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LA-603

Physics and Mathematics

UNITED STATES ATOMIC ENERGY COMMISSION

NEUTRON DIFFUSION IN A SPACE LATTICE OF FISSIONABLE AND ABSORBING MATERIALS

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Photostat Price $3.30

Microfilm Price $2.40

Available from the
Office of Technical Services
Department of Commerce
Washington 25, D. C.

August 27, 1946

Los Alamos Scientific Laboratory,
New Mexico

Technical Information Service Extension, Oak Ridge, Tenn.

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ABSTRACT

Methods are developed for estimating the effect on a critical assembly of fabricating it as a lattice rather than in the more simply interpreted homogeneous manner.

In experiments with critical assemblies it is often convenient to fabricate active material, tamper material, and absorbing material, such as boron, in the form of blocks or slabs and then to assemble these blocks or slabs in the form of some regular space lattice. From the point of view of a theoretical treatment it would, of course, be preferable if the assembly were composed of a homogeneous core and a homogeneous tamper. If the dimensions of a unit cell of the lattice are small compared with a neutron mean free path the assembly may be considered as practically homogeneous and so treated. It is the purpose of this report to develop methods for deciding how big the lattice size can be before a serious departure from homogeneity is introduced.

We propose to discuss the following idealized case in some detail. Suppose we have an infinite medium in which fission, elastic scattering and absorption can occur. Suppose that neutrons of only one velocity are present in the system and that the neutron mean free path is independent of position, it being equal to unity with the unit of length used. We then assume that $f(\underline{x})$, the average number of extra neutrons emitted per collision, is a function of position which varies periodically throughout the medium. Specifically, $1 + f(\underline{x})$ will have the form:

$$1 + f(\underline{x}) = \frac{\mu(\underline{x})}{\lambda} \tag{1}$$

The function $\mu(\underline{x})$ is assumed to have a space average value of unity so that $1/\lambda$ is the space average of the total number of neutrons emitted on the average per collision. We define a unit cell of the lattice by three vectors, $\underline{a}$, $\underline{b}$, and $\underline{c}$ and make the statement of periodicity, that:

$$\mu(\underline{x} + 1\underline{a} + m\underline{b} + n\underline{c}) = \mu(\underline{x}) \tag{2}$$

where 1,m,n, are integers. With these assumptions we can then write the following integral equation for the neutron density $\psi(\underline{x})$:

$$\lambda\psi(\underline{x}) = (1/4\pi) \int d\underline{x}' \frac{e^{-|x-x'|}}{|\underline{x} - \underline{x}'|^2} \mu(\underline{x}') \psi(\underline{x}') \tag{3}$$

If $\underline{R}$ is any displacement which keeps the value of $\mu(\underline{x})$ unchanged then we can rewrite Eq. 3 as:

$$\lambda\psi(\underline{x} + \underline{R}) = (1/4\pi) \int d\underline{x}' \frac{e^{-|x+R-x'|}}{|\underline{x} + \underline{R} - \underline{x}|^2} \mu(\underline{x}') \psi(\underline{x}') \tag{4}$$

If we now displace the origin of $\underline{x}$ by an amount $\underline{R}$ and use the periodicity of μ, we can rewrite Eq. 4 in the following way:

$$\lambda\psi(\underline{x} + \underline{R}) = (1/4\pi) \int d\underline{x}' \frac{e^{-|x-x'|}}{|\underline{x} - \underline{x}'|^2} \mu(\underline{x}') \psi(\underline{x}' + \underline{R}) \tag{5}$$

Comparing Eqs. 3 and 5 we see that if $\psi(\underline{x})$ is a solution of the integral equation, $\psi(\underline{x} + \underline{R})$ will also be a solution.

If, as is usual in the theory of metals, we properly choose the elementary solutions of the integral Eq. 3, it will be true that for some $\underline{k}$:

$$\psi(\underline{x} + \underline{R}) = e^{i\underline{k}\cdot\underline{R}} \psi(\underline{x}) \tag{6}$$

So that:

$$\psi(\underline{x}) = e^{i\underline{k}\cdot\underline{x}} \phi_k(\underline{x})$$

where

$$\phi_k(\underline{x} + \underline{R}) = \phi_k(\underline{x}) \tag{7}$$

A general solution of the integral equation can of course be built up by superposing solutions of the form Eq. 7.

