IMPROVEMENT OF EFFICIENCY IN
GENERATING RANDOM $U(1)$ VARIABLES
WITH BOLTZMANN DISTRIBUTION

Tetsuya Hattori
Faculty of Engineering, Utsunomiya University, Ishii-cho, Utsunomiya, Tochigi 321, Japan
e-mail address: hattori@tansei.cc.u-tokyo.ac.jp

Hideo Nakajima
Faculty of Engineering, Utsunomiya University, Ishii-cho, Utsunomiya, Tochigi 321, Japan
e-mail address: nakajima@kinu.infor.utsunomiya-u.ac.jp

July 9, 2018

Abstract
A method for generating random $U(1)$ variables with Boltzmann distribution is presented. It is based on the rejection method with transformation of variables. High efficiency is achieved for all range of temperatures or coupling parameters, which makes the present method especially suitable for parallel and pipeline vector processing machines. Results of computer runs are presented to illustrate the efficiency. An idea to find such algorithms is also presented, which may be applicable to other distributions of interest in Monte Carlo simulations.

Subject classification: 65C10, 81E25, 82A68.

Key words: Random number generation, Monte Carlo method, Spin system, Parallel processor.

1 Introduction.
Monte Carlo numerical integration method, or Monte Carlo simulation, has been widely used in the numerical study of quantum field theories with lattice formalism and statistical mechanics of spin systems. In performing Monte Carlo simulations, one must generate sequences of random numbers with given probability distributions. Each random number is used to 'update' a spin or a gauge variable. Probability distributions which appear in such calculations
have parameter dependences. These parameters carry the information of temperature and other thermodynamic quantities, and also that of the neighboring spin states.

For a fixed probability distribution there are algorithms (see, for example, [5] and references therein) which may be very efficient in generating random numbers. In Monte Carlo simulations, however, we have fluctuations in the neighboring spins, which results in changes of the parameters within a single program. One faces the problem of finding an algorithm suitable to a class of distributions parametrized by the parameters. These parameters are changed over a wide range, so that we must find a method which maintain high efficiency for all range of parameters, especially in the limit where a parameter tends to $\infty$ and the distribution becomes singular.

Another aspect which we consider, is the efficiency in parallel or pipeline vector processing. As far as we know, much of the currently available vector processors work efficiently when there are no ‘if-branches’ in the program.

We study a method based on a rejection method combined with a change of variables [1], which is an approach that is widely used. In the case of rejection method, to avoid ‘if-branches’ we have to fix the number of iterations of the rejection trials. It is particularly important to have high acceptance rate uniformly in the parameters.

The aim of the present study is to find a suitable method for generating a sequence of random $U(1)$ numbers which we use to update site or link variables of a canonical ensemble for $U(1)$ lattice gauge theories or $U(1)$ spin systems, from the point of view mentioned above. An example of a program for our proposal is given in appendix C.

In section 2 we set up the problem. In section 3 we give our strategy for the solution, and in section 4 we give an answer to the problem. We present the results of our efficiency tests of the algorithm in section 5.

2 Random $U(1)$ variable and rejection method.

In the following we call a sequence of random $U(1)$ numbers, a random $U(1)$ variable: A random $U(1)$ variable is a sequence of numbers (the angle variables)

$$\theta_1, \theta_2, \theta_3, \cdots,$$

whose distribution

$$P([\theta, \theta + d\theta]) = f_a(\theta) d\theta$$

is given by the density function

$$f_a(\theta) = N_a \exp(a \cos(\theta - \theta_0)),$$

where $N_a$ is a normalization constant. In the practical applications, the parameter $a$ is proportional to the inverse temperature $1/T$ or the inverse coupling
1/g^2, and both a and the constant \( \theta_0 \) contain the effect of interactions with other sites or link variables. By the shift of variable \( \theta' = \theta - \theta_0 \) if \( a > 0 \), and \( \theta' = \theta - \theta_0 - \pi \) if \( a < 0 \), we may assume without loss of generality that \( \theta_0 = 0 \) and \( a \geq 0 \). Hence

\[
f_a(\theta) = N_a \exp(a \cos \theta), \quad -\pi \leq \theta < \pi, \quad a > 0,
\]

\[
\frac{1}{N_a} = \int_{-\pi}^{\pi} \exp(a \cos \theta) \, d\theta.
\]

The right hand side of eq. (2) is (modulo constant) an integral representation of modified Bessel function \( I_0(a) \).

On computers we start with uniform random variables

\[
\omega_1, \, \omega_2, \, \omega_3, \cdots,
\]

with the probability distribution

\[
P([\omega, \omega + d\omega]) = d\omega, \quad 0 \leq \omega < 1.
\]

If we know an expression for a function \( X(\omega) \) expressible as a computer program of small time consumption such that the sequence

\[
\theta_i = X(\omega_i), \quad i = 1, 2, 3, \cdots,
\]

is the random \( U(1) \) variable \( [0, 1] \), then there is in principle no problem. Such a function \( X(x) \) is formally given by

\[
X(x) = F^{-1}(x);
\]

\[
F(t) = P([-\pi \leq \theta < t]) = \int_{-\pi}^{t} f_a(\theta) \, d\theta.
\]

(Here and in the following, \( F^{-1} \) is the inverse function of \( F \); \( F^{-1}(F(x)) = x \).) Unfortunately, we do not know a suitable expression of \( X(x) \) for random \( U(1) \) variables. (Note that we have the parameter \( a \) dependence.)

