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Method for Sampling from Fission Neutron Energy Spectra

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MASTER

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METHOD FOR SAMPLING FROM FISSION NEUTRON ENERGY SPECTRA

F. H. Froehner* and R. R. Spencer

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ABSTRACT

A simple method for fast and efficient sampling from the Watt fission neutron energy spectrum is described. As a limiting case the Maxwellian energy distribution can also be sampled. A short FORTRAN routine written for this purpose and results obtained with it are presented. The routine is shown to give accurate results, and requires < 1 ms/sample on a DEC KA-10 processor.

INTRODUCTION

Fission neutron spectra are often described by a formula employed e.g. by Watt¹ and by Cranberg et al.,²

$$\chi(E) dE = C e^{-E/A} \sinh \sqrt{BE} dE, \quad (1)$$

known as the Watt spectrum. In reactor physics and neutron metrology the need arises in Monte Carlo calculations to sample from this distribution. In what follows we show a way to accomplish this. The method is based on the facts that (i) the Watt spectrum can be considered as a Maxwellian energy spectrum seen from a moving (Galileo-transformed) reference system and (ii) that the Maxwellian energy spectrum corresponds to normally distributed Cartesian coordinates of the neutron velocity.

THEORETICAL DERIVATION OF THE WATT SPECTRUM

Consider fission fragments with lab velocity $\vec{v}_f$ emitting neutrons with a Maxwellian velocity distribution in the center-of-mass system,

$$p(\vec{v}_c) d^3v_c = \prod_{i=1}^3 \exp\left(-\frac{v_{ci}^2}{v_T^2}\right) \frac{dv_{ci}}{v_T \sqrt{\pi}} = \frac{1}{\pi^{3/2}} \exp\left(-\frac{v_c^2}{v_T^2}\right) \frac{d^3v_c}{v_T^3}. \quad (2)$$

The quantity v_T , the most probable speed, is related to the fission fragment temperature T (in energy units) by $mv_T^2/2 = T$, m being the neutron mass. The distribution of neutron velocities $\vec{v}$ in the laboratory system is obtained from (2) by Galileo transformation to the lab system, i.e. by substitution of $\vec{v}_c = \vec{v} - \vec{v}_f$, $d^3v_c = d^3v$, whence

$$p(\vec{v})d^3v = \frac{1}{\pi^{3/2}} \exp\left[-\left(\frac{\vec{v}-\vec{v}_f}{v_T}\right)^2\right] \frac{d^3v}{v_T^3}.$$

Using polar coordinates, $d^3v = v^2 dv d\mu d\phi$, with the polar axis parallel to $\vec{v}_f$, then integrating over angles and expressing everything in energies ($E = mv^2/2$, $E_f = mv_f^2/2$) one gets the Watt spectrum in the form

$$\chi(E) dE = \frac{1}{\sqrt{\pi}} e^{-E_f/T} e^{-E/T} \sinh \sqrt{\frac{4E_f E}{T^2}} \frac{dE}{\sqrt{TE_f}}. \quad (3)$$

Comparison with (1) yields

$$A = T = \frac{m}{2} v^2, \quad B = \frac{4E_f}{T^2} = \frac{4v_f^2}{Av_T^2}.$$

SAMPLING FROM THE WATT SPECTRUM

The interpretation of the Watt spectrum as a Galileo-transformed Maxwell energy spectrum suggests the following sampling procedure: Sampling thrice from the normal density function, $p(x) dx = \exp(-x^2) dx/\sqrt{\pi}$, one obtains relative c.m.s. velocity coordinates, $x_i = v_{ci}/v_T$, $i = 1, 2, 3$. With the 1-axis parallel to $\vec{v}_f$ the lab velocity coordinates are $v_1 = v_{c1} + v_f$, $v_2 = v_{c2}$, $v_3 = v_{c3}$, hence the lab energy is

$$E = \frac{m}{2} v_T^2 \left[\left(x_1 + \frac{v_f}{v_T}\right)^2 + x_2^2 + x_3^2 \right] = A \left[\left(x_1 + \frac{\sqrt{AB}}{2}\right)^2 + x_2^2 + x_3^2 \right]. \quad (4)$$

Many techniques are available for sampling from a normal density function. Perhaps the most lucid one is that of Box and Muller;³ one writes the joint

probability for obtaining x_1 in dx_1 , x_2 in dx_2 in terms of polar coordinates $x = \sqrt{(x_1^2 + x_2^2)}$, $\phi = \arctan(x_2/x_1)$,

$$\begin{aligned} p(x_1, x_2) dx_1 dx_2 &= \frac{1}{\pi} \exp(-x_1^2 - x_2^2) dx_1 dx_2 \\ &= -d(e^{-x^2}) d\left(\frac{\phi}{2\pi}\right), \quad 0 < x < \infty, \quad 0 < \phi < 2\pi. \end{aligned}$$

