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Random Selection from Trace-Biased Invariant Distributions of $SU(3)$ Matrices*

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The dependence of $SU(3)$ invariant measure on the real and imaginary parts of the $SU(3)$ matrix trace is derived and used to construct an algorithm for random selection of $SU(3)$ stepping matrices for Monte Carlo lattice gauge calculations. The algorithm generates an ensemble of trace-biased, but otherwise invariantly distributed $SU(3)$ matrices matched to prescribed values of the trace average and trace standard deviation, and depends on a prescribed shape parameter for added flexibility.

I. INTRODUCTION

The formulas for $SU(n)$ invariant measure and $SU(n)$ matrices in terms of polar parameters [1] are applied here to obtain a random sampling algorithm for $SU(3)$ stepping matrices for Monte Carlo lattice gauge calculations of quantum chromodynamics. The algorithm's purpose is to speed up the calculation of thermalized and uncorrelated ensembles of configurations of matrices attached to the lattice links.

The matrices would be sampled from a product distribution; the first factor is the

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invariant (Haar) measure for $SU(3)$, and the second biases the sample in the neighborhood of the unit matrix I. The degree of bias depends on adjustable parameters which would be optimized in numerical experiments on the system under study. The goal is to minimize the number of Monte Carlo sweeps required to generate thermalized and uncorrelated lattice configurations and so to minimize the computer time needed to generate a usable ensemble of configurations.

Numerical calculations of decorrelation rates and other criteria for this algorithm and comparisons with other algorithms will be described in a subsequent paper.

Let A be an $SU(3)$ matrix. Its distance $d(A, I)$ from the identity is represented conveniently by the trace metric

$$[d(A, I)]^2 = \text{trace}(A - I)(A^\dagger - I) = \text{trace}(2I - A - A^\dagger) = 2(3 - t)$$

where $t = \text{Real}(\text{trace}\, A)$. Thus, biasing A to the neighborhood of I may be done by biasing t to a neighborhood of 3.

Let A be represented in diagonal form:

$$A = V^{-1}(\boldsymbol{\rho}, \boldsymbol{\psi})\, D(\boldsymbol{\theta})\, V(\boldsymbol{\rho}, \boldsymbol{\psi}).$$

Here $D(\boldsymbol{\theta})$ is the diagonal matrix of eigenvalues $\exp(i\theta_i)$, $i = 1, 2, 3$, in any order. The eigenangles satisfy

$$\theta_1 + \theta_2 + \theta_3 = 2n\pi. \tag{1}$$

The diagonalizing matrix V can be taken as an $SU(3)$ matrix parameterized by three radial variables $\rho_{21}, \rho_{31}, \rho_{32}$ (or equivalently, the complementary variables $\bar{\rho}_{21} = (1 - \rho_{21}^2)^{1/2}$, etc.) and three phase variables $\psi_{21}, \psi_{31}, \psi_{32}$. This amounts to a specialization of V by the conditions det $V = +1$, V_{11} and $V_{33} = \text{real}$. The invariant $SU(3)$ measure $d\mu(A)$ factors into

$$d\mu(A) = d\nu(\boldsymbol{\rho}, \boldsymbol{\psi})\, d\lambda(\boldsymbol{\theta}),$$

where, up to an overall constant,

$$d\nu(\boldsymbol{\rho}, \boldsymbol{\psi}) = d(\bar{\rho}_{21})^2 d(\bar{\rho}_{31})^4 d(\bar{\rho}_{32})^2\, d\psi_{21}, d\psi_{31}, d\psi_{32}$$

and

$$d\lambda(\boldsymbol{\theta}) = \left| \sin\frac{(\theta_1 - \theta_2)}{2} \sin\frac{(\theta_2 - \theta_3)}{2} \sin\frac{(\theta_3 - \theta_1)}{2} \right|^2 d\theta_1\, d\theta_2.$$

To generate random matrices A, one would:

(a) Generate ρ and ψ variables distributed according to $d\nu(\boldsymbol{\rho}, \boldsymbol{\psi})$ and construct V according to the rules of [1]. For the explicit algorithm, see Section IV.

(b) Transform $d\lambda(\boldsymbol{\theta})$ from angle variables to trace variables and introduce a bias factor as a function of t. The trace variables will be generated randomly and the θ_i calculated from them. These are the tasks of the following sections.

(c) Finally, calculate A from $A = V^{-1}D(\boldsymbol{\theta})V$.

II. Trace Space for $SU(3)$

We shall map the manifold of eigenvalues θ_i to trace space. Take θ_1 and θ_2 as independent variables, with θ_3 dependent through (1). Triplets $(\theta_1, \theta_2, \theta_3)$ and $(\theta'_1, \theta'_2, \theta'_3)$ related by

$$\theta_i = \theta'_i - 2n_i\pi, \qquad i = 1, 2, 3 \tag{2}$$

represent the same point on the manifold.

