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

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The numerical sign problem has been a major obstacle to first-principles calculations of many important systems, including QCD at finite density. The *Worldvolume Hybrid Monte Carlo* method is a HMC algorithm which solves both the sign problem and the ergodicity problem simultaneously. In this algorithm, configurations explore the extended configuration space (worldvolume) that includes a region where the sign problem disappears and also a region where the ergodicity problem is mild. The computational cost of the algorithm is expected to be much lower than other related algorithms based on Lefschetz thimbles, because one no longer needs to calculate the Jacobian of the gradient flow of Picard and Lefschetz when generating a configuration. In this talk, after reviewing the basics of the method, we apply the method to complex scalar field theory at finite density, and report on the numerical results together with the computational cost scaling with the lattice volume.

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1. Introduction

The *numerical sign problem* is one of the major obstacles when performing first-principles calculations in various fields of physics. Typical examples include QCD at finite density, Quantum Monte Carlo simulations of quantum statistical system, finite θ vacuum, and the real-time dynamics of quantum fields.

There have been proposed various approaches to the sign problem, such as

- complex Langevin method [1–3]
- Lefschetz thimble method [4–6], from which were developed the generalized thimble method [7], the tempered Lefschetz thimble method [8–11], and the *Worldvolume HMC method* [12]
- path optimization method [13, 14]
- tensor network method [15, 16]

The main aim of my talk is to review the basics of the Worldvolume HMC (WV-HMC) method, and to argue that the computational cost for generating a configuration is cheap for local field theories. The argument is made for complex scalar field theory at finite density. The application to Yang-Mills theory is now on-going [18], based on the WV-HMC for group manifolds [19].

2. Basics of WV-HMC method

The WV-HMC method has been developed from the Lefschetz thimble method, which we explain first.

In the Lefschetz thimble method, we first complexify a dynamical variable $x = (x^i) \in \mathbb{R}^N$ to $z = (z^i = x^i + iy^i) \in \mathbb{C}^N$, where N is the number of DOF. We set an assumption (satisfied for most cases) for the action $S(x)$ and observables $\mathcal{O}(x)$ that $e^{-S(z)}$ and $e^{-S(z)}\mathcal{O}(z)$ are entire functions over $\mathbb{C}^N$. Then, thanks to Cauchy's theorem, integrals do not change under continuous deformations of the integration surface, $\Sigma_0 = \mathbb{R}^N \to \Sigma\ (\subset \mathbb{C}^N)$ as long as the boundary at $|x| \to \infty$ is fixed so as to make the integrals kept convergent:

$$\langle \mathcal{O}(x) \rangle \equiv \frac{\int_{\Sigma_0} dx\, e^{-S(x)}\, \mathcal{O}(x)}{\int_{\Sigma_0} dx\, e^{-S(x)}} = \frac{\int_{\Sigma} dz\, e^{-S(z)}\, \mathcal{O}(z)}{\int_{\Sigma} dz\, e^{-S(z)}}. \tag{1}$$

Thus, even when the integrals on Σ_0 suffer from the severe sign problem, the problem will be significantly reduced if $\mathrm{Im}\, S(z)$ is almost constant on Σ.

The prescription for such deformation is given by the *anti-holomorphic gradient flow* (see Fig. 1):

$$\dot{z}_t = \overline{\partial S(z_t)} \quad \text{with} \quad z_{t=0} = x. \tag{2}$$

This flow satisfies the property

$$[S(z_t)]^{\cdot} = \partial S(z_t) \cdot \dot{z}_t = |\partial S(z_t)|^2 \geq 0, \tag{3}$$

which means that $\mathrm{Re}\, S(z_t)$ increases along the flow except at critical points ζ,[1] while $\mathrm{Im}\, S(z_t)$ is always kept constant along the flow. So, if we define the *Lefschetz thimble* $\mathcal{J}$ associated with ζ

[1] ζ is said to be a critical point when the gradient of $S(z)$ vanishes there, $\partial S(\zeta) = 0$.

