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Applying the Worldvolume Hybrid Monte Carlo method to lattice gauge theories[†]

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The numerical sign problem remains one of the central challenges in computational physics. The Worldvolume Hybrid Monte Carlo (WV-HMC) method has recently been proposed as a reliable and computationally efficient algorithm that crucially avoids the ergodicity issues inherent in Lefschetz-thimble approaches. In these proceedings, after outlining the key ideas behind WV-HMC, we present its extension to group manifolds. This provides a rigorous framework for applying WV-HMC to lattice gauge theories.

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1. Introduction

The numerical sign problem is a major obstacle to first-principles computations of various physically important systems, including finite-density QCD, finite-θ Yang-Mills theory, strongly correlated electron systems, and real-time dynamics of quantum many-body systems.

For the last fifteen years, there have been attempts to construct a versatile solution to the sign problem, and various methods have been proposed. Among them, methods based on Lefschetz thimbles have attracted much attention because of their mathematical rigor rooted in Picard-Lefschetz theory [1–9]. There, the integration surface is continuously deformed within the complexified space, so that the oscillatory behavior is mild on the new integration surface. It, however, soon became clear that the original Lefschetz thimble method generally suffers from an ergodicity problem [5–7], due to the appearance of zeros of the Boltzmann weight on the deformed surface, which behave as infinitely high potential barriers for the Markov chain walker.

The first algorithm that simultaneously solves the sign and ergodicity problems was the *Tempered Lefschetz thimble (TLT) method* [10, 11], where the deformation parameter t (called the flow time) is treated as an extra dynamical variable, and the resulting extended configuration space provides a detour between two regions that are originally separated by the potential barriers. Although the TLT method has proven its versatility and reliability in various models [10, 12], it requires computing the Jacobian of the deformation every time two configurations are exchanged between adjacent replicas, in order to take into account the difference in volume elements of the replicas. The *Worldvolume Hybrid Monte Carlo (WV-HMC) method* was then invented to overcome this limitation [13] (see also Refs. [14–19]). There, the configuration space is extended to a continuous union of deformed surfaces (worldvolume), and one considers phase-space integrals over the tangent bundle of the worldvolume, which carries a natural symplectic structure. One no longer needs to compute the Jacobian in configuration generation because the phase-space volume element does not change in molecular dynamics (MD) if one employs a symplectic (and thus volume-preserving) integrator. The aim of the present paper is to generalize WV-HMC to group manifolds [20], an extension that provides a general setting for lattice gauge theories. The presentation closely follows that of Ref. [20].

In the following, we write $\langle X, Y\rangle \equiv \mathrm{Re}\,\mathrm{tr}\, X^\dagger Y$ for matrices X and Y.

2. Complex analysis on complexified groups

We first define the complexification $G^{\mathbb{C}}$ of a compact Lie group G. We assume that G is in a faithful unitary representation, so that the elements $U_0 \in G$ are expressed by unitary matrices, and thus the elements of its Lie algebra $\mathfrak{g}$ by anti-hermitian matrices. We denote a basis of $\mathfrak{g}$ by $\{T_a\}$ ($a = 1, \ldots, N$), which we normalize as $\mathrm{tr}\, T_a T_b = -\delta_{ab}$. Accordingly, we raise and lower indices with the rule $A_a = -A^a$. We introduce the right-invariant Maurer-Cartan 1-form on G by

$$\theta_0 \equiv dU_0\, U_0^{-1} = T_a\, \theta_0^a \quad (\theta_0^a\text{: real 1-form}), \tag{2.1}$$

from which the Haar measure (dU_0) on G is defined as

$$(dU_0) \equiv \theta_0^1 \wedge \cdots \wedge \theta_0^N. \tag{2.2}$$

We let $\mathfrak{g}^{\mathbb{C}}$ be the complexified Lie algebra constructed from $\mathfrak{g}$, and define the complexification $G^{\mathbb{C}}$ of G as[1]

$$G^{\mathbb{C}} \equiv \{U = e^{Z} e^{Z'} \cdots e^{Z''} \,|\, Z, Z', \dots, Z'' \in \mathfrak{g}^{\mathbb{C}}\}. \tag{2.3}$$