Set

$$T = \text{trace } A = t + iu, \tag{3}$$

so that

$$T = \exp(i\theta_1) + \exp(i\theta_2) + \exp(i\theta_3), \tag{4a}$$

$$t = \cos\theta_1 + \cos\theta_2 + \cos\theta_3 = \cos\theta_1 + \cos\theta_2 + \cos(\theta_1 + \theta_2), \tag{4b}$$

$$u = \sin\theta_1 + \sin\theta_2 + \sin\theta_3 = \sin\theta_1 + \sin\theta_2 - \sin\theta_1 + \theta_2). \tag{4c}$$

A complex T which is the trace of an SU_3 matrix will be said to be in the "allowed region" of the T plane. This means that a set of θ_i exist such that $\{T, \theta_1, \theta_2, \theta_3\}$ satisfy Eqs. (1) and (4).

When $\{T, \theta_1, \theta_2, \theta_3\}$ satisfy these conditions, then so do

$$\{T\exp\{\tfrac{2}{3}in\pi), \theta_1 + \tfrac{2}{3}n\pi, \theta_2 + \tfrac{2}{3}n\pi, \theta_3 + \tfrac{2}{3}n\pi\}$$

and

$$\{T^*, -\theta_1, -\theta_2, -\theta_3\}.$$

Therefore, the allowed region in T plane is symmetric under rotations by $2\pi/3$ and $4\pi/3$, and under reflection through the t axis.

The eigenangle manifold has the topology of the (2-dimensional) surface of a torus. To give it a concrete representation, we may consider it as a bounded region of the plane

$$\theta_1 + \theta_2 + \theta_3 = 0$$

drawn in a 3-dimensional Euclidean space by coordinate axes for $\theta_1, \theta_2, \theta_3$. The boundary points in this representation are not boundary points of the manifold as they are identified with other boundary points through condition (2). The 3-space is the union of six subspaces, one of which is defined by $\theta_1 \leqslant \theta_2 \leqslant \theta_3$, and the others by permutations of the θ_i in this condition. Then the θ-manifold in this concrete representation is likewise subdivided into six regions, with boundary lines between regions defined by equality of a pair of the θ_i.

Now t and u are symmetric functions of the θ_i, and each of these six regions of the θ-manifold is mapped continuously and one-to-one to the allowed region of the T-plane. Each point on the region's boundary is a map of a boundary point of one of the six regions in the manifold and hence associated with a value θ_0 common to a pair of the θ_i. Then the third angle is $2n\pi - 2\theta_0$. Therefore,

$$t = 2\cos\theta_0 + \cos 2\theta_0, \tag{5a}$$

$$u = 2\sin\theta_0 - \sin 2\theta_0, \tag{5b}$$

are parametric equations, with parameter θ_0, $0 \leqslant \theta_0 \leqslant 2\pi$, defining the boundary of the allowed region (see Fig. 1). Its shape is a cusp-triangle with the symmetry properties already noted. Gupta and Patel [3] have used graphs of this type. The ranges of the trace variables are

$$-3/2 \leqslant t \leqslant 3, \qquad -3\sqrt{3}/2 \leqslant u \leqslant 3\sqrt{3}/2.$$

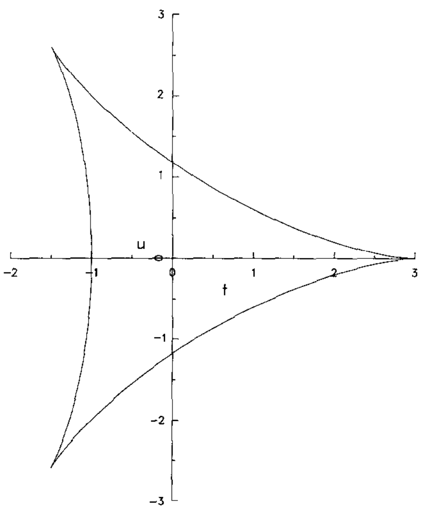

FIG. 1. The interior of the cusp triangle is the domain of points in the complex T-plane for which T is the trace of an $SU(3)$ matrix, where $T = t + iu = \text{Trace}(A)$.

To describe the boundary $u=u(t)$ near the maximum of t, set $\theta_0 \to 0$ in Eqs. (5) to get

$$t=3-3\theta_0^2+O(\theta_0^4),$$
$$u=\theta_0^3+O(\theta_0^5),$$

whence

$$u(t)=\pm(1-\tfrac{1}{3}t)^{3/2}+\text{higher order terms}$$

in the neighborhood of $t=3$. This corresponds to A near the unit matrix.