Usually the rejection method is adopted to solve the problem. The rejection method, combined with transformation of variables, is defined as follows. Let \( \tilde{f}(\theta) \) be some approximate density function to the density function \( f_a(\theta) \). We assume that the density functions are continuous. Note that they are normalized to satisfy \( \int_{-\pi}^{\pi} f(\theta) \, d\theta = 1 \). Suppose that there is a monotonic function \( h \) which satisfies

\[
h(0) = -\pi, \quad h(1) = \pi,
\]

and

\[
\tilde{f}(h(x)) h'(x) = 1, \quad 0 < x < 1,
\]

\( (4) \)
where \( h' \) is the derivative of \( h \), \( h' = \frac{dh}{dx} \). (For the moment, we suppress possible parameter dependences of \( \tilde{f} \) and \( h \).) Define a function \( g \) by

\[
g(x) = R(a) \frac{f_a(h(x))}{f(h(x))}, \quad 0 \leq x < 1,
\]

\[
R(a) = \min_{-\pi \leq \theta < \pi} \left\{ \frac{\tilde{f}(\theta)}{f_a(\theta)} \right\}.
\]

Let \( \omega_j \) and \( \omega'_j \) with \( j = 1, 2, 3, \ldots \), be two sequences of independent uniform random variables as in (3). Define a subsequence

\[
\tilde{\omega}_i = \omega_{j_i}, \quad i = 1, 2, 3, \ldots,
\]

of the sequence \( \{\omega_j\} \) by selecting the numbers \( j = j_i \) that satisfy

\[
\omega'_j \leq g(\omega_j).
\]

Then the sequence

\[
h(\tilde{\omega}_1), h(\tilde{\omega}_2), h(\tilde{\omega}_3), \ldots
\]

is the random \( U(1) \) variable we are looking for. We call the rate of picking up \( \tilde{\omega}_i \) out of \( \omega_j \) the acceptance rate. To achieve high efficiency, the acceptance rate should be high. It can be shown that the acceptance rate is equal to \( R(a) \) in eq. (6). The proof that the distribution of (7) is the one with the density function \( f_a \), and the proof that the acceptance rate is equal to \( R(a) \), are given in Appendix A.

Note that the density functions are non-negative functions and that the integrated values of \( \tilde{f} \) and \( f_a \) are normalized to unity, hence \( 0 \leq R(a) \leq 1 \), which should hold for an acceptance rate. Note also that if \( \tilde{f} \) is a good approximation to \( f_a \), then the function \( g \) is almost flat.

**Our problem is to find a good \( \tilde{f} \).**

### 3 Approximate distributions and the optimization of the acceptance rate.

In order to keep high efficiency, we must choose \( \tilde{f} \) with high acceptance rate \( R(a) \). To illustrate the implications of this statement, let us first consider the simplest choice of \( \tilde{f} \), the flat distribution. Hereafter, we refer to this choice as the ‘direct’ method.

The ‘direct’ method is defined by choosing \( \tilde{f} \) in eq. (4) to be a constant function;

\[
\tilde{f}(\theta) = \frac{1}{2\pi},
\]

\[
h(x) = (2x - 1)\pi.
\]
The acceptance rate is
\[ R(a) = \frac{1}{2\pi N_a \exp(a)}. \] (10)

For \( a \) near zero (‘high temperature’), the acceptance rate is high: 
\[ R(a) \approx 1 - a + \frac{3}{4} a^2, \ a \ll 1, \] while for large \( a \) (‘low temperature’), the acceptance rate becomes very small;
\[ R(a) \approx \frac{1}{\sqrt{2\pi a}}, \ a \gg 1. \]

In the limit \( a \to \infty \), the acceptance rate approaches zero. We have very slow effective generation of random \( U(1) \) variables for large values of \( a \) with the ‘direct’ method. In other words, the improvement of the efficiency of generating random \( U(1) \) variables, which we measure by time lapse per a random variable generation, depends basically on the improvement of the acceptance rate. The reason that the acceptance rate is small for large \( a \) is that for large \( a \) the original distribution \( f_a \) has a large peak at \( \theta = 0 \). The distribution becomes highly non-uniform and the flat (uniform) distribution \( \tilde{f} \) is not a good approximation.

As noted in the section 1 (see also section 5), it is even more important to keep high acceptance rate uniformly in \( a \) when we use parallel processing machines.

Our aim is to find a \( \tilde{f} \) which is a good approximation to the original distribution \( f_a \) for all values of \( a \), in particular, the \( a \to \infty \) limit. In a sense, this is to find a family of distributions which interpolates the flat distribution (\( a = 0 \)) and the delta function distribution (\( a = \infty \)) expressible as a simple computer program.

For large \( a \), the density function \( f_a \) has a sharp peak at \( \theta = 0 \). Therefore \( \tilde{f} \) should be a very good approximation at \( \theta = 0 \), while being not too bad an approximation at \( \theta = \pi \). Therefore it is desirable to have two free parameters for \( \tilde{f} \). Also since \( f_a \) is an even function, \( \tilde{f} \) is desired to be an even function. We also impose the condition that the corresponding function \( h \) in eq. (4) has an analytic expression. The simplest choice satisfying these conditions is the following \( \tilde{f}_{\alpha,\beta} \):

\[ \tilde{f}_{\alpha,\beta}(\theta) = \frac{\tilde{N}_{\alpha,\beta}}{2 \cosh(\alpha \theta) + 2 \beta}, \ \alpha > 0, \ \beta > -1, \] (11)

where \( \tilde{N}_{\alpha,\beta} \) is a normalization constant;

\[ \tilde{N}_{\alpha,\beta} = \begin{cases} \alpha \frac{\sqrt{\beta^2 - 1}}{2 \tanh^{-1}(A B)}, & \beta > 1, \\ \alpha \frac{1}{A}, & \beta = 1, \\ \alpha \frac{\sqrt{1 - \beta^2}}{2 \tan^{-1}(A B)}, & -1 < \beta < 1, \end{cases} \] (12)
where we put \( A = \tanh \frac{\pi \alpha}{2} \), and \( B = \sqrt{\frac{|\beta - 1|}{\beta + 1}} \). The corresponding function \( h \) in eq. (4) is;

