

region, it is impossible to claim that this region of the energy scale is unimportant. One should also note that for  $\sigma_a = 0.01$  barns, the smallest value used by GK,  $(\kappa/\Sigma_{tr})^2$  is of the order of 0.3 just below the Bragg cutoff. Hence, even for this small absorption, which is about what exists in natural beryllium, there is some doubt as to the validity of diffusion theory.

The GK paper presents values of diffusion parameters that are based upon the calculated dependence of  $\kappa^2$  on  $\Sigma_a$ . Since the calculations are based upon an invalid application of diffusion theory one must conclude that the derived parameters have little to do with reality and an agreement with experiment is most likely fortuitous.

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### Comments on Michael's Criticism of the Use of Diffusion Theory for the Study of Thermal Neutrons in Beryllium

In the preceding letter, Michael<sup>1</sup> has criticized our earlier paper<sup>2</sup> for using diffusion theory for the study of thermal neutrons in beryllium. There are two main points in his letter: a) he suggests an alternative approach to the problem—that of 'transport approximation,' and b) puts forward arguments to show that our use of diffusion theory was not justified.

Let us consider the first point first. According to Eqs. (1) or (2) of his letter, even the equilibrium neutron energy distribution will not be Maxwellian for the case  $\Sigma_a = 0$  (we use the notation of (Ref. 1)), except in the special case of completely isotropic scattering, when  $\Sigma_{tr}(E)$  is the same as  $\Sigma_s(E)$ . The two equations are quite inappropriate for multi-velocity problems and all conclusions that have been drawn from them are unreliable. The difficulty has arisen because Michael has applied the result of Rakavy and Yeiven's paper<sup>3</sup> to a case where it is not applicable. 'If these cautions are not observed it is easy to loose touch with reality.' Further to quote Davison<sup>4</sup>, '... the approximation (transport approximation) leads in general to rather poor results, as we might expect.' We feel that the suggestion by Michael, that one should solve his Eq. (1) by introducing an auxiliary eigenvalue, is not seriously meant.

In spite of the above, the point raised by him concerning the validity of using diffusion theory in the case of poisoned beryllium moderator is significant and needs some clarification.

It is well known that diffusion theory is a poor approximation for neutrons with energy just below the Bragg cutoff energy, because of their very low scattering cross section. However, since these neutrons form only a small fraction of the total number of neutrons (Table I), one expects  $\kappa^2$  calculated on the basis of diffusion theory to be essentially correct. According to diffusion theory

$$\kappa^2 = 3 \int \Sigma_a(E) \phi_0(E) dE / \int \frac{\phi_0(E) dE}{\Sigma_{tr}(E)}, \quad (1)$$

<sup>1</sup>PAUL MICHAEL, *Nucl. Sci. Eng.*, this issue, p. 93.

<sup>2</sup>P. S. GROVER and L. S. KOTHARI, *Nucl. Sci. Eng.*, **22**, 366 (1965).

<sup>3</sup>G. RAKAVY and Y. YEIVEN, *Nucl. Sci. Eng.*, **15**, 158 (1963).

<sup>4</sup>B. DAVISON and J. B. SYKES, *Neutron Transport Theory*, Oxford (1957), p. 241.

TABLE I  
Ratio, R, of Neutron Flux Below the Bragg Cut-off to the Total Neutron Flux

Absorption cross-section $\Sigma_a(E)$ <sup>a</sup> cm <sup>-1</sup>	R
( $\times 10^{-2}$ )	( $\times 10^{-2}$ )
0.12	2.5
0.50	3.5
0.84	4.4
1.20	6.5

<sup>a</sup> $(\Sigma_a(E))$  corresponds to velocity =  $2.22 \times 10^5$  cm/sec.

where  $\phi_0(E)$  is the asymptotic flux (large distances). If the diffusion theory breaks down in a small range of energy (below the Bragg cut-off),  $\phi_0(E)$  will be in error in that energy range, but since  $\kappa^2$  is defined as an integral over the entire energy spectrum, the error in  $\kappa^2$  will be small. Thus, there does not seem to be any ground for taking such a pessimistic view as Michael does—"the derived parameters have little to do with reality and agreement with experiment is most likely fortuitous." One can very well consider this agreement as corroborating the fact that diffusion theory works, even for cases where neutrons in a small energy range do not fulfill the conditions demanded by the diffusion theory.