Solving (5a) for the parameter, we get

$$\cos\theta_0=-\tfrac{1}{2}\pm\tfrac{1}{2}(3+2t)^{1/2}.$$

The positive square root is for the sides of the cusp triangle in Fig. 1 meeting at $t=3$, and the negative square root for the third side. Putting these solutions into (5b) we get

$$u=u_+(t), \qquad u=-u_+(t)$$

for the boundary curves meeting at $t=3$ and

$$u=u_-(t), \qquad u=-u_-(t),$$

for the boundary curve on the left, where

$$u_+(t)=[+2(3+2t)^{3/2}-t^2-12t-9]^{1/2}, \qquad -\tfrac{3}{2}\leqslant t\leqslant 3, \tag{6a}$$
$$u_-(t)=[-2(3+2t)^{3/2}-t^2-12t-9]^{1/2}, \qquad -\tfrac{3}{2}\leqslant t\leqslant -1. \tag{6b}$$

Note that $[u_-(t)]^2$ is defined for all t in $(-\tfrac{3}{2}, 3)$ and is negative for t in $(-1, 3)$. Note also that

$$[u_+(t)\,u_-(t)]^2=-(3-t)^3(1+t). \tag{7}$$

Then

$$u_+(t)=\left(\frac{(3-t)^3(1+t)}{2(3+2t)^{3/2}+t^2+12t+9}\right)^{1/2} \tag{8}$$

is an alternate to (6a) and a more practical formula for t close to 3. For example, if $t=2.7$, calculation of $u_+(t)$ from (6a) loses more than six significant figures.

III. Dependence of the Invariant Measure on the Trace Variables

Let $v(\boldsymbol{\theta})$ be the Vandermonde determinant of the eigenvalues of A:

$$v(\boldsymbol{\theta}) = \begin{vmatrix} 1 & 1 & 1 \\ \exp(i\theta_1) & \exp(i\theta_2) & \exp(i\theta_3) \\ \exp(2i\theta_1) & \exp(2i\theta_2) & \exp(2i\theta_3) \end{vmatrix}$$

$$= [\exp(i\theta_1) - \exp(i\theta_2)][(\exp(i\theta_2) - \exp(i\theta_3)][(\exp(i\theta_3) - \exp(i\theta_1)].$$

Then

$$|v(\boldsymbol{\theta})| = 8 \left| \sin\left(\frac{\theta_1 - \theta_2}{2}\right) \sin\left(\frac{\theta_2 - \theta_3}{2}\right) \sin\left(\frac{\theta_3 - \theta_1}{2}\right) \right|$$
$$= 2\ |\sin(\theta_1 - \theta_2) + \sin(\theta_2 - \theta_3) + \sin(\theta_3 - \theta_1)|. \tag{9}$$

Using the second form in (9), we verify that

$$\int |v(\boldsymbol{\theta})|^2 \frac{d\theta_1}{2\pi} \frac{d\theta_2}{2\pi} = 6.$$

We can now take over the part of $d\mu(A)$ depending on the unitary invariants of A and write it in normalized form

$$d\lambda(\boldsymbol{\theta}) = \frac{1}{6} |v(\boldsymbol{\theta})|^2 \frac{d\theta_1}{2\pi} \frac{d\theta_2}{2\pi}, \tag{10}$$

so that

$$\int d\lambda = 1. \tag{11}$$

To convert to trace variables, we have

$$|v(\boldsymbol{\theta})|^2 = \begin{vmatrix} 1 & 1 & 1 \\ \exp(i\theta_1) & \exp(i\theta_2) & \exp(i\theta_3) \\ \exp(2i\theta_1) & \exp(2i\theta_2) & \exp(2i\theta_3) \end{vmatrix} \cdot \begin{vmatrix} 1 & \exp(-i\theta_1) & \exp(-2i\theta_1) \\ 1 & \exp(-i\theta_2) & \exp(-2i\theta_2) \\ 1 & \exp(-i\theta_3) & \exp(-2i\theta_3) \end{vmatrix}$$

$$= \begin{vmatrix} 3 & T^* & (T^*)^2 - 2T \\ T & 3 & T^* \\ T^2 - 2T^* & T & 3 \end{vmatrix}$$

$$= -u^4 - 2(t^2 + 12t + 9)\,u^2 + (3 - t)^3(1 + t)$$

$$= [u_+^2(t) - u^2][u^2 - u_-^2(t)].$$

By explicit calculation from (4),

$$2dt\,du = 2\left|\frac{\partial(t, u)}{\partial(\theta_1, \theta_2)}\right| d\theta_1\, d\theta_2 = |v(\boldsymbol{\theta})|\, d\theta_1\, d\theta_2.$$