The last equality shows that $\exp(-x^2)$ and $\phi/(2\pi)$ are independent random variates, uniformly distributed between 0 and 1. One can therefore sample twice from the uniform distribution in this interval (i.e. with one of the usual random number generators) to get the random numbers r_1, r_2 . Solving $r_1 = \exp(-x^2)$ and $r_2 = \phi/(2\pi)$ for x and ϕ and going back to Cartesian coordinates one finds

$$x_1 = \sqrt{-\ln r_1} \cos 2\pi r_2, \quad x_2 = \sqrt{-\ln r_1} \sin 2\pi r_2.$$

These are two independent numbers of the normal density function. Sampling velocity coordinates in this way and noting $(x_1^2 + x_2^2) = -\ln r_3$, one finds from (4) the final result

$$\begin{aligned} E_1 &= A[(\sqrt{-\ln r_1} \cos 2\pi r_2 + \sqrt{AB}/2)^2 - \ln r_3], \\ E_2 &= A[(\sqrt{-\ln r_1} \sin 2\pi r_2 + \sqrt{AB}/2)^2 - \ln r_3]. \end{aligned} \tag{5}$$

Thus from 3 random numbers r_1, r_2, r_3 one gets 2 numbers E_1, E_2 of the Watt distribution (1). In the special case $v_f = 0$, i.e. $B = 0$, the Watt distribution reduces to the Maxwell energy distribution

$$\chi(E) dE = \frac{2}{\sqrt{\pi}} e^{-E/A} \sqrt{\frac{E}{A}} \frac{dE}{A}. \tag{6}$$

Therefore, the prescription (5) is valid for both. It should be mentioned that the prescription is related to one employed in the ESP Reactor Monte Carlo code (see Ref. 6).

So far the method involves no approximation and in this sense it is rigorous. It is also quite efficient since nothing is rejected if E is allowed to assume arbitrarily large values. In reality, of course, the fission neutron energy cannot exceed the total excitation energy available. It is therefore customary to use a cutoff (see e.g. Refs. 4 and 5) which is typically 10-20 times larger than T . This presents no difficulty for Monte Carlo sampling with the prescription (5). One simply rejects all E -values exceeding the cutoff. The fraction of energies thus rejected is so small (see Fig. 1) that the efficiency of the method is virtually unaffected within the limits of the statistical accuracies normally achieved in Monte Carlo calculations.

FORTTRAN ROUTINE

A simple FORTRAN routine which samples energies according to the prescription (5) is reproduced in Appendix A. The distribution of numbers of sampled energies is stored in an 18 group structure defined by the DATA instruction. Test calculations for a Watt and a Maxwellian distribution with the same average energy, $\bar{E} = 2.09$ MeV, are compared in Table I to their theoretical shapes as calculated from Eqs. (7) and (6), respectively. Each sampling calculation was run for $NH = 100,000$ pairs of energies; this required approximately 160 CPU seconds on a Digital Equipment Corporation KA-10 processor.

Fig. 1. Comparison of Monte Carlo sampled Watt and Maxwellian distributions in an 18 energy group structure with their respective analytic distributions.

TABLE I. Comparison of Sampled (P_i) and Calculated (N_i)
Normalized, Group Probabilities for Watt and Maxwell
Spectra. (Both spectra have the same average
energy, $\langle E \rangle = 2.09$ MeV.)

i	$E_{\max}^a$ (MeV)	P_i	N_i^b	$(P_i - N_i) / \sigma(P_i)^c$
Watt spectrum ($A = 1.010$ MeV, $B = 2.254$ MeV $^{-1}$)				
1	0.250000	0.047550	0.047823	-0.573
2	0.750000	0.159110	0.159152	-0.051
3	1.250000	0.165280	0.165122	0.190
4	1.750000	0.145820	0.145238	0.737
5	2.250000	0.119650	0.119207	0.611
6	2.750000	0.094390	0.093997	0.601
7	3.250000	0.073185	0.072150	1.778
8	3.750000	0.053430	0.054300	-1.729
9	4.250000	0.039560	0.040247	-1.576
10	4.750000	0.028550	0.029467	-2.462
11	5.250000	0.021390	0.021355	0.107
12	6.000000	0.021105	0.021282	-0.549
13	6.750000	0.012835	0.012759	0.301
14	7.500000	0.007620	0.007548	0.371
15	8.500000	0.005395	0.005427	-0.198
16	10.000000	0.003420	0.003347	0.560
17	20.000000	0.001710	0.001581	1.395
Maxwell spectrum ($A = 1.393$ MeV, $B = 0$)				
1	0.250000	0.050395	0.051412	-2.079
2	0.750000	0.165885	0.165914	-0.035
3	1.250000	0.167390	0.166583	0.967
4	1.750000	0.144020	0.143067	1.214
5	2.250000	0.114410	0.115583	-1.648
6	2.750000	0.091110	0.090342	1.193
7	3.250000	0.069380	0.069162	0.383
8	3.750000	0.051190	0.052197	-2.044
9	4.250000	0.039160	0.038985	0.404
10	4.750000	0.029145	0.028887	0.686
11	5.250000	0.021550	0.021270	0.861
12	6.000000	0.021505	0.021718	-0.656
13	6.750000	0.013660	0.013500	0.616
14	7.500000	0.008050	0.008333	-1.416
15	8.500000	0.006180	0.006332	-0.865
16	10.000000	0.004215	0.004260	-0.309
17	20.000000	0.002755	0.002454	2.566

^aMaximum energy of neutron energy group.