No one will dispute that the use of diffusion theory should not be pressed too far and that more elaborate transport-theory calculations should be done (anyway, not on the lines suggested by Michael but rather as done by Honeck<sup>5</sup>). It is, however, worthwhile to remember that there are other important approximations involved in all present-day calculations, for example, the use of a particular lattice model in calculating the scattering kernels, the use of incoherent approximation, expansion of highly angle-dependent kernels in terms of a few Legendre polynomials, etc. In view of these and because of its great simplicity, the use of diffusion theory need not be abandoned. On the other hand, it does have a distinct advantage in that the sharp peaks in the transport cross-section can be explicitly taken into account.

The one oversight in our paper<sup>2</sup> has been our failure to state explicitly that the limit set on  $\kappa^2$  by diffusion theory

$$\kappa^2 \leq 3 \Sigma_{tr}(E) \cdot (\Sigma_a(E) + \Sigma_s(E)) \Big|_{\min} \quad (2)$$

will not be valid for large  $\Sigma_a$ , for the simple reason that when the diffusion length becomes of the order of the average scattering mean free path, the theory itself will break down. Since the various parameters occurring in diffusion theory are quantities averaged over the equilibrium neutron-energy distribution, the validity of the theory should be judged by the criterion as to whether the average absorption mean free path far exceeds the average value of scattering mean free path. In other words, the condition for the validity of diffusion theory is<sup>6-8</sup>

$$\bar{\Sigma}_a \ll \bar{\Sigma}_s. \quad (3)$$

<sup>5</sup>HENRY HONECK, Brookhaven Conf. on Neutron Thermalization (1962).

<sup>6</sup>A. M. WEINBERG and L. C. NODERER, Report No. ORNL 51-5-98 (1951).

<sup>7</sup>A. M. WEINBERG and E. P. WIGNER, *The Physical Theory of Neutron Chain Reactors*, Chicago (1958); p. 191.

<sup>8</sup>A. D. GALANIN, *Thermal Reactor Theory*, Pergamon Press (1960); p. 15.

The average value of the neutron scattering cross section of beryllium is about  $0.84 \text{ cm}^{-1}$ , whereas the values of  $\bar{\Sigma}_a$  do not exceed  $0.93 \times 10^{-2} \text{ cm}^{-1}$ . (Except in one case in our second paper<sup>9</sup>, where we have used  $\bar{\Sigma}_a = 6.06 \times 10^{-2} \text{ cm}^{-1}$ . This case was studied simply to investigate the effect of samarium resonances on the equilibrium spectra.) Thus,  $\bar{\Sigma}_s$  is about a hundred times larger than  $\bar{\Sigma}_a$  and we feel the use of diffusion theory by us was not unjustified.

Thus, though Michael has raised an important point, in view of what has been said above it is difficult to agree with his conclusions.

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<sup>9</sup>P. S. GROVER and L. S. KOTHARI, *Nucl. Sci. Eng.*, to be published.

### Reply to a Note by Jeffery Lewins and a Simplified Development of the Maximum Principle

In our recent publication<sup>1</sup>, the time-optimal solution to the xenon shutdown problem was obtained by application of the techniques of Pontryagin, Boltyanskii, Gamkrelidze, and Mishchenko<sup>2</sup>. An important consideration in formulating this problem was the choice of direction of the canonical (adjoint) vector in the xenon-iodine state space at the intersection of the optimal trajectory and the target curve, labeled  $\Omega$  in Ref. 1. In his note, Lewins<sup>3</sup> incorrectly refers to this choice as a "supposition," whereas in Ref. 1, the unambiguous condition for the choice of sign of the xenon canonical variable  $p_2$  in reverse time is specified by the statement, "The initial conditions at  $T = 0$  [i.e., the intersection mentioned above] are determined by choosing a point  $x$  ( $T = 0$ )  $\in \Omega$  according to Eq. (15) and applying the additional conditions (11) and (18) . . ." (Paragraph 1, page 474, Ref. 1). Equation (18) is the statement of transversality, and Eq. (11) prescribes the Hamiltonian, which is a positive constant<sup>1,2</sup>. Hence, we did not rely on the condition of transversality alone as suggested by Lewins. The desired manipulation of these two conditions is presented by Lewins in his equation (4). The same result follows easily from our equations (11) and (18), and it was for this reason that we stated in Ref. 1, "Equations (11) and (18) combine to specify  $p(0)$  as an outwardly directed normal from  $\Omega$ ; i.e.,  $p_2(0) > 0$ ." (Paragraph 1, page 474 of Ref. 1).

