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CRITICAL SIZE AND MULTIPLICATION NUMBER FOR UNTAMPED RECTANGULAR BLOCK BY VARIATION METHOD

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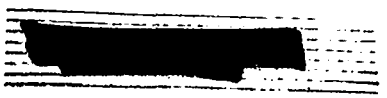
ABSTRACT

By the use of the integral variation method and a one-velocity-group theory, we compute critical sizes and multiplication numbers for rectangular parallelepipeds of square cross section. We do this by getting values for the size of the gadget versus $(1 + f)/(1 + \gamma)$, where f is the net number of neutrons produced in the gadget per (transport averaged) neutron collision process, and γ gives, in certain units, the multiplication rate of the neutrons in the gadget (cf. equations (1) and (2)). From these values the desired results on critical sizes and multiplication numbers follow at once.

We consider also the much simpler extrapolated end-point method of calculating these same quantities, in a form which applies to our problem. We then compare the results given by the two methods so as to compute correction curves to be applied to the extrapolated end-point results in order to obtain the variation method results. These corrections turn out to be very small and, for practical purposes, our conclusion is that the desired quantities for the rectangular parallelepiped are best computed by using the extrapolated end-point method (in the form given in Section IV) along with the c rrection curves of Figures 1 and 2.



CRITICAL SIZE AND MULTIPLICATION NUMBER FOR UNTAMPED RECTANGULAR BLOCK BY VARIATION METHOD

1. THE INTEGRAL VARIATION METHOD

Since the integral variation method for determining critical sizes and multiplication numbers is discussed elsewhere, cf. a forthcoming compendium by Frankel and Nelson, we shall not derive it here nor discuss its details. We shall simply set forth the method and apply it to the problem at hand.

We suppose we have a gadget of any size or shape which, for simplicity, we shall take as untamped (this is the only case which we shall consider). We consider all neutrons as being of one velocity, i.e. this is a one-group theory, so that there is a unique fission cross section σ_f, a unique absorption cross-section σ_a, a unique transport cross section σ_t, etc. Let ν as usual be the number of neutrons emitted per fission. Then we define f by

$$f = \frac{(\nu - 1)\sigma_f - \sigma_a}{\sigma_t} \tag{1}$$

that is, f is the net number of neutrons produced per (transport averaged) neutron collision process. This is clearly a physical constant depending on the nature of the gadget material.

If α gives the multiplication rate of the neutrons in the gadget, that is, $dn/dt = \alpha n$ (n is the neutron density), and V is the neutron velocity, then we define the quantity γ by

$$\gamma = \alpha/(\sigma_t V) \tag{2}$$

Thus γ gives essentially the multiplication rate, since it is proportional to α. We furthermore agree that, instead of measuring distances in units of the

mean free path $1/\sigma_t$, as is usually done, we shall measure them in units of $1/[\sigma_t (1 + \gamma)]$. We now define two integrals

$$I = \int \frac{e^{-r_{12}}}{4\pi r_{12}^2} n(1)\, n(2)\, dV_1\, dV_2 \tag{3}$$

$$N = \int n^2(1)\, dV_1 \tag{4}$$

where the numbers 1 and 2 each denote an arbitrary point in the gadget, r_{12} is the distance between the points 1 and 2 in units of $1/[\sigma_t (1 + \gamma)]$, n denotes the neutron density, and the integration is performed with the points 1 and 2 each moving over the entire gadget independently. The assertion of the integral variation method applied to a homogeneous gadget is then that of all the trial functions which can be substituted for n in (3) and (4), the true neutron density will make the ratio N/I a minimum, and that furthermore for this minimum:

$$(N/I)_{min} = \frac{1 + f}{1 + \gamma} \tag{5}$$

for the gadget in question. It turns out that the approach of the ratio N/I to its minimum, as various trial functions are used, is much more rapid than the approach of the trial functions to the true neutron distribution. This is very useful, since it means that even a fairly rough approximation to the neutron distribution gives a rather accurate value for $(N/I)_{min}$, and we are interested primarily in the ratio $(1 + f)/(1 + \gamma)$ rather than the actual neutron density. In practice it has been found that, if the minimization is performed using only parabolic trial functions, the values obtained for $(1 + f)/(1 + \gamma)$ for the interesting cases are correct to a small fraction of a percent; (indeed, even with a constant trial function the result has turned out to be in error by only five or ten percent at most.) In our application of this method we shall take our cue from previous work and use trial functions which are parabolic.

