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A MONTE CARLO DETERMINATION OF THE ESCAPE FRACTION FOR A SCATTERING SPHERICAL SHELL WITH CENTRAL POINT SOURCE

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PHYSICS

ABSTRACT

Two types of Monte Carlo procedures were developed for the computation of the fraction of monoenergetic neutrons, emanating from a central point source, which escape from the surface of a hollow spherical shell after any number ($\geqq 0$) of elastic collisions. The shell is composed of heavy nuclei with given elastic and inelastic cross sections and a given differential cross-section curve for elastic scattering angle. Both methods yield the distribution of escaped neutrons with respect to the number of elastic collisions suffered.

A computation of each type was made on the MANIAC for a particular shell, and an estimate of the escape fraction (.70871) was obtained, based on a total sample of 215,000 source neutrons. The result is in good agreement with that (.707) obtained by J. R. Beyster using a method of H. A. Bethe involving a modified transport theory.

A comparison of the statistical and transport methods in the case of a thicker shell should be of greater interest, and a problem of this kind is being done by Beyster.

1. Description of the Problem

A point source of N monoenergetic neutrons is placed at the center of a hollow spherical shell of radii $R_o < R_1$ cm. The shell consists of a medium of numerical density N_o nuclei per cubic centimeter. These nuclei possess elastic and inelastic scattering cross sections of σ_e and σ_i barns, respectively, with total cross section of $\sigma_t = \sigma_e + \sigma_i$. Inelastic collisions are regarded as absorptions, and the neutrons resulting from such collisions are not followed further. A differential elastic scattering cross section curve is given for $\sigma_e(\mu)$ (barns per steradian) so that

$$\sigma_e = 2\pi \int_{-1}^{1} \sigma_e(\mu) d\mu$$

and, given an elastic collision,

$$2\pi \int_{-1}^{\bar{\mu}} \sigma_e(\mu) d\mu \Big/ \sigma_e$$

represents the probability of scattering at a laboratory angle ψ with the line of flight, such that

$$-1 \leq \mu \equiv \cos\psi \leq \bar{\mu}$$

The nuclei are heavy, and no loss of neutron energy attends an elastic scattering.

The problem consists in computing the number of neutrons escaping from the outer surface of the shell. The distribution of escaped neutrons, with respect to number s of elastic collisions suffered ($s = 0, 1, 2, \cdots 10$, and $s \geq 11$), and with respect to the normal angle of escape, is also obtained.

2. Constants Used in the Problem

The setup is arranged so that arbitrary substitution of the variables mentioned may be made. The particular case considered here is the following:

σ_t	3.17 barns
σ_e	2.45 "
σ_i	.72 "
N_o	$.0845 \times 10^{24}$ cm^{-3}
R_o	6.0325 cm
R_1	10.16 cm

$\mu = \cos\psi$	$\sigma_e(\mu)$
1.0	1.44
.9	.782
.8	.480
.7	.302
.6	.196
.5	.125
.4	.0978
.3	.08
.2	.08
.1	.08
0	.0889
- .1	.0889
- .2	.0889
- .3	.0978
- .4	.0978
- .5	.0978
- .6	.1067
- .7	.1067
- .8	.1067
- .9	.1067
-1.0	.1067

3. Summary of Methods

A neutron in flight is described by three parameters: (a) the radial distance R (cm) from the center, (b) $\cos\theta$, where θ is the angle measured from the positive direction of the radius vector to the direction of the line of flight, (c) the number s of elastic collisions already undergone. For example, the initial values of these parameters are $R = R_0$, $\cos\theta = 1$, $s = 0$.

The fundamental principle of Monte Carlo is the following: let u be an arbitrary random variable, and P(v) the probability of an event with $u \leq v$. Choose r at random, uniformly on the interval $0 \leq r \leq 1$. Set $r = P(v)$ and solve for v. In this way, a random number r determines an event with $u = v$.

