RMHMC by embedding $SU(N)$ into $M_N(\mathbb{C})$

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1. Introduction

This note tries to spell out possible complexities, and how they may be overcome, in Luchang's idea of embedding $SU(N)$ in $M_N(\mathbb{C})$, the space of $N \times N$ complex matrices, for RMHMC/Fourier acceleration. The original note can be found in this link. This amazing idea was described elegantly already in the original note, and this note only includes minor modifications and additions of the detailed formulas to it.

2. Basic idea

In RMHMC, we would like to perform the Hamiltonian evolution with the nonseparable Hamiltonian of the form:

$$H(\pi, U) \equiv \frac{1}{2} \pi_a G_{ab}^{-1}(U) \pi_b + S(U) - \frac{1}{2} \log \det G(U), \tag{2.1}$$

where $U \in SU(N)$ and π_a the momentum in the Lie algebra. However, the constraint $U \in SU(N)$ enforces us to exponentiate the Lie algebra elements in the discretized integrators,

which induces nonlinear terms that break symplecticity because of the nonseparable nature of the kinetic term.

The idea is to put away the constraint $U \in SU(N)$ and instead work in the larger space $W \in M_N(\mathbb{C})$. We can then take as the dynamical variables the real and imaginary parts of the matrix elements: $W \equiv (w_{jk})$, $w_{jk} \equiv x_{jk} + iy_{jk}$, and use the symplectic integrators for x_{jk}, y_{jk} with the conventional linear form.

Nevertheless, we want to make the deviation from $SU(N)$ as small as possible to make it controllable. For this purpose, it is convenient to parametrize $W \in M_N(\mathbb{C})$ in the form of a polar decomposition:

$$W = e^{i\theta}\Phi U, \tag{2.2}$$

where Φ is an $N \times N$ hermitian matrix and $U \in SU(N)$. We will identify the $SU(N)$ part the physical gauge field. The uncompact nature of $M_N(\mathbb{C})$ is then fully described by Φ, and therefore we introduce the additional potential for Φ such as:

$$S_0(\Phi) \equiv \frac{\lambda}{2N} \operatorname{tr} \left[(\Phi - \mathbb{1}_N)(\Phi - \mathbb{1}_N)^\dagger \right] \tag{2.3}$$

with the tunable parameter $\lambda \in \mathbb{R}_{>0}$.

3. Uniqueness and sufficiency of the decomposition

To begin with, we clarify that the decomposition (2.2) well-determines the gauge field U and that the determined U spans the entire configuration space of the original theory.

As is well known, for an invertible matrix $W \in GL(N)$, the polar decomposition:

$$W = \Phi\Omega \tag{3.1}$$

is unique, where Φ is a positive hermitian matrix and $\Omega \in U(N)$. Since in the space of $W \in M_N(\mathbb{C})$ the matrices with $\det W = 0$ are measure zero, and furthermore since $\det W = 0$ will not happen in the vicinity of the unitary matrix, we may safely assume below that the decomposition (3.1) well-determines Φ and Ω even for $W \in M_N(\mathbb{C})$ for an appropriately chosen λ.

The remainder is to decompose $\Omega \in U(N)$ into $e^{i\theta} \in U(1)$ and $U \in SU(N)$. This is unique up to the center $\mathbb{Z}_N$ of $SU(N)$. In fact, suppose

$$\Omega = e^{i\theta}U, \tag{3.2}$$

then so as

$$\Omega = e^{i\theta'}U' \tag{3.3}$$

with

$$\theta' \equiv \theta + 2\pi n/N, \quad U' \equiv e^{-2\pi in/N}U \quad (n \in \mathbb{Z}). \tag{3.4}$$