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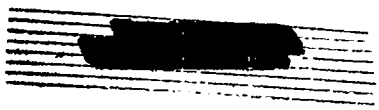
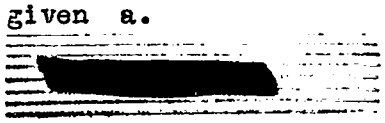


II. THE PROBLEM FOR RECTANGULAR PARALLELEPIPEDS

We are interested in critical sizes and multiplication numbers for various untamped rectangular parallelepipeds; we shall consider here only those cases in which at least two sides of the rectangular solid are of equal length. Let us denote the length of the equal sides by 2a, that of the remaining side by 2b. Our problems then are these: 1) Given the physical constant f, what is the critical size (i.e. $\gamma = 0$) for, say, a cube $a = b$, or for a solid for which $b/a = 2$, or one for which $b/a = 3$, or in general one for which $b/a = r$? 2) Given f and given a, what is the value of the multiplication number γ, for given values of $r = b/a$? Both of these problems are solved by obtaining curves of $\frac{1+f}{1+\gamma}$ vs. a for various values of $r = b/a$, according to the variation method of Section I. For, given f, to find the critical value of a for any particular type of solid (given by the value of r) we read off the graph the value of a associated with $\frac{1+f}{1+\gamma} = 1+f$ (since $\gamma = 0$), and this is our answer. As we remarked before, the values which we use for a and b are measured in units of $1/[\sigma_t(1+\gamma)]$; however, in the case of critical sizes, for which $\gamma = 0$, this means that we are measuring a and b in the usual way, that is, in units of the transport mean free path $1/\sigma_t$.

If on the other hand we are given a and f, and also r, we can read from our graph the value of $\frac{1+f}{1+\gamma}$, and consequently the value of the multiplication number γ. It is to be noted that since a and b are measured in units of $1/[\sigma_t(1+\gamma)]$ we do not know in this case what actual physical size our choice of a and b represents until after γ is determined. This however is no real difficulty, since for any given f and r we can by this method easily determine enough points on a graph of γ vs. a (in direct physical units) in the neighborhood of a given value of a, to be able to read off easily from the curve the correct value of γ for this given a.



As a matter of actual practice it would be rather difficult to determine enough points by our variation method to get good curves of $\frac{1+f}{1+\gamma}$ vs. a for various values of r. Fortunately it turns out that there is an easier procedure which we shall adopt. There is, as we shall discuss below in Section IV, an approximate method for getting $\frac{1+f}{1+\gamma}$ vs. a for given values of r, which is quite accurate and is very simple to apply. This is the extrapolated end-point method. We shall use our variation method to get curves for corrections to be applied to the results given by this extrapolated end-point method. Since the corrections are quite small, we get adequate correction curves by calculating only a few points with the variation method. This is then the attack on the problem which we shall adopt. For further discussion of this, see Sections IV and V.

III. APPLICATION OF THE VARIATION METHOD TO THIS PROBLEM

We can now proceed to use the variation method outlined in Section I to determine $(1+f)/(1+\gamma) = (N/I)_{min}$, for an arbitrary rectangular solid. For the present we shall let the sides of the solid be 2a, 2b, 2c, although in applying our results we shall always set a = c. Then we must evaluate

$$I = \int \frac{e^{-r_{12}}}{4\pi r_{12}^2} n(1)\, n(2)\, dV_1\, dV_2 \qquad (3)$$

$$N = \int n^2(1)\, dV_1 \qquad (4)$$

and minimize the ratio N/I for a chosen class of trial functions n. We shall use as our trial function the class

$$n(x,y,z) = n_1(x)n_2(y)n_3(z) = (1 - Px^2)(1 - Qy^2)(1 - Rz^2) \quad \begin{cases} -a \le x \le a \\ -b \le y \le b \\ -c \le z \le c \end{cases} \qquad (6)$$

where P,Q,R may be arbitrarily varied in the minimizing. It seems reasonable from the symmetry of the problem to use the separated form for n, $n = n_1(x)n_2(y)n_3(z)$; also the diffusion theory solution of the problem yields a separated form for the neutron density. We have furthermore previously noted, Section I, that parabolic trial functions yield very accurate results, and

since clearly we must use even functions here, we are therefore led to the form (6).

