

THE THEORY OF NEUTRON WAVE PROPAGATION

Thesis by

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ABSTRACT

The objectives of this thesis include the development of an exact theory of neutron wave propagation in non-multiplying media as well as the application of this theory to analyze current experimental work.

An initial study is made of the eigenvalue spectrum of the velocity-dependent Boltzmann transport operator for plane wave propagation in both noncrystalline and polycrystalline moderators. The point spectrum is discussed in detail, and a theorem concerning the existence of discrete eigenvalues for high frequency, high absorption, and/or small transverse dimensions is demonstrated. The limiting cases of low and high frequency behavior are analyzed. A physical interpretation of the discrete and continuum eigenfunctions (plane wave modes) is given, and the point spectrum existence theorem is explained in the light of such interpretations.

Using this spectral representation, a technique for solving full-range boundary value problems for a general noncrystalline scattering kernel is presented. Orthogonality and completeness of the eigenfunctions are demonstrated, and the problem of a plane source at the origin of an infinite medium is solved. This solution is compared with that obtained by a Fourier transform technique. A procedure for solving half-range boundary value problems is presented for a one-term separable kernel model. For purposes of illustration, the problem of an oscillating source incident upon the boundary of a half-space is solved. The difficulty in extending the half-range theory

to more general scattering models is discussed.

The second part of the thesis proceeds to demonstrate this theory in more detail by applying it to analyze recent neutron wave experiments in graphite and D_2O parallelepipeds. To facilitate the interpretation of the general solution, the inelastic scattering kernel is approximated by a separable kernel, while the elastic scattering is modeled with a Dirac δ -function. The eigenvalue spectrum is analyzed in some detail, revealing several interesting conclusions concerning the experimental data and methods of data analysis. Several modifications in experimental design and analysis are suggested.

The agreement of the theory with experiment is sufficient to warrant its application to the analysis of more complicated experiments (multiple-region, multiplying media, pulse propagation, etc.). Several suggestions for such extensions are indicated.

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I. INTRODUCTION

Neutron wave experiments involve the measurement of the response of the neutron density in a nuclear reactor or reactor materials to a modulated neutron source. This source creates a wave-like disturbance in the neutron distribution whose propagation through the medium depends upon material composition and geometry. By measuring the relative attenuation and phase lag of this disturbance at various locations within the medium, one can obtain information about the composition and neutron transport properties of the propagation material.

Such neutron wave experiments are expected to find application in a number of areas of reactor physics. At present these experiments are being used to measure the neutron transport properties of various moderator materials⁽¹⁻⁵⁾. A second possible area of application involves the measurement of the kinetic behavior and criticality of reactor systems by propagating neutron waves through a multiplying assembly. A third and perhaps more immediate area of application is to provide a clearer understanding of the transport process itself, since the propagation of these waves is an ideal example of non-equilibrium behavior in the linearized kinetic theory of gases.

The effectiveness with which such applications can be pursued depends both upon advances in the area of experimental techniques and upon more advanced theoretical models with which to interpret measured results. This thesis is concerned with research into the latter area.

A. PREVIOUS WORK IN THE THEORY OF NEUTRON WAVES

The theory of neutron wave experiments dates from the analysis of an oscillating absorber in a reactor core by Weinberg and Schweinler⁽⁶⁾ in 1948. This one-velocity diffusion theory analysis was later used to analyze the early wave experiments of Raievski and Horowitz⁽⁷⁾. However it was not until 1963 that Perez and Uhrig⁽⁸⁾ extended this theory to include energy dependence, using a Laguerre polynomial expansion in the energy variable. Subsequent work by Moore⁽⁹⁾ introduced the concept of the dispersion law for such wave propagation. In 1964 di Pasquantonio⁽¹⁰⁾ developed a monoenergetic P_1 theory which was later extended by Kunaish⁽¹¹⁾ to energy-dependent P_1 theory (again using Laguerre polynomial expansions). Recently Ohanian, Booth, and Perez⁽¹²⁾ have developed a more advanced energy-dependent diffusion theory which allows a more accurate modeling of the scattering kernel. Since this latter theory is customarily used to analyze the neutron wave experiment, it is described in more detail in Appendix A. Travelli⁽¹³⁾ has subsequently examined both one-velocity and multigroup transport models, including linearly anisotropic scattering effects. More recently Moore⁽¹⁴⁾ has dealt briefly with a velocity-dependent transport model using degenerate kernel expansions. However the status of the exact transport theory of neutron wave propagation remains rather primitive at this time.

B. RELATED WORK IN THE FIELD OF RAREFIED GAS DYNAMICS

Much of the kinetic theory of rarefied gases is applicable to the neutron wave problem since both a rarefied gas and a neutron gas are described by a similar linearized Boltzmann equation. The specific problem most analogous to neutron wave propagation has been the treatment of forced sound waves. The theory of such non-equilibrium behavior in rarefied gases has been, until recently⁽²²⁻²³⁾, considerably more advanced than its counterpart in neutron transport theory. The literature on this subject is quite extensive, and only the work most closely related to this thesis can be mentioned in the following brief review.

Of course the fundamental kinetic theory of gases can be traced back to the work of Boltzmann, Hilbert, Chapman, Enskog, Grad⁽¹⁵⁾, and others. Of more immediate interest to this thesis, however, was the work of Wang-Chang and Uhlenbeck⁽¹⁶⁾ in 1952 which amounted to an energy-dependent transport theory analysis of sound propagation. In this treatment, the particle distribution function was expanded in a truncated set of the natural eigenfunctions of the collision operator for Maxwell molecules, and the resulting determinant dispersion relation was then solved for the appropriate eigenvalues. Later work by Sirovich, Thurber, and Weitzner⁽¹⁷⁻¹⁸⁾ has relied on modeling of the collision operator (BKG models, etc.) to reduce the complexity of the Boltzmann equation to such an extent that it could be analyzed more easily by integral transform techniques. This modeling is similar to the degenerate kernel expansions⁽²⁰⁾ well-

known in neutron transport theory, except that it assumes a constant collision frequency (effectively a $1/v$ behavior of the total cross-section). Buckner and Ferziger⁽²¹⁾ have solved similar modeled problems using the Case method of elementary solutions⁽²⁴⁾. More recently Cercignani⁽²⁵⁾ has extended much of this theory to models with velocity-dependent collision frequency--but within the restrictions of a one-term separable kernel.

Perhaps the most comprehensive work in this area of kinetic theory can be found in the numerous papers of Grad. Of particular interest to this thesis is his recent work⁽¹⁹⁾ on high frequency sound propagation, the direct analogue of the neutron wave experiment, which includes a qualitative study of the eigenvalue spectrum for the problem.

C. STATEMENT OF THE THESIS PROBLEM

It will be demonstrated in detail in this thesis that the previous theories of neutron wave propagation fail in one approximation or another to describe the true character of the propagation process. While much of the theory in rarefied gas dynamics is more applicable, the specific nature of neutron scattering in matter makes it necessary to formulate an alternative, and in some respects a more advanced, theory. This is particularly necessary for the study of wave propagation in polycrystalline media.

The basic goal of this thesis, then, is a logical development of a general theory of neutron wave propagation. This theory will be

developed, insofar as possible, from the exact classical equation describing neutron transport--the Boltzmann equation. As mentioned earlier, motivation for such a theory has been provided not only by recent experimental work with modulated neutron sources, but as well by a desire for a deeper physical and mathematical understanding of the propagation of plane wave disturbances in the linearized kinetic theory of gases.

The propagation of thermal neutron waves in moderating media of both infinite and finite dimensions will be analyzed. Two basic techniques will be developed for the treatment of specific problems in wave propagation: a method using the spectral representation of the Boltzmann operator and an integral transform technique. While the latter technique appears easier for infinite medium problems, the more general applicability of the eigenfunction method will be indicated as well as its more direct physical interpretation.

The general mathematical theory of neutron wave propagation is developed in Part I of this thesis. In Part II the validity of the theory is demonstrated by applying it to understand existing neutron wave experiments as well as to suggest several more advanced experiments.

However it must be emphasized that the understanding and analysis of such experiments in themselves should not be regarded as a suitable goal for this thesis. Indeed such an analysis could probably be accomplished with much less effort using much less sophisticated models. Rather the more general theory is developed to add to the

growing understanding of non-equilibrium kinetic theory and to predict and understand phenomena which are not yet accessible to experimenters in neutron physics (and are of only marginal interest to reactor technology in general). Such motivation underlies much of the more advanced work⁽⁴²⁾ in neutron physics and is certainly not unique to neutron wave propagation. However rather than justifying the theory of neutron wave propagation merely for its own sake, we shall appeal to other very closely related areas in kinetic theory in which such analyses have much broader physical significance and importance to technology.

PART I

A GENERAL THEORY OF NEUTRON WAVE PROPAGATION

INTRODUCTION

The transport of neutrons in a homogeneous, nonmultiplying medium can be described by the linearized Boltzmann equation⁽²⁶⁾

$$\frac{\partial f}{\partial t} + \underline{v} \cdot \text{grad } f = -v \Sigma_t(v) f(\underline{r}, \underline{v}, t) + \int \int \int d^3 \underline{v}' \Sigma_s(\underline{v}' \rightarrow \underline{v}) f(\underline{r}, \underline{v}', t) + S(\underline{r}, \underline{v}, t) \quad (\text{II-1})$$

Here $f(\underline{r}, \underline{v}, t)$ is the neutron distribution function of space \underline{r} , velocity \underline{v} , and time t ; $S(\underline{r}, \underline{v}, t)$ is the source distribution; $\Sigma_t(v)$ is the macroscopic total cross-section; and $\Sigma_s(\underline{v}' \rightarrow \underline{v})$ is the differential scattering cross-section ("scattering kernel") for scattering from velocity \underline{v}' in $d^3 \underline{v}'$ to \underline{v} in $d^3 \underline{v}$.

This equation merely expresses a neutron balance condition, i. e. that the substantial derivative, $D/Dt = \partial/\partial t + \underline{v} \cdot \text{grad}$, of $f(\underline{r}, \underline{v}, t)$ is equal to the change in $f(\underline{r}, \underline{v}, t)$ due to collisions and source neutrons. In general $\Sigma_t(v)$ and $\Sigma_s(\underline{v}' \rightarrow \underline{v})$ are given functions which must be determined from either quantum-mechanical calculations or experimental investigations of neutron-nuclei scattering.