In other words,

$$U(N) \simeq U(1) \times SU(N)/\mathbb{Z}_N. \tag{3.5}$$

An obvious way to get a representative of the RHS of the isometry is:

$$i\theta \equiv \frac{1}{N} \log \det \Omega, \tag{3.6}$$

where we take the principal branch in the logarithm, and then set:

$$U \equiv e^{-i\theta}\Omega. \tag{3.7}$$

Since our action $S(U)$ is not necessarily $\mathbb{Z}_N$ symmetric, we need to carefully choose the integer $n \in \{0, \cdots, N-1\}$; otherwise, the action can have a discontinuous jump as we step over to a different $\mathbb{Z}_N$ sector. The identification of the appropriate $\mathbb{Z}_N$ sector should be possible when the discretized evolution well-approximates the continuous time limit, in which n is unambiguously determined by smoothness. In practice, it should be sufficient to trace the angle variable θ and to choose n such that the evolution looks most continuous. In the following, the map (2.2) is used under this understanding of the continuity of the Hamiltonian evolution, which makes the decomposition unique.

Having understood the uniqueness, its surjective property as a map $M_N(\mathbb{C}) \to SU(N)$ is obvious since it is sufficient to take $W \in SU(N) \subset M_N(\mathbb{C})$.

4. Definition of the integration measure in $M_N(\mathbb{C})$

In order to define the path integral in the larger space and to prove the equivalence to the original one, we first define an appropriate measure for $M_N(\mathbb{C})$ and its relation to the Haar measure of $SU(N)$. As Luchang correctly pointed out, the key point is to make it right-invariant under the multiplication of $U(N)$ matrices, which ensures, according to the form of the decomposition (2.2), the associated decomposition of the measure to be also right invariant, meaning that it does not depend on the physical gauge field U (and also θ).

We define such a measure by first defining the right-invariant metric tensor $\mathbf{g}$ (which turns out to be also left-invariant):

$$\mathbf{g} \equiv \mathrm{tr}\,[dW\,dW^\dagger]. \tag{4.1}$$

The one-form $dW \equiv (dw_{jk})$ is defined in the element basis as:

$$dw_{jk} = dx_{jk} + idy_{jk}, \tag{4.2}$$

and therefore:

$$\mathbf{g} = \sum_{j,k} [dx_{jk}^2 + dy_{jk}^2]. \tag{4.3}$$

The associated volume form can be thus derived to be:

$$(dW) \equiv \prod_{j,k} \left(dx_{jk} dy_{jk} \right). \tag{4.4}$$

In $SU(N)$, a convenient one-form basis is given by the Maurer-Cartan form:

$$\Theta \equiv iT_a \Theta_a = dU U^{-1}. \tag{4.5}$$

The generators T_a of $SU(N)$ are here taken to be hermitian and normalized as:

$$\mathrm{tr}\,[T_a T_b] = \delta_{ab}. \tag{4.6}$$

Θ_a is dual to the right-invariant derivative D_a:

$$D_a U = iT_a U, \tag{4.7}$$

i.e.,

$$dU = \Theta_a D_a U, \tag{4.8}$$

in accordance to eq. (4.5). The Haar measure is:

$$(dU) \equiv \prod_a \Theta_a \tag{4.9}$$

up to an irrelevant normalization constant.

With the traceless hermitian generators T_a, hermitian matrices can be expanded as:

$$\Phi = \phi_0 \mathbb{1}_N + \phi_a T_a. \tag{4.10}$$

The map (2.2) then induces the relation:

$$dW = ie^{i\theta}\Phi U d\theta + e^{i\theta} U d\phi_0 + e^{i\theta} T_a U d\phi_a + ie^{i\theta}\Phi T_a U \Theta_a. \tag{4.11}$$

The metric can be rewritten accordingly:

$$\mathbf{g} = \mathrm{tr}\,\Phi^2 d\theta^2 + 2\,\mathrm{tr}\,[T_a\Phi^2]d\theta\,\Theta_a + d\phi_0^2 + d\phi_a^2 + \mathrm{tr}\,[T_a T_b\Phi^2]\Theta_a\Theta_b. \tag{4.12}$$