\[
\begin{align*}
\alpha, \beta(\alpha, \beta) &= \begin{cases} \\
\frac{2}{\alpha} \tanh^{-1} \left( B^{-1} \tanh((2x - 1) \tanh^{-1}(AB)) \right), & \beta > 1, \\
\frac{2}{\alpha} \tanh^{-1} \left( (2x - 1) \alpha \right), & \beta = 1, \\
\frac{2}{\alpha} \tanh^{-1} \left( B^{-1} \tan((2x - 1) \tan^{-1}(AB)) \right), & -1 < \beta < 1,
\end{cases}
\end{align*}
\]

(13)

where \( A \) and \( B \) are as above.

The next step is to choose \( \alpha = \alpha(a) \) and \( \beta = \beta(a) \) as functions of \( a \). In principle, they should be chosen so as to optimize the acceptance rate \( R = R(a) \). Here, we search for a solution that satisfies a condition that the minimum in the definition of \( R(a) \) (i.e. in the right hand side of eq. (3)) is achieved at \( \theta = 0 \). We impose this condition to avoid ‘if-braches’ in the resulting computer program. If the minimum is attained at different values of \( \theta \), we will need if-braches according to the different values of \( \theta \).

We have an argument that the optimal solution under this condition, which we shall refer to as the ‘optimized cosh’ method, is given by choosing \( \alpha = \alpha(a) \) and \( \beta = \beta(a) \) in eq. (13) to satisfy the following:

\[
\begin{align*}
\alpha(a) &= \sqrt{3} a - 1, \quad \beta(a) = 2 - \frac{1}{a}, \quad \text{if } a \geq a^o, \\
\frac{\cosh(\pi \alpha(a)) - 1}{\alpha(a)^2} &= \frac{\exp(2a) - 1}{a}, \quad \beta(a) = \frac{\alpha(a)^2}{a} - 1, \quad \text{if } a^o > a \geq a^*.
\end{align*}
\]

(14) (15)

Here \( a^o \) and \( a^* \) are positive constants satisfying \( a^o > a^* \), uniquely determined by,

\[
\begin{align*}
\frac{\exp(2a^o) - 1}{a^o} &= \frac{\cosh(\pi \sqrt{3a^o} - 1) - 1}{3a^o - 1}, \\
\frac{\exp(2a^*) - 1}{a^*} &= \frac{\pi^2}{2}.
\end{align*}
\]

(16) (17)

Their numerical values are \( a^* \approx 0.799 \) and \( a^o \approx 5.04 \). The function \( g = g_a \) in eq. (3) is,

\[
g_a(x) = \exp(-a G_a(h_{\alpha(a), \beta(a)}(x)))
\]

(18)

with

\[
G_a(\theta) = 1 - \cos \theta - \frac{1}{a} \log \left( 1 + \frac{1}{1 + \beta(a)}(\cosh(\alpha(a) \theta) - 1) \right).
\]

(19)
For the parameter range of $0 < a < a^*$, we have to take a limit $\alpha \downarrow 0$ with 
\[
\frac{\alpha(a)^2}{1 + \beta(a)} \ \text{fixed to} \ 2\pi^{-2}(\exp(2a) - 1). 
\]
We have, in place of eq. (13),
\[
h_\gamma(x) = \frac{1}{\gamma} \tan((2x - 1)\tan^{-1}(\pi \gamma)) ,
\]
where $\gamma = \gamma(a)$ is
\[
\gamma(a) = \pi^{-1}\sqrt{\exp(2a) - 1}, \text{ if } 0 < a < a^*. 
\]
The function $g = g_a$ in eq. (5) is
\[
g_a(x) = \exp(-a G_a(h_\gamma(a)(x)))
\]
with
\[
G_a(\theta) = 1 - \cos \theta - \frac{1}{a} \log (1 + \gamma(a)^2 \theta^2). 
\]
The distribution is reduced to the Cauchy distribution:
\[
\tilde{f}_\gamma(\theta) = \frac{\tilde{N}_\gamma}{1 + \gamma^2 \theta^2},
\]
where
\[
\tilde{N}_\gamma = \frac{\gamma}{2\tan^{-1}(\pi \gamma)}. 
\]
See appendix B for the proof that these formulae correctly generate a random $U(1)$ variable, and arguments for our choice of the parameters.

The acceptance rate $R = R(a)$ for the ‘optimized cosh’ method is given by
\[
R(a) = \frac{\tilde{N}_a(\alpha, \beta)}{2 N_a \exp(a)(1 + \beta(a))}, \ \ a \geq a^* ,
\]
\[
= \frac{\gamma(a)}{2 N_a \exp(a)\tan^{-1}(\pi \gamma(a))}, \ \ a^* > a > 0 ,
\]
where $N_a$ and $\tilde{N}_a, \beta$ are defined in eq. (3) and eq. (12), respectively. Note the high acceptance rate for both small $a$ and large $a$:
\[
R(a) \approx 1 - \frac{1}{3}a + \frac{71}{180}a^2, \ \ a \ll 1 ,
\]
\[
R(a) \rightarrow \frac{\sqrt{2\pi}}{2 \log(2 + \sqrt{3})} \approx 0.95, \ \ a \rightarrow \infty. 
\]
See Fig. 1 for the acceptance rate for full range of $a$. The acceptance rate for the ‘optimized cosh’ method keeps more than 90% for all values of $a$, including the ‘zero temperature’ limit $a \rightarrow \infty$. 


