerically accessible.

<u>cor</u>	nplex Langevin Aarts	i 83, Klauder 83, 84, s-Seiler-Stamatescu 09, Aarts-James-Seiler-Stamatescu 09
•	real-time scalar field	Berges-Stamatescu 05, Berges-Borsanyi-Sexty-Stamatescu 07
•	real-time Yang-Mills	Berges-Borsanyi-Sexty-Stamatescu 07, Berges-Sexty-Stamatescu 08 Boguslavski-Hotzy-Müller 22
<u>cor</u>	ntour deformation	Witten 10, Cristoforetti-Di Renzo-Scorzato 12, Fujii-Honda-Kato-Kikukawa-Komatsu-Sano 13 Alexandru et al. 15, Fukuma-Umeda 17, Alexandru et al. 17, Fukuma-NM 20
•	real-time scalar field	Alexandru-Basar-Bedaque-Ridgway 17 Mou-Saffin-Tranberg-Woodward 19
•	real-time Yang-Mills	Kanwar-Wagman 21 cf. Hoshina-Fujii-Kikukawa 20
٠	real-time QM	Alexandru-Basar-Bedaque-Vartak-Warrington 16 Fujisawa-Nishimura-Sakai-Yosprakob 21

#### tensor renormalization group (TRG) Levin-Nave 06

• real-time scalar field **Takeda 19, 21** 

It is becoming of practical importance (not only of theoretical interest) to establish an appropriate way to evaluate real-time path integrals.

# Background (3/3)

#### QCD on the lattice: gauge field takes values on a compact group. Wilson 74

It has been discussed that real-time path integral requires care (especially in theories with compact variables):

• Need of *i*ε discussed in non-relativistic QM

Langguth-Inomata 79, Bohm-Junker 87

- The discretized path integral is not well-defined exactly on  $\varepsilon = 0$  for systems with compact variables.
- Need of  $i\varepsilon$  can be seen from the asymptotic expansion of the modified Bessel function  $I_n(z)$ .
- Unitarity and convergence in lattice gauge theory
  - Hoshina-Fujii-Kikukawa 20: developed Schwinger-Keldysh formalism with the transfer matrix respecting unitarity using character expansion.
  - Kanwar-Wagman 21: proposed alternative actions to the Wilson action removing divergences that existed in the character expansion action with contour deformation.

See also **Fatollahi 16** for a discussion on unitarity in theories with compact variables.

## Summary of this work (1/2)

We here would like to clarify that:

- We can use conventional lattice gauge theory actions (in particular, Wilson), but by properly implementing the *i*ε.
- It is here important that the  $i\varepsilon$  should be implemented both for timelike and spacelike plaquettes.

Use of *iε* to stabilize Complex Langevin: Berges-Borsanyi-Sexty-Stamatescu 07 See also Boguslavski-Hotzy-Müller 22

It should be noted that this subtlety is *not evident* in noncompact scalar field theories discretized with the ordinary differences into a Gaussian form.

We would further like to argue the reason why  $i\varepsilon$  becomes necessary in lattice gauge theories from the Feynman kernel derived in Hamiltonian formalism.

• Note that the plaquette action reproduces the continuum action only for continuous field configurations;

naive use of the plaquette action makes the phase factor associated with large fluctuations different from the continuum theory.

Consequently, it breaks the delicate cancelation in the real-time path integral for the large fluctuations.

• The  $i\varepsilon$  is required to manifestly suppress the contributions from these large fluctuations, as is the case in Euclidean path integral.

#### • Kanwar-Wagman 21's idea:

Deform the integration contour under  $\varepsilon > 0$  in a way that we can take  $\varepsilon \to 0$  limit on the deformed contour without divergences.

They addressed the unitarity of the real-time transfer matrix, and considered the  $i\varepsilon$  in the kinetic term in constructing the contour deformation analytically.

They showed that the deformation removes the problem of convergence together with the sign problem that works perfectly in 2D YM theory;

however, as we argue below, the asymptotic expansion analysis explains the need of  $i\varepsilon$  also for the spatial plaquettes in higher dimensions to obtain the continuum theory, in which case such analytic contour deformation is difficult to find.

The  $i\varepsilon$  for spatial plaquettes has a peculiar consequence:

It restricts the configuration space to have continuity to an extent, but prevents the transfer matrix from being unitary for finite *a*. We discuss possible consequences in quantum algorithms on the last slide.

• In this work, no Monte Carlo result is presented.

Construction of an algorithm and calculation in progress [NM+]

### Outline

• Introduction

#### <u>1D QM</u>

- Subtlety of real-time path integral in QM (review)
- $i\varepsilon$  from Hamiltonian formalism

#### <u>YM</u>

- Subtlety in lattice gauge theory
- *i*ε from Hamiltonian formalism
- Convergence properties of Wilson action
- Discussion

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## Example in quantum mechanics (review) (1/3)

#### The simplest example having the subtlety: particle in a periodic box

$$S(\phi) \equiv \frac{\beta}{2} \int_0^T dt \, (\partial_t \phi)^2, \qquad \phi$$
: angular variable on  $S^1$ 

particle 
$$x \equiv \frac{L}{2\pi}\phi$$
 with mass  $M \equiv (2\pi)^2\beta/L^2$ , L: spatial extent

<u>Hamiltonian</u>

$$H \equiv \frac{1}{2\beta} p_{\phi}^2 \qquad \left( p_{\phi}: \text{ conjugate momentum of } \phi \right)$$

#### momentum eigenstates: plane waves

$$e^{in\phi}$$
  $(n \in \mathbb{Z})$ 

energy eigenvalues

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

#### transition amplitude

$$A_{n_f,n_i}(T) \equiv \langle n_f | e^{-i\hat{H}T} | n_i \rangle = \delta_{n_f,n_i} \exp\left(-iE_{n_f}T\right)$$