The vector $\underline{k}$ is of course analagous to the wave number of the asymptotic infinite medium solution of the integral Eq. 3 in the elementary case where $\mu(\underline{x})$ is constant. In that case $\phi_k(\underline{x})$ is of course constant also. We shall find it convenient to deal directly with the periodic function ϕ_k rather than with the neutron density itself. To accomplish this we substitute Eq. 7 in Eq. 3 and obtain:

$$\lambda \phi_k(\underline{x})\, e^{i\underline{k}\cdot\underline{x}} = (1/4\pi) \int d\underline{x}' \, \frac{e^{-|\underline{x}-\underline{x}'|}}{|\underline{x}-\underline{x}'|^2} \mu(\underline{x}')\, e^{i\underline{k}\cdot\underline{x}'}\, \phi_k(\underline{x}') \tag{8}$$

which is conveniently rewritten:

$$\lambda \phi_k(\underline{x}) = (1/4\pi) \int d\underline{x}' \, \frac{e^{-|\underline{x}-\underline{x}'|}}{|\underline{x}-\underline{x}'|^2} e^{i\underline{k}\cdot(\underline{x}'-\underline{x})}\, \mu(\underline{x}')\, \phi_k(\underline{x}') \tag{9}$$

This equation is seen to be an integral equation for the function $\phi_k(\underline{x})$, the kernel of the integral equation containing the over-all wave-vector of the solution explicitly and being Hermitian, if the propagation vector $\underline{k}$ is real.

In order to illustrate the general method of procedure, and for use in investigating the approximate methods to be developed, we will solve a simple problem exactly. We assume for $\mu(\underline{x})$ the following:

$$\mu(\underline{x}) = 1 + \alpha \cos(2\pi x/a) = 1 + (\alpha/2)\, e^{2\pi i x/a} + (\alpha/2)\, e^{-2\pi i x/a} \tag{10}$$

It is also convenient, but not essential, to assume $\underline{k} = 0$. We then wish to find the value of λ required for criticality as a function of α and of a. As usual in a plane problem, we simplify the integral equation to the following:

$$\lambda \phi(x) = (1/2) \int_{-\infty}^{\infty} dx' \, E(|x - x'|)\, \mu(x')\, \phi(x') \tag{11}$$

We now expand $\phi(x)$ in a Fourier series and obtain:

$$\phi(x) = \sum_{n=-\infty}^{\infty} \phi_N e^{2\pi i n x/a} \tag{12}$$

We substitute the expression (Eq. 12) in the Eq. 11 and obtain:

$$\lambda \sum_n \phi_n e^{2\pi i n x/a} = \sum_n \phi_n (1/2) \int_{-\infty}^{\infty} dx' E(|x - x'|) e^{2\pi i n x'/a}$$
$$+ (\alpha/2) \sum_n \phi_n (1/2) \int_{-\infty}^{\infty} dx' E(|x - x'|) e^{2\pi i (n+1) x'/a}$$
$$+ (\alpha/2) \sum_n \phi_n (1/2) \int_{-\infty}^{\infty} dx' E(|x - x'|) e^{2\pi i (n-1) x'/a} \tag{13}$$

The integrals appearing in Eq. 13 can easily be done and we obtain, by shifting the summation index n:

$$\sum_n \lambda \phi_n e^{2\pi i n x/a} = \sum_n \lambda_n [\phi_n + (\alpha/2) \phi_{n-1} + (\alpha/2) \phi_{n+1}] e^{2\pi i n x/a} \tag{14}$$

where

$$\lambda_n = \frac{\tan^{-1}, 2\pi n/a}{2\pi n/a} \tag{15}$$

From Eq. 15 we finally get the following recursion relations for the ϕ_n:

$$\lambda \phi_n = \lambda_n [\phi_n + (\alpha/2) \phi_{n-1} + (\alpha/2) \phi_{n+1}] \tag{16}$$

If two of the neighboring ϕ_n are specified it is clear that we can solve for all of the ϕ_n. In general, as the magnitude of n gets very large ϕ_n will increase without limit. If the value of λ is properly chosen, however, then ϕ_n will converge to zero. Since the ϕ_n are the Fourier co-efficients of a smooth function $\phi(x)$ the ϕ_n must converge to zero for large n if we are to have a real solution of the integral equation. We can therefore proceed by assuming that ϕ_n is zero for sufficiently large n and determining λ from this requirement.