Thus, $1 - \exp(-N_0\sigma_t y)$ is the probability of a (first) collision at distance $\leq y$ from a given point of origin (σ_t in cm^2). We have therefore $r = 1 - \exp(-N_0\sigma_t y)$, or, equally well, $r = \exp(-N_0\sigma_t y)$, where r is random on $[0,1]$. Hence, the formula

$$y = (-\ln r)/N_o\sigma_t$$

gives the distance to the point of collision, the medium permitting. Comparison of y with the distance along the line of flight to the immediate boundary of the shell decides between collision and arrival at the boundary.

In the event that the boundary reached is the outer one, the neutron is classified as to its number s of elastic collisions, and the angular zone j in which falls its normal angle of escape. A tally of 1 is made in the counter for N_s (number of neutrons escaping with s collisions) and in that for E_j (number of neutrons escaping with normal angle in angular zone j; cf., the final section on results).

If the boundary reached is the inner boundary of the shell, the values of the neutron's parameters R, cos θ are computed at that position on its line of flight where it re-enters the shell, and one returns to the computation of y, based on this position as a new point of departure.

In case collision occurs within the shell, a new random number decides between elastic and inelastic scattering, according as

$$r < \sigma_e/\sigma_t \qquad \text{or} \qquad r > \sigma_e/\sigma_t$$

An inelastic collision is recorded by a tally of 1 in the counter for I (number of neutrons "absorbed" by inelastic collision), and the neutron is dropped from further consideration.

It remains to discuss the method of dealing with an elastic collision. Technically, one should set a new random number

$$r = 2\pi \int_{-1}^{\mu} \sigma_e(\mu)d\mu \Big/ \sigma_e$$

and solve for $\mu = \cos\psi$, to obtain the angle ψ of scattering from the line of flight. This involves the necessity of fitting the $\sigma_e(\mu)$ curve analytically, and an approximation method for μ, a cumbersome process when such approximations must be done hundreds of thousands of times. Moreover, in the Bethe method, which this computation was designed to check, integrations involving $\sigma_e(\mu)$ are performed using Simpson's rule on the 21 points listed in § 2. We therefore adopt the convention that the curve $\sigma_e(\mu)$ is <u>defined</u> by the 10 parabolic arcs fitting these 21 points under the Simpson rule method. A table was prepared on this basis for the probability a_i of a scattering with $\cos\psi = \mu \geq \mu_i$ for each of 32 strategically chosen values of μ_i on the interval (-1, 1). The table is presented on the next page.

A random number r then determines i by means of the inequality $a_{i-1} < r < a_i$, and the corresponding value of $\frac{\mu}{2}$ (on the $i^{\underline{th}}$ interval) is taken to be

$$\frac{\cos\psi}{2} = C_i + \frac{r - a_i}{a_i - a_{i-1}}(C_i - C_{i-1})$$

i	$\frac{\mu_i}{2} = C_i = \frac{\cos \psi_i}{2}$	a_i
0	.5000	0
1	.4875	.085 853
2	.4750	.159 724
3	.4625	.223 057
4	.4500	.277 268
5	.4375	.323 786
6	.4250	.364 042
7	.4125	.399 451
8	.4000	.431 457
9	.3750	.486 522
10	.3500	.530 176
11	.3250	.564 728
12	.3000	.592 484
13	.275	.614 869
14	.250	.632 702
15	.225	.647 388
16	.200	.660 330
17	.175	.672 108
18	.150	.682 745
19	.125	.692 811
20	.100	.702 877
21	.075	.713 039
22	.050	.723 200
23	.025	.733 647
24	.000	.744 664
25	-.100	.790 254
26	-.125	.802 032
27	-.150	.814 380
28	-.175	.827 014
29	-.200	.839 647
30	-.250	.864 534
31	-.300	.890 561
32	-.500	.999 9999 · · ·

The μ_i of the table are so chosen that the error involved in linear interpolation is kept to a minimum.

Figure 1 shows the quantities involved in an elastic collision C suffered by a neutron with point of origin R, cos θ, and implies the relations

$$R'^2 = R^2 + y^2 + 2Ry\cos\theta$$

$$\cos\alpha = \frac{R'^2 + y^2 - R^2}{2R'y}$$

$$\cos\theta' = \cos\alpha\cos\psi + \sin\alpha\sin\psi\cos\beta$$

The angle β is obtained by choosing another random number r, and setting $\beta = \pi r$.