We introduce the Maurer-Cartan 1-form on $G^{\mathbb{C}}$ by

$$\theta \equiv dU U^{-1} = T_a \, \theta^a \quad (\theta^a\text{: complex 1-form}), \tag{2.4}$$

from which we introduce the holomorphic N-form (dU) as

$$(dU) \equiv \theta^1 \wedge \cdots \wedge \theta^N. \tag{2.5}$$

We then have Cauchy's theorem on $G^{\mathbb{C}}$ [20]:

Theorem 1. *Let $\mathcal{D}$ be a domain in $G^{\mathbb{C}}$ and $f(U)$ be a holomorphic function on $\mathcal{D}$. Then, the integral I_Σ of $f(U)$ over a real N-dimensional oriented submanifold $\Sigma \subset \mathcal{D}$,*

$$I_\Sigma = \int_\Sigma (dU)\, f(U), \tag{2.6}$$

depends only on the boundary of Σ.

Here, a function $f = f(U)$ is said to be *holomorphic* if it depends holomorphically on the matrix elements U_{ij}.

3. WV-HMC for group manifolds

Our aim is to numerically evaluate the expectation value of an observable $O(U_0)$ defined by

$$\langle O \rangle \equiv \frac{\int_G (dU_0)\, e^{-S(U_0)}\, O(U_0)}{\int_G (dU_0)\, e^{-S(U_0)}}. \tag{3.1}$$

We complexify $G = \{U_0\}$ to $G^{\mathbb{C}} = \{U\}$ and assume that both $e^{-S(U)}$ and $e^{-S(U)}\, O(U)$ are holomorphic on $G^{\mathbb{C}}$ (which usually holds in cases of physical interest). By Cauchy's theorem, the expression above can be rewritten as a ratio of integrals over a new integration surface Σ that is obtained by a continuous deformation of G (see Fig. 1):

$$\langle O \rangle = \frac{\int_\Sigma (dU)\, e^{-S(U)}\, O(U)}{\int_\Sigma (dU)\, e^{-S(U)}}. \tag{3.2}$$

Thus, even when the original path integral on $\Sigma_0 = G$ suffers from a severe sign problem due to the highly oscillatory behavior of $e^{-i\, \mathrm{Im}\, S(U_0)}$, this problem can be significantly alleviated if $\mathrm{Im}\, S(U)$ is almost constant on the new integration surface Σ.

In this work, we generate such a deformation using the anti-holomorphic gradient flow:

$$\dot{U} = \xi(U)\, U \quad \text{with} \quad U|_{t=0} = U_0. \tag{3.3}$$

[1] For $G = SU(n)$ and its Lie algebra $\mathfrak{g} = \mathfrak{su}(n)$, their complexifications are given by $G^{\mathbb{C}} = SL(n, \mathbb{C})$ and $\mathfrak{g}^{\mathbb{C}} = \mathfrak{sl}(n, \mathbb{C})$.

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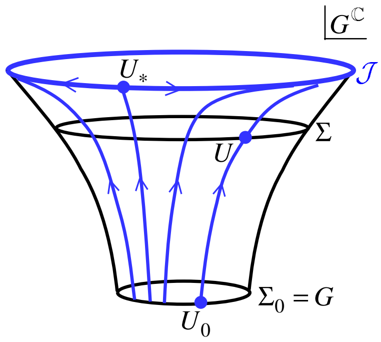

Figure 1: Deformation of $\Sigma_0 = G$ into a submanifold Σ within $G^{\mathbb{C}}$ [20]. The deformed surface Σ approaches a Lefschetz thimble $\mathcal{J}$, which consists of points flowing out from a critical point U_*.

Here, $\dot{U} \equiv dU/dt$, and the drift is given by

$$\xi(U) \equiv [DS(U)]^\dagger, \tag{3.4}$$

where we define the Lie-algebra-valued derivative $DS(U) \in \mathfrak{g}^{\mathbb{C}}$ through the variation [20]:

$$\delta S(U) = \mathrm{tr}\left[(\delta U U^{-1})\, DS(U)\right] = (\delta U U^{-1})^a\, D_a S(U). \tag{3.5}$$