To study the propagation of neutron waves, one examines the neutron distribution resulting from a modulated source with time behavior $e^{i\omega t}$ which is applied at a boundary of the system. In practice, this oscillating source is superimposed upon a static source, thus avoiding the conceptual difficulties of negative fluxes. Of primary interest will be the "steady-state" or long-time response of the neutron distribution to the oscillating component of the source after

all time transients have decayed away. Hence we shall only concern ourselves with solutions to (II-1) which have a time behavior of $e^{i\omega t}$.

Since it will usually be possible to choose a coordinate system along a wave vector \underline{k} when discussing plane wave solutions (II-1) of the form $\varphi(\underline{v})e^{-\underline{k} \cdot \underline{r} + i\omega t}$, it suffices to consider one-dimensional geometries such that (II-1) becomes

$$\begin{aligned} \frac{\partial f}{\partial t} + \mu v \frac{\partial f}{\partial x} + v \Sigma_t(v) f(x, \mu, v, t) \\ = \int_{-1}^{+1} d\mu' \int_0^{\infty} dv' v' \Sigma_s(v' \rightarrow v, \mu' \rightarrow \mu) f(x, \mu', v', t) + S(x, \mu, v) e^{i\omega t} \end{aligned} \quad (\text{II-2})$$

Here, of course, $v \equiv |\underline{v}|$ and $\mu \equiv \underline{v} \cdot \underline{k} / |\underline{v}| |\underline{k}|$ and the oscillating character of the source has been explicitly indicated.

The general theory of the propagation of wave-like disturbances in a neutron distribution will now be developed by considering the steady-state solutions to equation (II-2) subject to suitable boundary conditions. The only essential assumption is that the medium be non-multiplying, homogeneous (isotropic), and of time-independent composition.

From time to time more specific results will be obtained for more restrictive models. The additional assumptions to be made will usually involve approximating the form of the scattering kernel, e.g. by assuming isotropic scattering, degenerate kernels, etc. These assumptions will be made only when necessary, and unless otherwise

indicated, the theory developed in this first part of the thesis will be based on the model represented by equation (II-2) where $\Sigma_t(v)$ and $\Sigma_s(v' \rightarrow v, \mu' \rightarrow \mu)$ are regarded as essentially arbitrary functions.

II. A SPECTRAL ANALYSIS OF THE BOLTZMANN WAVE OPERATOR

A. INTRODUCTION

1. Reduction to an Eigenvalue Problem

Our primary goal, at least from a mathematical standpoint, is to obtain the steady-state solutions to equation (II-2) for various boundary and source conditions. A very powerful technique for obtaining these solutions involves the use of separation of variables to reduce equation (II-2) to an eigenvalue problem. To be more specific, consider solutions to the homogeneous Boltzmann equation

$$\begin{aligned} \frac{\partial f}{\partial t} + \mu v \frac{\partial f}{\partial x} + v \Sigma_t(v) f(x, \mu, v, t) \\ = \int_{-1}^{+1} d\mu' \int_0^{\infty} dv' v' \Sigma_s(v' \rightarrow v, \mu' \rightarrow \mu) f(x, \mu', v', t) \end{aligned} \quad (\text{II-3})$$

Guided by the harmonic time dependence of the source and the invariance under spatial translation of this homogeneous integro-differential equation, one seeks elementary solutions to (II-3) in the form of plane waves

$$f(x, \mu, v, t) = F(\kappa; \mu, v) e^{-\kappa x + i\omega t} \quad (\text{II-4})$$

where κ is an arbitrary complex constant, $F(\kappa; \mu, v)$ is an as yet undetermined function of (μ, v) , and ω is real and fixed at the source frequency.

Substituting this form of a solution into equation (II-3) yields

a restriction on κ and $F(\kappa; \mu, \nu)$

$$\begin{aligned} & [i\omega + \nu \Sigma_t(\nu) - \kappa \mu \nu] F(\kappa; \mu, \nu) \\ &= \int_{-1}^{+1} d\mu' \int_0^\infty d\nu' \nu' \Sigma_s(\nu' \rightarrow \nu, \mu' \rightarrow \mu) F(\kappa; \mu', \nu') \end{aligned} \quad (\text{II-5})$$

But recognize that this two-dimensional integral equation is just an eigenvalue problem for the eigenvalues κ and the corresponding eigenfunctions $F(\kappa; \mu, \nu)$.

It is convenient to transform (II-4) into a slightly different form by defining

$$\psi_\kappa(\mu, \nu) = \sqrt{\frac{\mu \nu}{M(\nu)}} F(\kappa; \mu, \nu)$$

$$\tilde{\Sigma}_s(\nu' \rightarrow \nu, \mu' \rightarrow \mu) = \sqrt{\frac{\nu' M(\nu')}{\nu M(\nu)}} \Sigma_s(\nu' \rightarrow \nu, \mu' \rightarrow \mu)$$

where $M(\nu)$ is the Maxwellian distribution. Then (II-5) becomes

$$\begin{aligned} & \left[\frac{i\omega}{\mu \nu} + \frac{\Sigma_t(\nu)}{\mu} \right] \psi_\kappa(\mu, \nu) \\ & - \int_{-1}^{+1} d\mu' \int_0^\infty d\nu' \frac{\tilde{\Sigma}_s(\nu' \rightarrow \nu, \mu' \rightarrow \mu)}{\sqrt{\mu' \mu}} \psi_\kappa(\mu', \nu') = \kappa \psi_\kappa(\mu, \nu) \end{aligned} \quad (\text{II-6})$$

One can use detailed balance⁽²⁶⁾

$$\nu' M(\nu') \Sigma_s(\nu' \rightarrow \nu, \mu' \rightarrow \mu) = \nu M(\nu) \Sigma_s(\nu \rightarrow \nu', -\mu \rightarrow -\mu')$$

and parity invariance to show that the kernel in (II-6) is now symmetric. Notice that we have also written (II-6) in the more standard

form of an eigenvalue problem

$$A\psi_K = \kappa\psi_K \quad (\text{II-6}')$$

where

$$A \equiv \underbrace{\left[\frac{i\omega}{\mu v} + \frac{\Sigma_t(v)}{\mu} \right]}_{A_1 \text{ Streaming Operator}} + \underbrace{\left[- \int_{-1}^{+1} d\mu' \int_0^\infty dv' \frac{\tilde{\Sigma}_s(v' \rightarrow v, \mu' \rightarrow \mu)}{\sqrt{\mu'\mu}} \right]}_{A_2 \text{ Scattering Operator}} \quad \text{Boltzmann Wave Operator} \quad (\text{II-7})$$

and $\psi_K(\mu, v)$ is the eigenfunction corresponding to the eigenvalue κ .

In principle then, if (II-6) could be solved for the eigenvalues and eigenfunctions of A , and it could then be demonstrated that these eigenfunctions formed a complete orthogonal set, one would have available an extremely powerful tool for treating problems involving not only infinite sourceless media, but also finite media and media containing distributed sources. To treat these latter problems one would merely expand their general solution in the eigenfunctions of A , and then use boundary conditions to evaluate the expansion coefficients. Thus in some sense, we have succeeded in reducing the problem of neutron wave propagation to a study of the eigenvalue spectrum of the Boltzmann wave operator A .

Now unfortunately (II-6) is more complicated than the standard eigenvalue problems of mathematical physics. The operator A is

- i) not completely continuous
- ii) unbounded

iii) non-self-adjoint.

A rigorous analysis of the spectrum of A is therefore quite difficult and involves rather deep mathematical concepts. A sketch of this analysis has been placed in Appendix B. The principal results will be presented and discussed in the remainder of this chapter.

2. Some Preliminary Concepts

First it is useful to summarize briefly some concepts from functional analysis^(27,28). We shall consider our operators defined on a Hilbert space \mathfrak{L}_2 (that is, a complete linear space whose metric is derived from a scalar product). To be more precise, define the sets

$$I_\mu \equiv \{ \mu : \mu \in [-1, +1] \}, \quad I_\nu \equiv \{ \nu : \nu \in [0, \infty) \}, \quad G \equiv I_\mu \otimes I_\nu$$

Now let $\mathfrak{L}_2(G)$ be the Hilbert space of complex-valued, square-integrable functions defined over G . The inner product will be chosen as

$$(f, g) \equiv \int_{-1}^{+1} d\mu \int_0^\infty d\nu \overline{f(\mu, \nu)} g(\mu, \nu) \quad (\text{II-8})$$

The vector norm is then

$$\|f\| = (f, f)^{1/2} \quad (\text{II-9})$$

while the operator norm is

$$\|A\| \equiv \left\{ \sup_{\varphi \in \mathfrak{L}_2(G)} \frac{\|A\varphi\|}{\|\varphi\|} \right\} \quad (\text{II-10})$$

Now to every operator A we can associate an eigenvalue spectrum $\sigma(A)$ by considering the problem

$$(A - \kappa)f = g \quad (\text{II-11})$$

We shall say that the inverse of $(A - \kappa)$ exists if for any $g \in R(A - \kappa)$, there exists a unique f such that (II-11) is satisfied. [Here $R(A - \kappa)$ denotes the range of $(A - \kappa)$.]

We define the resolvent set $\rho(A)$ of A as the set of all values of κ for which the inverse of $(A - \kappa)$ exists and is a bounded operator, while $R(A - \kappa) \equiv \mathfrak{L}_2(G)$. [A bounded operator A is one for which for any $\varphi \in \mathfrak{L}_2(G)$, there exists a $c < \infty$ such that $\|A\varphi\| < c\|\varphi\|$.] The complement of this open set $\rho(A)$ is defined to be the spectrum $\sigma(A)$ of A . That is, the spectrum of the operator A is the set of all κ such that $(A - \kappa)$ fails to have a bounded inverse. This spectrum can be decomposed into three disjoint sets:

- $\sigma_p(A)$: If the inverse of $(A - \kappa)$ does not exist, then κ is said to be in the point spectrum $\sigma_p(A)$.
- $\sigma_r(A)$: If the inverse of $(A - \kappa)$ exists, but $R(A - \kappa)$ is a proper subset of $\mathfrak{L}_2(G)$, then κ is said to be in the residual spectrum $\sigma_r(A)$.
- $\sigma_c(A)$: If the inverse of $(A - \kappa)$ exists, $R(A - \kappa) \equiv \mathfrak{L}_2(G)$, but the inverse of $(A - \kappa)$ is an unbounded operator, then κ is said to be in the continuous spectrum $\sigma_c(A)$.