In transforming (10) to trace variables, we multiply by six to account for the six-fold mapping of θ-space to T-space. The complete formula becomes

$$d\lambda(\boldsymbol{\theta}) \equiv d\lambda(t, u) = (2\pi^2)^{-1}\sqrt{(u_+^2(t) - u^2)(u^2 - u_-^2(t))}\, dt\, du \qquad (12)$$

with

$$-\tfrac{3}{2} \leqslant t \leqslant 3,$$

$$-u_-(t) \leqslant u \leqslant u_+(t) \qquad \text{for} \qquad -1 \leqslant t \leqslant 3,$$

$$-u_+(t) \leqslant u \leqslant -u_-(t) \qquad \text{and} \qquad u_-(t) \leqslant u \leqslant u_+(t)$$

for $-\frac{3}{2} \leqslant t \leqslant -1$. And (11) remains valid. Figure 2 shows a surface plot of the t, u distribution associated with invariant measure $d\mu(A)$.

Question about trace distributions and other distributions of unitary invariants can now be posed, and sometimes answered analytically. Suppose, for example, we ask for the distribution $G(t)\,dt$ of $t = \text{real (trace } A)$, where A is distributed according to $d\mu(A)$. The u-integration over (12) brings in the complete elliptic integrals $E(k)$ and $K(k)$. The formulas of Byrd and Friedman [2] are applicable.

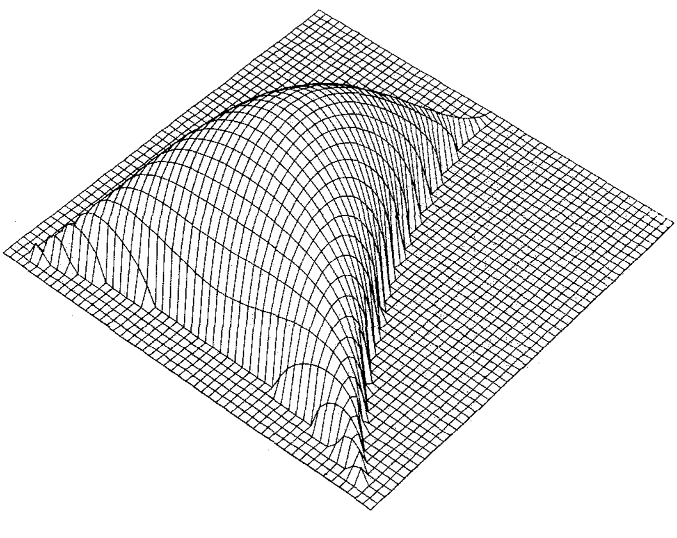

FIG. 2. Surface plot of $d\lambda(t, u)/dt\,du$, the part of the $SU(3)$ invariant measure dependent on the trace, $T = t + iu$, of an $SU(3)$ matrix.

For $-1 \leqslant t \leqslant 3$, we have

$$G(t) = 2 \int_{u=0}^{u=u_+(t)} \frac{d\lambda(t, u)}{dt}$$
$$= (3\pi^2)^{-1}(u_+^2 - u_-^2)^{1/2}[(u_+^2 + u_-^2)\, E(k) - u_-^2 K(k)]. \qquad (13a)$$

Here, $u_-^2 \leqslant 0$, and the modulus k is given by

$$k \equiv k(t) = u_+ (u_+^2 - u_-^2)^{-1/2}.$$

For $-\frac{3}{2} \leqslant t \leqslant -1$, we have

$$G(t) = 2 \int_{u=u_-(t)}^{u=u_+(t)} \frac{d\lambda(t, u)}{dt}$$
$$= (3\pi^2)^{-1} u_+ [(u_+^2 + u_-^2)\, E(k) - 2u_-^2 K(k)]. \qquad (13b)$$

In this case, $0 \leqslant u_-^2 \leqslant u_+^2$ and the modulus is given by

$$k \equiv k(t) = (u_+^2 - u_-^2)^{1/2}/u_+ .$$

Figure 3 shows $G(t)$. The maximum is 0.59072 at $t = -0.527$. By construction, $G(t)$ is normalized to

$$\int_{-3/2}^{3} G(t)\, dt = 1.$$

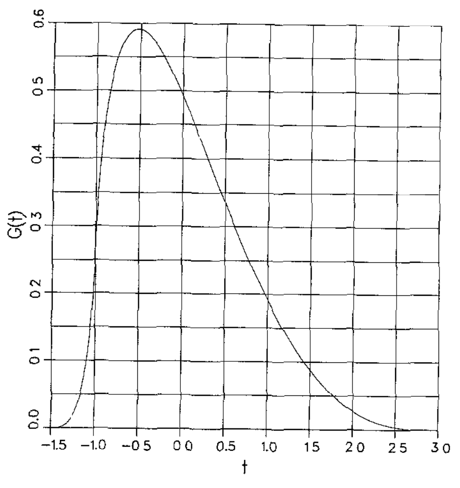

FIG. 3. Distribution of the real part t of the trace of $SU(3)$ matrices distributed according to the invariant measure.

