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PRELIMINARY STOCHASTIC ESTIMATES OF SLOWING DOWN OF FAST NEUTRONS IN H_2O

A.S. HOUSEHOLDER

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PRELIMINARY STOCHASTIC ESTIMATES OF SLOWING DOWN OF FAST NEUTRONS IN H_2O

In this report is described an application of the so-called Monte Carlo method to the estimations of certain quantities characterizing the slowing down of fast neutrons in water. The method as proposed by S. Ulam and J. von Neumann, is extremely simple. It amounts to setting up an abstract model to represent the actual events in the slowing down of the individual neutrons, and following a large number of ideal neutrons through these events. The statistics of this population of ideal neutrons are taken as estimates of the parameters of a large population of real neutrons.

It is clear that for reliable estimates a large population of a thousand or more is required. This means that one must generally resort to the use of machinery of at least the capacity of standard IBM. However, as a pilot study, a population of 100 neutrons, from a plane source of 10^7 ev, was followed using ordinary desk calculators. This is the study to be reported here. We begin by describing the method of computation.

<u>Degradation in Energy by Successive Collisions</u>. This can be discussed independently of the spatial changes. We therefore consider it first.

The collisions may be considered to be of three types: absorbing, elastic scattering with hydrogen, elastic scattering with oxygen. When a collision occurs, the probability that it is of one or another of

these types is represented by a ratio of cross-sections. Accordingly if A_o is the probability that the collision is absorbing; $A_1 - A_o$ the probability that it is an elastic collision with hydrogen, and $1-A_1$ the probability that it is an elastic collision with oxygen, we may decide the type of a particular collision by drawing a random number r_1 between zero and unity and noting whether $r_1 \leq A_o$, or $A_o < r_1 \leq A_1$, or $A_1 < r_1$.

Except for the first 6 neutrons, all random numbers used in this study were formed of random digits taken from Tippett's Tables of Random Sample Numbers. At first, however, these tables were not available and the first 3 of the last 5 digits were taken from 15 - place exponentials of the WPA Tables.

In Table I are given the values of A_o and A_1 as functions of energy, as well as the total mean free path utilized for determining the spatial variations.

[redacted]

TABLE I

E (ev)	λ (E)	A_o (E)	A_1 (E)
.025	.2519	.00597	.9656
.03163	.2705	.0053	.9629
.1	.3922	.00408	.9493
.3163	.5525	.00343	.9261
1.0	.6219	.00218	.9164
3.163	.6494	.00130	.9105
10	.6498	.000715	.9104
31.63	.6502	.00039	.9107
100.	.6502	.000195	.9105
316.3	.6502	.000130	.9104
1000.	.6502	.000065	.9103
1.778×10^3	.6649		.9109
3.163×10^3	.6662		.9127
5.623×10^3	.6812		.9128
10^4	.6988		.9084
1.778×10^4	.7331		.9090
3.163×10^4	.7911		.9019
5.623×10^4	.8569		.8912
10^5	1.004		.8735
1.778×10^5	1.137		.8755
3.163×10^5	1.496		.7929
5.623×10^5	1.943		.7772
10^6	2.199		.6597
1.778×10^6	4.098		.8196
3.163×10^6	5.438		.7287
5.623×10^6	7.294		.7294
6.00×10^6	8.306		.7210
6.80×10^6	8.795		.7054
7.68×10^6	9.970		.6660
8.73×10^6	10.68		.6419
9.89×10^6	11.50		.6141
10^7	11.50		.6141

Prepared by B. I. Spinrad

[redacted]

If the collision is scattering, a second random number r_2 determines the new energy as follows. Taking M = 1 or M = 16 as the case may be, we compute

$$\kappa^2 = 1 - 4r_2 M (M+1)^{-2} .$$

Then if E is the energy at which the collision occurred, E' the new energy,

$$E' = \kappa^2 E.$$

Starting with $E_0 = 10^7$ ev, all neutrons were continued either to absorption, or to the point where the energy dropped to 1 ev or lower.

<u>Statistics of the Degradation in Energy</u>. The distribution $f_n(u)$ in lethargy

$$u = \ln (E_0/E)$$

possessed by the neutrons remaining after the n-th collision was examined for each n up to and including 15. These were truncated distributions since neutrons with $E \leq 1$ were excluded. After the 16th collision only 78 neutrons remained at higher energies.

The lower moments of these distributions were computed and are given in Table II. No attempt was made to fit analytic curves, though, of course, the moments provide coefficients for the first terms of a Gram-Charlier series. The distributions look roughly Gaussian for the larger n's, and to exhibit the departure therefrom the values of the skewness and the kurtosis are also given in Table II. Also along with the values of the moments are tabulated their standard errors as estimated from the sample.

[redacted]

TABLE II

STATISTICS OF THE DISTRIBUTIONS IN LETHARGY

Col.	N	$\bar{u}$	$\sigma_{\bar{u}}$	μ_2	$\sigma_{\mu 2}$	μ_3	$\sigma_{\mu 3}$	sk	kur
1	100	0.78	0.10	1.00	0.28	2.29	1.07	2.28	5.79
2	100	1.58	0.14	1.85	0.38	3.17	1.61	1.26	2.17
3	100	2.55	0.18	3.16	0.55	5.52	3.70	0.98	1.09
4	100	3.32	0.21	4.32	0.72	7.85	3.11	0.87	0.78
5	100	4.16	0.26	6.46	1.07	14.41	5.29	0.88	0.74
6	100	5.07	0.26	6.56	0.94	10.92	3.81	0.65	0.05
7	100	6.07	0.29	8.34	1.17	13.88	4.70	0.58	-0.05
8	100	6.83	0.31	9.26	1.17	13.49	4.68	0.48	-0.40
9	100	7.51	0.32	10.37	1.27	13.92	5.04	0.42	-0.50
10	98	8.21	0.32	10.20	1.21	8.31	4.93	0.25	-0.62
11	95	8.73	0.33	10.01	1.14	5.27	4.49	0.17	-0.78
12	90	9.31	0.32	9.23	1.15	-0.51	4.94	-0.02	-0.60
13	88	10.02	0.32	8.69	1.09	-8.13	4.12	-0.32	-0.61
14	87	10.87	0.32	8.63	1.05	-9.09	3.97	-0.36	-0.71
15	82	11.48	0.32	8.36	1.21	-13.53	4.85	-0.56	-0.29