Langguth-Inomata 79 Kanwar-Wagman 21



Example in quantum mechanics (review) (2/3)

A naive discretization gives the path integral:

#### cf. Kanwar-Wagman 21

$$A_{n_{f},n_{i}}^{(\text{lat})}(T) \equiv \mathcal{N} \int (dU) e^{iS(U)} (U_{N}^{*})^{n_{f}} U_{0}^{n_{i}} \qquad \begin{pmatrix} T \equiv Na \\ U_{\ell} \equiv e^{i\phi_{\ell}} \\ \phi_{\ell} \equiv \phi(a\ell) \ (\ell = 0, \cdots, N) \end{pmatrix}$$

plaquette-like action

$$S(U) \equiv -\frac{\beta}{a} \sum_{\ell=0}^{N-1} \operatorname{Re} \left( U_{\ell+1} U_{\ell}^* \right) = -\frac{\beta}{a} \sum_{\ell=0}^{N-1} \cos(\phi_{\ell+1} - \phi_{\ell}) \,. \tag{4}$$



<u>Haar measure</u>

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

Fourier/character expansion:

cf. Kanwar-Wagman 21

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

$$I_n(z) \text{ modified Bessel function}$$
$$I_n(z) \equiv \int_{-\pi}^{\pi} \frac{d\phi}{2\pi} e^{-in\phi} e^{z\cos\phi}$$

<u>orthogonality</u>

$$\int dU \ U^n (U^m)^* = \delta_{nm}$$

$$\therefore \quad A_{n_f,n_i}^{(\text{lat})}(T) = \mathcal{N} \int (dU) \left( \prod_{\ell=0}^{N-1} \sum_{n_\ell \in \mathbb{Z}} I_{n_\ell} \left( -\frac{i\beta}{a} \right) U_{\ell+1}^{n_\ell} \left( U_{\ell}^{n_\ell} \right)^* \right) (U_N^*)^{n_f} U_0^{n_i}$$

$$= \mathcal{N} \left( \prod_{\ell=0}^{N-1} I_{n_\ell} \left( -\frac{i\beta}{a} \right) \right) \delta_{n_f,n_N} \cdots \delta_{n_0,n_i}$$

$$= \mathcal{N} \delta_{n_f,n_i} I_{n_f}^N \left( -\frac{i\beta}{a} \right)$$

Subtlety from the asymptotic expansion (1/2)

derived naive amplitude

$$A_{n_f,n_i}^{(\text{lat})}(T) = \mathcal{N}\delta_{n_f,n_i}I_{n_f}^N\left(-\frac{i\beta}{a}\right) \quad \checkmark \quad \text{analytic for all } \beta \in \mathbb{C} \text{ for finite } a,$$
  
but the situation changes in the limit  $a \to 0$ .  
Langguth-Inomata 79

asymptotic expansion of  $I_n(z)$   $(|z| \rightarrow \infty)$ 

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

$$\left[\begin{array}{c} +:-\frac{\pi}{2} < \arg z < \frac{3\pi}{2} \\ -:-\frac{3\pi}{2} < \arg z < \frac{\pi}{2} \end{array}\right]$$
For  $|\arg z| < \frac{\pi}{2}$ , 2nd term is completely ignorable.  
For  $\arg z = -\frac{\pi}{2}$  (naive real-time case), 2nd term equally contributes.

∴  $A_{n_f,n_i}^{(\text{lat})}(T)$  behaves differently depending on how we take  $a \to 0$  when using the real-time. Kanwar-Wagman 21

real-time,

continuum theory

Subtlety from the asymptotic expansion (2/2)

 $A_{n_f,n_i}^{(\text{lat})}(T) = \mathcal{N}\delta_{n_f,n_i}I_{n_f}^N\left(-\frac{i\beta}{a}\right) \to \mathcal{N}\delta_{n_f,n_i}I_{n_f}^N\left(-\frac{ie^{i\varepsilon}\beta}{a}\right)$ 

Indeed, we

 $A_{n_f,n_i}^{(\text{lat})}(T)$ 

The correct continuum limit is the one we obtain by introducing  $i\varepsilon$  ( $\varepsilon > 0$ ):

Langguth-Inomata 79 **Bohm-Junker 87** 

Z

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## Hamiltonian formalism (1/2)

It may be uncertain at which stage such  $i\varepsilon$  becomes required.

We here clarify these points from Hamiltonian formalism.

•  $\hat{U}$ ,  $\hat{p}_{\phi}$ : canonical operators  $\hat{U}$  is <u>not</u> the time evolution operator; rather  $\hat{U} \sim e^{i\hat{\phi}}$ 

٠

<u>commutation relation</u>  $[\hat{U}, \hat{p}_{\phi}] = \hat{U}$ 

- $|U\rangle$ : configuration basis  $\widehat{U} \mid U \rangle = U \mid U \rangle$
- $|n\rangle$ : momentum basis  $\langle U | n \rangle \equiv U^n$

Feynman kernel (a: time increment)

$$\langle U'|e^{-ia\widehat{H}}|U\rangle = \langle U'|e^{\frac{-ia}{2\beta}\widehat{p}_{\phi}^{2}}|U\rangle$$
  
insert  $1 = \sum_{n \in \mathbb{Z}} |n\rangle\langle n|$   
 $= \sum_{n \in \mathbb{Z}} \exp\left(\frac{-ia}{2\beta}n^{2} + in(\phi' - \phi)\right)$   $U = e^{i\phi}, U' = e^{i\phi'}$   
 $\phi, \phi' \in [-\pi, \pi)$ 

Judge-Lewis 63

Susskind-Glogower 64

review: Carruthers-Nieto 68

Hamiltonian formalism (2/2)

obtained kernel

$$\langle U'|e^{-ia\hat{H}}|U\rangle = \sum_{n\in\mathbb{Z}} e^{\frac{-ia}{2\beta}n^2} e^{in(\phi'-\phi)} = \vartheta\left(\frac{(\phi'-\phi)}{2\pi}, \frac{-a}{2\pi\beta}\right) \qquad \qquad \vartheta(v,\tau) \equiv \sum_{n\in\mathbb{Z}} e^{\pi in^2\tau} e^{2\pi inv}$$
(analytic for Im  $\tau > 0$ )

not well-defined as an ordinary function, but has a definite meaning as a distribution. See, e.g., Iwanami III p.46 Sincere thanks to Yoshio Kikukawa and referee of PTEP.