The whole difficulty here of course is in evaluating the integral (3). There are several possible approaches to this, but the scheme which seems best is one based on some ideas due to Feynman. To begin with, let us write (3) as

$$I = \int dV_1\, dV_2\, n\,(\underline{r}_1)\, n\,(\underline{r}_2)\, e^{-\rho}/\rho^2 \tag{7}$$

where we are now using vectorial notation for the points in space and where $\underline{\rho} = \underline{r}_1 - \underline{r}_2$, $\rho = |\underline{\rho}|$. We want next to make a Fourier expansion of $e^{-\rho}/\rho^2$. Let the components of $\underline{\rho}$ be $(\rho_x, \rho_y, \rho_z,)$. Now we want an $f(\underline{k})$ so that

$$\frac{e^{-|\underline{\rho}|}}{|\underline{\rho}|^2} = \int_{-\infty}^{\infty} d\,\underline{k}\, f\,(\underline{k})\, e^{\,i\,\underline{k}\,\cdot\,\underline{\rho}} \tag{8}$$

Hence we must have

$$f\,(\underline{k}) = \frac{1}{8\pi^3} \int_{-\infty}^{\infty} d\rho_x\, d\rho_y\, d\rho_z\, \frac{e^{-|\underline{\rho}|}}{|\underline{\rho}|^2}\, e^{-i\,\underline{k}\,\cdot\,\underline{\rho}}$$

We introduce polar coordinates whose polar axis is along the direction of $\underline{k}$, and using $k = |\underline{k}|$, we have

$$f\,(\underline{k}) = \frac{1}{8\pi^3} \int_{\text{space}} \rho^2 d\rho\, \sin\theta d\theta d\varphi\, \rho^{-2}\, e^{-\rho}\, e^{-ik\rho\cos\theta}$$

Integrating, and using Peirce 506 (integrating 506 first with respect to m), we got

$$f\,(\underline{k}) = \frac{1}{2\pi^2}\, \frac{\tan^{-1} k}{k} \tag{9}$$

Hence, from (7) and (8), we have

$$I = \int dV_1\, dV_2\, n\,(\underline{r}_1)\, n\,(\underline{r}_2) \int_{-\infty}^{\infty} d\,\underline{k}\, f\,(\underline{k})\, e^{\,i\,\underline{k}\cdot(\underline{r}_1 - \underline{r}_2)}$$

where $f\,(\underline{k})$ is given by (9). Changing the order of integration and substituting from (6) for n we get

$$I = \int_{-\infty}^{\infty} d\underline{k}\, f(\underline{k}) \int_{-a}^{a}\int_{-a}^{a} dx_1\, dx_2 \left\{(1 - Px_1^2)(1 - Px_2^2)\, e^{i k_x x_1}\, e^{-i k_x x_2}\right\} \cdot \tag{10}$$

$$\int_{-b}^{b}\int_{-b}^{b} dy_1\, dy_2 \left\{\quad\right\} \int_{-c}^{c}\int_{-c}^{c} dz_1\, dz_2 \left\{\quad\right\}$$

where the integrand in the y and z integrals is exactly the same as in the x integrals except that P, x and k_x are replaced by Q, y and k_y, and by R, z and k_z respectively. What we have accomplished by the Fourier expansion then is to get our function of the space coordinates x_1, ---z_2 completely separable, so that the integration over these coordinates is now very easy to perform.