4 Proposed algorithm.

The acceptance rate for the ‘optimized cosh’ method is high, but to obtain the parameter $\alpha(a)$ for $a^* \leq a < a^o$, one has to solve a transcendent equation eq. (15). Also, one has to use different formulae for $0 < a < a^*$, $a^* \leq a < a^o$, and $a^o < a$, which will cause ‘if-branches’ that will considerably lower the efficiency when using with vectorized processors.

One may, for example, use Newton method to solve equations numerically, but here instead we approximate the function $\alpha(a)$ in eq. (15) directly by a function which is explicitly expressible on computer programs without using if-branches for all $a$, and designed to keep high acceptance rate. The if-branches are avoided in such a way that we have $-1 < \beta < 1$ for all $a \in (0, \infty)$.

We shall give an example of realistic choice.

1. Define $\alpha(a)$ and $\beta(a)$ by,

   \[
   \alpha(a) = \min\{\sqrt{\frac{2}{1+\beta}} a^2, \max\{\sqrt{\epsilon a}, \delta(a)\}\}, \\
   \beta(a) = \max\left\{\frac{\alpha(a)^2}{a}, \frac{\cosh(\pi \alpha(a)) - 1}{\exp(2a) - 1}\right\} - 1,
   \]

   where

   \[
   \delta(a) = 0.35 \max\{0, a - a^*\} + 1.03 \sqrt{\max\{0, a - a^*\}},
   \]

   and $\epsilon = 0.001$. $a^* = 0.798953686083986$ is the constant defined by eq. (17).

2. Define functions $h_{\alpha,\beta}$ and $g_a$ by

   \[
   h_{\alpha,\beta}(x) = \frac{2}{\alpha} \tanh^{-1}\left(\sqrt{1+\beta} \tan((2x - 1) \tan^{-1}(\sqrt{1+\beta} (\tanh(\frac{\pi \alpha(a)}{2}))))\right),
   \]

   and

   \[
   g_a(x) = \exp(-a G_a(h_{\alpha(a),\beta(a)}(x)))
   \]

   with

   \[
   G_a(\theta) = 1 - \cos \theta - \frac{1}{a} \log \left(1 + \frac{1}{1 + \beta(a)} (\cosh(\alpha(a) \theta) - 1)\right).
   \]

3. Let $\omega_j$ and $\omega'_j$ with $j = 1, 2, 3, \ldots$, be two sequences of independent random variables uniformly distributing in $[0, 1)$. Define a subsequence

   \[
   \tilde{\omega}_i = \omega_{j_i}, \quad i = 1, 2, 3, \ldots,
   \]

   of the sequence $\{\omega_j\}$ by selecting the numbers $j = j_i$ that satisfy

   $\omega'_j \leq g_a(\omega_j)$.
The sequence
\[ h_{\alpha(a),\beta(a)}(\tilde{\omega}_1), h_{\alpha(a),\beta(a)}(\tilde{\omega}_2), h_{\alpha(a),\beta(a)}(\tilde{\omega}_3), \ldots, \]
is the random \( U(1) \) variable, a sequence whose distribution is
\[ P([\theta, \theta + d\theta]) = N_a \exp(a \cos \theta) d\theta, \quad -\pi \leq \theta < \pi, \quad a > 0, \]
\[ \frac{1}{N_a} = \int_{-\pi}^{\pi} \exp(a \cos \theta) d\theta. \]

We will refer to this choice as the ‘proposed cosh’ method. One can explicitly check that the choice of parameters satisfies \(-1 < \beta(a) < 1\) for all \( a \in (0, \infty) \).

The functions \( h_{\alpha,\beta} \) and \( g_a \) therefore are obtained from section 3. One can see that this choice of parameters satisfies the conditions (32), (33), and (34), which implies that the ‘proposed cosh’ method correctly generates \( U(1) \) random variables. The acceptance rate \( R(a) \) for ‘proposed cosh’ method is given in Figure 1. Note that the acceptance rate is high for all values of \( a \). The minimum of \( R(a) \) for ‘proposed cosh’ method is \( R(a = \infty) \approx 0.88 \).

5 Efficiency test.

We will show our results of efficiency test for ‘proposed cosh’ method.

In Monte Carlo simulations, we try to generate a number in the random \( U(1) \) variable, for each trial update of a site or link variable. As explained in section 2, this is to generate two independent uniform random number \( \omega_j \) and \( \omega_j' \) and decide whether to accept or reject \( h(\omega_j) \). We may alternatively decide to try at most \( n \)-times, namely to try \( \omega_j, \omega_{j+1}, \ldots, \omega_{j+n-1} \), before deciding that this site variable was not updated. (We shall call this number \( n \), the iteration number, and call this one set of trial, an update.) This will effectively improve the acceptance rate to
\[ R_n = 1 - (1 - R)^n, \quad (25) \]
where \( R \) is the original acceptance rate. On the other hand, this will increase the time consumption per update by an average rate of roughly \( R^{-1} \) when \( n(1 - R)^n \ll 1 \).

In other words, one must consider the possibility of iterating an algorithm with low acceptance rate but high speed, such as iterating the ‘direct’ method. Improvement of the efficiency resides in a balance of high acceptance rate and simple (fast) program.

Efficiency is a measure of average speed of producing random \( U(1) \) variable. From the above consideration on Monte Carlo updates, we may define the efficiency by the average time consumption for an update with iteration number \( n \) chosen so that the effective acceptance rate \( R_n \) exceeds some fixed rate, say,
\[ R_n > 0.9. \quad (26) \]
This definition is useful when considering Monte Carlo calculations.