We notice that Eq. 16 is unchanged by the substitution of $-n$ for n, and we can therefore argue that the solutions of Eq. 16 must be either even or odd in n. The odd solution can be ruled out because it would require that ϕ_0 be zero, which implies that the neutron density averages to zero. We therefore lose nothing by assuming that ϕ_n is equal to ϕ_{-n}. Consideration of Eq. 16 with n set equal to zero yields the condition:

$$\lambda\phi_0 = \lambda_0\phi_0 + \alpha\lambda_0\phi_1$$

or

$$(\lambda - \lambda_0)\phi_0 = \alpha\lambda_0\phi_1$$

$$\phi_1/\phi_0 = (\lambda - \lambda_0)/\alpha\lambda_0 \tag{17}$$

We then write the remaining equations (16) in the following form:

$$\phi_1 = \frac{\lambda_1}{\lambda - \lambda_1}\frac{\alpha}{2}\phi_0 + \frac{\lambda_1}{\lambda - \lambda_1}\frac{\alpha}{2}\phi_2$$

$$\phi_2 = \frac{\lambda_2}{\lambda - \lambda_2}\frac{\alpha}{2}\phi_1 + \frac{\lambda_2}{\lambda - \lambda_2}\frac{\alpha}{2}\phi_3 \tag{18}$$

For convenience we abbreviate the co-efficients as follows:

$$\phi_1 = a_1\phi_0 + b_1\phi_2$$

$$\phi_2 = a_2\phi_1 + b_2\phi_3 \text{ etc.} \tag{19}$$

We then divide all of the equations by ϕ_0 and call the ratio $\phi_n/\phi_0 \sim R_n$, where R_0 equals unity.

We now solve these equations for R_1 by assuming that all the ϕ_n beyond a certain point are equal to zero and then taking into account more and more of the ϕ_n. If we first decide to neglect R_2 and all R_n beyond, we obtain:

$$R_1 = a_1 \tag{20}$$

If we now neglect all R_n except R_1 and R_2 we clearly obtain:

$$R_1 = a_1 + b_1R_2$$

$$R_2 = a_2R_1$$

whence:

$$R_1 = a_1 + a_2b_1R_1 \tag{21}$$

$$R_1 = a_1/(1 - a_2b_1)$$

It is then easily seen that inclusion of higher and higher R_n will give values for R_1 that are successive approximations to the value of the continued fraction:

$$R_1 = \cfrac{a_1}{1 - \cfrac{a_2b_1}{1 - \cfrac{a_3b_2}{a - a_4b_3}}} \qquad (22)$$

We now insert the values which we have for a_n and b_n and set the resulting continued fraction equal to the value of R_1 given in Eq. 17. We thus obtain the following secular equation for λ:

$$\frac{\lambda - \lambda_0}{\alpha\lambda_0} = \cfrac{\frac{\alpha}{2}\frac{\lambda_1}{\lambda - \lambda_1}}{1 - \cfrac{\frac{\alpha^2}{4}\frac{\lambda_1}{\lambda - \lambda_1}\frac{\lambda_2}{\lambda - \lambda_2}}{1 - \frac{\alpha^2}{4}\frac{\lambda_2}{\lambda - \lambda_2}\frac{\lambda_3}{\lambda - \lambda_3}}} \qquad (23)$$

This may conveniently be rewritten in the more symmetrical form:

$$\cfrac{1 - \frac{\alpha^2}{4}\frac{\lambda_0}{\lambda - \lambda_0}\frac{\lambda_1}{\lambda - \lambda_1}}{1 - \frac{\alpha^2}{4}\frac{\lambda_1}{\lambda - \lambda_1}\frac{\lambda_2}{\lambda - \lambda_2}} = \frac{1}{2} \qquad (24)$$

For a given value of the λ_n are determined. If the value of α is then given λ can be found by a small amount of trial and error. The continued fraction in Eq. 24 fortunately converges exceedingly rapidly for reasonable values of a and α.

We should make sure that the Eq. 24 gives λ correctly in the limit $\alpha = 0$ or $a = 0$. If either a or α approaches zero the medium approaches

homogeneity and λ should approach unity. If a is very small λ_0 will be equal to unity and all the higher λ_n will be zero. Equation 24 then reduces to:

$$\lambda = 1 + (\alpha^2/2)\ \lambda_1/(\lambda - \lambda_1) \tag{25}$$

From this we see that λ approaches unity as a approaches zero. It is furthermore clear that if α approaches zero, Eq. 25 will again hold and λ must again approach unity so that we have verified that Eq. 24 has the correct limiting behavior.

We now wish to work out an approximate procedure for calculating λ, which will be reasonably accurate and simple for an arbitrary function $\mu(\underline{x})$. If the wave vector $\underline{k}$ is real, Eq. 9 can be arranged to have a Hermitian kernel. We multiply each side of Eq. 9 by $\sqrt{\mu(\underline{x})}$ and rewrite it as follows:

$$\lambda \phi_k(\underline{x})\ \sqrt{\mu(\underline{x})} = (1/4\pi) \int d\underline{x}'\ \frac{e^{-|\underline{x}-\underline{x}'|}}{|\underline{x}-\underline{x}'|^2} \times e^{i\underline{k}\cdot(\underline{x}'-\underline{x})}\ \sqrt{\mu(\underline{x})\mu(\underline{x}')}\ \phi_{\underline{k}}(\underline{x}')\ \sqrt{\mu(\underline{x}')} \tag{26}$$