For the integration over the space coordinates we use the typical formula

$$\int_{-a}^{a} dx_1\, (1 - Px_1^2)\, e^{i k_x x_1} = \frac{2 \sin k_x a}{k_x} - P\left\{\frac{2a^2 \sin k_x a}{k_x} + \frac{4a \cos k_x a}{k_x^2} - \frac{4 \sin k_x a}{k_x^3}\right\}$$

This gives us

$$I = 64 \int_{-\infty}^{\infty} d\underline{k}\, f(\underline{k}) \left\{\frac{\sin k_x a}{k_x} - P\left[(k_x^2 a^2 - 2)\frac{\sin k_x a}{k_x^3} + \frac{2a \cos k_x a}{k_x^2}\right]\right\}^2 \tag{11}$$

$$\left\{Q, k_y, b\right\}^2 \left\{R, k_z, c\right\}^2$$

The brackets $\left\{Q, k_y, b\right\}$ and $\left\{R, k_z, c\right\}$ denote the same function as the first bracket with P, k_x, a replaced by the corresponding quantities in the other brackets.

In order to perform the integrations over the k's it would be useful to get the integrand to separate into a function of k_x times a function of k_y times

a function of k_z. This product form already exists except for the function

$$f(\underline{k}) = \frac{1}{2\pi^2} (\tan^{-1} k)/k = \frac{1}{2\pi^2} (\tan^{-1} \sqrt{k_x^2 + k_y^2 + k_z^2})/\sqrt{k_x^2 + k_y^2 + k_z^2}.$$

We can get $f(\underline{k})$ into the desired form by making the expansion (due to Feynman)

$$\frac{\tan^{-1} k}{k} = \int_0^\infty e^{-k^2 y} F(y)\, dy = \int_0^\infty e^{-k_x^2 y}\ e^{-k_y^2 y}\ e^{-k_z^2 y} F(y)\, dy \qquad (12)$$

where

$$F(y) = \frac{1}{\sqrt{y}} \frac{\sqrt{\pi}}{2} Er(\sqrt{y}) = \frac{1}{\sqrt{y}} \int_{\sqrt{y}}^\infty e^{-t^2} dt \qquad (13)$$

(The correctness of this expansion can be readily checked). Hence

$$I = \frac{32}{\pi^2} \int_0^\infty F(y)dy \int_{-\infty}^\infty dk_x dk_y dk_z\ e^{-k_x^2 y} \left\{ P, k_x, a \right\}^2 e^{-k_y^2 y} \left\{ Q, k_y, b \right\}^2 e^{-k_z^2 y} \left\{ R, k_z, c \right\}^2 \qquad (14)$$

where the brackets $\left\{\ \right\}$ are the same as above in (11). The integrations over the k's can be performed by fairly straightforward, although rather lengthy, methods. We shall omit the details of this and simply write down the results. If we perform these integrations, and also replace y by x^2 in (14) we get as our final result the following:

Letting

$$E(x) = \int_0^x e^{-x^2} dx \qquad (15)$$

$$Er(x) = \frac{2}{\sqrt{\pi}} \int_x^\infty e^{-x^2} dx \qquad (16)$$

and setting

$$K_o(x) = 2E(1/x) - x(1 - e^{-1/x^2}) \tag{17}$$

$$K_1(x) = (4x^2 + 4/3)E(1/x) + \frac{2x(4x^2+1)}{3} e^{-1/x^2} - \frac{2x(4x^2+3)}{3} \tag{18}$$

$$K_2(x) = (4x^2/3 + 2/5)E(1/x) + (16x/15)\left[x^4 + x^2 + (3/16)\right] e^{-1/x^2} - x(16x^4/15 + 1) \tag{19}$$

then

$$I = \frac{8abc}{\pi}\int_0^\infty dx\, Er(x)\left\{K_o(x/a) - a^2PK_1(x/a) + a^4P^2K_2(x/a)\right\}\left\{K_o(x/b) - b^2QK_1(x/b) + b^4Q^2K_2(x/b)\right\}\left\{K_o(x/c) - c^2RK_1(x/c) + c^4R^2K_2(x/c)\right\} \tag{20}$$

It also follows immediately, after substituting in (4) from (6) and integrating, that

$$N = 8abc\left(1 - \frac{2}{3}Pa^2 + \frac{1}{5}P^2a^4\right)\left(1 - \frac{2}{3}Qb^2 + \frac{1}{5}Q^2b^4\right)\left(1 - \frac{2}{3}Rc^2 + \frac{1}{5}R^2c^4\right) \tag{21}$$

The integration of (20) can not be carried out analytically, so we must resort to numerical means.