In fact,

• As a function:



Inclusion of large n components makes the quantity oscillatory and singular.

Jacobi  $\vartheta$  function:

- As a distribution:
  - state space = span $\{U^n\}_{n \in \mathbb{Z}}$

- Trivially, 
$$\int dU' \langle n | U' \rangle \langle U' | e^{-ia\hat{H}} | U \rangle$$
$$= e^{\frac{-ia}{2\beta}n^2} e^{-in\phi}$$

establishes the meaning as a distribution

which is a well-defined number for given n and  $\phi$ 

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Meaning of  $i\varepsilon$  (1/4)

In the previous naive path integral, we replaced the kernel by

$$\langle U'|e^{-ia\widehat{H}}|U\rangle = \sum_{n\in\mathbb{Z}} \exp\left(\frac{-ia}{2\beta}n^2 + in(\phi'-\phi)\right)$$

**Poisson resummation** 

$$= e^{i\pi/4} \sqrt{\frac{2\pi\beta}{-a}} \sum_{w \in \mathbb{Z}} \exp\left(i\frac{\beta}{2a}(\phi' - \phi + 2\pi w)^2\right)$$



previous replacement

$$\stackrel{\checkmark}{\rightarrow} e^{i\pi/4} \sqrt{\frac{2\pi \beta}{-a}} e^{\frac{i\beta}{a} \left[1 - \operatorname{Re}(U'U^*)\right]}$$

This replacement *cannot* be justified as a relation between distributions. In fact, for an infinitesimal *a* (as we have just seen):

$$\int dU' (U'^{*})^{n} \cdot e^{\frac{i\beta}{a} \left[1 - \operatorname{Re}(U'U^{*})\right]} = e^{-in\phi} e^{\frac{i\beta}{a}} I_{n} \left(\frac{-i\beta}{a}\right)$$

$$\stackrel{\uparrow}{} \sim e^{-in\phi} \left[1 - \left(n^{2} - \frac{1}{4}\right)\frac{ia}{2\beta} - i(-1)^{n} e^{\frac{2i\beta}{a}} \left(1 + \left(n^{2} - \frac{1}{4}\right)\frac{ia}{2\beta}\right)\right]$$

$$\sim e^{-in\phi} \left[e^{-\frac{ia}{2\beta}(n^{2} - \frac{1}{4})} - i(-1)^{n} e^{\frac{2i\beta}{a}} e^{\frac{ia}{2\beta}(n^{2} - \frac{1}{4})}\right] \qquad (\text{ ignored irrelevant overall constants})$$
which is different from the original case:
$$\int dU' (U'^{*})^{n} \langle U'| e^{-ia\hat{H}} | U \rangle = e^{-in\phi} e^{\frac{-ia}{2\beta}n^{2}}$$

Meaning of  $i\varepsilon$  (2/4)

• However, the replacement *can* be justified under the *i*ε:

$$\int dU' \, (U'^*)^n \cdot e^{i\pi/4} \sqrt{\frac{2\pi e^{i\varepsilon\beta}}{-a}} e^{\frac{ie^{i\varepsilon\beta}}{a} \left[1 - \operatorname{Re}(U'U^*)\right]} = e^{i\pi/4} \sqrt{\frac{2\pi e^{i\varepsilon\beta}}{-a}} e^{-in\phi} e^{\frac{ie^{i\varepsilon\beta}}{a}} I_n \left(\frac{-ie^{i\varepsilon\beta}}{a}\right)$$
$$\sim e^{-in\phi} \left[1 - \left(n^2 - \frac{1}{4}\right) \frac{ia}{2e^{i\varepsilon\beta}}\right]$$
$$\sim e^{-in\phi} e^{\frac{-ia}{2e^{i\varepsilon\beta}} \left(n^2 - \frac{1}{4}\right)}$$

cf. With the original kernel:

$$\int dU' \langle n' | U' \rangle \langle U' | e^{-ia\hat{H}} | U \rangle \Big|_{\beta \to e^{i\varepsilon}\beta} = e^{-in'\phi} e^{\frac{-ia}{2e^{i\varepsilon}\beta}n^2}$$

The difference is the constant shift of the zero-point energy that does not depend on  $\phi$  and n. The shift factor can be absorbed in the overall constant of the path integral.

and we did absorb this constant into  ${\mathcal N}$  in the previous argument.  $\Big]$ 

: We have the following equality as distribution for an infinitesimal a:

$$\left\langle U'|e^{-ia\widehat{H}}|U\rangle\right|_{\beta\to e^{i\varepsilon}\beta} = e^{\frac{-ia}{8e^{i\varepsilon}\beta}} e^{i\pi/4} \sqrt{\frac{2\pi e^{i\varepsilon}\beta}{-a}} e^{\frac{ie^{i\varepsilon}\beta}{a}\left[1-\operatorname{Re}(U'U^*)\right]}$$
  
energy shift factor

# Meaning of $i\varepsilon$ (3/4)

Where and why did the  $i\varepsilon$  and the normalization constant come in?