IV. Approximation for Generation of Stepping Matrices

To generate random stepping matrices for an SU_3 gauge theory Monte Carlo calculation, one could first consider distributions

$$d\lambda(t, u) \times \text{bias factor } (= \text{function of } t) \tag{14}$$

which bias the selection of trace variables for the random SU_3 matrices toward a neighborhood of $t = 3$. The bias should depend on a few adjustable parameters to be tuned for specific applications. The bias might be further optimized by giving it a u-dependence; we have not investigated this. Random sampling of the distributions should be easy and fast on a computer. While the expression (12) for $d\lambda(t, u)$ is rather cumbersome, it admits simple approximations for such purposes.

We suppose, for practical purposes, that the bias factor is very small for $t < 0$. Then we need to approximate $d\lambda(t, u)$ well for positive t only.

First, define a normalized u variable by

$$\hat{u} = u/u_+(t) \tag{15}$$

so that $-1 \leqslant \hat{u} \leqslant 1$ for $t > -1$. Then $d\lambda$ takes the form

$$d\lambda = (2\pi^2)^{-1}\alpha(t)(1 - \tfrac{1}{3}t)^3\sqrt{1 - \hat{u}^2}\,\sqrt{r(t)\,\hat{u}^2 + 1}\,dt\,d\hat{u} \tag{16}$$

where, recalling Eqs. (6), (7),

$$\begin{aligned} r(t) &= |u_+/u_-|^2 = |u_+u_-|^2/|u_-|^4 \\ &= (3 - t)^3(1 + t)/[2(3 + 2t)^{3/2} + t^2 + 12t + 9]^2 \end{aligned}$$

and

$$\begin{aligned} \alpha(t) &= 27\,|u_+^2 u_-|/(3 - t)^3 \\ &= 27(1 + t)/[2(3 + 2t)^{3/2} + t^2 + 12t + 9]^{1/2}. \end{aligned}$$

For $t \geqslant 0$, $(r(t)\,\hat{u}^2 + 1)^{1/2}$ varies from a minimum of 1 (for $\hat{u} = 0$) to a maximum of 1.035 (for $\hat{u} = 1$, $t = 0$). This $3\frac{1}{2}\%$ variation is irrelevant for Monte Carlo strategies. Accordingly, the second square root in (16) can be approximated by unity. The factor $\alpha(t)$ is a well-behaved function for positive t whose trend is as follows:

$$\begin{aligned} \alpha(t)/\alpha(3) &= 1.000 \quad \text{for} \quad t = 3, \\ &= 0.906 \quad \text{for} \quad t = 2, \\ &= 0.781 \quad \text{for} \quad t = 1, \\ &= 0.590 \quad \text{for} \quad t = 0. \end{aligned}$$

Therefore, in place of (14), we could generate distributions of the form

$$dF(t)\,\sqrt{1 - \hat{u}^2}\,d\hat{u}, \tag{17}$$

where the slow variation of $\alpha(t)$ is absorbed into the tunable variation of $F(t)$. A specific $F(t)$ is proposed in the next section.

V. A Biased Distribution for t = Real (Trace A)

In line with the preceeding discussion, we could begin a generation of a stepping matrix A by generating two real variables $\hat{u}$ and t according to distributions $(1-\hat{u}^2)^{1/2}\,d\hat{u}$ and $dF(t)$, respectively, where $dF(t)/dt$ goes like $(3-t)^3$ near $t=3$. If the $(3-t)^3$ factor is not present, too much computer time and Monte Carlo sweep time may be expended on stepping matrices so close to the identity that the steps move too slowly. The approach is similar to that set forth in [1] for $SU(2)$ stepping matrices.

Assume that the t-distribution is normalized to 1, and let $\bar{t}$, σ be its average and standard deviation:

$$\int dF(t)=1, \qquad \int t\,dF(t)=\bar{t} \qquad \int (t^2-\bar{t}^2)\,dF(t)=\sigma^2. \tag{18}$$

We seek a prescription for $F(t)$ which allows $\bar{t}$ and σ (and perhaps some shape parameters) to be preset, and which can still be programmed efficiently on a computer. One can then seek to optimize the choices of $\bar{t}$, σ, and any other parameters by numerical experiments, with physical judgments guiding extension of results to lattices of different dimension and different spacing.