This equation can be derived from a simple variational principle and λ can be written as the maximum of the following expression:

$$U = \frac{\int d\underline{x} \int d\underline{x}'\ \phi_k^*(\underline{x})\ \mu(\underline{x})\ (1/4\pi)\ \frac{e^{-|\underline{x}-\underline{x}'|}}{|\underline{x}-\underline{x}'|^2}\ e^{i\underline{k}\cdot(\underline{x}'-\underline{x})}\ \phi_k(\underline{x}')\ \mu(\underline{x})}{\int d\underline{x}\ \phi_k^*(\underline{x})\ \phi_k(\underline{x})\ \mu(\underline{x})} \tag{27}$$

The maximum will be reached when ϕ_k is an actual solution of Eq. 9. If the variation of $\mu(\underline{x})$ is not too violent, $\phi_k(x)$ will be approximately constant. We, therefore, place, $\phi_k(\underline{x})$ and $\phi_k^*(\underline{x})$ equal to unity and investigate the agreement between the value of U thus obtained and the correct value of λ. It is, of course, clear that the value of U thus obtained will always be lower than the correct value of λ. We write λ for this approximate value and obtain:

$$\lambda = \frac{\int d\underline{x} \int d\underline{x}'\ (1/4\pi)\ \frac{e^{-|\underline{x}-\underline{x}'|}}{|\underline{x}-\underline{x}'|^2}\ e^{i\underline{k}\cdot(\underline{x}'-\underline{x})}\ \mu(\underline{x})\ \mu(\underline{x}')}{\int d\underline{x}\ \mu(\underline{x})} \tag{28}$$

Each integral in Eq. 28 is taken over all space. The result of the integration over $\underline{x}'$ in the numerator will be a function periodic with the periodicity of the lattice. The integration over $\underline{x}$ in the numerator and denominator can then be extended over a unit cell of the lattice.

In order to obtain the expression (Eq. 28) for λ in a somewhat more usable form, we expand $\mu(\underline{x})$ in a Fourier series:

$$\mu(\underline{x}) - \sum_{\underline{K}} \mu_{\underline{K}} e^{i\underline{K}\cdot\underline{x}} \tag{29}$$

The $\underline{K}$ form a denumerable set and are of the form:

$$\underline{K} = 2\pi(p\underline{\alpha} + q\underline{\beta} + r\underline{\gamma}) \tag{30}$$

Here p, q, r, are integers and $\underline{\alpha}$, $\underline{\beta}$, $\underline{\gamma}$ are the defining vectors of a lattice in $\underline{K}$ space. This new lattice is reciprocal to the lattice defined by $\underline{a}$, $\underline{b}$, $\underline{c}$, in the $\underline{x}$ space in the following sense:

$$\underline{\alpha}\cdot\underline{b} = \underline{\alpha}\cdot\underline{c} = 0 \qquad \underline{\alpha}\cdot\underline{a} = 1 \tag{31}$$

and cyclically for $\underline{\beta}$, $\underline{\gamma}$. The conditions (Eq. 31) are obviously satisfied by the choice:

$$\underline{\alpha} = \frac{\underline{b}\times\underline{c}}{\underline{a}\cdot(\underline{b}\times\underline{c})} \tag{32}$$

and similarly for $\underline{\beta}$, and $\underline{\gamma}$. Any $\underline{K}$ satisfying Eq. 30 has the property that:

$$\underline{K}\cdot(1\underline{a} + m\underline{b} + n\underline{c}) = 2\pi x \text{ (an integer)} \tag{33}$$

Therefore, every term in the expansion (Eq. 29) is periodic with a periodicity which is that of $\mu(\underline{x})$.

We now insert the expansion (Eq. 29) in the Eq. 28 for λ. It is necessary to remember that:

$$(1/4\pi)\int d\underline{x}' \frac{e^{-|\underline{x}-\underline{x}'|}}{|\underline{x}-\underline{x}'|^2} e^{i\underline{k}\cdot\underline{x}'} = \frac{\tan^{-1}|\underline{k}|}{|\underline{k}|} e^{i\underline{k}\cdot\underline{x}} \tag{34}$$

and also that $\mu_K^* = \mu_{-K'}$ since $\mu(\underline{x})$ is real. We obtain:

$$\lambda = \frac{\int d\underline{x} \sum_K \sum_{K'} \mu_K^* e^{-i\underline{K}\cdot\underline{x}} e^{-i\underline{k}\cdot\underline{x}} \mu_{K'} e^{i\underline{K}'\cdot\underline{x}} e^{i\underline{k}\cdot\underline{x}} \frac{\tan^{-1}|\underline{K}' + \underline{k}|}{|\underline{K}' + \underline{k}|}}{\int d\underline{x}\, \mu(\underline{x})} \tag{35}$$