We note that this is not the only possible definition of efficiency. Alternatively, one may use the criteria to iterate until a variable is updated. In appendix A of [2] this criteria is adopted to measure the speed of their methods. However, except for the discreetness of iteration number (and modulo multiplication of a constant), the two criteria essentially measure the same quantity, so the conclusion will not change.

The best possible choice depends on the machine to be used. We checked our choice in section 4 by HITACHI S820 in Computer Centre of University of Tokyo, which uses a pipelined vector processor. We measured the efficiency of generating random $U(1)$ variable defined as above, with average taken over $4 \times 10^6$ updates. The ‘proposed cosh’ method (without iteration) has acceptance rate of more than 90% for $a \leq 8$. We compared the speed of ‘proposed cosh’ method with the iterated ‘direct’ method for $a \leq 8$, with the condition that the number of iteration is chosen to keep the acceptance rate to be more than 90%.

The measured acceptance rates were in good agreement with the theoretical predictions in section 3 and in Figure 1 (within 0.1% accuracy).

The results of the efficiency test is given in Figure 2, which shows that the ‘proposed cosh’ method is efficient for all values of $a$, especially for large $a$. Note that for the ‘direct’ method, the CPU time increases as $a$ increases, which is due to the decrease in the acceptance rate $R(a)$. Since $R(a) \rightarrow 0$ as $a \rightarrow \infty$, the CPU time for the ‘direct’ method will tend to $\infty$ as $a \rightarrow \infty$. The acceptance rate for the ‘proposed cosh’ method is greater than 0.88647 for all values of $a$, consequently the CPU time is bounded for all $a$, and furthermore, the method is suitable for vector processors.

6 Concluding remarks.

We have shown a simple method for generating random $U(1)$ variables. Our method, based on rejection algorithm, achieves high acceptance rate and low time consumption for all values of the parameter $a$, including the ‘low temperature limit’, $a \rightarrow \infty$ (section 4). The only requirement on the hardware for our method to be efficient, is that the computer is quick in calculating elementary functions such as $\exp(x)$, $\tan(x)$, and their inverse functions. Many present day computers which are equipped with co-processors for floating point calculations are suitable for our methods. Our method which keeps uniformly high acceptance rate for all values of $a$, is particularly suitable to parallel or pipeline vector processors.

From the general consideration given in section 3, the use of the ‘cosh’ distribution and the Cauchy distribution which we proposed as approximate distributions, will be efficient for generating random variables taking values in a finite interval (e.g. $[-\pi, \pi]$) and whose distribution $f_a(\theta)$ is an even function and takes maximum at $\theta = 0$, and behaves like $f_a(\theta) \approx \text{const.} - a\theta^2$ near $\theta = 0$,
with a parameter $a > 0$ that controls the sharpness of the peak. This is a common feature of weight functions for statistical mechanical systems with one component spins and link variables.

We would like to mention a couple of methods which appears in the literature, both of which are based on rejection methods, but use different approximate distributions $\tilde{f}$. The approximate distribution adopted in [4] is

$$\tilde{f}(\theta) = \tilde{N}_a \exp(a\left(1 - \frac{2}{\pi}|\theta|\right)), $$

where $\tilde{N}_a$ is a normalization constant. The acceptance rate $R(a)$ for this choice is, from eq. (2),

$$R(a) = \frac{1}{N_a \exp(a) \frac{\pi}{2} (1 - \exp(-2a))},$$

where $N_a$ is as in eq. (2) and $c = \frac{2}{\pi} \sin^{-1}\left(\frac{2}{\pi}\right) + \sqrt{1 - \left(\frac{2}{\pi}\right)^2} - 1 \approx 0.2105$ is a positive constant. In particular, at ‘low temperature’ $a \gg 1$,

$$R(a) \approx \sqrt{\frac{2a}{\pi}} \exp(-ca),$$

which rapidly approaches 0 as $a \to \infty$. Therefore this choice suffers from the same problem as with ‘direct’ method that as $a \to \infty$, the CPU-time to keep 90% effective acceptance rate tends to $\infty$. In fact, we have performed an efficiency test as explained in section 5 for this choice of approximate distribution, and found that for $a > 3$, the ‘proposed cosh’ method is faster.

The approximate distribution of [2] is the Gaussian distribution which, in our notation, is

$$\tilde{f}(\theta) = \tilde{N}_a \exp(-\alpha(a) \theta^2),$$

where

$$\frac{1}{\tilde{N}_a} = \int_{-\infty}^{\infty} \exp(-\alpha(a) \theta^2) d\theta,$$

is a normalization constant, and $\alpha(a) = \frac{2}{\pi^2} \max(a, \frac{1}{4}).$ (To be precise, they adopt ‘direct’ method for small $a$ and Gaussian distribution for large $a$. We focus our attention on the large $a$ case where the simple ‘direct’ method is not effective.) [2] quotes [3] for an algorithm of generating the Gaussian random variable.

The original distribution $f_a(\theta)$ is now considered as a distribution on $\theta \in \mathbb{R}$, where $f_a(\theta) = 0$ if $|\theta| > \pi$. The formula similar to eq. (6) (with $-\pi \leq \theta < \pi$ replaced by $\theta \in \mathbb{R}$) holds in the present case, and the acceptance rate $R(a)$ for the Gaussian distribution is,

$$R(a) = \frac{1}{N_a \exp(a) \sqrt{\frac{2a}{\pi^3}}},$$
where $N_a$ is as in eq. (2). This coincides with the results in [2]. At $a \to \infty$, $R(a) \to \frac{2}{\pi} \approx 0.6366$. Since $R(a)$ does not tend to zero, the effective CPU-time consumption is bounded for all range of $a$, which is of course a nice feature shared with our methods. The acceptance rate of ‘proposed cosh’ method is considerably higher than that of the Gaussian method for all values of $a$. As for a quantitative comparison of CPU-time consumption, [2] compares the CPU-time between the ‘direct’ method and the Gaussian method, and finds that (with their machine) for $a > 1.5$ the Gaussian method becomes faster than the ‘direct’ method, and slows down somewhat as $a$ is increased further. (Roughly 12% decrease in speed from $a = 1.5$ to $a = \infty$.) As can be seen from Figure 2, at $a = 1.5$ the ‘proposed cosh’ method is already faster (the ratio in speed is roughly 1.6) than the ‘direct’ method, and it practically does not slow down if $a$ is increased. (A rough estimate shows that only 3% decrease in speed occurs from $a = 1.5$ to $a = \infty$.) Therefore we may conclude that the ‘proposed cosh’ method is faster than the Gaussian method for $a > 1.5$.