For any given a,b,c now we can compute the various integrals involved in (20) and thus get I as a polynomial in P,Q,R. N is already such a polynomial. The ratio of these polynomials, N/I, can then be minimized with respect to P,Q,R. As has been said before, we have considered in the applications only cases in which a = c, which implies of course that in our trial functions we should set R = P. It was found in practice that the minimizing could be accomplished most easily by a trial and error method, rather than by equating $(\partial/\partial P)(N/I)$ and $(\partial/\partial Q)(N/I)$ to zero. This was largely due to the fact that the actual value of the minimum was rather insensitive to the particular choice of P and Q; this of course also speaks well for the probable accuracy of the result achieved using parabolic trial functions. The results

are given in Table I, which gives $\frac{1+f}{1+\gamma}$ against certain values of a (listed as $a_{variation}$) in the case of a cube, in the case where $b = 2a$, $c = a$, and in the case where $b = \infty$, $c = a$. From this table we get at once, clearly, f as a function of a for the critical case $\gamma = 0$, and the multiplication number γ as a function of a for any desired f. The remaining two columns of the table are explained in Section IV below.

IV. THE EXTRAPOLATED END-POINT METHOD

There is an approximate method which is very easy to apply and which enables us to compute with very good accuracy the same quantities obtained by the variation method used above. This is the extrapolated end-point method. This method is described in considerable detail elsewhere by Nelson and Frankel (LA-8), and we shall merely set it forth as a recipe for computing $(1+f)/(1+\gamma)$ vs. a here. Given $(1+f)/(1+\gamma)$, we want to compute a. The scheme as applied to our problem is the following:

We solve the diffusion equation for the neutron density n:

$$\nabla^2 n = -k^2 n \quad \text{inside gadget} \quad \begin{cases} -a \le x \le a \\ -b \le y \le b \\ -c \le z \le c \end{cases} \qquad (22)$$

$$n = 0 \quad \text{outside gadget}$$

where k is determined by

$$\frac{\tan^{-1} k}{k} = \frac{1+\gamma}{1+f} \qquad (23)$$

The fundamental solution is then

$$\begin{aligned} n &= \cos k_1 x \cdot \cos k_2 y \cdot \cos k_3 z \quad \text{inside gadget} \\ n &= 0 \quad \text{outside gadget} \end{aligned} \qquad (24)$$

where

$$k_1^2 + k_2^2 + k_3^2 = k^2 \qquad (25)$$

In order to satisfy the condition that the neutron density be continuous everywhere, we should get for the sides of the solid: $a = \pi/2k_1$, $b = \pi/2k_2$, $c = \pi/2k_3$. The extrapolated end-point method asserts that a much better

approximation to the integral theory solution of the problem is given by adding a correction term to each of these values. This correction is of amount $x_o = \chi(1+\gamma)/(1+f)$, where χ is a function of $(1+\gamma)/(1+f)$ and is given by the graph of Figure 3; for the derivation of this curve cf. Report LA-8. Thus we have for the half-sides of the solid

$$\begin{aligned} a &= \pi/(2k_1) + x_o \\ b &= \pi/(2k_2) + x_o \\ c &= \pi/(2k_3) + x_o \end{aligned} \tag{26}$$

As before, these lengths are in units of $1/[\sigma_t(1+\gamma)]$. Of course these values for the sides are not determinate, since the k_1, k_2, k_3 are not uniquely determined by (25). We must specify two more conditions. This is accomplished by setting $c = a$, as in our previous work, and letting $b = ra$ where r is fixed in advance. If this is done the equation for a becomes

$$1/(a+x_o)^2 + 0.5/(ra+x_o)^2 = 2k^2/\pi^2 \tag{27}$$

Equation (27) can be solved for a for any choice of r and any given $(1+f)/(1+\gamma)$. For the cases $r=1$, $r=2$, $r=\infty$, the values of a determined by this extrapolated end-point method for certain values of $(1+f)/(1+\gamma)$ (i.e. those obtained using the variation method described above) are shown in Table I. If we assume that the variation method is exact, since its errors are probably of the order of a fraction of a percent, we can compute for each point in our table a percentage correction p to be applied to a_{ext} to get a_{var}. This is given in the fourth column of the table.