^bObtained by precise numerical integration of the distribution function over the group energy interval.

^c $\sigma(P_i) = \sqrt{P_i(1-P_i)/\# \text{ of Trials}}$

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APPENDIX A. FORTRAN Test Program

THIS ROUTINE SAMPLES NEUTRON ENERGIES FROM EITHER
 A MAXWELLIAN($B=0.0$) OR A WATT-CRANBERG DISTRIBUTION
 ($E>0.0$); TWO ENERGIES ARE RETURNED FOR EACH SET
 OF THREE RANDOM NUMBERS CHOSEN. RESULTS ARE COMPARED
 IN AN 18 GROUP ENERGY STRUCTURE WITH PROBABILITIES OBTAINED
 FROM THE DISTRIBUTION FUNCTION BY NUMERICAL INTEGRATION.

RAN(D) IS THE DEC SYSTEM-10 RANDOM NUMBER GENERATOR;
 FOR OTHER COMPUTERS AN APPROPRIATE SUBROUTINE SHOULD
 BE SUBSTITUTED

COMMON/WAT/EB(18),WT(18),P(18),CHI(18),DP(18)
 COMMON/SIM/NI,FN(4001),SM
 DATA(EB(I),I=1,18)/.25,.75,1.25,1.75,2.25,2.75,3.25,3.75,
 14.25,4.75,5.25,6.,6.75,7.5,8.5,10.,20.,99.999/

TYPE 30
 30 FORMAT(' A=,F5.3,',\$)
 ACCEPT 31,A
 31 FORMAT(F5.3)
 TYPE 40
 40 FORMAT(' B=,F5.3,',\$)
 ACCEPT 41,B
 41 FORMAT(F5.3)
 X=SQRT(A*B)/2.
 TYPE 50
 50 FORMAT(' # HISTORIES,16,',\$)
 ACCEPT 51,NH
 51 FORMAT(I6)
 DO 4 K=1,NH
 R1=RAN(D)
 R2=RAN(D)
 R3=RAN(D)
 Z=SQRT(-ALOG(R1))
 S=6.28319*R2
 ALOGR3=ALOG(R3)
 E1=A*((Z*COS(S)+X)**2-ALOGR3)
 E2=A*((Z*SIN(S)+X)**2-ALOGR3)
 DO 1 I=1,18
 IF(E1.LE.EB(I))WT(I)=WT(I)+1.
 IF(E1.LE.EB(I))GO TO 2
 1 CONTINUE
 2 DO 3 J=1,18
 IF(E2.LE.EB(J))WT(J)=WT(J)+1.
 IF(E2.LE.EB(J))GO TO 4
 3 CONTINUE
 4 CONTINUE
 SUM=0.
 DO 5 L=1,18
 5 SUM=SUM+WT(L)
 EL0=0.
 TYPE 32
 32 FORMAT(' NO. OF SIMPSON INTERVALS=(16)',\$)
 ACCEPT 33,NI
 33 FORMAT(I6)
 DO 6 M=1,18
 P(M)=WT(M)/SUM
 DP(M)=SQRT(P(M)*(1.-P(M))/SUM)
 DLE=EB(M)-EL0

APPENDIX A -continued-

```

DLEE=DLE/FLOAT(2*NI)
NMAX=2*NI+1
EN=ELO
IF(E.NE.0.)GO TO 8
C   MAXWELL FUNCTION
DO 9 N=1,NMAX
FN(N)=EXP(-EN/A)*SQRT(EN/A)/A
9 EN=EN+DLEE
CALL SIMPSN
CHI(M)=SM*1.12838*DLEE/3.
ELO=EB(M)
GO TO 11
C   WATT-CRANBERG FUNCTION
8 DO 10 N=1,NMAX
RT=SQRT(E*EN)
FN(N)=EXP(-EN/A)*SINH(RT)
10 EN=EN+DLEE
CALL SIMPSN
C=0.56419*EXP(-A*B/4.)/SQRT(E*A**3/4.)
CHI(M)=SM*C*DLEE/3.
ELO=EB(M)
11 CONTINUE
DP(M)=(P(M)-CHI(M))/DP(M)
TYPE 7,M,EB(M),P(M),CHI(M),DP(M)
7 FORMAT(14,3F10.6,F8.3)
6 CONTINUE
END

C
C
SUBROUTINE SIMPSN
C
COMMON/SIM/NI,Y(4001),SM
C
SM=Y(1)
DO 1 I=1,NI
J=2*I
1 SM=SM+Y(J)*4.+Y(J+1)*2.
SM=SM-Y(2*NI+1)
RETURN
END

```


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