Acknowledgements.

We would like to thank Prof. Y. Oyanagi for very helpful discussions and encouragements. We would also like to thank Prof. A. D. Sokal for instructive comments and bringing basic references to our attention.

A

In this Appendix, we prove the statements in section 2.

Let $p$ be the density function for the distribution of the random variable (7):

$$p(\theta) \, d\theta = \text{Prob}[ h(\tilde{\omega}_i) \in [\theta, \theta + d\theta] ],$$

where

$$\text{Prob}[ P(i) ] \equiv \lim_{N \to \infty} \frac{1}{N} \# \{ 1 \leq i \leq N \mid P(i) \}.$$  

The statement $p = f_a$ is proved as follows. By eq. (4) we have

$$h^{-1}(\theta + d\theta) = h^{-1}(\theta) + \frac{1}{h'(h^{-1}(\theta))} d\theta = h^{-1}(\theta) + \tilde{f}(\theta) \, d\theta,$$

hence

$$p(\theta) \, d\theta = \text{Prob}[ \tilde{\omega}_i \in [h^{-1}(\theta), h^{-1}(\theta) + \tilde{f}(\theta) \, d\theta] ].$$  \hfill (27)
Fix $0 \leq x < 1$. By definition we have $0 \leq g(x) \leq 1$. Since $\omega_j^i$, $j = 1, 2, 3, \ldots$, is a uniform random variable, we see that the conditional acceptance rate for $\omega_i$ under the condition that $\omega_i \in [x, x + dx]$, is $g(x)$. Therefore,

$$P \{ \omega_i \in [x, x + dx] \} = P \{ \omega_i \in [x, x + dx] \} \times g(x) \propto g(x) dx,$$

where we also used the fact that $\omega_i$, $i = 1, 2, 3, \ldots$, is a uniform random variable. Insert this equation in eq. (27) and use eq. (5) to obtain

$$p(\theta) d\theta \propto g(h^{-1}(\theta)) \tilde{f}(\theta) d\theta \propto f_a(\theta) d\theta.$$

Since $f_a$ is correctly normalized, we have $p(\theta) = f_a(\theta)$. This completes the proof.

The proof that the acceptance rate is equal to $R$ in eq. (6) is as follows. For each $x$ with $0 \leq x < 1$, the conditional acceptance rate for $\omega_i$ under the condition that $\omega_i \in [x, x + dx]$, is $g(x)$. Therefore

$$\text{The acceptance rate} = \int_0^1 g(x) dx$$

$$= R \int_0^1 \frac{f_a(h(x))}{f(h(x))} dx$$

$$= R \int_{-\pi}^\pi \frac{f_a(\theta)}{\tilde{f}(\theta)} \tilde{f}(\theta) d\theta = R.$$

This completes the proof.

**B**

In this Appendix, we give a proof that the ‘optimal cosh’ method in section 3 correctly gives the random $U(1)$-variables, and also we give the argument for the choice of the parameters.

We consider the case $a > a^*$. The proof for the case $0 < a \leq a^*$ is similar.

By explicit calculation, one sees that $h_{\alpha,\beta}$ of eq. (13) satisfies eq. (4). Therefore it suffices to show that eq. (18) satisfies eq. (5) with eq. (6).

Define,

$$G(\theta) = \frac{1}{a} \log \left\{ \frac{\tilde{f}(\theta) f_a(0)}{f_a(\theta) \tilde{f}(0)} \right\}$$

$$= 1 - \cos \theta - \frac{1}{a} \log \left( \frac{1}{1 + \beta} \cosh(\alpha \theta) + \beta \right).$$

($G$ depends on three free parameters $a$, $\alpha$, and $\beta$. We suppress the parameter dependences for the moment.) Then eq. (18) and eq. (5) imply

$$g(x) = \exp\{-a (G(h(x)) - \min_{\theta \in [-\pi,\pi]} G(\theta))\},$$

(30)
and
\[
R(a) = \frac{\tilde{f}(0)}{Na \exp(a)} \exp\{a \min_{\theta \in [-\pi, \pi]} G(\theta)\}.
\]

Comparing eq. (29) with eq. (18), one sees that the results in section θ are correct if
\[
\min_{\theta \in [-\pi, \pi]} G(\theta) = 0.
\] (31)

**Proposition.** Let \(a > 0\), \(\alpha > 0\), and \(\beta > -1\). If \(G\) satisfies the three conditions
\[
G''(0) = 1 - \frac{a^2}{a + \beta} \geq 0,
\] (32)
\[
G^{(4)}(0) = -1 - \frac{a^4(\beta - 2)}{a(1 + \beta)^2} \geq 0,
\] (33)
\[
G(\pi) = 2 - \frac{1}{a} \log \left( \frac{\cosh(\pi \alpha + \beta)}{1 + \beta} \right) \geq 0,
\] (34)
then \(G\) satisfies
\[
G(x) \geq 0, \quad -\pi \leq x \leq \pi.
\] (35)

Assume for the moment that this Proposition is true. It is easy to see by explicit calculations that \(\alpha = \alpha(a)\) and \(\beta = \beta(a)\) defined by eq. (14) or eq. (15) satisfy the conditions (32), (33), and (34), and \(\alpha(a) > 0\) and \(\beta(a) > -1\), for all \(a > a^*\). Since
\[
G(0) = 0,
\]
the Proposition implies that eq. (31) is satisfied for all \(a > a^*\).