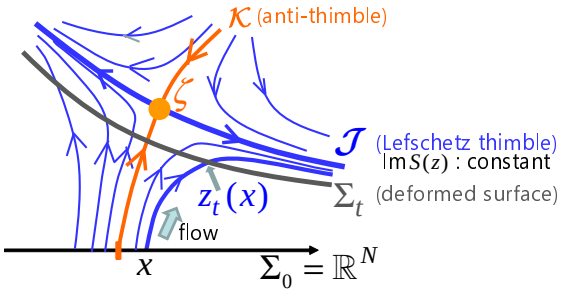

Figure 1: Deformation of integration surface.

as the union of the flows coming out of ζ, then $\mathrm{Im}\, S(z)$ is constant over $\mathcal{J}$, $\mathrm{Im}\, S(z) = \mathrm{Im}\, S(\zeta)$ $(\forall z \in \mathcal{J})$. Thus, when Σ_t approaches a Lefschetz thimble as in Fig. 1, the oscillatory integrals are expected to be tamed on Σ_t if we take a sufficiently large flow time t.

However, this is not the end of the story. Actually, there comes out another problem at large t, the *ergodicity problem*. To see this, we consider the Boltzmann weight of the form $e^{-S(x)} = e^{-\beta x^2/2}(x-i)^\gamma$ with $\beta \gg 1$ and $\gamma \in \mathbb{Z}_{>0}$ (see Fig. 2). In this case, in addition to two

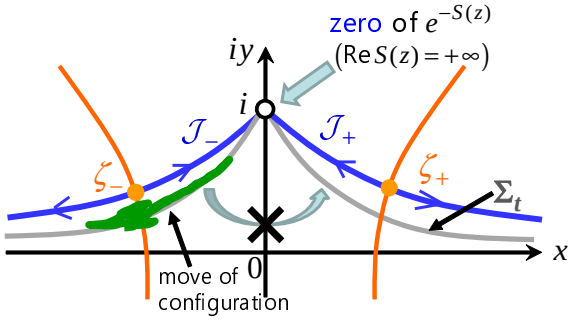

Figure 2: Ergodicity problem in the Lefschetz thimble method.

critical points $\zeta_\pm$ and their associated thimbles $\mathcal{J}_\pm$, we have a zero of $e^{-S(z)}$ at $z = i$, where $\mathrm{Re}\, S(z)$ diverges. Thus, when we consider MC processes on Σ_T at a large flow time T, it is very hard for configurations to move from a branch to another branch stochastically.

The solution proposed in Refs. [8] and [9] is to temper the system with the flow time, which then prompts the equilibration on Σ_T (see Fig. 3). This *tempered Lefschetz thimble method* is the first algorithm that solves the sign and ergodicity problems simultaneously. The disadvantage is its high numerical cost $O(N^3)$, which comes from the computation of the Jacobian matrix $J \equiv (\partial z^i/\partial x^a)$ $(i, a = 1, \ldots, N)$.

To overcome this, we invented the *Worldvolume Hybrid Monte Carlo* (WV-HMC) method [12], which is a HMC algorithm on a continuous accumulation of integration surfaces, $\mathcal{R} \equiv \bigcup_{0 \le t \le T} \Sigma_t$ (see Fig. 4). The computational cost is much reduced, because we no longer need to compute the Jacobian matrix in the configuration generation, and also because the autocorrelation is reduced due to the use of HMC. We call the region $\mathcal{R}$ the *worldvolume* because it can be regarded as an orbit of integration surface in the "target space" $\mathbb{C}^N = \mathbb{R}^{2N}$.[2]

[2]We borrowed terminology from string theory, where an orbit of a particle is called a worldline, that of a string a

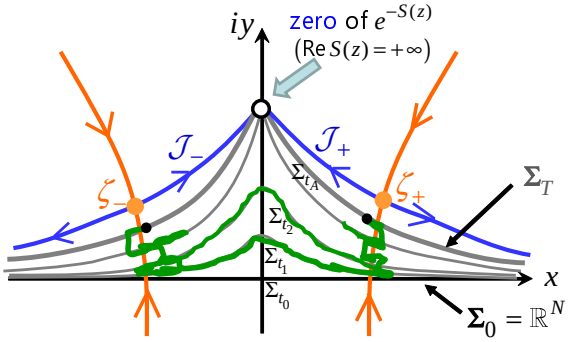

Figure 3: Tempered Lefschetz thimble method [8].