Notice that

$$\sigma(A) = \sigma_p(A) \cup \sigma_c(A) \cup \sigma_r(A)$$

With this background, we shall now proceed to study the eigenvalue spectrum $\sigma(A)$ of A . It is convenient to study the cases of noncrystalline and polycrystalline moderators separately because of the significant differences in the form of A for each case.

B. NONCRYSTALLINE MEDIA

1. Introduction

For noncrystalline media, the total cross-section $\Sigma_t(v)$ is a continuous, monotonically decreasing function of v . For low v , $\Sigma_t(v) \sim a/v$, diverging as $v \rightarrow 0$. For high v , $\Sigma_t(v)$ approaches a constant, Σ_M .

The behavior of the scattering kernel $\Sigma_s(v' \rightarrow v, \mu' \rightarrow \mu)$ for high (v, v') coincides with that of a rigid sphere monatomic gas. For intermediate and low (v, v') this behavior is much more sensitive to the detailed mechanism of molecular binding. However several general statements can be made concerning the symmetrized scattering operator

$$\tilde{\mathfrak{S}} \equiv \int_{-1}^{+1} d\mu' \int_0^{\infty} dv' \tilde{\Sigma}_s(v' \rightarrow v, \mu' \rightarrow \mu) .$$

- i) monatomic gas: Detailed calculations by Dorfman⁽²⁹⁾ have demonstrated that while $\tilde{\Sigma}_s(v' \rightarrow v, \mu' \rightarrow \mu)$ is not square-integrable, its third iterate is square-integrable. This is sufficient to imply that $\tilde{\mathfrak{S}}$ is a completely continuous operator.

- ii) solids in the incoherent approximation¹: Kuscer and Corngold⁽³⁰⁾

¹Solid media for which coherent scattering can be neglected.

have shown that the angle-integrated scattering kernel $\tilde{\Sigma}_s(v',v)$ is square-integrable for low and intermediate (v,v') . Since it must reduce to the monatomic gas kernel at high (v,v') , they conclude that $\tilde{\mathfrak{S}}$ is completely continuous in this case.

iii) liquids: These authors⁽³⁰⁾ have found that the kernel for liquids also possesses a divergence at low (v,v') . However it is conjectured that an iterate of the kernel is square-integrable, thus insuring complete continuity of $\tilde{\mathfrak{S}}$.

Hence we shall characterize the noncrystalline moderators by a smooth, monotonically decreasing $\Sigma_t(v)$ and a completely continuous scattering operator $\tilde{\mathfrak{S}}$.

2. Classification of the Wave Operator A

We have separated the operator A into a multiplicative operator A_1 and an integral operator A_2

$$A = \left[\frac{i\omega}{\mu v} + \frac{\Sigma_t(v)}{\mu} \right] \cdot + \left[- \int_{-1}^{+1} d\mu' \int_0^{\infty} dv' \frac{\tilde{\Sigma}_s(v' \rightarrow v, \mu' \rightarrow \mu)}{\sqrt{\mu' \mu}} \cdot \right] \equiv A_1 + A_2 \quad (\text{II-7})$$

One can demonstrate the following properties for each of these operators (see Appendix B):

The Streaming Operator: $A_1 \equiv \left[\frac{i\omega}{\mu v} + \frac{\Sigma_t(v)}{\mu} \right]$

It is obvious that A_1 is not self-adjoint $[(f, A_1 g) \neq (A_1 f, g)]$. However A_1 is a normal operator $[A_1^\dagger A_1 = A_1 A_1^\dagger]$. Furthermore A_1 is unbounded since the divergence of $\Sigma_t(v)$ as $v \rightarrow 0$ means that

there exist functions $f(\mu, \nu) \in \mathcal{L}_2(G)$ such that $\|A_1 f\| \not\leq M \|f\|$ for any M .

The Scattering Operator: $A_2 \equiv - \int_{-1}^{+1} d\mu' \int_0^\infty dv' \frac{\tilde{\Sigma}_s(v' \rightarrow \nu, \mu' \rightarrow \mu)}{\sqrt{\mu' \mu}} .$

This operator is obviously symmetric and thus self-adjoint.

It is demonstrated in Appendix B that $\frac{\tilde{\Sigma}_s(v' \rightarrow \nu, \mu' \rightarrow \mu)}{\sqrt{\mu' \mu}}$ is not square-integrable. However there is some reason to hope that an iterate of this kernel is square-integrable provided $\tilde{\Sigma}$ is completely continuous. Thus we shall assume that A_2 is a completely continuous operator.

3. The Spectrum $\sigma(A)$ of A

We can now examine the spectrum of $A = A_1 + A_2$ where A_1 is a normal, unbounded, multiplicative operator and A_2 is a self-adjoint, completely continuous integral operator. This analysis is rather long and is presented in detail in Appendix B. The results of the analysis can be summarized in the following theorem²:

THEOREM I: The Boltzmann wave operator A for noncrystalline media decomposes the spectral κ -plane as follows:

$$\sigma_c(A) = C \text{ where } C \equiv \left\{ \kappa : \kappa = \frac{i\omega}{\mu\nu} + \frac{\Sigma_t(\nu)}{\mu}, \mu \in [-1, +1], \nu \in [0, \infty) \right\}$$

$\sigma_p(A)$: A point set lying in those regions of the first and third quadrants such that $\kappa \notin C$.

²In this theorem and in Theorems II and III it has been convenient to assume that there are no point eigenvalues imbedded in $\sigma_c(A)$ [i.e., (II-14) and (II-30) possess no nontrivial solutions for $\kappa \in C \cup \Gamma$]. This assumption can be relaxed with only slight complication in the analysis⁽³⁷⁾.

$\sigma_r(A)$: An empty set.

$\rho(A)$: All other points of the κ -plane not contained in the spectrum $\sigma(A)$.

Proof: Given in Appendix B.

A sketch of the spectral plane is given in Figure 1. More detailed diagrams of $\sigma_c(A)$ for typical moderators are given on p. 30.

By returning to (II-5), one can give a more detailed expression for the point spectrum $\sigma_p(A)$. Begin by defining an effective emission density

$$f(\kappa; \mu, \nu) \equiv \int_{-1}^{+1} d\mu' \int_0^{\infty} d\nu' \nu' \Sigma_s(\nu' \rightarrow \nu, \mu' \rightarrow \mu) F(\kappa; \mu', \nu') \quad (\text{II-12})$$

so that (II-5) can be rewritten as

$$[i\omega + \nu \Sigma_t(\nu) - \kappa \mu \nu] F(\kappa; \mu, \nu) = f(\kappa; \mu, \nu) \quad (\text{II-13})$$

(which is equivalent to $(A - \kappa)\psi_\kappa = 0$ and thus should yield the discrete eigenvalues). To derive the characteristic equation defining the discrete spectrum, restrict $\kappa \notin C$ and divide through in (II-13) by $[i\omega + \nu \Sigma_t(\nu) - \kappa \mu \nu]$. Then multiply through by $\nu' \Sigma_s(\nu' \rightarrow \nu, \mu' \rightarrow \mu)$, integrate over μ' and ν' , and use (II-12) to obtain

$$f(\kappa; \mu, \nu) = \int_{-1}^{+1} d\mu' \int_0^{\infty} d\nu' \left\{ \frac{\nu' \Sigma_s(\nu' \rightarrow \nu, \mu' \rightarrow \mu)}{[i\omega + \nu \Sigma_t(\nu) - \kappa \mu' \nu']} \right\} f(\kappa; \mu', \nu') \quad \kappa \notin C \quad (\text{II-14})$$

This integral equation represents an associated eigenvalue problem determining the discrete eigenvalues $\kappa_j \in \sigma_p(A)$ and the "associated