[redacted]

To simplify these computations the range of u was divided into class intervals of unit length for $n \geq 3$, and half-unit lengths for $n = 1, 2$, with the subsequent application of Sheppard's corrections.

It is of interest to note that the increase in $\bar{u}$, the mean lethargy is almost strictly linear in the number of collisions, with an average value of 0.77. At the same time the skewness shifts continuously from positive to negative values, as does the kurtosis ("peakedness"). The latter, however, shows a less consistent trend at larger values of n, due perhaps partly to the truncation. For so small a population one must not expect any high degree of reliability. The estimates of the standard errors of the mean run generally below 10%, but those for the second and third moments are considerably higher.

<u>The Distribution in z</u>. Knowing the scattering nucleus and the initial and final energies at any collision, one can compute the cosine of the scattering angle uniquely by the formula

$$\omega = \left[(M+1)\kappa - (M-1)\kappa^{-1}\right]/2, \kappa > 0,$$

where κ^2 has been previously computed and M is the atomic weight of the nucleus. A random number r_3 determines the azimuth πr_3 of scattering, whence the new direction cosine μ' is obtainable from the old, μ, by means of the spherical law of cosines:

$$\mu' = \mu\,\omega + \sqrt{1-\mu^2}\,\sqrt{1-\omega^2}\,\cos \pi r_3.$$

A fourth random number r_4 (again lying on the interval from 0 to 1) determines the length ρ of the free flight between collisions by

$$\rho = -\lambda(E) \ln r_4.$$

This is equivalent to drawing ρ from the distribution $\lambda^{-1}\exp(-\rho/\lambda)$. The change in z is then $\Delta z = \mu\rho$. This completes the description of the computation from collision to collision. There remains only the observation that since the source was supposed isotropic, the initial direction cosine μ was obtained from a random number r by means of the formula

$$\mu = 1 - 2r.$$

The distributions in z were taken as follows. For a given level of energy, each neutron was located at the point of the collision where it first dropped to an energy below this level. Thus there is a z for each neutron associated with this energy. These distributions were formed for energies expressed in integral powers of 10 down to the zeroth. The second moments of these distributions represent the ages, except for a constant factor.

The distributions look fairly Gaussian. Asymmetries are to be expected as a result of sampling errors, so that non-null values are found for the odd moments. However, since these are expected to vanish with large N, the moments about the mean provide the best estimates of the statistical parameters, and these are the moments recorded in Table III. Along with the second and fourth moments are tabulated the estimates of the standard error of the second moments, and the values of the kurtosis. The mean and the skewness are not tabulated since they have no theoretical significance.

[redacted]

TABLE III

STATISTICS OF THE DISTRIBUTION IN z

$\log_{10}E$	μ_2	σ_{μ_2}	$10^{-5}\mu_4$	Kur
6	100	21	0.56	2.5
5	439	85	9.15	1.8
4	446	91	10.20	2.1
3	458	90	10.12	1.8
2	456	90	10.14	1.9
1	449	90	10.08	2.0
0	457	89	10.04	1.8

[redacted]

The computations were made as before by dividing the range into class intervals, and applying Sheppard's corrections to the results. The class intervals here were taken 5 cm. long in all cases. Since no absorptions occurred, N = 100 for all distributions.

The variation of the second moment with energy is not what one would expect, the increase being too small as the energy drops to 10^6 ev, and too great as it drops from 10^6 to 10^5. Actually most of this increase is found to occur in the range from 10^6 to 3×10^5. The only explanation seems to be in terms of an unexpectedly high sampling error.

<u>Discussion of the Method.</u> A total of 1992 collisions were computed, averaging very nearly 20 per neutron. The calculations were carried to 3 figures, and after some practice it was possible to complete about 3 or more neutrons per day, or about 8 collisions per hour. This represents the time required for the accumulation of a population, and does not include the subsequent statistical analysis of the results -- plotting of histograms, computation of moments and their standard errors, etc. This analysis is itself a task of considerable, though lesser, magnitude.

At the same time it may be pointed out that the population can be utilized in a variety of ways. We have here obtained two distinct series of distribution; in space, for fixed energies, and in lethargy (equivalent to energy) for fixed collision number. We have considered only the case of an infinite medium. If one were interested in similar statistics for a finite slab the same population would serve, after one had weeded out all collisions following a crossing of the boundary.

The same population could be used again if one were interested in studying an extended source. One has only to add to all z's of each neutron an initial z_o determined by a new random number in accordance with the assumed distribution of the sources.

This possibility of using the same basic population for a large family of problems is one of the most appealing features of this method. To take advantage of it, it is of course necessary to record, in readily available form, a sufficient amount of the computational work.

The foregoing results are not presented with any claim to reliability, since it is clear that the population is too small. They are presented merely as the results of a small scale experiment in Monte Carlo techniques.