This flow equation leads to the monotonicity relation

$$[S(U)]^{\cdot} = \mathrm{tr}\,[(\dot{U}\,U^{-1}) DS(U)] = \mathrm{tr}\left[(DS(U))^\dagger\,(DS(U))\right] \geq 0, \tag{3.6}$$

which shows that the real part $\mathrm{Re}\,S(U)$ always increases along the flow [except at critical points where $DS(U)$ vanishes], while the imaginary part $\mathrm{Im}\,S(U)$ remains constant. The Lefschetz thimble $\mathcal{J}$ associated with a critical point U_* is defined as the set of points flowing out of U_* (see Fig. 1). Since $\mathrm{Im}\,S(U)$ is invariant along the flow, it is constant over $\mathcal{J}$. Thus, the oscillatory behavior of the integrands in Eq. (3.2) is expected to be significantly mitigated if the integration surface is deformed with a sufficiently large flow time t so that it reaches the vicinity of $\mathcal{J}$.

Sampling on a deformed surface Σ corresponds to a group-manifold extension of the generalized thimble method of Alexandru et al. [8].[2] However, as mentioned in Sect. 1, integration over Σ will introduce ergodicity issues when the flow time is taken to be sufficiently large to reduce the oscillatory behavior of $e^{-i\,\mathrm{Im}\,S(U)}$. This motivates us to extend WV-HMC to group manifolds.

The prescription for introducing WV-HMC to group manifolds is the same as in the flat case. We first note that when we set the deformed surface to $\Sigma = \Sigma_t$ (the deformed surface at flow time t), both the numerator and the denominator of Eq. (3.2) do not depend on t due to Cauchy's theorem. Thus, we can take averages over t separately with an arbitrary common weight $e^{-W(t)}$ as in Ref. [13] [we denote (dU) along Σ_t by $(dU)_{\Sigma_t}$ to specify where it lives]:

$$\langle O \rangle = \frac{\int_{\Sigma_t} (dU)_{\Sigma_t}\, e^{-S(U)}\, O(U)}{\int_{\Sigma_t} (dU)_{\Sigma_t}\, e^{-S(U)}} = \frac{\int dt\, e^{-W(t)} \int_{\Sigma_t} (dU)_{\Sigma_t}\, e^{-S(U)}\, O(U)}{\int dt\, e^{-W(t)} \int_{\Sigma_t} (dU)_{\Sigma_t}\, e^{-S(U)}}. \tag{3.7}$$

[2] An HMC algorithm on Σ in flat space was developed in Refs. [21, 22] and Ref. [16], which we call the *generalized thimble Hybrid Monte Carlo* (GT-HMC). A group-manifold extension of GT-HMC (along with WV-HMC) is presented in Ref. [20].

This can be regarded as a ratio of integrals over the *worldvolume* $\mathcal{R}$ defined by

$$\mathcal{R} \equiv \bigcup_t \Sigma_t = \{U(t, U_0) \in G^{\mathbb{C}} \,|\, t \in \mathbb{R},\, U_0 \in G\}, \tag{3.8}$$

where $U(t, U_0)$ denotes the configuration reached at flow time t starting from the initial configuration U_0. One can effectively constrain the extent of $\mathcal{R}$ in the t-direction within a finite interval $[T_0, T_1]$ by adjusting $W(t)$ [16]. The lower cutoff T_0 is chosen such that ergodicity issues are absent at $t \sim T_0$, while the upper cutoff T_1 is chosen such that oscillatory integrals are sufficiently tamed at $t \sim T_1$. The expectation value (3.7) is thus expressed as a ratio of the reweighted averages over $\mathcal{R}$ [20],

$$\langle O \rangle = \frac{\langle \mathcal{F}(U)\, O(U) \rangle_{\mathcal{R}}}{\langle \mathcal{F}(U) \rangle_{\mathcal{R}}} \tag{3.9}$$

$$\langle g(U) \rangle_{\mathcal{R}} \equiv \frac{\int_{\mathcal{R}} |dU|_{\mathcal{R}}\, e^{-V(U)}\, g(U)}{\int_{\mathcal{R}} |dU|_{\mathcal{R}}\, e^{-V(U)}}. \tag{3.10}$$

Here, $|dU|_{\mathcal{R}}$ is the invariant measure on $\mathcal{R}$, and $V(U)$ and $\mathcal{F}(U)$ are the potential and the associated reweighting factor [20]:[3]

$$V(U) \equiv \mathrm{Re}\, S(U) + W(t(U)), \quad \mathcal{F}(U) \equiv \frac{dt\, (dU)_{\Sigma_t}}{|dU|_{\mathcal{R}}}\, e^{-i\, \mathrm{Im}\, S(U)}. \tag{3.11}$$