We call the volume of the unit cell V and remember that the average of $\mu(\underline{x})$ is unity. Also we have:

$$\int e^{i(\underline{K}'-\underline{K})\cdot\underline{x}}\, d\underline{x} = 0 \qquad \underline{K} = \underline{K}'$$
$$= V \qquad \underline{K} = \underline{K}' \tag{36}$$

Equation 35 then becomes:

$$\lambda = \frac{\sum_K \sum_K \mu_K^* \mu_K \frac{\tan^{-1}|\underline{K}' + \underline{k}|}{|\underline{K}' + \underline{k}|} V \int_{\underline{K}\underline{K}'}}{V}$$

or

$$\lambda = \sum_K |\mu_K|^2 \frac{\tan^{-1}|\underline{K} + \underline{k}|}{|\underline{K} + \underline{k}|} \tag{37}$$

Since the average of $\mu(\underline{x})$ is unity, μ_0 is also equal to unity. We can then write Eq. 37 as:

$$\lambda = \frac{\tan^{-1}|\underline{k}|}{|\underline{k}|} + \sum_{K\neq 0} |\mu_K|^2 \frac{\tan^{-1}|\underline{K} + \underline{k}|}{|\underline{K} + \underline{k}|} \tag{38}$$

The quantity λ is, therefore equal to the value which it would have for homogeneous system plus a positive correction, due to the inhomogenity. This says, in other words, that $1/(1 + f)$ is greater for criticality in the inhomogeneous case, or that $1 + f$ is less, which implies that making the material non-uniform increases its activity. It can be seen in the following way that this statement is correct. Consider a homogeneous mixture of fissionable and absorbing materials combined in such proportions that the mixture neither absorbs nor reproduces. If we take the same materials in the same proportions,

but in the form of an inhomogeneous lattice rather than a mixture, we can make the size of a single piece of the fissionable material such that this piece will be super-critical. This is, of course, an extreme case. The slightest disturbance of the homogenity will increase the activity of the system. This will be so since in the homogeneous arrangement the absorption of one neutron yields one neutron on the average. In any inhomogeneous arrangement the neutron density would be higher in the places rich in fissionable material than in the absorbing regions. This means that a larger fraction of neutrons will be absorbed in fission than previously and the system will be supercritical.

The expression 38 gives a value of λ, which is too low. Therefore the correction to the homogeneous value of λ is certainly positive but somewhat larger than given by Eq. 38.

The expression 38 is convenient but has, thus far, no rigorous foundation if $\underline{k}$ is not real. We proceed to derive this equation in such a way that the restriction to real values of $\underline{k}$ can be removed. We can write Eq. 9 as follows:

$$\phi(\underline{x}) = (1/4\pi)\int d\underline{x}' \frac{e^{-|\underline{x}-\underline{x}'|}}{|\underline{x}-\underline{x}'|^2} e^{i\underline{k}\cdot(\underline{x}'-\underline{x})} \frac{\mu(\underline{x}')}{\lambda} \phi(\underline{x}') \tag{39}$$

We also write the integral equation for ϕ_n in the case where the vector $\underline{k}$ has the opposite direction to that in Eq. 39 and $\mu(\underline{x})$ is equal to unity. We write $\phi = \phi_0$ and $\lambda = \lambda_0$ and obtain:

$$\phi_0(\underline{x}) = (1/4\pi)\int d\underline{x}' \frac{e^{-|\underline{x}-\underline{x}'|}}{|\underline{x}-\underline{x}'|^2} e^{-i\underline{k}\cdot(\underline{x}'-\underline{x})} (1/\lambda_0)\ \phi_0(\underline{x}') \tag{40}$$

We multiply Eq. 39 by $(1/\lambda_0)\ \phi_0(\underline{x})$ and Eq. 40 by $(\mu(\underline{x})/\lambda)\phi(\underline{x})$ and integrate over $\underline{x}$. We interchange the dummy variables $\underline{x}$ and $\underline{x}'$ in the integrations on the right hand side of the first expression and note that the right hand sides of the two expressions are now equal. We therefore obtain the exact equation:

$$\int d\underline{x} \left[\frac{1}{\lambda_0} - \frac{\mu(\underline{x})}{\lambda}\right] \phi_0(\underline{x})\ \phi(\underline{x}) = 0 \tag{41}$$

The function $\phi_0(\underline{x})$ is really constant and can be taken equal to unity. We obtain:

$$\lambda = \lambda_0 \frac{\int d\underline{x}\, \mu(\underline{x})\, \phi(\underline{x})}{\int d\underline{x}\, \phi(\underline{x})} \tag{42}$$