Let r and s be selected randomly from the uniform distribution on (0, 1). Let b, w, and n be real positive parameters, as specified below. Let t be determined by solving

$$s=\exp\{-[(3-t)/(b+wr^n)]^4\}. \tag{19}$$

This defines t as a variable on $(-\infty, 3)$ but in practice, values of t less than -1 will occur infrequently and can be dropped, or reset to $t=-1$.

Then the effective t-distribution is $dF(t)$, where

$$F(t)=\int_{r=0}^{1} \exp\{-[(3-t)/(b+wr^n)]^4)\,dr.$$

This satisfies the first condition of (18) and dF/dt goes like $(3-t)^3$ near $t=3$. We define two constants related to the Γ function

$$c_1=\int_{\infty}^{0} z\,d[\exp(-z^4)]=\Gamma(\tfrac{5}{4})=0.90640\ 24771$$

and

$$c_2=\int_{\infty}^{0} z^2 d[\exp(-z^4)]=\tfrac{1}{2}\sqrt{\pi}=0.88622\ 69255,$$

then

$$\bar{t} = 3 - c_1[b + w/(n+1)], \tag{20a}$$

$$\sigma^2 = \frac{c_2 - c_1^2}{c_1^2}(3 - \bar{t})^2 + \frac{c_2 n^2 w^2}{(2n+1)(n+1)^2}. \tag{20b}$$

The distribution becomes more sharply peaked in the neighborhood of $t = \bar{t}$ as n increases, and has a longer tail. Reasonable shapes are given for, e.g., $1 \leqslant n \leqslant 10$.

Given values of $\bar{t}$ and σ, Eqs. (20) can be solved to fix w and then b:

$$w^2 = \left(\sigma^2 - \frac{(c_2 - c_1^2)(3 - \bar{t})^2}{c_1^2}\right)\frac{(2n+1)(n+1)^2}{c_2 n^2}, \tag{21a}$$

$$b = (3 - \bar{t})/c_1 - w/(n+1). \tag{21b}$$

For a given $\bar{t}$ in this scheme, there is a minimum value of σ, namely the value that makes $w = 0$ in Eq. (21a).

Finally, when t and $\hat{u}$ are generated (and the rare events $t < -1$ are discarded), then Eq. (8) and $u = u_+(t)\hat{u}$ yield u.

Figure 4 shows illustrative trace distributions with $\bar{t} = 2.0$, several σ values, and $n = 1$. Figure 5 shows the effect of changing n.

Eigenangles from Trace Variables

We must also determine (efficiently) the eigenangles or, better, the pairs $(\cos\theta_i, \sin\theta_i)$ from t and u. The characteristic equation

$$\begin{aligned}\det(xI - A) &= [x - \exp(i\theta_1)][x - \exp(i\theta_2)][x - \exp(i\theta_3)] \\ &= x^3 - Tx^2 + T^*x - 1 = 0\end{aligned}$$

can be solved for the θ_i when T is given. A more direct approach is to form and solve a real cubic equation whose roots y_i are trigonometric functions, e.g., $y_i = \sin\theta_i$, $i = 1, 2, 3$. Then, the sum of the roots is u. From

$$t^2 + u^2 = 3 + 2\sum_{i<j}(\cos\theta_i\cos\theta_j + \sin\theta_i\sin\theta_j)$$

and

$$t = \sum_{i<j}\cos(\theta_i + \theta_j) = \sum_{i<j}(\cos\theta_i\cos\theta_j - \sin\theta_i\sin\theta_j),$$

an expression for $\sum_{i<j}\sin\theta_i$ is obtained. Also

$$\begin{aligned}tu &= \tfrac{1}{2}\sum_i \sin 2\theta_i + \sum_{i<j}\sin(\theta_i + \theta_j) \\ &= -2\sin\theta_1\sin\theta_2\sin\theta_3 - u,\end{aligned}$$