V. CONCLUSIONS AND SUMMARY

The most useful product of the work described here is the set of curves of p versus a_{ext} and p versus $\frac{1+f}{1+\gamma}$ for the cases $b=a$, $b=2a$, $b=\infty$ (cf. Figures 1 and 2). In the first place a_{ext} is exceedingly easy to compute, since all that is required is to solve (27) for a. In the second place the values of a_{ext} are quite close to those of a_{var} (cf. Table I). This means

that the inaccuracies in p due to the fact that the curves are drawn through only three points, although relatively large compared with p, are absolutely very small and have negligible effect on the final answer.

We can summarize our results then as follows: Given $(1+f)/(1+\gamma)$, given that $c = a$, and given $r = b/a$, to compute a we first compute a_{ext} using (23) and (27) and then correct this result to get a_{var} using the graph of p, either Figure 1 or Figure 2. The curves given in these graphs are only for the cases $r = 1$, $r = 2$, $r = \infty$, but it is clear that an adequate interpolation can be made for any intermediate cases. (We have not been interested in this work in the cases for which $r < 1$). The values of a which we get will be in units of $1/[\sigma_t(1+\gamma)]$ and the actual physical size of a can be determined only when the value of γ is specified (we can assume that the physical constant σ_t is known).

We might be given the converse problem, for given a (that is, a_{var}) to determine $(1+f)/(1+\gamma)$. This is readily done as we shall see below if a is given in units of $1/[\sigma_t(1+\gamma)]$. However in general a will be given in some more direct physical way; even so, if σ_t and $1+\gamma$ are given, so that the object is to determine f, we can at once proceed to get a in the desired units, determine $(1+f)/(1+\gamma)$ (see below) and hence f. If, as is most likely, f and σ_t are given, and it is desired to compute γ, our best hope is to guess at the neighborhood in which the answer lies, take several values of γ and hence $(1+f)/(1+\gamma)$ in this neighborhood, and compute a from these, as described above, in direct physical units; thus we get a graph of a vs. $(1+f)/(1+\gamma)$ from which the value of $(1+f)/(1+\gamma)$, and hence γ, for the specified a can be read off at once.

We must finally justify our above statement that if we are given a_{var} in units of $1/[\sigma_t(1+\gamma)]$, then $(1+f)/(1+\gamma)$ is readily determined. We must first guess at the appropriate value of p (this is easy to do adequately well

even though p is plotted against a_{ext} instead of a_{var}, since a_{ext} will not differ much from a_{var}) and determine from it the value of a_{ext}. We then place this value in (27) and use a trial and error method to solve for $(1+\delta')/(1+f)$ from (27) and (23).

TABLE I

$a_{variation}$	$\frac{1+f}{1+\gamma}$	$a_{ext.\ end\ point}$	$p = \frac{a_{var} - a_{ext.}}{a_{ext}}$ 100%
		Cube: a = b = c	
.80	2.0409	.7831	2.16%
1.50	1.4634	1.4819	1.22%
2.30	1.2527	2.2810	0.83%
		2 x 1 x 1 Rectangular Solid c = a b = 2a	
.70	1.9870	.6862	2.01%
1.20	1.4974	1.1859	1.19%
2.00	1.2429	1.9896	0.52%
		Infinite Rectangular Solid c = a b = ∞	
.62	1.9669	.6129	1.16%
1.10	1.4798	1.0907	0.85%
1.80	1.2464	1.7901	0.55%

Graph of p vs. a_{ext} for Untamped Rectangular Solids of Square Cross Section (cf. page 12)