The reweighted averages $\langle \cdots \rangle_{\mathcal{R}}$ can be rewritten as integrals over the tangent bundle of $\mathcal{R}$,

$$T\mathcal{R} = \{(U, \pi) \,|\, U \in \mathcal{R},\, \pi \in T_U \mathcal{R}\}, \tag{3.12}$$

as in the flat case [16] (see also Ref. [13]),

$$\langle g(U) \rangle_{\mathcal{R}} = \frac{\int_{T\mathcal{R}} d\Omega_{\mathcal{R}}\, e^{-H(U,\pi)}\, g(U)}{\int_{T\mathcal{R}} d\Omega_{\mathcal{R}}\, e^{-H(U,\pi)}}, \tag{3.13}$$

$$H(U, \pi) = \frac{1}{2} \langle \pi, \pi \rangle + V(U). \tag{3.14}$$

Here, we have introduced a symplectic structure on $T\mathcal{R}$ with the symplectic 2-form $\omega_{\mathcal{R}} = d\, \langle \pi, \theta_{\mathcal{R}} \rangle$ ($\theta_{\mathcal{R}}$ denoting θ along $\mathcal{R}$), and set the symplectic volume form $d\Omega_{\mathcal{R}}$ as [20]

$$d\Omega_{\mathcal{R}} = \frac{\omega_{\mathcal{R}}^{N+1}}{(N+1)!}. \tag{3.15}$$

In the rest of this section, we construct a Markov chain on $T\mathcal{R}$ that has the equilibrium distribution $\propto e^{-H(U,\pi)}$. To this end, we first *define* Hamiltonian dynamics on the tangent bundle of $G^{\mathbb{C}}$, $TG^{\mathbb{C}} \equiv \{(U, \pi) \,|\, U \in G^{\mathbb{C}},\, \pi \in T_U G^{\mathbb{C}}\}$, using the first-order action [20]

$$I[U(s), \pi(s)] = \int ds\, \bigl[\langle \pi, \mathring{U} U^{-1} \rangle - H(U, \pi)\bigr], \tag{3.16}$$

[3] The function $t(U)$ returns the flow time t for configuration $U = U(t, U_0)$. If we introduce vectors $E_b \equiv T_a E^a_b$ from the Jacobian matrix E^a_b in the linear relation $\theta^a|_{\Sigma_t} = E^a_b\, \theta^b_0$, the reweighting factor can be expressed as $\mathcal{F}(U) = \alpha^{-1}\, (\det E/\sqrt{\gamma})\, e^{-i\, \mathrm{Im}\, S(U)}$ with $\gamma_{ab} = \langle E_a, E_b \rangle$. $\alpha \equiv \sqrt{\langle \xi_n, \xi_n \rangle}$ is the norm of the normal component $\xi_n \in N_U \Sigma_t$ of ξ. The potential $V(U)$ is a real-valued function, and its derivatives are defined by $\delta V = \mathrm{tr}\, \bigl[(\delta U U^{-1})\, DV + (\delta U U^{-1})^\dagger\, (DV)^\dagger\bigr]$. See Ref. [20] for details.

where $\mathring{U} \equiv dU/ds$. The first term $\langle \pi, \mathring{U} U^{-1} \rangle$ corresponds to the symplectic potential $a = \langle \pi, \theta \rangle$ of the symplectic 2-form $\omega = da = d\langle \pi, \theta \rangle$, for which the Poisson brackets take the form [20]

$$\{U_{ij}, \pi^\dagger_{kl}\} = 2\left(\delta_{il}\, U_{kj} - \frac{1}{n}\, U_{ij}\, \delta_{kl}\right), \quad \{\pi_{ij}, \pi_{kl}\} = 2\,(-\delta_{il}\, \pi_{kj} + \pi_{il}\, \delta_{kj}), \quad \cdots \tag{3.17}$$

One can check that the obtained Hamilton's equations [20]

$$\mathring{U} = \pi\, U, \quad \mathring{\pi} = -2\,[DV(U)]^\dagger + [\pi, \pi^\dagger] \tag{3.18}$$

are indeed written as $\mathring{U} = \{U, H\}$, $\mathring{\pi} = \{\pi, H\}$.