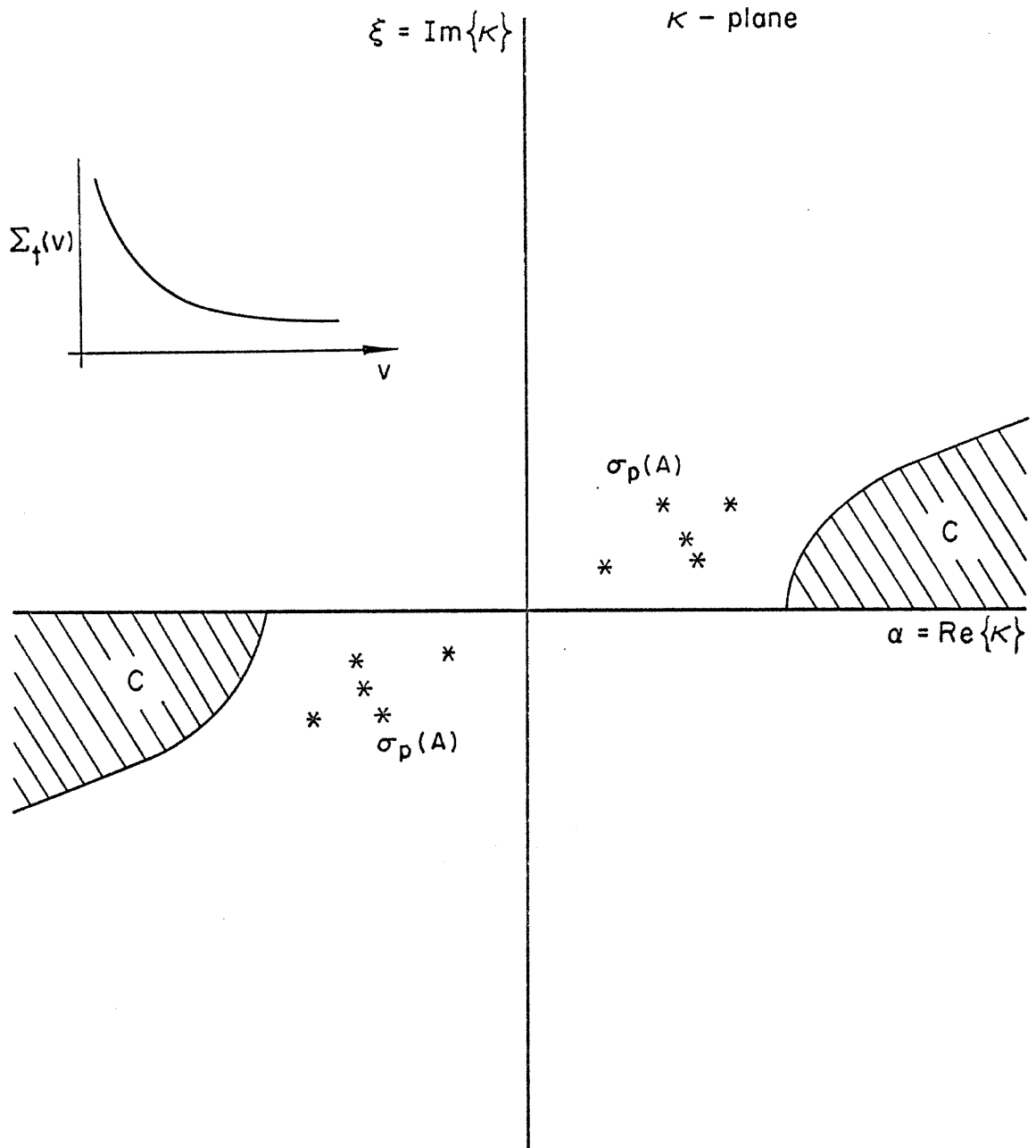


Figure 1. A Sketch of the Spectral κ -Plane for Noncrystalline Media

eigenfunctions" $f(k; \mu, \nu)$. In future discussions, equations such as (II-14) which define the point spectrum will be referred to as the "dispersion law" or "dispersion relation" for the system of interest.

It will be convenient to rederive the dispersion law under the assumption of isotropic scattering in the Lab system, i.e.

$\Sigma_s(\nu' \rightarrow \nu, \mu' \rightarrow \mu) = \frac{1}{2} \Sigma_s(\nu', \nu)$. Then if one defines

$$N(k; \nu) \equiv \int_{-1}^{+1} d\mu F(k; \mu, \nu) ,$$

(II-13) can be rearranged and integrated over μ to obtain

$$N(k; \nu) = \frac{1}{2k\nu} \ln \left[\frac{i\omega + \nu \Sigma_t(\nu) + k\nu}{i\omega + \nu \Sigma_t(\nu) - k\nu} \right] \int_0^\infty d\nu' \nu' \Sigma_s(\nu', \nu) N(k; \nu') \quad (\text{II-15})$$

$k \notin \mathbb{C}$

as the associated eigenvalue problem corresponding to (II-14).

These dispersion laws (II-14) and (II-15) will be discussed in more detail in section (II-E).

4. The Eigenfunctions of A

We shall now derive the form of the eigenfunctions corresponding to $\sigma(A)$.

Discrete Eigenfunctions: $k \notin \mathbb{C}$

These can be found directly from (II-13) as

$$F(k_j; \mu, \nu) = \frac{f(k_j; \mu, \nu)}{i\omega + \nu \Sigma_t(\nu) - k_j \mu \nu} \quad k_j \in \sigma_p(A) \quad (\text{II-16})$$

where the $f(\kappa_j; \mu, \nu)$ and κ_j must be found by solving (II-14). Note that since the kernel of (II-14) is square-integrable for $\kappa \notin C$, $f(\kappa_j; \mu, \nu)$ will certainly be contained⁽²⁸⁾ in $\mathfrak{L}_2(G)$, thus implying $F(\kappa_j; \mu, \nu) \in \mathfrak{L}_2(G)$ as expected. Now it may happen that (II-14) possesses solutions which are in $\mathfrak{L}_2(G)$ even for $\kappa \in C$. Since this means that there exist nontrivial f such that $(A - \kappa)f = 0$ for $\kappa \in C$, these would correspond to point eigenvalues imbedded in the continuous spectrum $\sigma_c(A)$. However such "imbedded" eigenvalues should more properly be regarded as a special subset of the essential spectrum (which contains all limit points of $\sigma(A)$) and will be considered in more detail below.

Continuum Eigenfunctions: $\kappa \in C$

We recognize that the eigenfunctions corresponding to the continuous spectrum will not be contained in $\mathfrak{L}_2(G)$. Thus our Hilbert space must be extended to include more general functions--and, in particular, distributions in the sense of Schwartz⁽²⁸⁾--when discussing the continuum eigenfunctions.

Generalizing the work of Case⁽²⁴⁾ and Bednarz & Mika⁽³¹⁾ suggests the form of the eigenfunctions corresponding to $\kappa \in C$

$$F(\kappa; \mu, \nu) = \frac{f(\kappa; \mu, \nu)}{i\omega + \nu \Sigma_t(\nu) - \kappa \mu \nu} + \lambda(\kappa) \delta [(\mu, \nu) - (\mu, \nu)_\kappa] \quad \kappa \in C \quad \text{(II-17)}$$

where $(\mu, \nu)_\kappa$ denotes the ordered pair such that

$$i\omega + \nu \Sigma_t(\nu) - \kappa \mu \nu = 0$$

is satisfied for a given κ . Here $\lambda(\kappa)$ is, as yet, unspecified.

Notice that one can distinguish two sub-classes of continuous spectra:

- a) $\kappa \in \mathbb{C}$, $\lambda(\kappa) \neq 0$: This case corresponds to what is usually called the continuous spectrum.
- b) $\kappa \in \mathbb{C}$, $\lambda(\kappa) = 0$: These κ must be isolated (by the identity theorem of pseudo-analytic functions), correspond to square-integrable eigenfunctions, and hence are the "imbedded" point eigenvalues referred to earlier. We will show later that $\lambda(\kappa) = 0$ implies the dispersion law (II-14) is satisfied for some $\kappa \in \mathbb{C}$.

Now it is hoped that the spectral representation of the general solution to our original problem, (II-2), can be written as an expansion in these eigenfunctions

$$f(x, \mu, \nu, t) = \sum_{\kappa_j \in \sigma_p(A, \omega)} a_j F(\kappa_j; \mu, \nu) e^{-\kappa_j x + i\omega t} + \iint_{C(\omega)} A(\kappa) F(\kappa; \mu, \nu) e^{-\kappa x + i\omega t} d\kappa \quad (\text{II-18})$$

where the frequency dependence of the eigenvalue spectrum $\sigma(A)$ has been explicitly indicated. However several questions must be answered before one can make use of (II-18). First one must investigate the question of completeness of the eigenfunctions

$\{F(\kappa; \sigma, \nu); \kappa \in \sigma(A)\}$; that is, one must determine for what class of functions an expansion such as (II-18) is possible. Of comparable importance is a prescription for the evaluation of the expansion coefficients a_j and $A(\kappa)$ for given boundary and source conditions. As we shall see in more detail in Chapters III and IV, the questions of completeness and coefficient evaluation are intimately related and are quite different for full- and half-range expansion problems.

C. POLYCRYSTALLINE MEDIA

1. Introduction

The form of the wave operator A is somewhat different for polycrystalline materials such as graphite or beryllium. There are essentially two major variations from noncrystalline media: $\Sigma_t(v)$ is no longer smooth and monotonic in v and indeed can exhibit essentially discontinuous behavior; in addition, the scattering operator $\tilde{\mathcal{S}}$ is no longer completely continuous. Both of these effects are due to the diffraction of the neutron wave function by the ordered crystal lattice.

To be more precise, we note that in general one can write

$$\Sigma_s(v' \rightarrow v, \mu' \rightarrow \mu) = \Sigma_i(v' \rightarrow v, \mu' \rightarrow \mu) + \Sigma_e(v' \rightarrow v, \mu' \rightarrow \mu)$$

where $\Sigma_i(v' \rightarrow v, \mu' \rightarrow \mu)$ is that portion of the kernel due to inelastic scattering. It is reasonable to assume that the operator associated with incoherent inelastic scattering is completely continuous since it is similar to those discussed in our treatment of noncrystalline media. The operator corresponding to coherent inelastic scattering will not be completely continuous. However since we expect this type of scattering to contribute very little to the total scattering cross-section, we shall henceforth ignore coherent inelastic scattering.

Now $\Sigma_e(v' \rightarrow v, \mu' \rightarrow \mu)$ is due to elastic scattering and can be written⁽²⁶⁾ as

$$\begin{aligned}
 \Sigma_e(\mathbf{v}' \rightarrow \mathbf{v}, \mu' \rightarrow \mu) &= \frac{\Sigma_{\text{inc}}}{4\pi} e^{-2w_D} \delta(E' - E) \\
 &\quad \text{incoherent elastic} \\
 &\quad + \frac{\Sigma_{\text{coh}} (2\pi)^3}{4\pi V_0} \sum_{\underline{\tau}} \delta(\underline{\kappa} - \underline{\tau}) e^{-2w_D} \delta(E' - E) \\
 &\quad \quad \quad \text{coherent elastic} \\
 &= \left[\frac{\Sigma_{\text{inc}}}{4\pi} e^{-2w_D} + \frac{\Sigma_{\text{coh}} (2\pi)^3}{4\pi V_0} \sum_{\underline{\tau}} \delta(\underline{\kappa} - \underline{\tau}) e^{2w_D} \right] \delta(E' - E)
 \end{aligned} \tag{II-19}$$

where w_D is the Debye-Waller factor, V_0 is the unit cell volume, $\underline{\tau}$ is the reciprocal lattice vector, and $\underline{\kappa}$ is the momentum transfer vector.

We shall rewrite (II-19) as

$$\Sigma_e(\mathbf{v}' \rightarrow \mathbf{v}, \mu' \rightarrow \mu) = \Sigma_e(\mathbf{v}) P(\mu' \rightarrow \mu) \delta(\mathbf{v}' - \mathbf{v}) \tag{II-20}$$

It is obvious that $\Sigma_e(\mathbf{v}' \rightarrow \mathbf{v}, \mu' \rightarrow \mu)$ is not square-integrable due to the $\delta(\mathbf{v}' - \mathbf{v})$ term. [By definition, elastic scattering from a solid implies essentially no energy change because the mass of the polycrystal is many orders of magnitude larger than that of the neutron.]