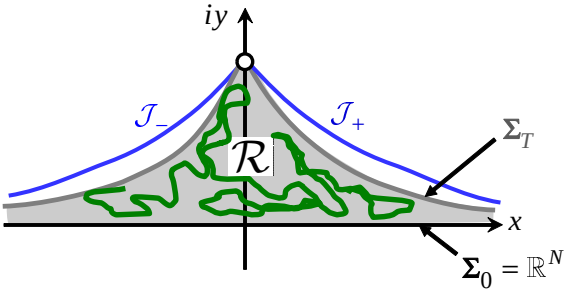

Figure 4: Worldvolume HMC [12].

The basic idea in the algorithm is as follows:

$$\begin{aligned}\langle O(x)\rangle &\equiv \frac{\int_{\Sigma_0} dx\, e^{-S(x)} O(x)}{\int_{\Sigma_0} dx\, e^{-S(x)}} = \frac{\int_{\Sigma_t} dz_t\, e^{-S(z_t)} O(x)}{\int_{\Sigma_t} dz_t\, e^{-S(z_t)}} \\ &= \frac{\int_0^T dt\, e^{-W(t)} \int_{\Sigma_t} dz_t\, e^{-S(z_t)} O(x)}{\int_0^T dt\, e^{-W(t)} \int_{\Sigma_t} dz_t\, e^{-S(z_t)}} = \frac{\int_{\mathcal{R}} dt\, dz_t\, e^{-W(t)}\, e^{-S(z_t)} O(x)}{\int_{\mathcal{R}} dt\, dz_t\, e^{-W(t)}\, e^{-S(z_t)}}. \end{aligned} \tag{4}$$

From the first line to the second line, we have used the fact that the numerator and the denominator are both independent of flow time t, so that we can make an average over t for each of them with an arbitrary weight $e^{-W(t)}$.[3]

Note that our worldvolume $\mathcal{R}$ is an $(N+1)$-dimensional submanifold in the target space $\mathbb{C}^N = \mathbb{R}^{2N}$ (see Fig. 5). A configuration on $\mathcal{R}$ can be specified by either of its target-space coordinates $z \in \mathbb{C}^N$ or a pair of the flow time and initial configuration, (t, x). Accordingly, there can be two ways in introducing a HMC algorithm [12], one is (1) the *target-space picture* which treats a Markov chain of the form $\{z, z', z', \ldots\}$, and the other is (2) the *parameter-space picture* whose Markov chain takes the form $\{(t,x), (t',x'), \ldots\}$. At first sight, (2) may seem simpler and easier to implement, but actually (1) is faster and more solid as an algorithm, and we use it in the following discussions.[4]

worldsheet, and that of a membrane (surface) a worldvolume.

[3] $W(t)$ is chosen such that the appearance probabilities are almost the same at different t [12]. Statistical analysis method for the WV-HMC is established in Ref. [20].

[4] Recently, the second picture is further pursued in Ref. [21].

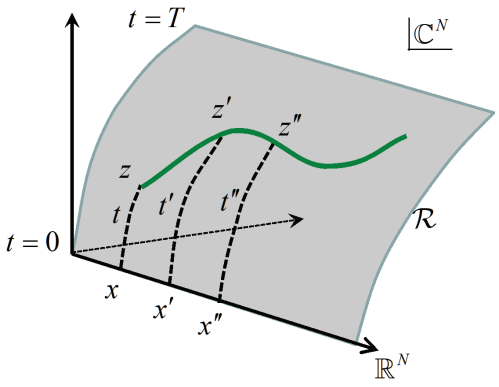

Figure 5: Two pictures in WV-HMC [12].

We close this section with a discussion on the computational cost of WV-HMC. The expensive steps can be classified into the following three parts.
(i) configuration flow:

$$\dot{z}_i = \overline{\partial_i S(z)}, \tag{5}$$

whose computational cost is $O(N)$.
(ii) vector flow:

$$\dot{v}_i = \overline{\partial_i \partial_j S(z)\, v_j}. \tag{6}$$

The computational cost is $O(N^2)$ when the Hessian matrix $H_{ij}(z) = \partial_i \partial_j S$ is dense, but it becomes $O(N)$ when the Hessian matrix $H_{ij}(z)$ is sparse, as in local field theories (with the absence of fermion determinant).
(iii) RATTLE:[5]