We then define the MD evolution operator of step size $\Delta s = \epsilon$ on $TG^{\mathbb{C}}$ as

$$T \equiv e^{-(\epsilon/2)\{*,K\}}\, e^{-\epsilon\{*,V\}}\, e^{-(\epsilon/2)\{*,K\}}, \tag{3.19}$$

which differs from the continuous evolution operator $e^{-\epsilon\{*,H\}}$ by $O(\epsilon^3)$. A straightforward calculation [20] shows that a single MD step $(U, \pi) \to (U', \pi') \equiv (T(U), T(\pi))$ is given by

$$\pi_{1/2} = \pi - \epsilon\, [DV(U)]^\dagger, \tag{3.20}$$

$$U' = e^{\epsilon\,(\pi_{1/2} - \pi^\dagger_{1/2})}\, e^{\epsilon\, \pi^\dagger_{1/2}}\, U, \tag{3.21}$$

$$\pi' = e^{\epsilon\,(\pi_{1/2} - \pi^\dagger_{1/2})}\, \pi_{1/2}\, e^{-\epsilon\,(\pi_{1/2} - \pi^\dagger_{1/2})} - \epsilon\, [DV(U')]^\dagger. \tag{3.22}$$

One can prove [20] that this is (a) exactly reversible with

$$U \leftrightarrow U', \quad \pi \leftrightarrow -\pi', \quad \pi_{1/2} \leftrightarrow -e^{\epsilon\,(\pi_{1/2} - \pi^\dagger_{1/2})}\, \pi_{1/2}\, e^{-\epsilon\,(\pi_{1/2} - \pi^\dagger_{1/2})}, \tag{3.23}$$

(b) symplectic, $\omega' = \omega$, and (c) approximately preserving $H(U, \pi)$ as $H(U', \pi') = H(U, \pi) + O(\epsilon^3)$.

Once consistent MD [Eqs. (3.20)–(3.22)] is defined on $TG^{\mathbb{C}}$, constrained MD on $T\mathcal{R}$ can be constructed using the RATTLE algorithm [23, 24] (see Ref. [20] for details),[4]

$$\pi_{1/2} = \pi - \epsilon\, [DV(U)]^\dagger - \lambda, \tag{3.24}$$

$$U' = e^{\epsilon\, (\pi_{1/2} - \pi^\dagger_{1/2})}\, e^{\epsilon\, \pi^\dagger_{1/2}}\, U, \tag{3.25}$$

$$\pi' = e^{\epsilon\, (\pi_{1/2} - \pi^\dagger_{1/2})}\, \pi_{1/2}\, e^{-\epsilon\, (\pi_{1/2} - \pi^\dagger_{1/2})} - \epsilon\, [DV(U')]^\dagger - \lambda', \tag{3.26}$$

where the Lagrange multipliers $\lambda \in N_U\mathcal{R}$ and $\lambda' \in N_{U'}\mathcal{R}$ are determined such that $U' \in \mathcal{R}$ and $\pi' \in T_{U'}\mathcal{R}$, respectively. This MD step is again (a) reversible [Eq. (3.23) together with interchange $\lambda \leftrightarrow \lambda'$], (b) symplectic, $\omega'_{\mathcal{R}} = \omega_{\mathcal{R}}$ (thus volume preserving, $d\Omega'_{\mathcal{R}} = d\Omega_{\mathcal{R}}$), and (c) approximately preserving $H(U, \pi)$ to the same precision.

We can now define the Markov chain on $T\mathcal{R}$ as consisting of two stochastic processes [20]:
(1) Heat bath for π:

$$P_{(1)}(U', \pi' \,|\, U, \pi) = e^{-(1/2)\,\langle \pi', \pi' \rangle}\, \delta_{\mathcal{R}}(U',\, U), \tag{3.27}$$

[4]The gradient of the potential can be set to the following form [20]: $[DV(U)]^\dagger = (1/2)\left[\xi + (W'(t)/\alpha^2)\, \xi_n\right]$.