#### have a detailed look in the derivation

We can safely introduce  $i\varepsilon$  in the kernel  $\langle U'|e^{-ia\hat{H}}|U\rangle$ and regard the original one as its  $\varepsilon \to +0$  limit:

$$\langle U'|e^{-ia\widehat{H}}|U\rangle = \sum_{n\in\mathbb{Z}} \exp\left(\frac{-ia}{2\beta}n^2 + in(\phi'-\phi)\right)$$
$$= \lim_{\varepsilon \to +0} \langle U'|e^{-ia\widehat{H}}|U\rangle|_{\beta \to e^{i\varepsilon}\beta}$$

Under  $\varepsilon > 0$ ,  $\langle U' | e^{-ia\hat{H}} | U \rangle |_{\beta \to e^{i\varepsilon_{\beta}}}$  is a well-defined function and has a sharp peak around U = U':

Poisson resummation



become a distributional equality for an infinitesimal a

Meaning of  $i\varepsilon$  (4/4)

Finally, we derive the relation:

$$e^{\frac{i\pi}{4}}\sqrt{\frac{2\pi e^{i\varepsilon\beta}}{-a}}\exp\left(i\frac{e^{i\varepsilon\beta}}{2a}[\phi'-\phi]^2\right) = e^{\frac{-ia}{8e^{i\varepsilon\beta}}}e^{i\pi/4}\sqrt{\frac{2\pi e^{i\varepsilon\beta}}{-a}}e^{\frac{ie^{i\varepsilon\beta}}{a}[1-\cos(\phi'-\phi)]}$$
shift factor

• Again since  $\varepsilon > 0$ , the integral has a sharp peak at  $\phi' - \phi = 0$ . This allows us to expand the exponent in the powers of  $[\phi' - \phi]$ :

$$e^{\frac{ie^{i\varepsilon}\beta}{a}[1-\cos(\phi'-\phi)]} = e^{\frac{ie^{i\varepsilon}\beta}{2a}[\phi'-\phi]^2 - \frac{ie^{i\varepsilon}\beta}{24a}[\phi'-\phi]^4 + \cdots}$$

• The higher order terms only shifts the overall constant:

$$\int_{-\pi}^{\pi} \frac{d\phi'}{2\pi} e^{-in\phi'} e^{\frac{ie^{i\varepsilon}\beta}{2a}[\phi'-\phi]^2 - \frac{ie^{i\varepsilon}\beta}{24a}[\phi'-\phi]^4 + \cdots}$$

 $\phi^{\prime\prime} \equiv [\phi^{\prime} - \phi]$ , extend the integration region

$$\approx e^{-in\phi} e^{-\frac{ia}{2\beta}n^2} \int_{-\infty}^{\infty} \frac{d\phi''}{2\pi} e^{\frac{ie^{i\varepsilon}\beta}{2a}\phi''^2} \left(1 - \frac{ie^{i\varepsilon}\beta}{24a}\phi''^4 + \cdots\right)$$

The remaining integral is independent of n and  $\phi$ , and therefore an irrelevant constant:

$$\int_{-\infty}^{\infty} \frac{d\phi''}{2\pi} e^{\frac{ie^{i\varepsilon}\beta}{2a}\phi''^2} \left(1 - \frac{ie^{i\varepsilon}\beta}{24a}\phi''^4 + \cdots\right) \approx \left(1 + \frac{ia}{8e^{i\varepsilon}\beta}\right) \sqrt{\frac{-a}{2\pi i e^{i\varepsilon}\beta}} \\ \approx e^{\frac{ia}{8e^{i\varepsilon}\beta}} \sqrt{\frac{-a}{2\pi i e^{i\varepsilon}\beta}}$$

• Correcting this factor gives the desired distributional relation.

## Remarks (1/1)

Note the ordering of the limit.
 Since the distributional relation is for an infinitesimal *a* under ε > 0:

$$\langle U'|e^{-ia\widehat{H}}|U\rangle = \lim_{\varepsilon \to +0} e^{\frac{-ia}{8e^{i\varepsilon_{\beta}}}} e^{i\pi/4} \sqrt{\frac{2\pi e^{i\varepsilon_{\beta}}}{-a}} e^{\frac{ie^{i\varepsilon_{\beta}}}{a}} [1 - \operatorname{Re}(U'U^*)],$$

we first take  $a \rightarrow 0$  keeping  $\varepsilon > 0$ .

• Accordingly, we take  $\varepsilon \rightarrow +0$  outside the path integral once written by the plaquette-like action:

$$A_{n_{f},n_{i}}(T) = \mathcal{N}\lim_{\epsilon \to +0} \lim_{a \to 0} \int (dU) e^{-\frac{i\beta}{a}\sum_{\ell=0}^{N-1} \operatorname{Re}(U_{\ell+1}U_{\ell}^{*})} (U_{N}^{*})^{n_{f}} U_{0}^{n_{i}}$$

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Lattice gauge theory case (1/3)

<u>Wilson action in 4D Minkowski spacetime</u> (assume gauge group= $SU(N_c)$ ) Wilson 74 Berges-Borsanyi-Sexty-Stamatescu 07

$$S(U) \equiv \beta_t \sum_{x,i} \left[ 1 - \frac{1}{N_c} \operatorname{Re} \operatorname{tr} \left[ U_{x,i} U_{x+i,t} U_{x+t,i}^{\dagger} U_{x,t}^{\dagger} \right] \right] - \beta_s \sum_{x,i < j} \left[ 1 - \frac{1}{N_c} \operatorname{Re} \operatorname{tr} \left[ U_{x,i} U_{x+i,j} U_{x+j,i}^{\dagger} U_{x,j}^{\dagger} \right] \right]$$
$$\left[ \beta_t \equiv \frac{a}{a_0} \frac{2N_c}{g^2}, \qquad \beta_s \equiv \frac{a_0}{a} \frac{2N_c}{g^2} \right]$$