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Thus, as advertised above, the decomposition of the measure can be done with the Jacobian that only depends on Φ:

$$(dW) = \sqrt{\det g(\Phi)}\, d\theta\, d\phi_0 \left(\prod_a d\phi_a \right) \left(\prod_a \Theta_a \right), \tag{4.13}$$

where the determinant is given by:

$$\det g(\Phi) = \det \begin{pmatrix} \operatorname{tr}\Phi^2 & \operatorname{tr}[T_b\Phi^2] & & \\ \operatorname{tr}[T_a\Phi^2] & (1/2)\operatorname{tr}[\{T_a,T_b\}\Phi^2] & & \\ & & 1 & \\ & & & \mathbb{1}_{N^2-1} \end{pmatrix} \tag{4.14}$$

$$= \det \begin{pmatrix} \operatorname{tr}\Phi^2 & \operatorname{tr}[T_b\Phi^2] \\ \operatorname{tr}[T_a\Phi^2] & (1/2)\operatorname{tr}[\{T_a,T_b\}\Phi^2] \end{pmatrix}. \tag{4.15}$$

5. Path integral in the larger space

It is now easy to relate the original path integral:

$$Z_{SU(N)} \equiv \int (dU)\, e^{-S(U)} \tag{5.1}$$

to the path integral in the larger space:

$$Z_{M_N(\mathbb{C})} \equiv \int (dW)\, e^{-S(U)-S_0(\Phi)}, \tag{5.2}$$

where U is regarded as a function of W through the map (2.2). The integration domain of W is restricted s.t. the scale part Φ gives $\det\Phi \geq 0$, which is not important in the following. Plugging the expressions (2.3) and (4.13) into eq. (5.2), we find:

$$Z_{M_N(\mathbb{C})} = (2\pi) \int (dU)\, e^{-S(U)} \int_{\det\Phi\geq 0} d\phi_0 \left(\prod_a d\phi_a \right) \sqrt{\det g(\Phi)}\, e^{-S_0(\Phi)}$$

$$= (2\pi) Z_{SU(N)} \int_{\det\Phi\geq 0} d\phi_0 \left(\prod_a d\phi_a \right) \sqrt{\det g(\Phi)}\, e^{-S_0(\Phi)}. \tag{5.3}$$

The factorized integral is bounded from above:

$$\int_{\det\Phi\geq 0} d\phi_0 \left(\prod_a d\phi_a \right) \sqrt{\det g(\Phi)}\, e^{-S_0(\Phi)} \leq \int d\phi_0 \left(\prod_a d\phi_a \right) \sqrt{\det g(\Phi)}\, e^{-S_0(\Phi)}, \tag{5.4}$$

and the bound is a Gaussian integral over a function that is $O(\phi^{N^2})$ and thus has a finite value. In other words, the two partition functions are related by a finite overall constant.

The above shows that we can calculate the expectation values of the observables $\mathcal{O}(U)$ in the larger path integral and the nontrivial Jacobian factor will automatically drop out to ensure them to be the same as those of the original physical system.

6. Jacobian matrix and the RMHMC Hamiltonian

Having established the equivalence, we can focus on writing down the RMHMC algorithm by taking $w_{jk} = x_{jk} + i y_{jk}$ as dynamical variables. In this section, we describe a simple choice of the Hamiltonian for the RMHMC.

The basis of the tangent vectors that is conjugate to $\{dx_{jk}, dy_{jk}\}$ is $\{\partial_{x_{jk}}, \partial_{y_{jk}}\}$. Accordingly, we can expand the momentum π in the form:

$$\pi \equiv \pi_{jk}^x \partial_{x_{jk}} + \pi_{jk}^y \partial_{y_{jk}}. \tag{6.1}$$

We have another one-form basis $\{d\theta, \Theta_a, d\phi_0, d\phi_a\}$, which has the conjugate basis $\{\partial_\theta, D_a, \partial_{\phi_0}, \partial_{\phi_a}\}$:

$$\pi \equiv \pi_\theta \partial_\theta + \pi_a D_a + \rho_0 \partial_{\phi_0} + \rho_a \partial_{\phi_a}. \tag{6.2}$$

π_a is the momentum conjugate to the physical variables that we would like to accelerate.