In fact if one considers the elastic coherent scattering in detail, even the angular scattering probability $P(\mu' \rightarrow \mu)$ will contain delta functions in angle and thus will not be square-integrable in μ . However to allow further analysis, we shall be forced to treat elastic coherent scattering in an approximate fashion by assuming that $P(\mu' \rightarrow \mu) \in \mathcal{L}_2(I_\mu)$. Hopefully this approximation will not invalidate the qualitative results obtained in the following analysis⁽²²⁾.

2. Classification of the Wave Operator A

Using (II-20), we can write the symmetrized wave operator for polycrystalline media as

$$\begin{aligned}
 A = & \underbrace{\left[\frac{i\omega}{\mu v} + \frac{\Sigma_t(v)}{\mu} \right]}_{A_1} + \underbrace{\left[- \int_{-1}^{+1} d\mu' \int_0^\infty dv' \frac{\tilde{\Sigma}_1(v' \rightarrow v, \mu' \rightarrow \mu)}{\sqrt{\mu' \mu}} \right]}_{A_2} \\
 & + \underbrace{\left[- \Sigma_e(v) \int_{-1}^{+1} d\mu' \frac{\tilde{P}(\mu' \rightarrow \mu)}{\sqrt{\mu' \mu}} \right]}_{A_3} \quad \text{(II-21)}
 \end{aligned}$$

Now as before, A_1 is an unbounded, non-self-adjoint, but normal operator. A_2 is again self-adjoint and completely continuous. We have only to consider A_3 .

The Elastic Scattering Operator: $A_3 \equiv -\Sigma_e(v) \int_{-1}^{+1} d\mu' \frac{\tilde{P}(\mu' \rightarrow \mu)}{\sqrt{\mu' \mu}}$.

Now A_3 is certainly bounded and self-adjoint. It is not completely continuous however because of the $\delta(v' - v)$ term which yields a multiplicative operator in v .

3. The Spectrum $\sigma(A)$ of A

Now we examine the spectrum of $A = A_1 + A_2 + A_3$. The details are given once again in Appendix B, and the resulting spectral theorem is:

THEOREM II: The Boltzmann wave operator A for polycrystalline media decomposes the spectral κ -plane as follows:

$$\sigma_c(A) = C \cup \Gamma \text{ where } C \equiv \left\{ \kappa : \kappa = \frac{i\omega}{\mu\nu} + \frac{\Sigma_t(\nu)}{\mu}, \mu \in [-1, +1], \nu \in [0, \infty) \right\}$$

and Γ is the set of all κ such that

$$h(\kappa; \mu) = \nu \Sigma_e(\nu) \int_{-1}^{+1} d\mu' \left[\frac{P(\mu' \rightarrow \mu)}{i\omega + \nu \Sigma_t(\nu) - \kappa \mu' \nu} \right] h(\kappa; \mu') \quad \nu \in [0, \infty) \quad (\text{II-22})$$

possesses non-trivial solutions $h(\kappa; \mu)$.

- $\sigma_p(A)$: A point set lying in those regions of the first and third quadrants such that $\kappa \notin C \cup \Gamma$.
- $\sigma_r(A)$: An empty set.
- $\rho(A)$: All other points of the κ -plane not contained in the spectrum $\sigma(A)$.

Proof: See Appendix B.

A sketch of the spectral plane for polycrystalline media is given in Figure 2. A few comments concerning such diagrams are necessary. It has been assumed throughout this chapter that the frequency ω was real and fixed. However when one actually performs a wave experiment, the source frequency ω is varied as an independent experimental parameter, and the subsequent behavior of the eigenvalues is observed. It is important to recognize that both the point spectrum $\sigma_p(A)$ and the continuous spectrum $\sigma_c(A)$ are dependent upon ω . Thus as one varies ω , $\sigma(A)$ changes position in the κ -plane.

Whenever the eigenvalue spectrum is sketched in the κ -plane, $\sigma_c(A)$ will usually be depicted for a given fixed frequency. However

it will be useful on occasion to study the spectrum for all ω . Then it will be convenient to plot the spectrum using frequency-dependent coordinates. An inverted spectral diagram will then be used such that one plots

$$v_{\text{ph}} = \frac{\omega}{\xi} = \frac{\omega}{\text{Im}\{\kappa\}} \quad \text{vs.} \quad L \equiv \frac{1}{\alpha} = \frac{1}{\text{Re}\{\kappa\}}$$

Notice that v_{ph} can be interpreted as the phase velocity of the corresponding plane wave mode, while L is its corresponding attenuation length.

The following diagrams depict C for various materials, both in the first quadrant of the κ -plane and on the inverted diagram.

Theorem II indicates that the operator A_3 adds a new region Γ to the continuous spectrum $\sigma_c(A)$. To demonstrate that this set is given by the equation (II-22), one studies the eigenvalue problem

$$[A_1 + A_3]\varphi_\kappa(\mu, \nu) = \kappa\varphi_\kappa(\mu, \nu)$$

or equivalently

$$[i\omega + \nu\Sigma_t(\nu) - \kappa\nu]H(\kappa; \mu, \nu) = \nu\Sigma_e(\nu) \int_{-1}^{+1} d\mu' P(\mu' \rightarrow \mu) H(\kappa; \mu', \nu) \quad (\text{II-23})$$

since it is shown in Appendix B that $\sigma_c(A) = \sigma_c(A_1 + A_3)$. Note that ν appears in (II-23) only as a parameter. Thus (II-23) may be regarded as an effective one-velocity problem for each value of $\nu \in [0, \infty)$. If