#### Lattice gauge theory case (2/3)



Lattice gauge theory case (3/3) NM 22

#### Boltzmann weight

$$e^{iS(U)} \propto e^{\frac{-i\beta_t}{N_c}\sum_{x,i} \operatorname{Re}\operatorname{tr}\left[U_{x,i}U_{x+i,t}U_{x+t,i}^{\dagger}U_{x,t}^{\dagger}\right] + \frac{i\beta_s}{N_c}\sum_{x,i< j} \operatorname{Re}\operatorname{tr}\left[U_{x,i}U_{x+i,j}U_{x+j,i}^{\dagger}U_{x,j}^{\dagger}\right]}$$

#### character expansion

$$e^{i(-1)^r \left(\frac{\beta_r}{N_c}\right) \operatorname{Re} \operatorname{tr} U} = \sum_{R:\operatorname{irrep}} d_R c_R (i(-1)^r \beta_r) \chi_R(U)$$
$$c_R (i(-1)^r \beta_r) = \sum_{n \in \mathbb{Z}} \det_{1 \le j,k \le N_c} I_{\ell_k - k + j + n} \left(\frac{i(-1)^r \beta_r}{N_c}\right)$$

• Since  $\beta_r \to \infty$  in the continuum limit of asymptotically free theories, we again confront the problem of the asymptotic expansion of  $I_n(z)$ .

In fact, if exactly using the Minkowski signature on lattice, the appropriate continuum limit will not be obtained. **cf. Hoshina-Fujii-Kikukawa 20 Kanwar-Wagman 21** 

• For this, we introduce slight imaginary parts:

 $\beta_t \rightarrow e^{i\varepsilon} \beta_t$ ,  $\beta_s \rightarrow e^{-i\varepsilon} \beta_s$ 

The sign for the timelike plaquette can be justified by Hamiltonian formalism below.

The sign for the spacelike plaquettes can then be chosen from Lorentz invariance (or repeating the similar argument in the spatial direction).

In this way, we can obtain the correct asymptotic behavior of the Boltzmann weight not only for the (0, i) components but also for the (i, j) components.

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### Hamiltonian formalism for Wilson theory (review) (1/3)

We show that  $i\varepsilon$  has the same role as in the QM system [gauge group= SU(2) for simplicity]

We consider the formal  $a_0 \rightarrow 0$  limit keeping the spatial spacing *a* finite (...only gives a meaning of  $i\varepsilon$  in the timelike plaquettes from this argument).

Hamiltonian Kogut-Susskind 75

$$H \equiv \frac{g^2}{2a} \sum_{\mathbf{x},i} \left( p_{\mathbf{x},i}^a \right)^2 + V(U) \qquad \left( V(U) \equiv \frac{2N_c}{ag^2} \sum_{\mathbf{x},i< j} \left( 1 - \frac{1}{N_c} \operatorname{Re} \operatorname{tr} \left[ U_{\mathbf{x},i} U_{\mathbf{x}+i,j} U_{\mathbf{x}+j,i}^{\dagger} U_{\mathbf{x},j}^{\dagger} \right] \right) \right)$$

temporal gauge

$$U_{x,t} = 1 \ (\forall x)$$

At time slice t, DOF=spatial link variables  $U_{x,i}$ .

To describe fluctuations from  $U_{\mathbf{x},i}$ ,

$$e^{i\theta^a_{\mathbf{x},i}T^a} U_{\mathbf{x},i} \qquad \left[ \operatorname{tr} T^a T^b = \frac{1}{2} \delta^{ab} \right]$$



#### Lagrangian

$$L \equiv \frac{a}{a_0^2} \frac{2N_c}{g^2} \sum_{\mathbf{x},i} \left( 1 - \frac{1}{N_c} \operatorname{Re} \operatorname{tr} \left[ U_{\mathbf{x},i} U_{\mathbf{x},i}^{\dagger} e^{i\theta_{\mathbf{x},i}^a(a_0)T^a} \right] \right) - V(U)$$
$$\approx \frac{a}{2g^2} \sum_{\mathbf{x},i} \left( \dot{\theta}_{\mathbf{x},i}^a \right)^2 - V(U)$$

conjugate momentum

$$p_{\mathbf{x},i}^a \equiv \frac{a}{g^2} \dot{\theta}_{\mathbf{x},i}^a$$

## Hamiltonian formalism for Wilson theory (review) (2/3)

 $\widehat{U}_{\mathbf{x},i}$ ,  $\hat{p}^a_{\mathbf{x},i}$ : canonical operators

 $[\widehat{U}_{\mathbf{x},i}, \ \widehat{p}^{a}_{\mathbf{x},i}] = \widehat{U}_{\mathbf{x},i}$ 

configuration basis

Kogut-Susskind 75 Creutz 77

$$|U\rangle \equiv \prod_{\mathbf{x},i} |U_{\mathbf{x},i}\rangle, \qquad \widehat{U}_{\mathbf{x},i}|U_{\mathbf{x},i}\rangle = U_{\mathbf{x},i}|U_{\mathbf{x},i}\rangle$$

dual basis (returns matrix elements in irreps)

**Chin-Van Roosmalen-Umland-Koonin 85** 

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

$$\langle U_{\mathbf{x},i} | j, m, m' \rangle \equiv D_{m,m'}^{j} (U_{\mathbf{x},i})$$
  
matrix element in spin-*j* rep

completeness relation (: Peter-Weyl theorem)

$$1 = \sum_{\{j_{\mathbf{x},i}, m_{\mathbf{x},i}, m'_{\mathbf{x},i}\}} \left( \underbrace{\prod_{\mathbf{x},i} (2j_{\mathbf{x},i}+1)}_{\text{dim of irreps}} \right) |\{j_{\mathbf{x},i}, m_{\mathbf{x},i}, m'_{\mathbf{x},i}\} \rangle \langle\{j_{\mathbf{x},i}, m_{\mathbf{x},i}, m'_{\mathbf{x},i}\}|$$