where $\delta_{\mathcal{R}}(U',\,U)$ is the delta function on $\mathcal{R}$.[5] $\pi' \in T_U\mathcal{R}$ can be generated by drawing $\tilde{\pi} \in T_U G^{\mathbb{C}}$ from the Gaussian distribution $\propto e^{-(1/2)\langle\tilde{\pi},\tilde{\pi}\rangle}$ and projecting it onto $T_U\mathcal{R}$.
(2) MD followed by Metropolis test:[6]

$$\begin{aligned}&P_{(2)}(U',\pi'\,|\,U,\pi)\\&= \min\bigl(1, e^{-[H(U',\pi')-H(U,\pi)]}\bigr)\,\delta_{T\mathcal{R}}\bigl((U',\pi'),\,T^{N_{\rm MD}}(U,\pi)\bigr)\ \ \text{for}\ \ (U',\pi')\neq(U,\pi).\end{aligned} \tag{3.28}$$

Here, $\delta_{T\mathcal{R}}(U,\pi)$ is the symplectic delta function with respect to the symplectic volume form $d\Omega_{\mathcal{R}}$, and $N_{\rm MD}$ is the number of MD steps.

Since our observables depend only on U, the above algorithm can be viewed as a stochastic process on U alone as in the standard HMC algorithm [25]:

- Step 1 (momentum refresh): Given $U \in \mathcal{R}$, generate $\tilde{\pi} \in T_U G^{\mathbb{C}}$ from the Gaussian distribution $\propto e^{-(1/2)\langle\tilde{\pi},\tilde{\pi}\rangle}$, and project it onto $T_U\mathcal{R}$ to obtain $\pi = \Pi_{\mathcal{R}}\,\tilde{\pi}$.
- Step 2 (MD): Evolve $(U,\pi) \to (U',\pi')$ by repeatedly performing the update (3.24)–(3.26).
- Step 3 (Metropolis test): Accept the proposed U' with probability $\min\bigl(1, e^{-[H(U',\pi')-H(U,\pi)]}\bigr)$.

4. Numerical tests: one-site model

The one-site model for a compact group $G = SU(n)$ is defined by the action

$$S(U) \equiv \beta e(U)\ \ \text{with}\ \ e(U) \equiv -\frac{1}{2n}\,\mathrm{tr}\,(U + U^{-1}). \tag{4.1}$$

We take β to be purely imaginary, which makes the Boltzmann weight a pure phase factor of constant modulus. In the following numerical tests, we take $e(U)$ as the observable.

The variation of the action is given by ($\mathcal{P}$ denotes the traceless projector)

$$\delta S(U) = -\frac{\beta}{2n}\,\mathrm{tr}\,[\delta U U^{-1}(U - U^{-1})] = -\frac{\beta}{2n}\,\mathrm{tr}\,[\delta U U^{-1}\mathcal{P}(U - U^{-1})]. \tag{4.2}$$

Comparing this with $\delta S(U) = \mathrm{tr}\,[\delta U U^{-1} DS(U)]$, we obtain

$$DS(U) = -\frac{\beta}{2n}\,\mathcal{P}(U - U^{-1}), \tag{4.3}$$

and therefore

$$\xi(U) = [DS(U)]^\dagger = -\Bigl[\frac{\beta}{2n}\,\mathcal{P}(U - U^{-1})\Bigr]^\dagger. \tag{4.4}$$

This defines the flow of a configuration,

$$\dot{U} = \xi(U)\,U\ \ \text{with}\ \ U|_{t=0} = U_0. \tag{4.5}$$

[5]When $U \in \mathcal{R}$ is parametrized as $U = U(t, U_0)$, the delta function is proportional to $\delta(t'-t)\,\delta(U_0',\,U_0)$, where $\delta(U_0',\,U_0)$ is the bi-invariant delta function associated with the Haar measure (dU_0) on G. Jacobian factors can be neglected in the argument for detailed balance of MD [20].

[6]The transition probability for $(U',\pi') = (U,\pi)$ is determined by the normalization $\int d\Omega'_{\mathcal{R}}\,P_{(2)}(U',\pi'\,|\,U,\pi) = 1$.