To obtain the relation between the two expansion coefficients, let us rewrite the relation (4.11) in the matrix form:

$$
\begin{bmatrix} dx_{jk} & dy_{jk} \end{bmatrix} = \begin{bmatrix} d\theta & \Theta_a & d\phi_0 & d\phi_a \end{bmatrix} \times
$$
$$
\times \begin{bmatrix} -\sin\theta \operatorname{Re}(\Phi U)_{jk} - \cos\theta \operatorname{Im}(\Phi U)_{jk} & \cos\theta \operatorname{Re}(\Phi U)_{jk} - \sin\theta \operatorname{Im}(\Phi U)_{jk} \\ -\sin\theta \operatorname{Re}(\Phi T_a U)_{jk} - \cos\theta \operatorname{Im}(\Phi T_a U)_{jk} & \cos\theta \operatorname{Re}(\Phi T_a U)_{jk} - \sin\theta \operatorname{Im}(\Phi T_a U)_{jk} \\ \cos\theta \operatorname{Re}(\Phi U)_{jk} - \sin\theta \operatorname{Im}(\Phi U)_{jk} & \sin\theta \operatorname{Re} U_{jk} + \cos\theta \operatorname{Im} U_{jk} \\ \cos\theta \operatorname{Re}(T_a U)_{jk} - \sin\theta \operatorname{Im}(T_a U)_{jk} & \cos\theta \operatorname{Re}(T_a U)_{jk} + \cos\theta \operatorname{Im}(T_a U)_{jk} \end{bmatrix}
$$
$$
\equiv \begin{bmatrix} d\theta & d\phi_0 & d\phi_a & \Theta_a \end{bmatrix} J(\theta, U, \Phi). \tag{6.3}
$$

We then have:

$$
\begin{bmatrix} \partial_{x_{jk}} \\ \partial_{y_{jk}} \end{bmatrix} = J(\theta, U, \Phi)^{-1} \begin{bmatrix} \partial_\theta \\ D_a \\ \partial_{\phi_0} \\ \partial_{\phi_a} \end{bmatrix}. \tag{6.4}
$$

Though the kinetic term for the unphysical sector can be taken arbitrarily, for simplicity, we take the Hamiltonian:

$$H_{M_N(\mathbb{C})} \equiv \frac{1}{2\mu_\theta^2}\pi_\theta^2 + \frac{1}{2}\pi_a G_{ab}^{-1}(U)\pi_b + \frac{1}{2\mu^2}(\rho_0^2 + \rho_a^2) + S(U) + S_0(\Phi) - \frac{1}{2}\log\det G(U), \tag{6.5}$$

with the tunable parameters μ_θ and μ. The Jacobian matrix $J(\theta, U, \Phi)$ mixes the physical and unphysical modes according to the transformation law (6.3). We write the corresponding expression in the x_{jk}, y_{jk} basis simply as:

$$H_{M_N(\mathbb{C})}(\pi, W) = \frac{1}{2}\pi_I \tilde{G}_{JK}^{-1}(W)\pi_J + S(U) + S_0(W) - \frac{1}{2}\log\det\tilde{G}(U), \tag{6.6}$$

where we absorbed the normalization constants into the determinant and the index I runs all the $2N^2$ elements $(w_I) \equiv (x_{jk}, y_{jk})$.