It remains to prove the Proposition.

**Proof of the Proposition.** Since \(G\) is an even function, it is sufficient to prove \(G(x) \geq 0\) for \(0 \leq x \leq \pi\).

From (32) and (33) it follows that \(\alpha^2(2 - \beta) \geq \beta + 1\). The equality holds if and only if \(a(\beta + 1) = \alpha^2\) and \(\alpha^2 = 3a - 1\), which, with (34) implies \((3a - 1)(\exp(2a) - 1) \geq a(\cosh(\pi \sqrt{3a - 1}) - 1)\). This is equivalent to \(a > a^* (> 3/2)\), where \(a^*\) is defined by eq. (16). Therefore, if we define a set \(D\) by
\[
D = D_1 \cup D_2,
\]
\[
D_1 \equiv \{(a, \alpha, \beta) \in (0, \infty)^2 \times (-1, \infty) | \alpha^2(2 - \beta) > \beta + 1 \geq \alpha^2/a \},
\]
\[
D_2 \equiv \{(a, \alpha, \beta) \in (0, \infty)^2 \times (-1, \infty) | \alpha^2 = 3a - 1, \beta + 1 = \alpha^2/a, a > 3/2 \},
\]
it is sufficient to prove that for all \((a, \alpha, \beta) \in D\) and \(0 \leq x \leq \pi\), (34) implies \(G(x) \geq 0\).
Step 1. Fix \((a, \alpha, \beta) \in D\). Put \(g(x) \equiv G'(x)\). (This \(g\) has nothing to do with \(g\) in eq. (30).) Then we have
\[
f(x) \equiv g(x) + g''(x) = \frac{\alpha^5 \sinh(\alpha x)}{a(\beta + \cosh(\alpha x))^3} \cosh(\alpha x - 1),
\]
where
\[
h(y) \equiv -y^2 + (\beta - 2a^{-2}(\beta + 1))y + \alpha^{-4}(\beta + 1)(\alpha^2(2 - \beta) - (\beta + 1)).
\]
Since \((a, \alpha, \beta) \in D\), we see that there exists one and only one positive root \(y = y_0\) of \(h(y) = 0\) and that
\[
h(y) > 0, \quad \text{if} \quad 0 < y < y_0,
\]
\[
h(y) < 0, \quad \text{if} \quad y > y_0.
\]
Therefore if we let \(x = x_0\) to be the unique positive solution to the equation \(\alpha^{-2}(\cosh(\alpha x) - 1) = y_0\), we have
\[
f(x) > 0, \quad \text{if} \quad 0 < x < x_0, \quad \text{(37)}
\]
\[
f(x) < 0, \quad \text{if} \quad x > x_0. \quad \text{(38)}
\]
Note that \(g(0) = 0\) and \(g'(0) \geq 0\) if \((a, \alpha, \beta) \in D\). From eq. (30) and eq. (37) we therefore conclude
\[
g(x) > 0, \quad \text{if} \quad 0 < x \leq x_0 \text{ and } 0 < x < \pi. \quad \text{(39)}
\]
(The conclusion may be easily understood if one notes that eq. (36) is an equation of motion of harmonic oscillation with external force \(f\).)

The equations (36), (38), (39), imply
\[
G'(x) = g(x) > 0, \quad \text{if} \quad 0 < x \leq x_0 \text{ and } 0 < x < \pi. \quad \text{(40)}
\]
\[
g(x) + g''(x) < 0, \quad \text{if} \quad x > x_0. \quad \text{(41)}
\]

Step 2. Fix \(\alpha > 0\) and \(t \equiv a\alpha^{-2}(\beta + 1) \geq 1\), and let \(a\) vary with the restriction \((a, \alpha, \beta) \in D\). The allowed region of \(a\) differs by the values of \(t\) and \(\alpha\):

1. \(t > 1\), or \(t = 1\) and \(\alpha \leq \sqrt{t}/2\).

   In this case, \((a, \alpha, \beta) \in D\) is equivalent to \(a > (\alpha^2 + 1)/3\).

2. \(t = 1\) and \(\alpha > \sqrt{t}/2\).

   In this case, \((a, \alpha, \beta) \in D\) is equivalent to \(a \geq (\alpha^2 + 1)/3\).
Note that \( g(x) = g_a(x) \) is continuous (uniformly continuous on compact sets in \((0, \pi]\) w.r.t. \( x \)) and increasing in \( a \), and \( x_0 = x_0(a) \) is continuous in \( a \). Also, 

\[
\lim_{a \to \infty} g(x) = \sin x
\]

uniformly on compact sets in \((0, \pi]\).

We claim that for every \( a \) (such that \((a, \alpha, \beta) \in D)\), and for any \( x_1 \) and \( x_3 \) satisfying \( g_a(x_1) > 0, \ g_a(x_3) > 0 \), and \( 0 < x_1 < x_3 \leq \pi \), we have \( g_a(x) > 0, \ x \in [x_1, x_3] \).