Sides are of length 2b, 2a, 2a in units of $1/\sigma_t(1+\gamma)$

a_{ext} = value of a calculated by extrapolated end-point method

p = % correction to a_{ext} in order to get a_{var}

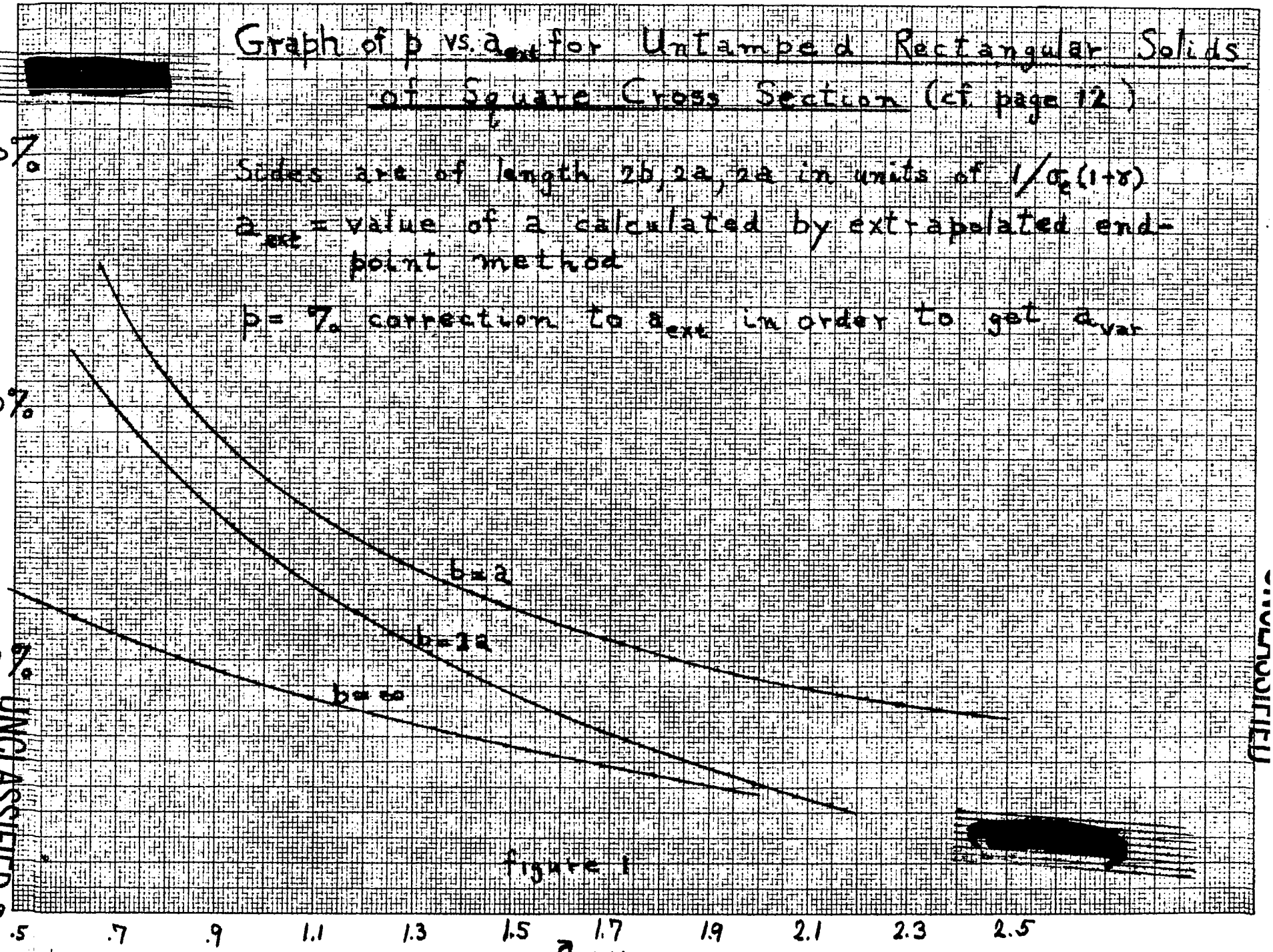


figure 1

Graph of ρ vs. $\frac{1+\xi}{1+\gamma}$ for Untamped Rectangular Solids of Square Cross Section (cf. page 12)