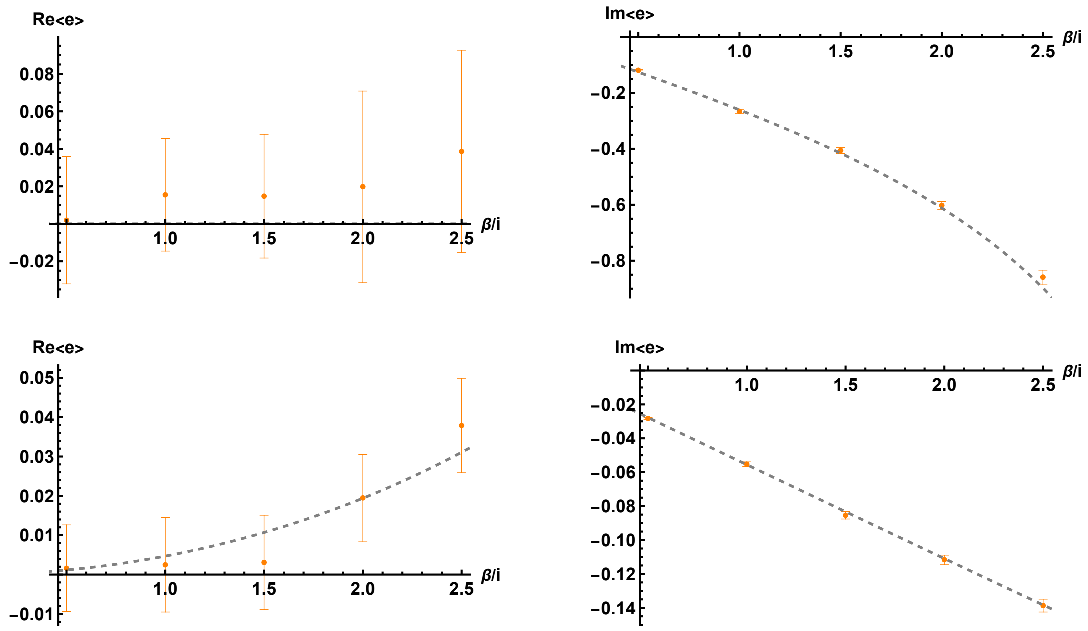

Figure 2: Real and imaginary parts of $\langle e \rangle$ in the one-site model for $\beta \in i\,\mathbb{R}$ with $G = SU(2)$ [top] and $G = SU(3)$ [bottom] [20]. The dashed lines represent the analytical results (for $G = SU(2)$, $\langle e \rangle = -I_2(\beta)/I_1(\beta)$, for which $\mathrm{Re}\,\langle e \rangle = 0$).

We numerically integrate the flow equation using an adaptive version of the Runge-Kutta-Munthe-Kaas algorithm [26, 27].

To estimate the observable, we introduce boundaries at $T_0 = 0$ and $T_1 = 0.5$ and set the MD step size to $\Delta s = \epsilon = 0.01$ with $N_{\mathrm{MD}} = 50$ steps per trajectory. We generate 5500 configurations using WV-HMC, with the first 500 configurations discarded. Figure 2 shows the real and imaginary parts of the energy density $\langle e \rangle$ for various values of $\beta \in i\,\mathbb{R}$ [20] with $G = SU(2)$ [top] and $G = SU(3)$ [bottom]. The results are in good agreement with the analytical values.

5. Conclusions and outlook

We have demonstrated that the WV-HMC algorithm can be extended to group manifolds [20] in such a way that reversibility, symplecticity, and approximate energy conservation are all realized as in the standard HMC algorithm using the leapfrog integrator. The key ingredient is to formulate the algorithm using phase-space integrals over the tangent bundle of the worldvolume, which naturally carries a symplectic structure. We have validated the correctness of the algorithms through numerical simulations of the one-site model.

The present formalism can be directly applied to lattice gauge theories without any modification to the algorithmic structure. The compact group G becomes a product group $G = \prod_{x,\mu} G_{x,\mu}$ [e.g., $G_{x,\mu} = SU(n)$ at each link (x,μ)], and the corresponding Lie algebra is given by $\mathfrak{g} = \bigoplus_{x,\mu} \mathfrak{g}_{x,\mu} = \bigoplus_{x,\mu,a} \mathbb{R}\,(T_{x,\mu})_a$ with the commutation relations $[(T_{x,\mu})_a, (T_{y,\nu})_b] = \delta_{xy}\,\delta_{\mu\nu}\,C_{ab}{}^{c}\,(T_{x,\mu})_c$. A study of lattice gauge theories with complex actions is now in progress and will be reported in forthcoming publications.

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