7. RMHMC in $M_N(\mathbb{C})$

We now have a path integral (5.2) over $2N^2$ real variables $(w_I) = (x_{jk}, y_{jk})$ with the flat measure (4.4). We are thus ready to write down the RMHMC with the Hamiltonian (6.6). We show below the algorithm with the simple implicit leapfrog:

1. Suppose we have a configuration W.

2. Generate π_I with the distribution:

$$w_{\text{init}}(\pi; W) \equiv \sqrt{\frac{\det \tilde{G}(W)}{(2\pi)^{2N^2}}} \times e^{-(1/2)\pi_I \tilde{G}_{IJ}^{-1}(W)\pi_J}, \tag{7.1}$$

   which is normalized against the flat measure:

$$(d\pi) \equiv \prod_I d\pi_I. \tag{7.2}$$

3. Integrate the leapfrog multiple times to get a new phase space configuration (π', W'):

$$\pi_I^{1/2} = \pi_I - \frac{\epsilon}{2}\partial_{w_I} H(\pi^{1/2}, W), \tag{7.3}$$

$$w_I^{1/2} = w_I + \frac{\epsilon}{2}\partial_{\pi_I} H(\pi^{1/2}, W), \tag{7.4}$$

$$w_I' = w_I^{1/2} + \frac{\epsilon}{2}\partial_{\pi_I} H(\pi^{1/2}, W'), \tag{7.5}$$

$$\pi_I' = \pi_I^{1/2} - \frac{\epsilon}{2}\partial_{w_I} H(\pi^{1/2}, W'). \tag{7.6}$$

4. Accept/reject with the probability:

$$\min\left(1, e^{-H_{M_N(\mathbb{C})}(\pi', W') + H_{M_N(\mathbb{C})}(\pi, W)}\right). \tag{7.7}$$

   This algorithm satisfies the detailed balance for the equilibrium distribution:

$$w_{\text{eq}}(W) \equiv \frac{1}{Z_{M_N(\mathbb{C})}} \times e^{-S(U) - S_0(W)}. \tag{7.8}$$

Indeed, the probability of getting the configuration W' accepted from W is:

$$P_{\text{accept}}(W' \leftarrow W) \equiv \int (d\pi')(d\pi) \, \min\left(1, e^{-H_{M_N(\mathbb{C})}(\pi', W') + H_{M_N(\mathbb{C})}(\pi, W)}\right) \times \tag{7.9}$$

$$\times \, \delta\left((\pi', W'), \Psi_{\text{MD}}(\pi, W)\right) w_{\text{init}}(\pi; W), \tag{7.10}$$

where $\Psi_{\text{MD}}(\pi, W)$ stands for the outcome of the symplectic integrator. As usual, using that

$$w_{\text{init}}(\pi; W) w_{\text{eq}}(W) = \frac{1}{(2\pi)^{N^2} Z_{M_N(\mathbb{C})}} e^{-H_{M_N(\mathbb{C})}(\pi, W)}, \tag{7.11}$$

we have:

$$P_{\text{accept}}(W' \leftarrow W)w_{\text{eq}}(W)$$

$$= \frac{1}{(2\pi)^{N^2} Z_{M_N(\mathbb{C})}} \int (d\pi')(d\pi) \, \min\left(e^{-H_{M_N(\mathbb{C})}(\pi',W')}, e^{-H_{M_N(\mathbb{C})}(\pi,W)}\right) \times \delta\left((\pi',W'), \Psi_{\text{MD}}(\pi,W)\right)$$

$$= \frac{1}{(2\pi)^{N^2} Z_{M_N(\mathbb{C})}} \int (d\pi')(d\pi) \, \min\left(e^{-H_{M_N(\mathbb{C})}(\pi',W')}, e^{-H_{M_N(\mathbb{C})}(\pi,W)}\right) \times \delta\left((-\pi,W), \Psi_{\text{MD}}(-\pi',W')\right)$$

$$= \frac{1}{(2\pi)^{N^2} Z_{M_N(\mathbb{C})}} \int (d\pi)(d\pi') \, \min\left(e^{-H_{M_N(\mathbb{C})}(\pi,W)}, e^{-H_{M_N(\mathbb{C})}(\pi',W')}\right) \times \delta\left((\pi,W), \Psi_{\text{MD}}(\pi',W')\right)$$

$$= P_{\text{accept}}(W \leftarrow W')w_{\text{eq}}(W'). \tag{7.12}$$