We would also like to comment on a second statement in Lewin's note. In the paragraph containing his equation (4), he states, ". . . that since the bracket (in Eq. (4)) vanishes for operations on the xenon boundary, the sign is then immaterial and  $H$  is zero." This statement is puzzling since a) the bracket in his equation (4) refers to the intersection

of the optimal trajectory with the target curve  $\Omega$ , which has nothing to do with the xenon boundary, defined in Ref. 1 by  $x_2 = x_{2,\text{max}}$ , and b) the corner conditions<sup>2</sup> require that  $H$  remain continuous at the intersection of an optimal trajectory with the boundary. Hence,  $H$  cannot equal zero on the boundary, since it is a positive constant off the boundary.

In the last paragraph of Lewin's note, he suggests changing the direction of the canonical variable and the optimization theorem to resolve an alleged conflict ". . . with our usual ideas of perturbation theory and the importance of a source of iodine or xenon." However, he adds that this will not affect our solution to the shutdown problem. Since we concur that the suggested change will leave the present results unaffected, we feel that there is no need for further comment.

Having dealt in detail with the specific comments of Lewins, we now return to the initial question regarding the sense of the adjoint vector  $p$ . We would like to present a simple geometric demonstration of the Maximum Principle for time optimal problems to show the manner in which the direction of  $p$  is related to the theory. The following development appeals to us as an excellent heuristic argument, but it is not to be construed as a rigorous derivation of either the Maximum Principle or the transversality condition. (We are indebted to Arthur M. Hopkin, University of California (Berkeley), for this model.)

In Fig. 1, let the initial point  $O$  be the origin. The target line is  $\Omega$ . The contours  $S_\tau$  (assumed convex) enclose all points in the  $(x_1, x_2)$  phase plane that can be attained from  $O$  using any allowable control scheme during the time interval  $0 \leq t \leq \tau$ . In Fig. 1, we observe:

- the points on  $S_{t_1}$  can be reached in time  $t_1$  only by employing time optimal control
- if  $T$  is the minimum time from  $O$  to the target  $\Omega$ , then  $S_T$  is tangent to  $\Omega$  at the point where the target is attained.

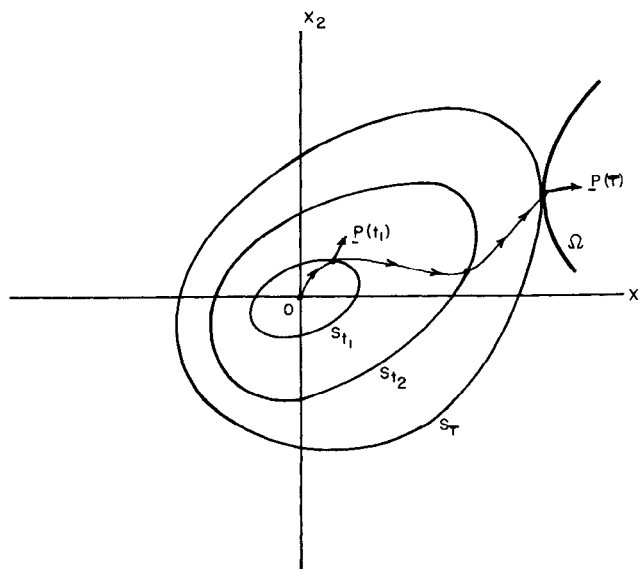


Fig. 1. Time-optimal trajectory from  $O$  to  $\Omega$ . System equations:

$$\frac{dx}{dt} = f(x, u); \quad 0 < t_1 < t_2 < T$$

for  $u$  in the allowable control space.

<sup>1</sup>J. J. ROBERTS and H. P. SMITH, Jr., "Time Optimal Solution to the Reactivity-Xenon Shutdown Problem," *Nucl. Sci. Eng.*, **22**, 470 (1965).

<sup>2</sup>L. S. PONTRYAGIN, V. G. BOLTYANSKII, R. G. GAMKRELIDZE and E. F. MISHCHENKO, *The Mathematical Theory of Optimal Processes*, (L. W. NEUSTADT, ed.), Interscience Publishers, New York, (1963).

<sup>3</sup>J. LEWINS, "A Note on the Adjoint Function in the Time Optimal Xenon Shutdown Problem," *Nucl. Sci. Eng.*, **23**, 404 (1965).