# Hamiltonian formalism for Wilson theory (review) (3/3)

For finite  $\eta_{\mathbf{x},i}^{a}$ , Kogut-Susskind 75  $\langle U_{\mathbf{x},i} | e^{i\eta_{\mathbf{x},i}^{a}\hat{p}_{\mathbf{x}}^{a}} | j, m, m' \rangle = \left( T e^{i\int_{0}^{1} ds \, \eta_{\mathbf{x},i}^{a} \, \mathcal{P}^{a}(s\eta_{\mathbf{x},i}^{a})} \langle U_{\mathbf{x},i} | \right) | j, m, m' \rangle$  (*T*: time-ordered product)  $= \left[ T e^{i\int_{0}^{1} ds \, \eta_{\mathbf{x},i}^{a} \, \mathcal{P}^{a}(s\eta_{\mathbf{x},i}^{a})} D^{j}(U_{\mathbf{x},i}) \right]_{m,m'}$   $\mathcal{P}^{a}(\theta)$ : differential operators s.t.  $\mathcal{P}^{a}(\theta) e^{i\theta^{a}T^{a}} = T^{a} e^{i\theta^{a}T^{a}}$  $\left[ \begin{array}{c} \mathcal{P}^{1}(\theta) \equiv \frac{1}{2i} \left[ \sin\psi \cos\phi \frac{\partial}{\partial\chi} + (\cot\chi \cos\psi \cos\phi + \sin\phi) \frac{\partial}{\partial\psi} + (\cot\psi \cos\phi - \cot\chi \frac{\sin\phi}{\sin\psi}) \frac{\partial}{\partial\phi} \right] \\ \mathcal{P}^{2}(\theta) \equiv \frac{1}{2i} \left[ \sin\psi \sin\phi \frac{\partial}{\partial\chi} + (\cot\chi \cos\psi \sin\phi - \cos\phi) \frac{\partial}{\partial\psi} + (\cot\psi \sin\phi + \cot\chi \frac{\cos\phi}{\sin\psi}) \frac{\partial}{\partial\phi} \right] \\ \mathcal{P}^{3}(\theta) \equiv \frac{1}{2i} \left[ \cos\psi \frac{\partial}{\partial\chi} - \cot\chi \sin\psi \frac{\partial}{\partial\psi} - \frac{\partial}{\partial\phi} \right] \\ \end{array} \right]$ 

In particular,  $\left(\mathcal{P}^{a}(\theta)\right)^{2} \geq 0$  is the minus of the Laplacian and

...

 $(\mathcal{P}^{a}(0))^{2} = (i^{-1}\partial_{\theta}a)^{2}$ . Menotti-Onofri 81 Chin-Van Roosmalen-Umland-Koonin 85

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

#### Meaning of $i\varepsilon$ from Hamiltonian formalism (1/3) NM 22

#### <u>Feynman kernel</u> ( $a_0$ : time increment)

$$\begin{split} \langle U' | e^{-ia_0 \hat{H}} | U \rangle &= \langle U' | e^{\frac{-ia_0 g^2}{2a} \sum_{\mathbf{x},i} (\hat{p}_{\mathbf{x},i}^a)^2} e^{-ia_0 V(\hat{U})} | U \rangle \\ \text{insert complete set} \\ &\stackrel{\downarrow}{=} \prod_{\mathbf{x},i} \left[ \sum_{j_{\mathbf{x},i}} (2j_{\mathbf{x},i} + 1) \chi_{j_{\mathbf{x},i}} (U'_{\mathbf{x},i} U_{\mathbf{x},i}^{\dagger}) e^{\frac{-ia_0 g^2}{2a} j_{\mathbf{x},i} (j_{\mathbf{x},i} + 1)} \right] e^{-ia_0 V(U)} \end{aligned}$$

maximal torus of timelike plaquettes:  $\delta \phi_{\mathbf{x},i} \in [-\pi,\pi)$ 

$$U'_{\mathbf{x},i}U^{\dagger}_{\mathbf{x},i} \sim \operatorname{diag}(e^{i\delta\phi_{\mathbf{x},i}}, e^{-i\delta\phi_{\mathbf{x},i}})$$

: [bracket part] (dropping the subscripts x, i)

$$\begin{bmatrix} \chi_{j}(U'U^{\dagger}) = \frac{\sin[\delta\phi(2j+1)]}{\sin\delta\phi} \end{bmatrix} = \sum_{j} (2j+1) \chi_{j}(U'U^{\dagger}) e^{\frac{-ia_{0}g^{2}}{2a}j(j+1)}$$

$$= -\sum_{j} \frac{1}{\sin\delta\phi} \frac{d}{d\delta\phi} \cos[\delta\phi(2j+1)] \cdot e^{\frac{-ia_{0}g^{2}}{2a}j(j+1)}$$

$$= -\frac{1}{2} \frac{1}{\sin\delta\phi} e^{i\frac{a_{0}g^{2}}{8a}} \frac{d}{d\delta\phi} \sum_{n\geq 1} \left[ e^{-i\frac{a_{0}g^{2}}{8a}n^{2}+in\delta\phi} + e^{-i\frac{a_{0}g^{2}}{8a}n^{2}-in\delta\phi} \right]$$

$$= -\frac{1}{2} \frac{1}{\sin\delta\phi} e^{i\frac{a_{0}g^{2}}{8a}} \frac{d}{d\delta\phi} \sum_{n\geq 1} e^{-i\frac{a_{0}g^{2}}{8a}n^{2}+in\delta\phi}$$
again theta function!