Sides of solid are of length $2b, 2a, 2a$ in units of $1/\sigma_c(1+\gamma)$

Denote by $a_{ext.}$ the value of a from extrapolated end-point method

ρ = % correction to $a_{ext.}$ in order to get $a_{var.}$

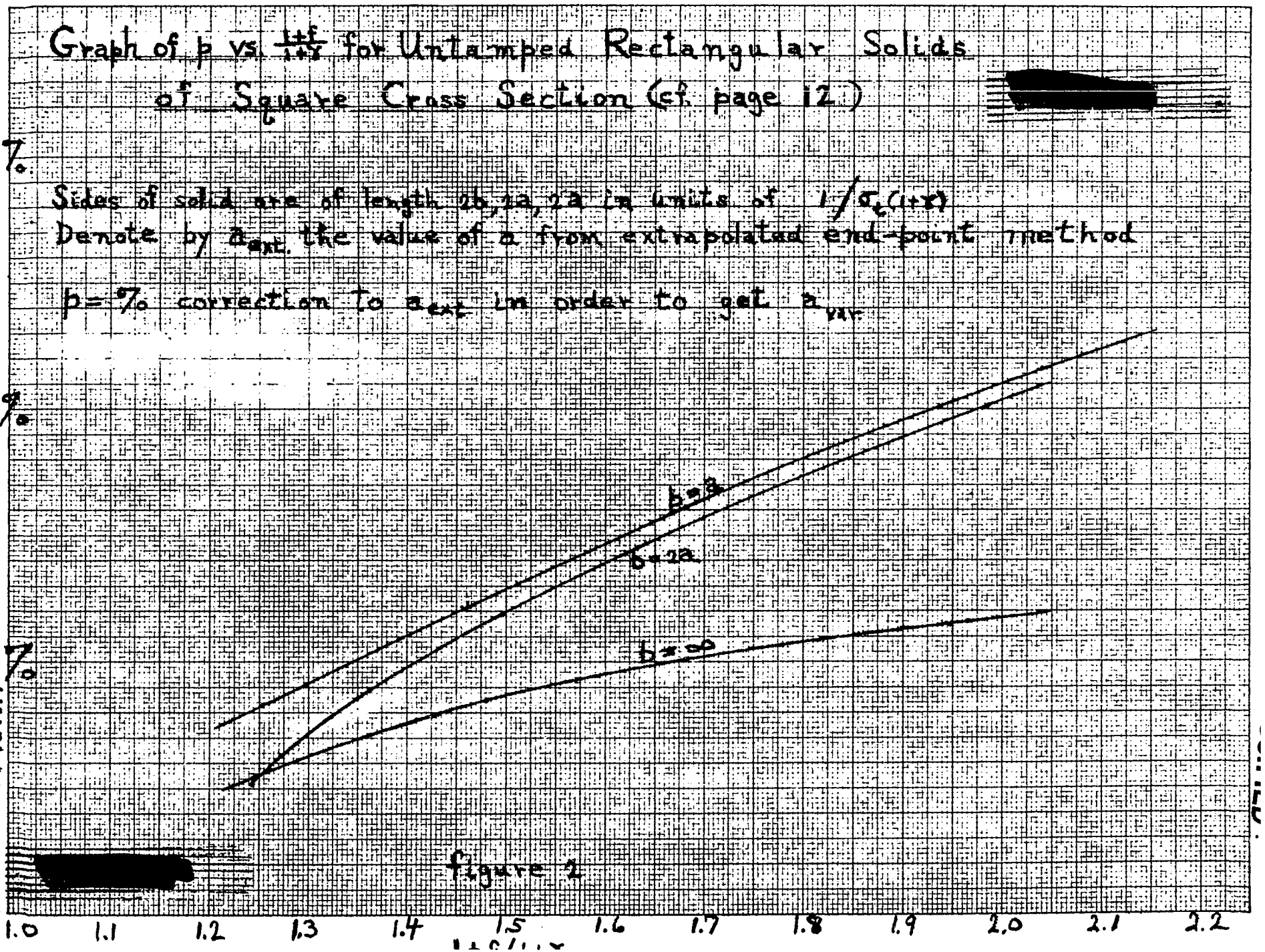


Figure 2

KEUFFEL & ESSER CO., N. Y. NO. 349H-14
Millimeters, 5 mm. lines accented, cm. lines heavy.
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figure 3