Assume this is wrong: Assume that for \( a = a_0 \) and \( 0 < x_1 < x_2 < x_3 \leq \pi \) we have \( g_{a_0}(x_1) > M, \ g_{a_0}(x_2) \leq 0, \) and \( g_{a_0}(x_3) > M \), where \( M \) is a positive constant. Since \( g_a(x) \) is increasing in \( a \), we have 

\[
g_a(x_1) > M, \ g_a(x_3) > M, \ a \geq a_0.
\]

Put 

\[
q(a) \equiv \min_{x_1 \leq x \leq x_3} g_a(x).
\]

Then \( q(a) \) is continuous in \( a \) and \( \lim_{a \to \infty} q(a) > 0 \). Therefore there exists \( a_1 \geq a_0 \) such that \( q(a_1) = 0 \), which further implies that \( g_{a_1}(x) \geq 0, \ x_1 \leq x \leq x_3 \), and that there exists \( x_4 \) satisfying \( x_1 < x_4 < x_3 \) and \( g_{a_1}(x_4) = 0 \). In particular, \( g_{a_1}(x_4) = 0 \) and \( g''_{a_1}(x_4) \geq 0 \) hold, which contradicts eq. (40) and eq. (41).

Hence the claim is proved.

**Step 3.** Fix \((a, \alpha, \beta) \in D\). From the claim and eq. (40) we see that either \( g(x) = G'(x) > 0 \) for \( 0 < x < \pi \), or there exists \( x' \) such that \( 0 < x' < \pi \), and \( g(x) > 0 \) for \( 0 < x < x' \), and \( g(x) < 0 \) for \( x' < x \leq \pi \). Hence \( G(x) \) is either increasing in \( 0 < x < \pi \) or has just one peak and no valley. Since \( G(0) = 0 \) and \( G(\pi) \geq 0 \), we have \( G(x) > 0, \ 0 < x < \pi \). This completes the proof.

We now turn to the argument for the choice of the parameters. We want to choose the parameters so that the acceptance rate is as large as possible. As stated at the end of section 3, it is better to have as flat \( g(x) \) as possible, hence a flat \( G(x) \). Thus we require \( G''(0) = 0 \). We impose the condition that the minimum of \( R(a) \) is achieved at \( \theta = 0 \). Note that this is equivalent to assuming eq. (35). As a necessary condition, we have \( G^{(4)}(0) \geq 0 \) and \( G(\pi) \geq 0 \). (By the Proposition, we know that these are sufficient to ensure eq. (35).) As we want to have flat \( G(x) \), it should be best to have either \( G^{(4)}(0) = 0 \) or \( G(\pi) = 0 \). If one draws a graph of these three conditions, in \((\alpha, \beta)\)-plane, one easily sees that the choice given in the section 3 is the one that we are looking for.

**C**

In this Appendix, we give a sample FORTRAN program for generating random \( U(1) \) variables, using ‘proposed cosh’ method. When the subroutine U1RND
is called with the parameter $a$ as the first argument, it returns a random $U(1)$ variable as the second argument.

Note that this sample program is different from the program used to test the efficiency discussed in section 3, where we modified the program in favor of a pipelined vector processor.

```fortran
SUBROUTINE U1RND(A,G)
C VARIABLES FOR U(1) RANDOM NUMBERS
REAL PI,A,AS,EPS,DEL,ALP,BET,DAP,DL1,DL2,BT1,H,G,CH,H1
PARAMETER (PI=SNGL(3.14159265358979D0))
PARAMETER (AS=SNGL(0.798953686083986D0))
PARAMETER (EPS=0.001, DL1=0.35, DL2=1.03)
C VARIABLES FOR UNIFORM RANDOM NUMBERS
INTEGER C30,CRND,IRND
REAL RND
REAL*8 C31
PARAMETER (C30=2**30, C31=2D0**31, CRND=48828125)
DATA IRND/1000001/
C
DAP=MAX(0,A-AS)
DEL=DL1*DAP+DL2*SQRT(DAP)
ALP=MIN(SQRT(A*(2-EPS)), MAX(SQRT(EPS*A),DEL))
BET=MAX(ALP*ALP/A, (COSH(PI*ALP)-1)/(EXP(2*A)-1)-1)
BT1=SQRT((1+BET)/(1-BET))
C
1 CONTINUE
C
R=IRND/C31
IRND=IRND*CRND
IF (IRND .LT. 0) IRND=(IRND+C30)+C30
C
H1=BT1*TAN(((2*R-1)*ATAN(TANH(PI*ALP/2)/BT1))
H=ALOG(((1+H1)/(1-H1))/ALP
G=EXP(-A*(1-COS(H)))*(COSH(ALP*H)+BET)/(1+BET)
C
R=IRND/C31
IRND=IRND*CRND
IF (IRND .LT. 0) IRND=(IRND+C30)+C30
C
IF (G .LT. R) GOTO 1
RETURN
END
```
References

[1] J. W. Butler, in *Symposium on Monte Carlo Methods*. ed. H. A. Meyer, (John Wiley, New York, 1956).

[2] R. G. Edwards, J. Goodman, A. D. Sokal, *Nucl. Phys.* B354 (1991) 289-327.

[3] D. E. Knuth, *The Art of Computer Programming Volume II*, 2nd ed. (Addison-Wesley 1981).

[4] K. J. Moriarty, *Phys. Rev.* D25 (1982) 2185-2193.

[5] T. Tsuda, *Monte Carlo methods and simulation (In Japanese)*, (Baihukan, Tokyo, 1969).
Figure captions.

Figure 1: Acceptance rate $R(a)$: ‘direct’ method (lowest curve), ‘optimized cosh’ method (highest curve), and ‘proposed cosh’ method (curve in between).

Figure 2: Time consumption $T$ to keep 90% acceptance rate $R(a) > 0.9$. Iterated ‘direct’ method (+) and ‘proposed cosh’ method (◦). $T$ is in arbitrary unit.