Using these formulas, one obtains the new values of R', θ', and s' (= s + 1) of the neutron parameters for the new point of departure C, and returns to the y formula again.

4. Results

The problem was run on the MANIAC using a source of 115000 neutrons. Of these, 81505 escaped, the remainder (33495) being "absorbed" in inelastic collisions. This gives an escape fraction of .7087. The distribution of escaped neutrons according to number s of elastic collisions suffered prior to escape is shown in the following table

s	N_s	$N_s/\Sigma N_s$
0	38 119	.4677
1	23 215	.2848
2	10 543	.1294
3	4 811	.0590
4	2 410	.0296
5	1 237	.0152
6	596	.0073
7	289	.0035
8	137	.0017
9	75	.0009
10	44	.0005
s ≥ 11	29	.0004
Total =	81 505	1.0000

One sees that the average number of collisions for an escaping neutron is

$$\frac{\sum_s sN_s}{\Sigma N_s} = 1.0145$$

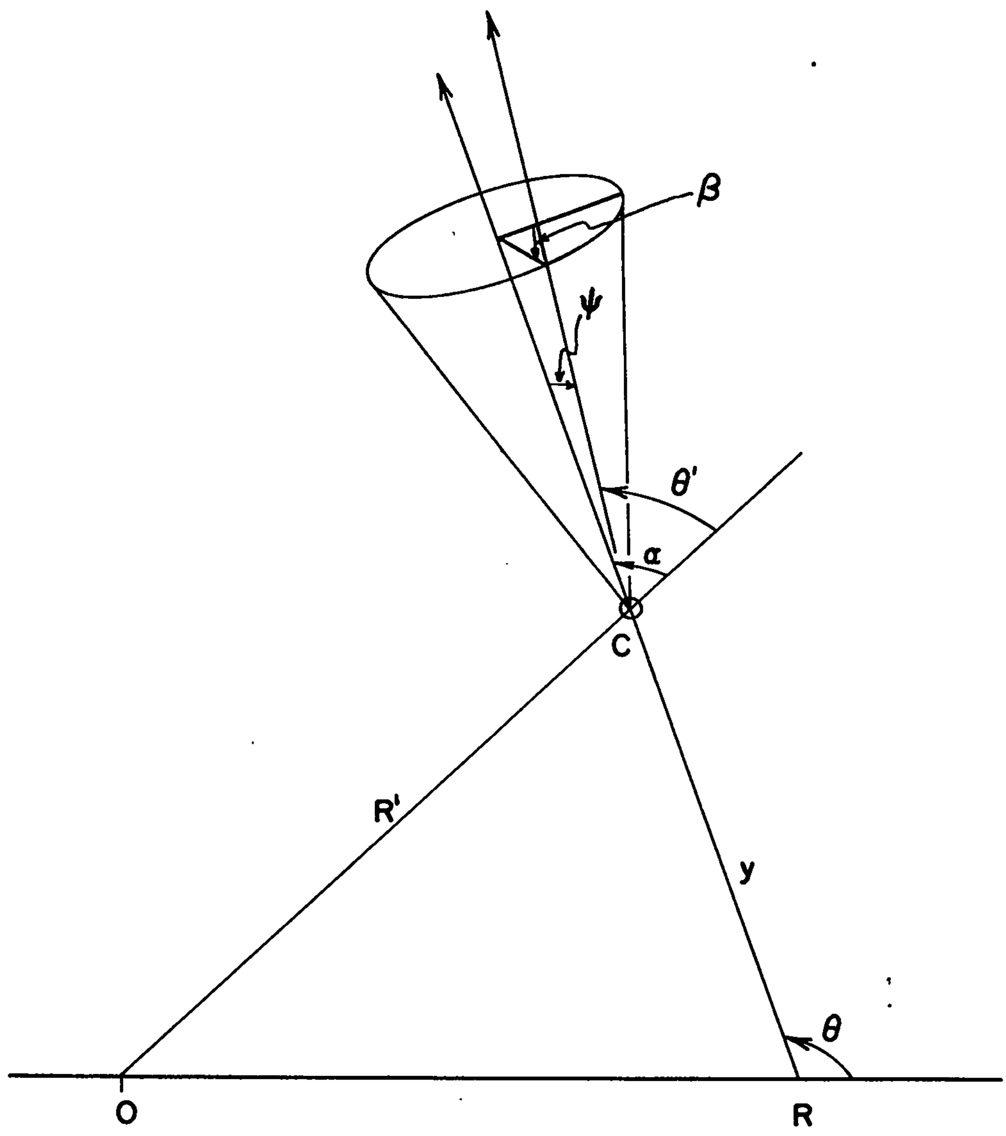

Figure 1

It is also to be noted that 38119/115000 = .3314696 of the source neutrons escaped without collision, a figure that is in excellent agreement with the probability of such escape:

$$e^{-N_o \sigma_t (R_1 - R_o)} = e^{-.0845 \times 3.17 \times 4.1275} = e^{-1.10561}$$

$$= \underline{.331009}$$

The (normal) angular distribution of escape is shown below:

j	θ range	E_j	$E_j/\Sigma E_j = A_j$
1	$(0^o, 5^o)$	39059*	.4792
2	$(5^o, 10^o)$	2788	.0342
3	$(10^o, 20^o)$	8920	.1094
4	$(20^o, 30^o)$	9554	.1172
5	$(30^o, 45^o)$	11506	.1412
6	$(45^o, 60^o)$	6587	.0808
7	$(60^o, 90^o)$	3091	.0379
	Total	81505	

* Of these, 38119 were unscattered and have angle $\theta = 0^o$.

APPENDIX

A SEMI-DETERMINISTIC METHOD AND ITS RESULTS