$$z' = z + \Delta s\, \pi - \Delta s^2\, \overline{\partial V(z)} - \lambda, \tag{7}$$

$$\pi_{1/2} = (z' - z)/\Delta s, \tag{8}$$

$$\tilde{\pi}' = \pi_{1/2} - \Delta s\, \overline{\partial V(z')}, \tag{9}$$

$$\pi' = \Pi'_{\mathcal{R}} \tilde{\pi}'. \tag{10}$$

Here, Δs is the step size in the molecular dynamics, $V(z) \equiv \mathrm{Re}\, S(z) + W(t(z))$ is the potential, and $\Pi'_{\mathcal{R}}$ is the projection onto $T_{z'}\mathcal{R}$. The Lagrange multiplier $\lambda \in N_z\mathcal{R}$ is determined such that $z' \in \mathcal{R}$, which is equivalent to the condition that there exists a triplet $h \in \mathbb{R}$, $u \in \mathbb{R}^N$, and $\lambda \in N_z\mathcal{R}$ such that the following equation is satisfied (see Fig. 6):

$$z_t(x) + \Delta s\, \pi - \Delta s^2\, \overline{\partial V(z)} - \lambda = z_{t+h}(x + u). \tag{11}$$

This can be solved by Newton's method with an iterative linear solver (such as BiCGStab) that uses

[5] The RATTLE algorithm [22, 23] was first introduced to the thimble method in [6], where HMC updates are made on a single dominant thimble. This method was generalized to HMC updates on a deformed surface Σ_t in [24] (see also [11]).

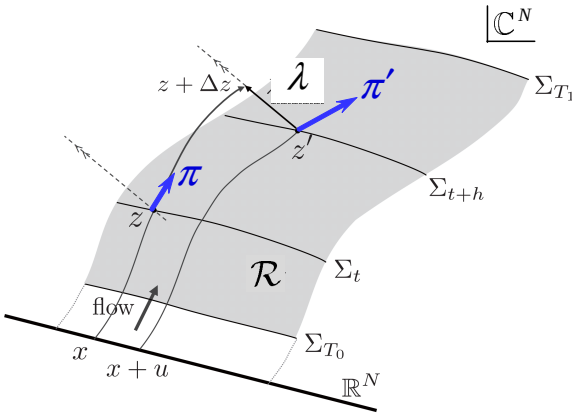

Figure 6: RATTLE algorithm in WV-HMC $\left(\Delta z \equiv \Delta s\, \pi - \Delta s^2\, \overline{\partial V(z)}\right)$ [12].

only configuration flows and vector flows. Thus, the computational cost for RATTLE is $O(N)$ for local field theories.

We thus conclude that the total computational cost at each molecular dynamics step should be $O(N)$ for local field theories.

3. Application of WV-HMC method to complex scalar field theory at finite density

Denoting a complex scalar field $\varphi(x)$ by two real scalar fields as $\varphi(x) = (1/\sqrt{2})\,[\varphi_1(x) + i\varphi_2(x)]$, the continuum action is given by

$$S(\varphi) = \int d^d x \left[|\partial_\nu \varphi|^2 + m^2\,|\varphi|^2 + \lambda\,|\varphi|^4 + \mu(\varphi^* \partial_0 \varphi - \partial_0 \varphi^* \varphi)\right] \quad (x_0\text{: Euclidean time}). \tag{12}$$

Treating the chemical potential μ as a complex gauge field, the lattice action is given by (see [17])

$$S(\varphi) \equiv \sum_n \Big[(2d + m^2)\,|\varphi_n|^2 + \lambda\,|\varphi_n|^4 - \sum_{\nu=0}^{d-1} \big(e^{\mu\,\delta_{\nu,0}}\,\varphi_n^*\,\varphi_{n+\nu} + e^{-\mu\,\delta_{\nu,0}}\,\varphi_n\,\varphi_{n+\nu}^*\big)\Big]. \tag{13}$$