Meaning of  $i\varepsilon$  from Hamiltonian formalism (2/3) NM 22

• To rewrite the expression with the Wilson action, we introduce the  $i\varepsilon$ :

$$e^{-i\frac{a_0g^2}{8a}n^2 + in\delta\phi} \to e^{-ie^{-i\varepsilon}\frac{a_0g^2}{8a}n^2 + in\delta\phi}$$
  
$$\cdot -\frac{1}{2}\frac{1}{\sin\delta\phi}e^{i\frac{a_0g^2}{8a}}\frac{d}{d\delta\phi}\sum_{n\in\mathbb{Z}}e^{-ie^{-i\varepsilon}\frac{a_0g^2}{8a}n^2 + in\delta\phi}$$
  
$$\approx -\frac{1}{2}\frac{1}{\sin\delta\phi}e^{ie^{-i\varepsilon}\frac{a_0g^2}{8a}}\frac{d}{d\delta\phi}e^{\frac{i\pi}{4}}\sqrt{\frac{8\pi a}{-e^{-i\varepsilon}a_0g^2}}\exp\left[ie^{i\varepsilon}\frac{2a}{a_0g^2}(\delta\phi)^2\right]$$

Poisson resummation & dropped the winding contributions

٠

- Thanks to  $\varepsilon > 0$ , finite contribution comes from the fluctuations of order  $\delta \phi = O(a_0)$ .
  - (Up to a shift of the zero-point energy, and for an infinitesimal  $a_0$ ):

$$\operatorname{const} \cdot \frac{\delta \phi}{\sin \delta \phi} \exp\left[i e^{i\varepsilon} \frac{2a}{a_0 g^2} (\delta \phi)^2\right] = \operatorname{const'} \cdot \exp\left[-i e^{i\varepsilon} \frac{2a}{a_0 g^2} \operatorname{tr}\left[U' U^{\dagger}\right]\right]$$

## Meaning of $i\varepsilon$ from Hamiltonian formalism (3/3) NM 22

• Combining everything together, we have the path integral expression:

$$\begin{aligned} A_{\psi_f,\psi_i}(T) &\equiv \langle \psi_f \left| e^{-i\widehat{H} T} \left| \psi_i \right\rangle \\ &\approx \mathcal{N}' \lim_{\varepsilon \to +0} \int \left( \prod_{\ell=0}^N dU_\ell \right) \exp i \sum_{\ell=0}^{N-1} \begin{bmatrix} -e^{i\varepsilon} \frac{2a}{a_0 g^2} \sum_{\mathbf{x},i} \operatorname{tr} \left[ U_{\ell+1,\mathbf{x},i} U_{\ell+1,\mathbf{x},i}^{\dagger} \right] \\ &+ \frac{2a_0}{a g^2} \sum_{\mathbf{x},i < j} \frac{1}{N_c} \operatorname{Re} \operatorname{tr} \left[ U_{\ell,\mathbf{x},i} U_{\ell,\mathbf{x}+i,j} U_{\ell,\mathbf{x}+j,i}^{\dagger} U_{\ell,\mathbf{x},j}^{\dagger} \right] \end{bmatrix} \psi_f^*(U_N) \psi_i(U_0) \end{aligned}$$

- Despite the complications related to the field theory, the basic structure is the same as in the quantum mechanical model:
  - Since the plaquette action can reproduce the continuum action only for smooth configurations, its naive application to the real-time path integral makes the phase factor associated with large fluctuations different from the continuum theory.
  - The  $i\varepsilon$  is required to manifestly suppress the contributions from these large fluctuations in the path integral.

#### Remarks (1/1) NM 22

• Since we only have considered the formal  $a_0 \rightarrow 0$  limit, the  $i\varepsilon$  for the spatial plaquettes have 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 functions of the form  $I_n\left(\frac{2ia_0}{ag^2}\right)$ , for which we can apply the expansion of  $I_n(z)$  around zero:

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

- : characters coming from the spatial plaquettes are analytic in the limit  $a_0 \rightarrow 0$  for a fixed a, giving no complication.
- The subtlety for the spatial plaquettes arises when we take the continuum limit taking  $a_0 \rightarrow 0$  and  $a \rightarrow 0$  at the same time, making  $g^2$  run according to the renormalization group equation.

In this treatment, which is required in extracting the continuum physics, the arguments of the Bessel functions diverge both in timelike and spacelike plaquettes.

 $\therefore$  We need to incorporate  $i\varepsilon$  also for the spatial plaquettes.

### Outline

• Introduction

#### <u>1D QM</u>

- Subtlety of real-time path integral in QM (review)
- *iε* from Hamiltonian formalism

#### <u>YM</u>

- Subtlety in lattice gauge theory
- *iε* from Hamiltonian formalism
- Convergence properties of Wilson action
- Discussion

#### Wilson 2D (1/1)

To check the convergence properties in  $\varepsilon \rightarrow 0$ , we consider the  $SU(N_c = 2,3)$  Wilson theory in 2D:

cf. Kanwar-Wagman 21

$$S(U) \equiv \beta_t e^{i\varepsilon} \sum_{x,i} \left[ 1 - \frac{1}{N_c} \operatorname{Re} \operatorname{tr} \left[ U_{x,i} U_{x+i,t} U_{x+t,i}^{\dagger} U_{x,t}^{\dagger} \right] \right] \quad \left( \begin{array}{c} \text{uniform spacetime: } a_0 = a \\ \beta_t \equiv \frac{2N_c}{(ag)^2} \end{array} \right)$$

g = 1, time and spatial volume=infinity below

$$\frac{W_A : \ell \times \tau \text{ Wilson loop (physical area } A \equiv \ell \tau a^2)}{\langle W_A \rangle} = N_c \left(\frac{c_{\text{fund}} \left(-i e^{i\varepsilon} \beta_t\right)}{c_{\text{triv}} \left(-i e^{i\varepsilon} \beta_t\right)}\right)^{\ell \tau}$$

Gross-Witten 80 Wadia 80

the continuum limit is known from the analysis of the heat-kernel action:

$$\langle W_A \rangle \rightarrow N_c \ e^{-i\left(\frac{N}{4}\right)\left(1-\frac{1}{N^2}\right)g^2A}$$

Menotti-Onofri 81 Kanwar-Wagman 21

# SU(2) (1/3) NM 22

 $\langle W_{A=1} \rangle$  for various  $\varepsilon$  (calculated directly using the modified Bessel functions  $I_n(z)$ )



• For relatively large *a*, the unwanted part of the asymptotic expansion contributes and gives oscillatory behavior.