This gives a simple expression for λ, except that an exact expression for $\phi(\underline{x})$ is necessary. We proceed by approximating $\phi(\underline{x})$ by a method of iteration. We insert a constant for $\phi(\underline{x})$ on the right hand side of Eq. 39 and take the result as an improved expression for $\phi(\underline{x})$. This gives:

$$\phi(\underline{x}) = (1/4\pi) \int d\underline{x}' \frac{e^{-|\underline{x}-\underline{x}'|}}{|\underline{x}-\underline{x}'|^2} e^{i\underline{k}\cdot(\underline{x}'-\underline{x})}\, \mu(\underline{x}') \tag{43}$$

We then insert the Fourier expansion Eq. 29 for $\mu(x)$ and do the indicated integrations. This yields:

$$\begin{aligned}\phi(\underline{x}) &= \sum_{\underline{K}} \mu_{\underline{K}} (1/4\pi)\, e^{-i\underline{k}\cdot\underline{x}} \int d\underline{x}' \frac{e^{-|\underline{x}-\underline{x}'|}}{|\underline{x}-\underline{x}'|^2} e^{i(\underline{k}+\underline{K})\cdot\underline{x}'} \\ &= \sum_{\underline{K}} \mu_{\underline{K}}\, e^{i\underline{K}\cdot\underline{x}} \frac{\tan^{-1}|\underline{k}+\underline{K}|}{|\underline{k}+\underline{K}|}\end{aligned} \tag{44}$$

We then insert this in Eq. 42, together with the Fourier expansion Eq. 29 for $\mu(\underline{x})$. This yields:

$$\lambda = \frac{\lambda_0 \sum_{\underline{K}} \sum_{\underline{K}'} \mu^*_{\underline{K}'} \mu_{\underline{K}} \frac{\tan^{-1}|\underline{k}+\underline{K}|}{|\underline{k}+\underline{K}|} \int d\underline{x}\, e^{i(\underline{K}-\underline{K}')\cdot\underline{x}}}{\sum_{\underline{K}} \mu_{\underline{K}} \frac{\tan^{-1}|\underline{k}+\underline{K}|}{|\underline{k}+\underline{K}|} \int d\underline{x}\, e^{i\underline{K}\cdot\underline{x}}} \tag{45}$$

If the integrations are then extended over a unit cell with V equal to the volume of the cell, we obtain:

$$\begin{aligned}\lambda &= \frac{\lambda_0 \sum_{\underline{K}} \sum_{\underline{K}'} \mu^*_{\underline{K}'} \mu_{\underline{K}} \frac{\tan^{-1}|\underline{k}+\underline{K}|}{|\underline{k}+\underline{K}|} V\delta_{\underline{K}\underline{K}'}}{\sum_{\underline{K}} \mu_{\underline{K}} \frac{\tan^{-1}|\underline{k}+\underline{K}|}{|\underline{k}+\underline{K}|} V\delta_{\underline{K},0}} \\ &= \frac{\lambda_0 \sum_{\underline{K}} |\mu_{\underline{K}}|^2 \frac{\tan^{-1}|\underline{k}+\underline{K}|}{|\underline{k}+\underline{K}|}}{\mu_0 \frac{\tan^{-1}|\underline{k}|}{|\underline{k}|}}\end{aligned} \tag{46}$$

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Remembering that $\lambda_0 = \frac{\tan^{-1}|\underline{k}|}{|\underline{k}|}$ and $\mu_0 = 1$, we finally obtain:

$$\lambda = \sum_{\underline{K}} |\mu_{\underline{K}}|^2 \frac{\tan^{-1}|\underline{k}+\underline{K}|}{|\underline{k}+\underline{K}|} \tag{47}$$

This equation is formally identical with Eq. 37 but there is now no restriction to real values of $\underline{k}$. If $\underline{k}$ is imaginary, however, it is not clear that the true λ is higher than that given by Eq. 47. If the accuracy of Eq. 47 is good for real $\underline{k}$, however, we would expect it to be good for imaginary $\underline{k}$. Suppose we assume $\underline{k} = i\,\underline{h}$ where $\underline{h}$ is a real vector. In Eq. 47 $|\underline{K}+\underline{k}|$ means the square root of the scalar product of the vector with itself, not with its complex conjugate. Remembering this, we obtain:

$$\lambda = \sum_{\underline{K}} |\mu_{\underline{K}}|^2 \frac{\tan^{-1}\sqrt{(i\underline{h}+\underline{K})\cdot(i\underline{h}+\underline{K})}}{\sqrt{(i\underline{h}+\underline{K})\cdot(i\underline{h}+\underline{K})}}$$