This can be rewritten to the following form by introducing (ξ_n, η_n) with $\varphi_n = (1/\sqrt{2})\,(\xi_n + i\eta_n)$:

$$\begin{aligned} S(\xi,\eta) = \sum_n \Big[& \frac{2d+m^2}{2}\,(\xi_n^2 + \eta_n^2) + \frac{\lambda}{4}\,(\xi_n^2 + \eta_n^2)^2 - \sum_{i=1}^{d-1} (\xi_{n+i}\xi_n + \eta_{n+i}\eta_n) \\ & - \cosh\mu\,(\xi_{n+0}\xi_n + \eta_{n+0}\eta_n) - i\sinh\mu\,(\xi_{n+0}\eta_n - \eta_{n+0}\xi_n)\Big]. \end{aligned} \tag{14}$$

We complexify $(\xi,\eta) \in \mathbb{R}^{2V}$ to $(z,w) \in \mathbb{C}^{2V}$ (V: lattice volume) with the flow equation

$$\dot{z}_n = \overline{\partial S(z,w)/\partial z_n}, \quad \dot{w}_n = \overline{\partial S(z,w)/\partial w_n}. \tag{15}$$

We are now in a position to apply to this model the general prescription described in the previous section. The computational cost scaling for two-dimensional square lattices is given in Fig. 7, which shows that it is linear in V at large lattice sizes, as expected.

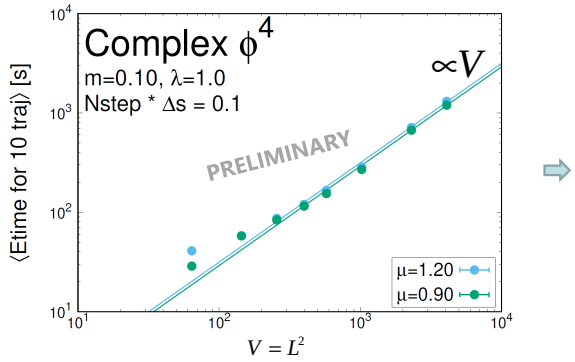

Figure 7: Computational cost scaling for two-dimensional square lattices. DOF is given by $N = 2V$.

The WV-HMC also works for group manifolds [19]. As a simple example, let us consider the one-site model with a purely imaginary coupling:

$$S(U) \equiv \beta\, e(U) \equiv \frac{\beta}{2N} \operatorname{tr}\,(2 - U - U^{-1}), \tag{16}$$

where $U \in G = SU(N)$ and $\beta \in i\mathbb{R}$. The numerical estimates of the energy density $\langle e \rangle$ with $N = 2$ are given in Fig. 8 for various β, which demonstrates the perfect agreement with the analytic result, $\langle e \rangle_{\text{exact}} = 1 - I_2(\beta)/I_1(\beta)$ ($I_n(\beta)$ is the modified Bessel function of the first kind).

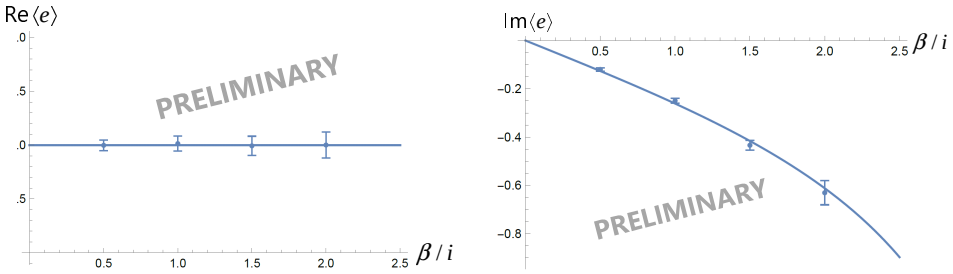

Figure 8: Estimates of $\langle e \rangle$ of the one-site model [19]. The sold lines are analytic results.

4. Summary and outlook

We have argued that the WV-HMC is a promising method towards solving the sign problem, and discussed that it allows a coding to reduce the computational cost to $O(V)$ (V: lattice volume) for local field theories. We exemplified the expected computational cost scaling for complex scalar field theory at finite density.

Our group has started applying the algorithm to QCD, encouraged by the success of extending the WV-HMC to a path integral over a group manifold [19], which can be readily applied to Yang-Mills theories [18]. In parallel with this research, we believe that it should be important to keep improving the algorithm itself.

A particularly important project in the near future should be the development of MC calculations for the real-time dynamics of quantum fields. Once accomplished, this will give us a tool for first-

principles calculations of nonequilibrium processes, such as those in the early universe and heavy ion collision experiments.

Acknowledgments

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