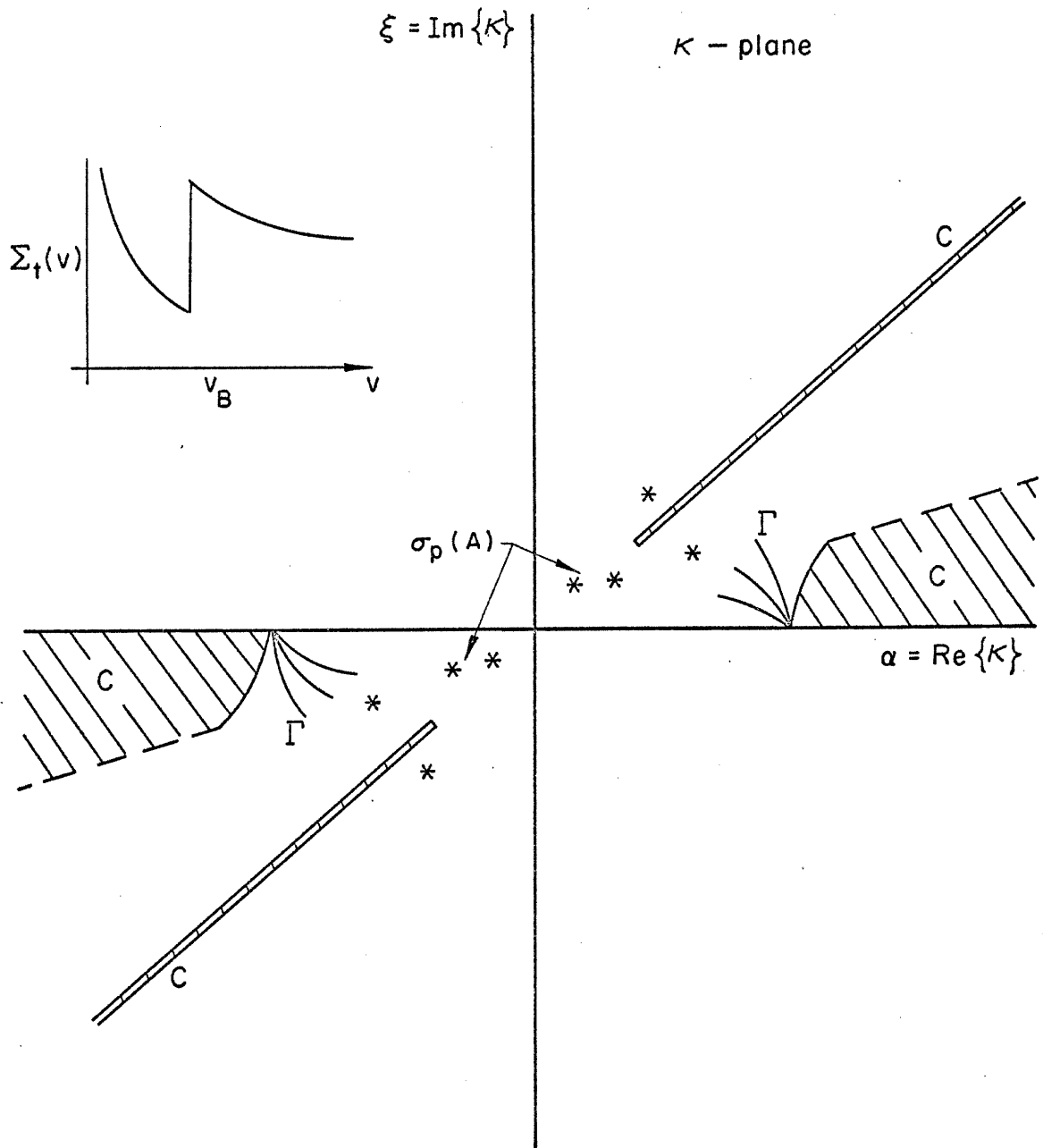


Figure 2. A Sketch of the Spectral κ -Plane for Polycrystalline Media

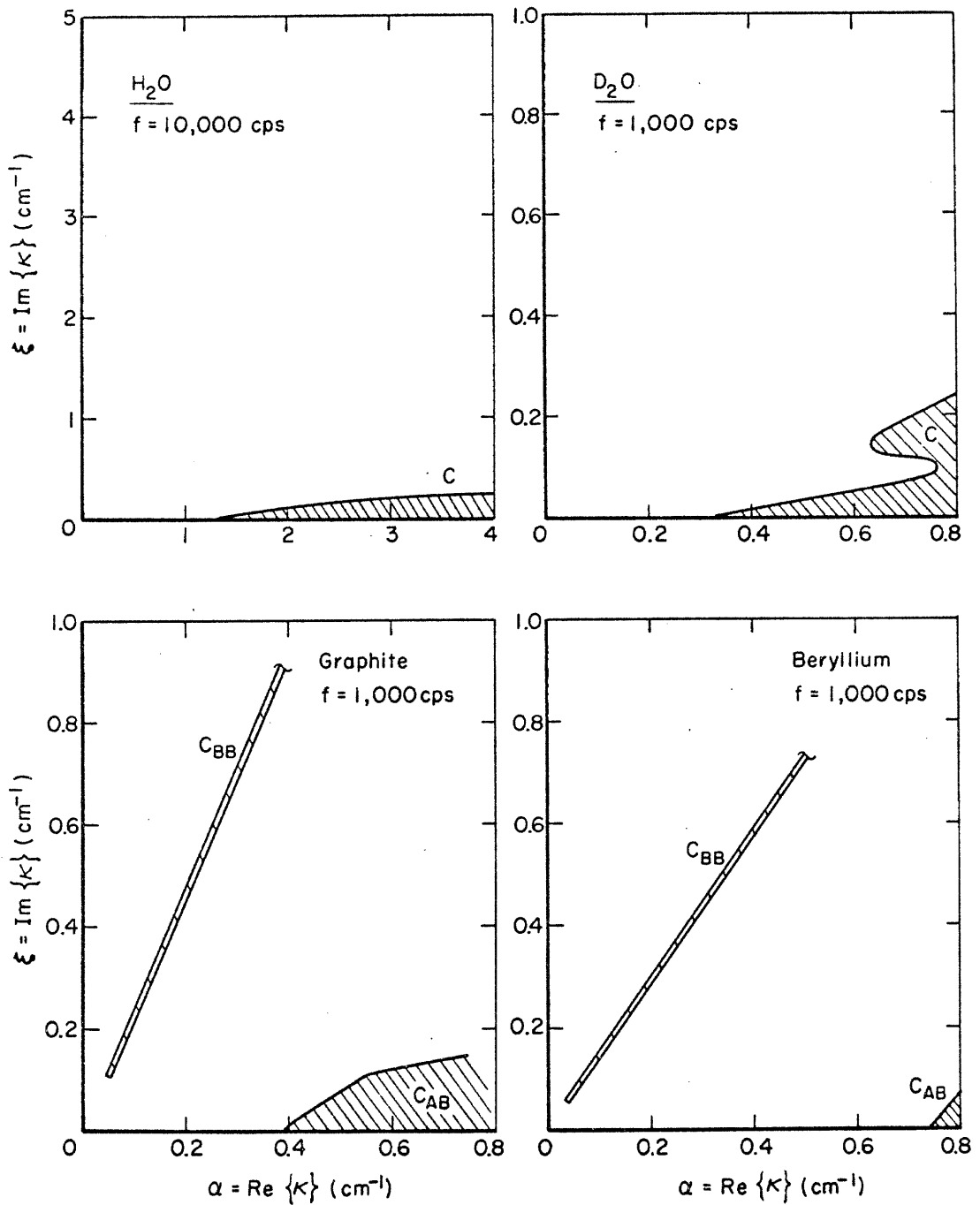


Figure 3. Plots of C for Typical Moderators

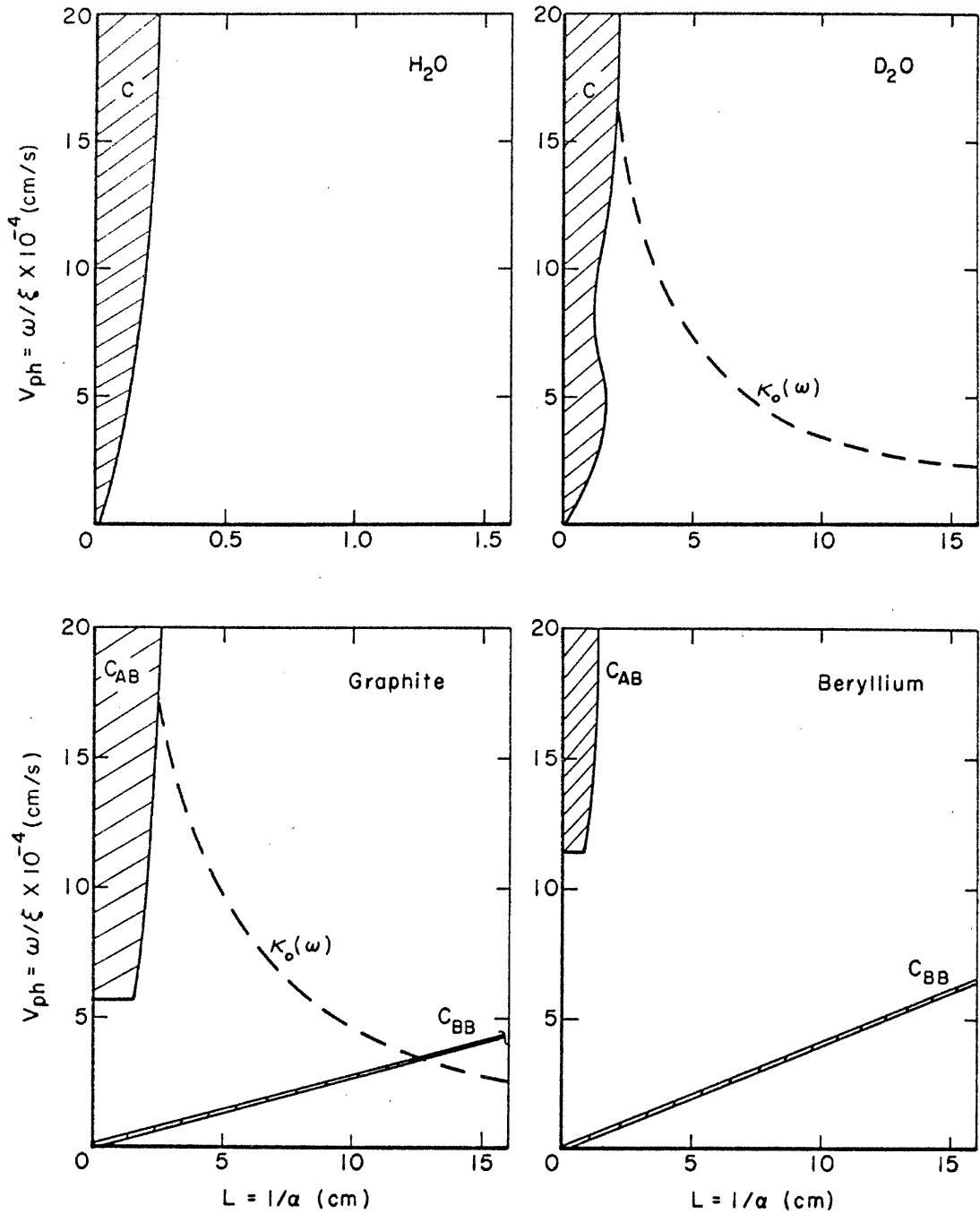
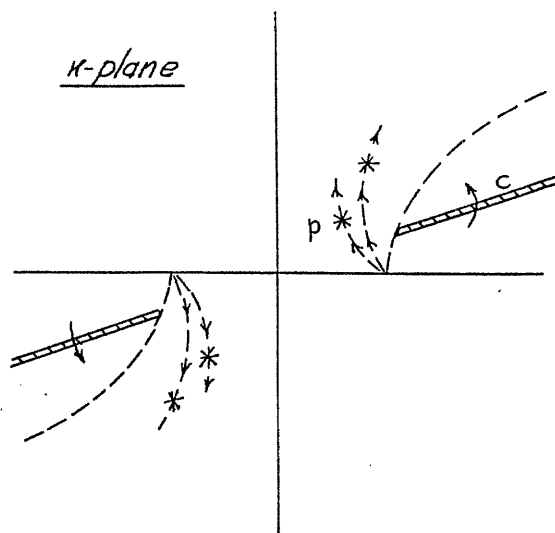


Figure 4. The Inverted Spectral Plane for Typical Moderators

one analyzes the eigenvalue spectrum of (II-23) treating v as fixed, then $\sigma_c(A_1 + A_3)$ can be generated by letting v vary between 0 and ∞ .

Since $P(\mu' \rightarrow \mu)$ is assumed to be $\mathcal{L}_2(I_\mu)$, equation (II-23) will have both a point spectrum p , as well as a continuous spectrum given by $c \equiv \left\{ k = \frac{i\omega}{\mu v} + \frac{\Sigma_t(v)}{\mu}, \mu \in [-1, +1] \right\}$ for each value of $v \in [0, \infty)$. To generate the total continuous spectrum of $A_1 + A_3$, one lets v vary, sweeping out not only the previous

continuum C , but in addition a sequence of curves Γ from the point spectrum of (II-23) for fixed v . In the usual manner one can derive the characteristic relation for the "discrete eigenvalues" of (II-23) by restricting $k \notin c$, dividing through by $[i\omega + v\Sigma_t(v) - k\mu v]$, multiplying by $P(\mu' \rightarrow \mu)$, and inte-



grating over μ to find that Γ is the set of all k such that (II-22) is satisfied. Of course this is just the dispersion relation for an effective one-velocity problem, allowing for anisotropic scattering. In general one expects that (II-23) will have an infinite point spectrum p (see Mika⁽³²⁾) resulting in an infinite number of curves in Γ . One also expects that p will possess a limit point contained in c , giving rise to the conjecture that the curves in Γ tend to merge into an area as they approach C .