$$= \sum_{\underline{K}} |\mu_{\underline{K}}|^2 \frac{\tan^{-1} i\sqrt{(\underline{h}-i\underline{K})\cdot(\underline{h}-i\underline{K})}}{i\sqrt{(\underline{h}-i\underline{K})\cdot(\underline{h}-i\underline{K})}}$$

$$= \sum_{\underline{K}} |\mu_{\underline{K}}|^2 \frac{\tanh^{-1}\sqrt{(\underline{h}-i\underline{K})\cdot(\underline{h}-i\underline{K})}}{\sqrt{(\underline{h}-i\underline{K})\cdot(\underline{h}-i\underline{K})}} \tag{48}$$

This sum is obviously real since $\mu^*_{\underline{K}} = \mu_{-\underline{k}'}$. It can be written:

$$= \frac{\tanh^{-1}|\underline{h}|}{|\underline{h}|} + \sum_{\underline{K}\neq 0} |\mu_{\underline{K}}|^2 \; 1/2 \; \frac{\tanh^{-1}\sqrt{(\underline{h}-i\underline{K})\cdot(\underline{h}-i\underline{K})}}{\sqrt{(\underline{h}-i\underline{K})\cdot(\underline{h}-i\underline{K})}}$$

$$+ \frac{\tanh^{-1}\sqrt{(\underline{h}+i\underline{K})\cdot(\underline{h}+i\underline{K})}}{\sqrt{(\underline{h}+i\underline{K})\cdot(\underline{h}+i\underline{K})}} = \frac{\tanh^{-1}|\underline{h}|}{|\underline{h}|}$$

$$+ \sum_{\underline{K}\neq 0} |\mu_{\underline{K}}|^2 \, R\left\{\frac{\tanh^{-1}\sqrt{(\underline{h}+i\underline{K})^2}}{\sqrt{(\underline{h}+i\underline{K}^2)}}\right\} \tag{49}$$

In Eq. 49, R {w} means the real part of w. The principal branch of the function $\tanh^{-1}$ is always required.

We now wish to check the accuracy of Eq. 47 by comparing the value of λ calculated by the exact Eq. 24 with the approximate value of λ. We assume, as we did in the derivation of Eq. 24 that $\underline{k}$ is equal to zero. The symbol used in Eq. 47 now are specialized to the following:

$$\mu(\underline{x}) = 1 + \alpha \cos(2\pi x/a) = 1 + (\alpha/2)\, e^{2\pi i x/a} + (\alpha/2)\, e^{-2\pi i x/a}$$

$$\mu_0 = 1$$

$$\mu_1 = \alpha/2 \qquad |\underline{K}_{-1}| = 2\pi/a$$

$$\mu_{-1} = \alpha/2 \qquad |\underline{K}_{-1}| = 2\pi/a$$

$$\mu_K = 0 \text{ otherwise} \tag{50}$$

Equation 47 therefore yields:

$$\lambda = 1 + 2\,(\alpha^2/4)\,\frac{\tan^{-1}(2\pi/a)}{2\pi/a} = 1 + (\alpha^2/2)\,\lambda_1 \tag{51}$$

If we assume $(\alpha^2/4)\,[\lambda_1/(\lambda - \lambda_1)]\,\lambda_2/(\lambda - \lambda_2) \ll 1$ in Eq. 24 we obtain:

$$\lambda = 1 + (\alpha^2/2)\,\lambda_1/(\lambda - \lambda_1) \tag{52}$$

In this equation λ will be nearly unity, and if we assume that λ_1 is much less than unity we obtain:

$$\lambda = 1 + (\alpha^2/2)\,\lambda_1 \tag{53}$$

which agrees with Eq. 49. The validity of these approximations can be seen from the following examples. We write $\lambda = 1 + \Delta\lambda$ and calculate $\Delta\lambda$ for various values of a and α by Eq. 47 (or Eq. 51 for this special case) and by the exact Eq. 24. We also give $(\Delta\lambda)/\alpha^2)$, which is independent of α in the approximation leading to Eq. 47, and may be expected to be nearly independent of α in reasonable cases with the use of the exact Eq. 24.