: Given a, in turn, we need to prepare  $\varepsilon$  large enough s.t. the unphysical part can be neglected.

For the studied range of a,  $\beta_t \sin \varepsilon \gtrsim 4.5$  (for SU(2)).

• Instead of implementing  $i\varepsilon$ , we can expand the action with characters and replace  $I_n(z)$  with the physical part of its asymptotic expansion in advance.

Corresponding result (with  $\varepsilon = 0$ ) is shown with **————** for the region where the asymptotic expansion gives a sufficient convergence up to machine precision.

SU(2) (2/3) NM 22

 $a \rightarrow 0$  limits for each  $\varepsilon$ 



We fit five points  $a = 0.1, 0.15, \dots, 0.3$  for each  $\varepsilon$  with the linear function of  $a^2$ .

 $\varepsilon \rightarrow +0$  extrapolation of the  $a \rightarrow 0$  limits



We fit with quadratic and cubic functions of  $\varepsilon$ . Cubic result: central value; the difference from the quadratic value: estimate of the sys error.

obtained estimate: $\lim_{a \to 0, \varepsilon \to +0} \langle W_A = 1 \rangle \approx 1.86146(93) - 0.7331(36)i$ analytical value: $\lim_{a \to 0, \varepsilon \to +0} \langle W_A = 1 \rangle = 1.8610 - 0.7325i$ agree within the error [31/36]

#### SU(2) (3/3) NM 22

#### finite *a* effects (under $\varepsilon = 0.1$ )



#### finite $\varepsilon$ effects









### SU(3) (1/1) NM 22

 $\langle W_{A=1} \rangle$  for various  $\varepsilon$ 



(The asymptotic expansion does not converge up to machine precision in the studied range of a.)



fitted range of  $a: a = 0.1, 0.125, \cdots, 0.2$ 

[33/36]



### Outline

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# Discussion (1/3)

#### Summary

- We can use the conventional lattice gauge theory actions (in particular, Wilson), but by properly implementing the *i*ε.
- It is important that we implement  $i\varepsilon$  both for timelike and spacelike plaquettes.

#### Outlook

• As mentioned,  $\varepsilon$  should be prepared s.t.  $\beta_t \sin \varepsilon \ge 4.5$  (SU(2)),  $\beta_t \sin \varepsilon \ge 15$  (SU(3))

Since the characters are expressed solely with  $\beta_r$ ,

these values should give a rough estimate of the required  $\varepsilon$  also in higher dimensions.

The large bounds are however unpleasant for 4D because of critical slowing down.

A similar situation occurs for the character-replaced action:

The (divergent) asymptotic expansion gives a sufficient approximation up to machine precision only for a comparably large  $\beta_r$  (especially for SU(3)).

#### Possible detours? NM+ in progress

- Since the problem is the oscillation that vanishes in  $a \rightarrow 0$ , we can add a counterterm to cancel the oscillation, or average the estimates in the  $\beta$  direction by a few periods, varying  $\beta$  in the simulation. **cf. Fukuma-NM 21**
- We can also develop a systematic way to truncate the character expansion, in which case we do not need ε → 0 extrapolation [however there is a caveat (next page)].



## Discussion (2/3) NM in progress

If we use the character-replaced action, the exponential factor is common to all irreps *R* and will be cancelled in expectation values.

$$I_n(z)\Big|_{\text{relevant}} \sim \frac{e^z}{\sqrt{2\pi z}} \sum_{k \ge 0} \frac{\Gamma(n+k+1/2)}{k! \,\Gamma(n-k+1/2)} \left(-\frac{1}{2z}\right)^k \quad \left(\frac{1}{z} = \mp \frac{g^2}{2i}\right)$$

Then the remainder is a power series of  $g^2$ .

Correspondingly, the expectation value of an observable will be expressed as a power series of  $g^2$ . The result seems to be a perturbative expansion.

If this is the case, the character-replaced action may not be a good option for performing *fully non-perturbative* calculation, though it should give practically good estimates.

On the other hand, this situation is the same in the Euclidean path integral.  $\therefore$  Non-perturbative effects  $e^{O(-1/g^2)}$  seem to be hidden in the difference between  $I_n(z)$  and its asymptotic expansion.



cf. Fukaya-Onogi-Yamaguchi 17 Fukaya-Furuta-Matsuo-Onogi-Yamaguchi-Yamashita 19 Fukaya-Kawai-Matsuki-Mori-Nakayama-Onogi-Yamaguchi 19

#### Discussion (3/3)NM in progress

The  $i\varepsilon$  for spatial plaquettes has a peculiar consequence that ٠ it prevents the transfer matrix from being unitary for finite a Type equation here.no matter how we write the kinetic term.

In quantum computation (QC), we construct an algorithm that corresponds to the time evolution:

 $\langle U'|e^{-ia_0\widehat{H}}|U\rangle = \langle U'|e^{\frac{-ia_0g^2}{2a}\sum_{\mathbf{x},i}(\widehat{p}^a_{\mathbf{x},i})^2}e^{-ia_0V(\widehat{U})}|U\rangle,$ 

whose asymptotic behavior is different in the continuum spacetime limit w/ or w/o  $i\varepsilon$ .

Since the ordinary scope of QC is restricted to unitary evolutions, we may avoid using the plaguette discretization in QC by, e.g., moving to momentum space lattice. Kogut-Lagae 93, 94

It is also theoretically interesting to consider causality ٠ from the lattice-oriented picture for the  $i\varepsilon$ ;

it may be notable that the situation is similar to the relation between the admissibility condition and the reflection positivity. Luscher 99 Creutz 04 Fukaya-Onogi 03

Thank you.