To determine the effects of the elastic scattering on the point spectrum, we can derive the dispersion law for polycrystalline media. Equation (II-13) now becomes

$$[i\omega + v\Sigma_t(v) - \kappa\mu v] F(\kappa; \mu, v) = \bar{f}_i(\kappa; \mu, v) + v\Sigma_e(v) \bar{f}_e(\kappa; \mu, v) \quad (\text{II-24})$$

$$\text{where } \bar{f}_i(\kappa; \mu, v) \equiv \int_{-1}^{+1} d\mu' \int_0^\infty dv' v' \Sigma_i(v' \rightarrow v, \mu' \rightarrow \mu) F(\kappa; \mu', v')$$

$$\bar{f}_e(\kappa; \mu, v) \equiv \int_{-1}^{+1} d\mu' P(\mu' \rightarrow \mu) F(\kappa; \mu', v) \quad (\text{II-25})$$

As before, divide through by $[i\omega + v\Sigma_t(v) - \kappa\mu v]$, multiply by $v'\Sigma_i(v' \rightarrow v, \mu' \rightarrow \mu)$ and integrate over μ and v to find, using (II-25),

$$\begin{aligned} \bar{f}_i(\kappa; \mu, v) &= \int_{-1}^{+1} d\mu' \int_0^\infty dv' \left\{ \frac{v'\Sigma_i(v' \rightarrow v, \mu' \rightarrow \mu)}{[i\omega + v'\Sigma_t(v') - \kappa\mu'v']} \right\} \bar{f}_i(\kappa; \mu', v') \\ &+ \int_{-1}^{+1} d\mu' \int_0^\infty dv' \left\{ \frac{v'\Sigma_i(v' \rightarrow v, \mu' \rightarrow \mu) v'\Sigma_e(v')}{[i\omega + v'\Sigma_t(v') - \kappa\mu'v']} \right\} \bar{f}_e(\kappa; \mu', v') \end{aligned}$$

$$\kappa \notin C \quad (\text{II-26})$$

To obtain a second relation between $\bar{f}_i(\kappa; \mu', v)$ and $\bar{f}_e(\kappa; \mu, v)$, divide (II-24) again by $[i\omega + v\Sigma_t(v) - \kappa\mu v]$, multiply by $P(\mu' \rightarrow \mu)$, and integrate over μ , using (II-25) to obtain

$$\begin{aligned} \bar{f}_e(\kappa; \mu, v) &= \int_{-1}^{+1} d\mu' \left\{ \frac{P(\mu' \rightarrow \mu)}{[i\omega + v\Sigma_t(v) - \kappa\mu'v]} \right\} \bar{f}_i(\kappa; \mu', v) \\ &+ v\Sigma_e(v) \int_{-1}^{+1} d\mu' \left\{ \frac{P(\mu' \rightarrow \mu)}{[i\omega + v\Sigma_t(v) - \kappa\mu'v]} \right\} \bar{f}_e(\kappa; \mu', v) \quad \kappa \notin C \end{aligned}$$

$$(\text{II-27})$$

Now (II-27) and (II-26) represent a rather complicated pair of coupled integral equations for $f_i(k; \mu, v)$ and $f_e(k; \mu, v)$. Together they define the new dispersion law for the discrete eigenvalues. To simplify further, note that for $k \notin \Gamma$ we can formally invert (II-27) as

$$f_e(k; \mu, v) = \mathfrak{L}_e^{-1} \left\{ \int_{-1}^{+1} d\mu' \left[\frac{P(\mu' \rightarrow \mu)}{[i\omega + v \Sigma_t(v) - k\mu'v]} \right] f_i(k; \mu', v) \right\} \quad (\text{II-28})$$

where we define

$$\mathfrak{L}_e \{ \varphi(\mu, v) \} \equiv \varphi(\mu, v) - v \Sigma_e(v) \int_{-1}^{+1} d\mu' \left[\frac{P(\mu' \rightarrow \mu)}{[i\omega + v \Sigma(v) - k\mu'v]} \right] \varphi(\mu', v) \quad (\text{II-29})$$

Now substitute (II-28) into (II-26), and use the fact that

$$\begin{aligned} & \mathfrak{L}_e \left\{ f_i(k; \mu, v) + v \Sigma_e(v) \mathfrak{L}_e^{-1} \left[\int_{-1}^{+1} d\mu' \left[\frac{P(\mu' \rightarrow \mu)}{[i\omega + v \Sigma_t(v) - k\mu'v]} \right] f_i(k; \mu', v) \right] \right\} \\ &= \mathfrak{L}_e \{ f_i(k; \mu, v) \} + [1 - \mathfrak{L}_e] f_i(k; \mu, v) = f_i(k; \mu, v) \end{aligned}$$

to rewrite the final form of the dispersion law for crystalline media as

$$f_i(k; \mu, v) = \int_{-1}^{+1} d\mu' \int_0^\infty dv' \left\{ \frac{v' \Sigma_i(v' \rightarrow v, \mu' \rightarrow \mu)}{[i\omega + v' \Sigma_t(v') - k\mu'v']} \right\} \mathfrak{L}_e^{-1} \{ f_i(k; \mu', v') \} \quad k \notin C \cup \Gamma \quad (\text{II-30})$$

A similar expression can be derived for the case of isotropic scattering, i.e. $\Sigma_i(v' \rightarrow v, \mu' \rightarrow \mu) \equiv \frac{1}{2} \Sigma_i(v', v)$; $P(\mu' \rightarrow \mu) \equiv \frac{1}{2}$. Then

$$f_e(k, \mu, v) = \int_{-1}^{+1} d\mu' F(k; \mu', v) = N(k; v)$$

and

$$\mathcal{L}_e^{-1} \{f_i(k; \mu, v)\} \rightarrow [\Lambda_e(k; v)]^{-1} f_i(k; \mu, v)$$

where we have defined the "elastic dispersion law"

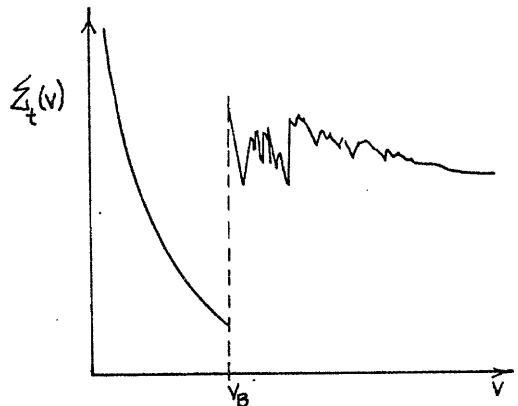
$$\Lambda_e(k; v) = 1 - \frac{v \Sigma_e(v)}{2} \int_{-1}^{+1} \frac{d\mu}{i\omega + v \Sigma_t(v) - k\mu v} \quad (\text{II-31})$$

One can immediately recognize the analogue to (II-15) as

$$N(k; v) = \frac{1}{\Lambda_e(k; v)} \frac{1}{2kv} \ln \left[\frac{i\omega + v \Sigma_t(v) + kv}{i\omega + v \Sigma_t(v) - kv} \right] \int_0^\infty dv' v' \Sigma_i(v', v) N(k; v') \quad (\text{II-32})$$

as the dispersion law for polycrystalline media under the assumption of isotropic scattering. Note that if $\Sigma_e(v) \equiv 0$, then equations (II-30) and (II-32) reduce to (II-14) and (II-15), respectively--the dispersion laws for noncrystalline media.

One other feature of the theory in polycrystalline media might be mentioned at this point. In general, the total cross-section for elastic scattering is actually discontinuous at a certain speed, v_B , corresponding to the fact that neutrons of wavelength ($\lambda \sim 1/v$) greater than the lattice



dimensions can no longer suffer coherent elastic scattering in the crystal. This jump in the cross-section is commonly referred to as the Bragg cutoff, while the velocity v_B will be called the Bragg velocity. Of course there will be similar jumps at shorter wavelengths comparable to multiples of lattice dimensions, but the dominant effect occurs at v_B . Such behavior produces rather interesting consequences as we shall see later.

4. The Eigenfunctions of A

As before, we can derive the form of the eigenfunctions corresponding to $\sigma(A)$:

Discrete Eigenfunctions:

Using equation (II-24) and (II-28), we find that the discrete eigenfunctions can be written as

$$F(\kappa_j; \mu, \nu) = \frac{\mathfrak{L}_e^{-1} \{ \tilde{f}_i(\kappa_j; \mu, \nu) \}}{i\omega + \nu \Sigma_t(\nu) - \kappa_j \mu \nu} \quad \kappa_j \in \sigma_p(A) \quad (\text{II-33})$$

Notice that these are similar to the eigenfunctions for noncrystalline media (II-16) with the exception of the inverted operator \mathfrak{L}_e^{-1} .

Continuum Eigenfunctions:

The usual eigenfunctions corresponding to $\kappa \in C$ become

$$F(\kappa; \mu, \nu) = \frac{\mathfrak{L}_e^{-1} \{ \tilde{f}_i(\kappa; \mu, \nu) \}}{[i\omega + \nu \Sigma_t(\nu) - \kappa \mu \nu]} + \lambda(\kappa) \delta[(\mu, \nu) - (\mu, \nu)_\kappa] \quad \kappa \in C \quad (\text{II-34})$$

where the notation is similar to that in equation (II-17).

However there are also eigenfunctions corresponding to those $\kappa \in \Gamma$.

After some manipulation, one can show that these take the form

$$F(\kappa; \mu, \nu) = \frac{\mathcal{L}_e^{-1}\{f_i(\kappa; \mu, \nu)\}}{[i\omega + \nu \Sigma_t(\nu) - \kappa \mu \nu]} + \frac{\nu \Sigma_e(\nu)}{[i\omega + \nu \Sigma_t(\nu) - \kappa \mu \nu]} \gamma(\kappa) \delta(\nu - \nu_\kappa) \quad \kappa \in \Gamma, \quad (\text{II-35})$$

where for a given $\kappa \in \Gamma$, (II-22) is satisfied for $\nu = \nu_\kappa$.

D. MULTIDIMENSIONAL TRANSPORT EFFECTS

1. Introduction

Thus far the analysis has been restricted to the propagation of plane neutron waves in an infinite medium. However most neutron wave experiments involve the excitation of such waves in parallelepiped geometries. While it is reasonable to treat these geometries as infinite in length (neglecting wave reflections from the far boundary), the effects of finite transverse dimension cannot be so easily ignored.