$\Delta\lambda$ Eq. 24	$\Delta\lambda$ Eq. 47	a	α	$\Delta\lambda/\alpha^2$ Eq. 24	$\Delta\lambda/\alpha^2$ Eq. 47
0.000500	0.000494	0.1	0.2	0.0125	0.0124
0.00316	0.00310	0.1	0.5	0.0125	0.0124
0.0125	0.0124	0.1	1.0	0.0125	0.0124
0.00270	0.00237	0.5	0.2	0.0675	0.0593
0.0165	0.0148	0.5	0.5	0.0660	0.0593
0.0629	0.0593	0.5	1.0	0.0629	0.0593
0.00576	0.00450	1.0	0.2	0.144	0.112
0.0348	0.0281	1.0	0.5	0.139	0.112
0.126	0.112	1.0	1.0	0.126	0.112

It is to be noticed that the approximate $\Delta\lambda$ is always less than the exact $\Delta\lambda$, as expected. For a lattice with periodic length considerably less than a mean free path (a = 0.1), $\mu(\underline{x})$ can oscillate between zero and two (α = 1.0) without introducing any appreciable error in the approximate value of $\Delta\lambda$. The approximate form gives a good idea of the size of the effect even when the periodic length becomes a mean free path.

It might be expected that if $\mu(x)$ departs little from unity and has a short periodic length, a first-order perturbation calculation of λ should suffice. This is not true and, in fact, several different values for λ can be obtained by doing the perturbation calculation in several seemingly equivalent ways. It seems, in fact, that the calculation is essentially second order and this can be seen from the following considerations. We write the equation whose kernel is adjoint to that of Eq. 9:

$$\lambda\overline{\phi_k}(\underline{x}) = (1/4\pi)\int \overline{d\underline{x}'}\,\frac{e^{-|x-x'|}}{|\underline{x}-\underline{x}'|^2}\,e^{-i\underline{k}\cdot(\underline{x}'-\underline{x})}\;\mu(\underline{x})\;\overline{\phi_k}(\underline{x}') \tag{54}$$

We consider first a case with $\mu(\underline{x})$ equal to unity (the unperturbed case) and then change $\mu(\underline{x})$ to $1 + \Delta\mu(\underline{x})$. The eigenvalue will change to $\lambda + \Delta\lambda$ where $\Delta\lambda$ is given by the usual first order perturbation calculation:

$$\Delta\lambda = \frac{\int \overline{d\underline{x}}\int \overline{d\underline{x}}\;\;\overline{\phi}_k(\underline{x})\;(1/4\pi)\;\frac{e^{-|\underline{x}-\underline{x}'|}}{|\underline{x}-\underline{x}'|^2}\,e^{i\underline{k}\cdot(\underline{x}'-\underline{x})}\;\Delta\mu(\underline{x}')\;\phi_k(\underline{x}')}{\int d\underline{x}\;\overline{\phi_k}(\underline{x})\;\phi_k(\underline{x})} \tag{55}$$

We use Eq. 54 to do one integration and obtain:

$$\Delta\lambda = \frac{\lambda\int d\underline{x}\;\overline{\phi_k}(\underline{x})\;\overline{\phi_k}(\underline{x})\;\Delta\mu(\underline{x})}{\int d\underline{x}\;\overline{\phi_k}(\underline{x})\;\phi_k(\underline{x})} \tag{56}$$

We insert for $\overline{\phi_k}$ and ϕ_k the unperturbed $\overline{\phi_k}$ and ϕ_k which are constants, and we obtain:

$$\frac{\overline{\Delta\lambda}}{\lambda} = \frac{\int d\underline{x}\,\overline{\Delta}\,\mu(\underline{x})}{\int d\underline{x}} \qquad \overline{\Delta\mu} = 0 \tag{57}$$

The result of the first-order perturbation calculation is, therefore, that the eigenvalue is unchanged. We must then go, either to a second order

calculation or use one of the treatments which have been given. It should be pointed out that the first order calculation will give correct answers in problems where $\Delta\mu$ is not assumed to be zero on the average. It is only in cases where no change is made in the total amount of active material that a second order calculation may be necessary.

The treatment which we have developed is certainly not capable of giving the critical mass of a lattice assembly. It does enable us to estimate the approximate effect of the inhomogenity. We can state some obviously necessary and obviously sufficient conditions that a given assembly to essentially homogeneous. We require that for the given λ of the core or tamper that the propogation vectors of the infinite medium plane wave solutions should have magnitudes which are essentially independent of direction. We further require that this magnitude shall be different from that for the corresponding homogeneous medium by only a small fraction of itself. We can further argue that the effect on the critical size produced by the inhomogenity will be of the order of magnitude of the effect on the magnitude of the vector $\underline{k}$.

If the inhomogeneities are not too large excellent approximations to the critical mass of an inhomogeneous core can be obtained by replacing the core by an "equivalent" homogeneous one. The "equivalence" being determined by making the homogeneous material such that an infinite medium of it would have the same λ for the important K values as does an infinite medium of inhomogeneous material as developed by the methods of this report.

Inhomogeneities of mean free path present problems which have not been solved. Inhomogeneities in a system in which many neutron velocities are involved present interesting problems which have only been partly solved in some especially simple cases.