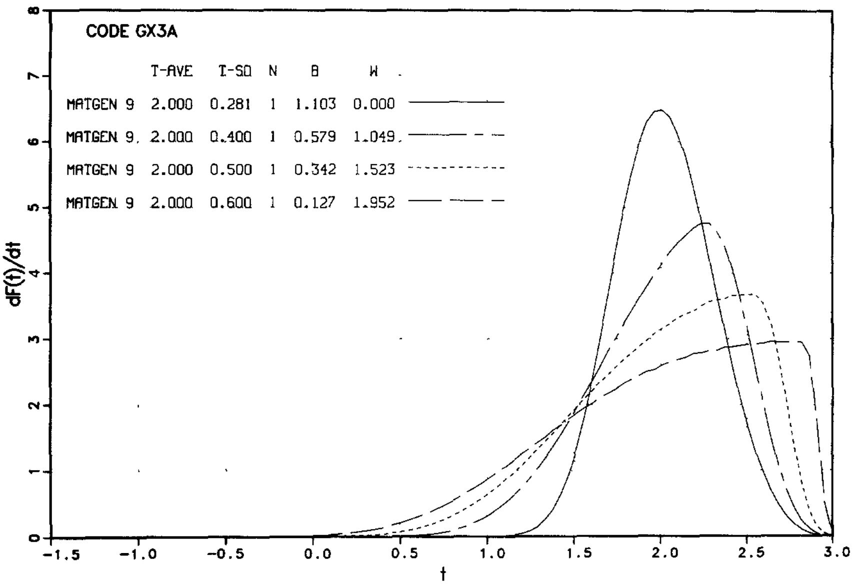

FIG. 4. t-distributions generated by the algorithm for $SU(3)$ stepping matrices, with average trace $\bar{t} = 2.0$, several standard deviations σ, and shape parameter $n = 1$.

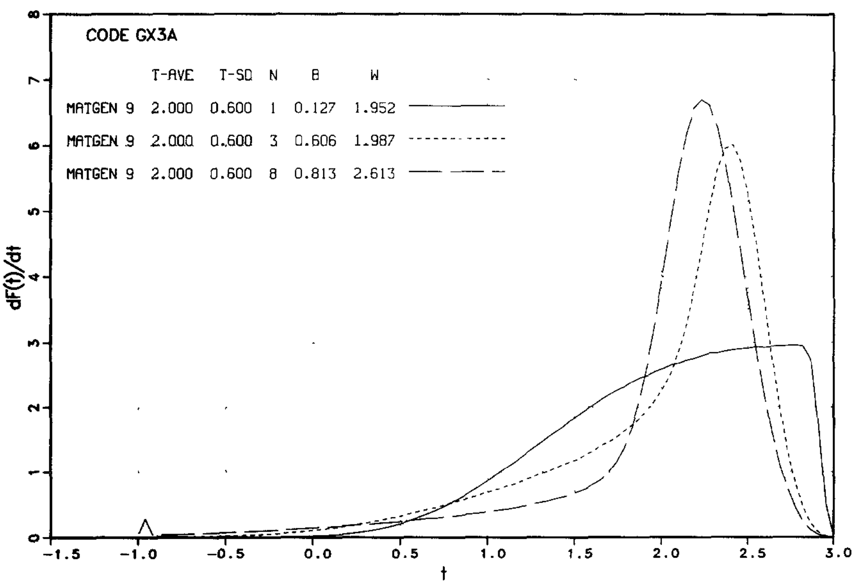

FIG. 5. t-distributions for $\bar{t} = 2.0$, showing the effect on shape of different n-values.

where the last step depends on Eq. (1). Then the desired equation is

$$y^3 + uy^2 + \tfrac{1}{4}(t^2 - 2t - 3 + u^2)\, y + \tfrac{1}{2}u(1+t) = 0.$$

Let γ_1 be any angle such that

$$\cos \gamma_1 = \frac{-u[u^2 + 9(3+t)(1+t)]}{[u^2 + 3(3-t)(1+t)]^{3/2}}. \tag{22}$$

Let $\gamma_2 = \gamma_1 + 2\pi$, $\gamma_3 = \gamma_1 + 4\pi$. Then the Cardan solution to the cubic in y is

$$y_i \equiv \sin \theta_i = \tfrac{1}{3}u + \tfrac{1}{3}[u^2 + 3(3-t)(1+t)]^{1/2} \cos(\tfrac{1}{3}\gamma_i), \qquad i = 1, 2, 3. \tag{23a}$$

In addition, again from (4),

$$\begin{aligned}
&\frac{\sin\theta_1 - \sin\theta_2 - \sin\theta_3}{1 + \cos\theta_1 + \cos\theta_2 + \cos\theta_3} \\
&\quad = \frac{2\sin(\frac{1}{2}\theta_1)\cos(\frac{1}{2}\theta_1) - 2\sin\frac{1}{2}(\theta_2+\theta_3)\cos\frac{1}{2}(\theta_2-\theta_3)}{2\cos(\frac{1}{2}\theta_1^2) + 2\cos\frac{1}{2}(\theta_2+\theta_3)\cos\frac{1}{2}(\theta_2-\theta_3)} \\
&\quad = \tan(\tfrac{1}{2}\theta_1) = \frac{1-\cos\theta_1}{\sin\theta_1}.
\end{aligned}$$

Therefore, for any θ_i and without computation of a square root,

$$\cos\theta_i = 1 - \frac{\sin\theta_i(2\sin\theta_i - u)}{1+t}, \tag{23b}$$

and, if the eigenangles themselves are desired,

$$\theta_i = 2 \arctan\left(\frac{2\sin\theta_i - u}{1+t}\right). \tag{23c}$$

When $T = t + iu$ is given and $1 + t \neq 0$, these equations are efficient prescriptions for the sines and cosines of the eigenangles, and the angles themselves, without ambiquity of sign.