As a check, to some extent independent of the first method already described, the procedure was modified in the following "semi-deterministic" way. Neutrons were again started from the source, and allowed to scatter according to total cross section σ_t. However, upon collision, instead of throwing to decide between inelastic and elastic collision, and losing the neutron in the former case, the neutron is assigned a weight $\left(\frac{\sigma_e}{\sigma_t}\right)^s = \chi^s$, where s is the total number of "total cross section collisions" suffered. The neutron escaping with parameter s is now regarded as χ^s neutrons escaping after s elastic collisions. Thus if M_s is the number of neutrons escaping under this scheme after s collisions based on σ_t alone, from a source of strength N, we have

$$\Sigma M_s = N$$

$$\chi^s M_s = N_s$$

where N_s is the number of neutrons escaping after s elastic collisions in the sense of the first problem described. Thus $\Sigma \chi^s M_s / N$ is the escape fraction in this new method.

A sample of N = 100 000 neutrons was processed in this way, with results as presented on the following page.

Hence our best value for the escape fraction would seem to be

$$\frac{70868.19030 + 81505}{100\,000 + 115\,000} = .70871$$

based on a sample of 215000 neutrons.

s	χ^s	M_s	$\chi^s M_s = N_s$
0	1	33319	33319
1	.77 28 71	26107	20177.3
2	.59 73 29 58	15222	9092.6
3	.46 16 58 71	9025	4166.5
4	.35 68 02 63	5773	2059.8
5	.27 57 62 41	3725	1027.2
6	.21 31 28 77	2419	515.6
7	.16 47 21 05	1524	251.0
8	.12 73 08 12	1010	128.6
9	.09 83 92 754	622	61.2
10	.07 60 44 906	492	37.4
11	.05 87 72 903	273	16.0
12	.04 54 23 872	192	8.7
13	.03 51 06 793	98	3.4
14	.02 71 33 022	69	1.9
15	.02 09 70 326	45	.9
16	.01 62 07 357	28	.35
17	.01 25 26 196	20	---
18	.00 96 81 134	15	---
19	.00 74 82 267	7	---
20	.00 57 828 28	7	---
$s \rightarrow$ 21	.00 44 693 80	8	---

Total = 70868.19030

Escape fraction = .70868