In the special case $1 + t = 0$, let θ_1, be any angle satisfying $\sin\theta_1 = \frac{1}{2}u$. Then the angles can be taken as θ_1, $(\pi - \theta_1)$, and π. The sines and cosines are, respectively, $\sin\theta_1$, $\sin\theta_1$, 0, and $\cos\theta_1$, $-\cos\theta_1$, -1.

VI. Summary of the Algorithm

The steps of the algorithm to generate a trace-biased but otherwise invariantly distributed ensemble of $SU(3)$ matrices with prescribed trace average $\bar{t}$, trace standard deviation σ, and shape parameter n are here assembled in the proper sequence.

In what follows, r, s, and subscripted rs are random variables sampled from the uniform distribution on (0, 1):

(1) Calculate b and w from Eqs. (21).

(2) Choose r and s randomly on (0, 1), and calculate t from Eq. (19), i.e., $t = 3 - (b + wr^n)(-\log s)^{1/4}$. Any t less than -1 should be dropped or redefined to be -1.

(3) Choose $\hat{u}$ randomly from the distribution $(1-\hat{u}^2)^{1/2}\, d\hat{u}$. It is probably adequate to replace this by $(1-\hat{u})^{1/2}\, d\hat{u}$. Then we can set $d(1-\hat{u})^{3/2} = dr_1$, $\hat{u} = 1 - (r_1)^{2/3} = 1 - [\mathrm{Max}(r_a, r_b, r_c)]^2$. Then set $\hat{u} \to \pm\hat{u}$; the two signs are equiprobable.

(4) Calculate $u = u_+(t)\hat{u}$ and $\sin\theta_i$, $\cos\theta_i$, $i = 1, 2, 3$, from Eqs. (8), (22), and (23). Then apply a random permutation (one of the six permutations on three objects) on the ordering of the θ_i. If this is not done, the $\sin\theta_i$ obtained by the solution to the cubic equation as given above will not be randomly ordered in magnitude. The diagonal matrix $D(\boldsymbol{\theta}_i)$ is not known.

(5) Set $\psi_{21} = 2\pi r_2$, $\psi_{31} = 2\pi r_3$, $\psi_{32} = 2\pi r_4$. Also, $\bar{\rho}_{21} = \mathrm{Max}(r_5, r_6)$, $\bar{\rho}_{31} = \mathrm{Max}(r_7, r_8, r_9, r_{10})$, and $\bar{\rho}_{32} = \mathrm{Max}(r_{11}, r_{12})$. For each $\bar{\rho}$, calculate the complement: $\rho = (1 - (\bar{\rho})^2)^{1/2}$. The $\bar{\rho}$s and ψs will be distributed according to $dv(\boldsymbol{\rho}, \boldsymbol{\psi})$.

(6) Set $V_{11} = \bar{\rho}_{31}\bar{\rho}_{21}$, $V_{21} = \bar{\rho}_{31}\rho_{21}\exp(i\psi_{21})$, $V_{31} = \rho_{31}\exp(i\psi_{31})$, $V_{32} = \bar{\rho}_{31}\rho_{32}\exp(i\psi_{32})$, $V_{33} = \bar{\rho}_{31}\bar{\rho}_{32}$.

(7) Utilize the orthogonality of the first and third columns of V and the cross-product relations for the rows of V to get the remaining elements of V, specifically,

$$V_{13} = (V_{21}^* V_{32}^* - V_{11} V_{31}^* V_{33})(\bar{\rho}_{31})^{-2},$$

$$V_{23} = (-V_{11} V_{32}^* - V_{21} V_{31}^* V_{33})(\bar{\rho}_{31})^{-2},$$

$$V_{12} = (V_{23} V_{31} - V_{21} V_{33})^*, \qquad V_{22} = (V_{33} V_{11} - V_{31} V_{13})^*.$$

(8) Calculate $A = V^{-1} D(\boldsymbol{\theta}) V$. This can be rephrased (with $I =$ unit matrix) as

$$A = V^{-1}[D(\boldsymbol{\theta}) - I\exp(i\theta_2)]\, V + I\exp(i\delta_2). \tag{24}$$

If the first two rows of A are calculated by Eq. (24) and the third row calculated from $\mathbf{A}_3 = (\mathbf{A}_1 + \mathbf{A}_2)^*$, the computation of A is shortened, and the computations of V_{12} and V_{22} are unnecessary.

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