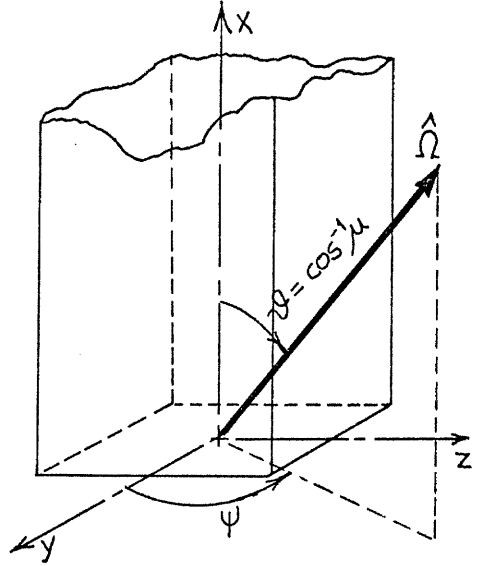
We shall now proceed to indicate the necessary modifications in the analysis of $\sigma(A)$. Choose the indicated coordinate system to rewrite the Boltzmann equation (II-1) as

$$\begin{aligned} \frac{\partial f}{\partial t} + \mu \nu \frac{\partial f}{\partial x} + \nu \sqrt{1 - \mu^2} \left(\cos \psi \frac{\partial f}{\partial y} + \sin \psi \frac{\partial f}{\partial z} \right) + \nu \Sigma_t(\nu) f(\underline{r}, \mu, \psi, \nu, t) \\ = \int_0^\infty dv' \int d\hat{\Omega}' v' \Sigma_s(\nu' \rightarrow \nu, \hat{\Omega} \cdot \hat{\Omega}') f(\underline{r}, \mu', \psi', \nu', t) \end{aligned} \quad (\text{II-36})$$

To treat the spatial dependence in the transverse y-z dimensions, it is convenient to use "asymptotic reactor theory"⁽³³⁾. That is, we assume a plane wave ansatz of the form

$$f(\underline{r}, \mu, \psi, \nu, t) = F(\rho; \mu, \psi, \nu) e^{-\rho x} e^{i(B_y y + B_z z)} e^{i\omega t}$$

where B_y , B_z , and ω are real and fixed, while ρ and $F(\rho; \mu, \psi, \nu)$ are as yet unspecified. Substituting this ansatz into the Boltzmann equation (II-36), we arrive at the eigenvalue problem for ρ , the spatial eigenvalue for finite transverse dimensions,



$$[i\omega + \nu \Sigma_t(\nu) + i\nu \sqrt{1 - \mu^2} (B_y \cos \psi + B_z \sin \psi) - \rho \mu \nu] F(\rho; \mu, \psi, \nu) = \mathfrak{S} F \quad (\text{II-37})$$

Of course for infinite transverse dimensions, $B_y, B_z \rightarrow 0$ and (II-37) reduces to (II-5) [and thus $\rho \rightarrow \kappa$].

2. The Spectrum $\sigma(A_T)$ of A_T

We can identify the Boltzmann wave operator for finite transverse dimensions, A_T , as

$$A_T \equiv \left[\frac{i\omega}{\mu\nu} + \frac{\Sigma_t(\nu)}{\mu} + i \frac{\sqrt{1 - \mu^2}}{\mu} (B_y \cos \psi + B_z \sin \psi) \right] + \left[- \int d\hat{\Omega}' \int_0^\infty dv' \frac{\tilde{\Sigma}_s(\nu' \rightarrow \nu, \hat{\Omega} \cdot \hat{\Omega}')}{\sqrt{\mu'\mu}} \right] \quad (\text{II-38})$$

The analysis of the eigenvalue spectrum of A_T is quite similar to that presented in Appendix B. Only the results of this analysis shall

be presented here:

THEOREM IIIa: The Boltzmann wave operator A_T for noncrystalline media of finite transverse dimension decomposes the spectral ρ -plane as follows:

$$\sigma_c(A_T) = C_T \text{ where } C_T \equiv \left\{ \rho : \rho = \frac{\Sigma_t(v)}{\mu} + i \left[\frac{\omega}{\mu v} + \frac{\sqrt{1-\mu^2}}{\mu} (B_y \cos \psi + B_z \sin \psi) \right], \right. \\ \left. \mu \in [-1, +1], \psi \in [0, 2\pi], v \in [0, \infty) \right\}$$

$\sigma_p(A_T)$: A point set lying in those regions of the first and third quadrants in which $\rho \notin C_T$.

$\sigma_r(A_T)$: An empty set.

$\rho(A_T)$: All other points in the ρ -plane not contained in the spectrum $\sigma(A_T)$.

Proof: Similar to those presented in Appendix B.

THEOREM IIIb: The Boltzmann wave operator A_T for polycrystalline media of finite transverse dimension decomposes the spectral ρ -plane as follows:

$$\sigma_c(A_T) = C_T \cup \Gamma \text{ where } \\ C_T \equiv \left\{ \rho : \rho = \frac{\Sigma_t(v)}{\mu} + i \left[\frac{\omega}{\mu v} + \frac{\sqrt{1-\mu^2}}{\mu} (B_y \cos \psi + B_z \sin \psi) \right], \right. \\ \left. \mu \in [-1, +1], \psi \in [0, 2\pi], v \in [0, \infty) \right\}$$

and Γ_T is the set of all ρ such that

$h(\rho; \mu, \psi)$

$$= v \Sigma_e(v) \int d\hat{\Omega}' \left[\frac{P(\hat{\Omega}' \rightarrow \hat{\Omega})}{[i\omega + v \Sigma_t(v) + iv\sqrt{1-\mu^2}(B_y \cos \psi + B_z \sin \psi) - \rho\mu v]} \right] h(\rho; \mu', \psi')$$

$$\text{all } v \in [0, \infty) \quad (\text{II-39})$$

possesses non-trivial solutions $h(\rho; \mu, v)$.

$\sigma_p(A_T)$: A point set lying in those regions of the first and third quadrants in which $\rho \in C_T \cup \Gamma_T$.

$\sigma_r(A_T)$: An empty set.

$\rho(A_T)$: All other points of the ρ -plane not contained in $\sigma(A_T)$.

Proof: Similar to those presented in Appendix B.

In Figure 5 we have sketched $\sigma_c(A_T)$ for $B_y = B_z \neq 0$. Notice that for polycrystalline media, the sub-Bragg continuum C_{BB} billows out into an area. This expansion of a line continuum into an area continuum occurs even for $\omega = 0$, giving rise to area continua in the static diffusion length problem for systems of finite transverse dimensions.

Now although one can easily derive the associated equations for discrete eigenvalues analogous to (II-14) and (II-30), it is particularly revealing to consider the case of noncrystalline media and isotropic scattering. Then one can show⁽³³⁾ that the associated eigenvalue problem for $\sigma_p(A_T)$ becomes

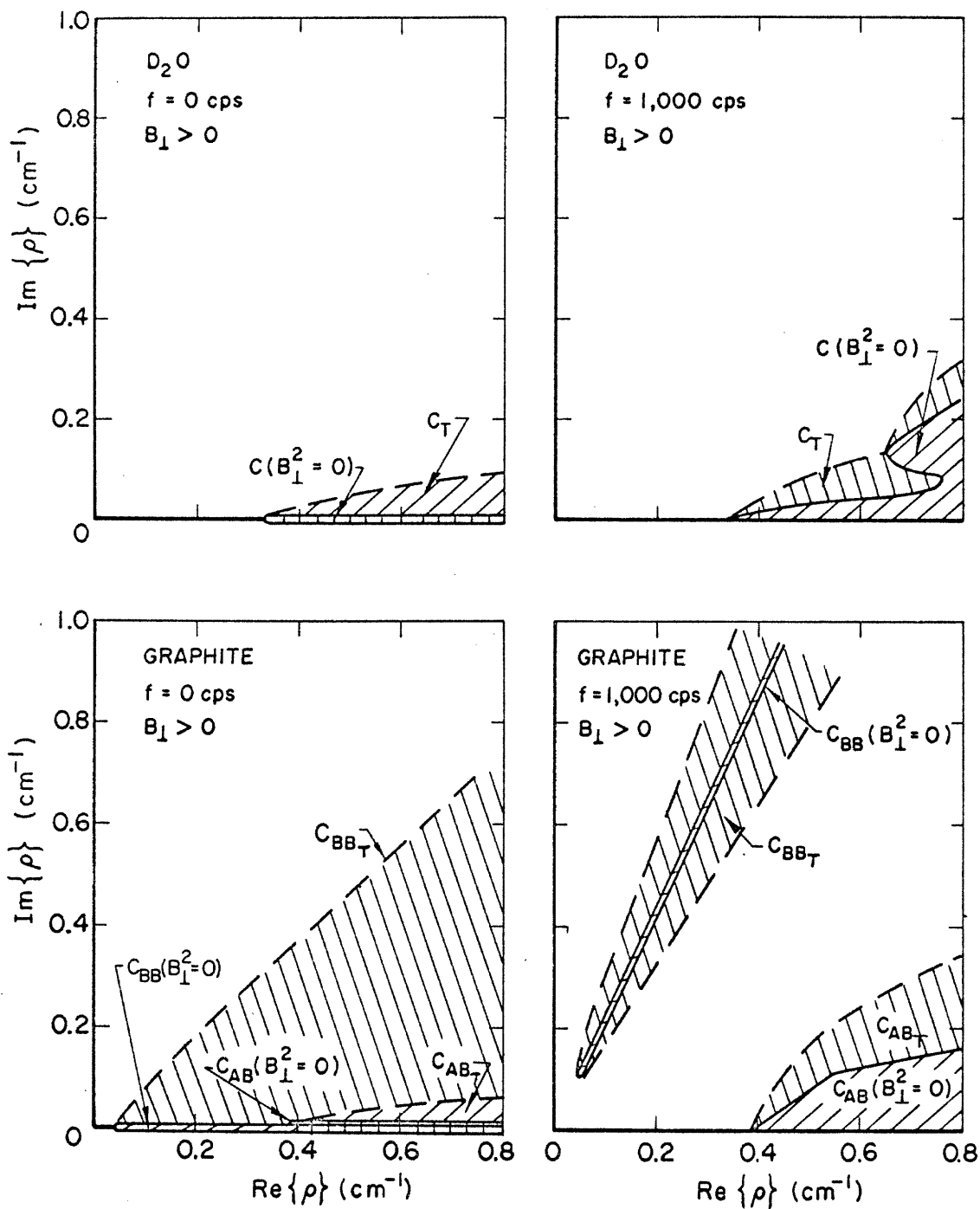


Figure 5. The Spectral ρ -Plane for Systems of Finite Transverse Dimension.

$$N(\rho;v) = \frac{1}{2v\sqrt{\rho^2 - B_{\perp}^2}} \ln \left[\frac{i\omega + v\Sigma_t(v) + v\sqrt{\rho^2 - B_{\perp}^2}}{i\omega + v\Sigma_t(v) - v\sqrt{\rho^2 - B_{\perp}^2}} \right] \int_0^{\infty} dv' v' \Sigma_s(v', v) N(\rho;v')$$

where $B_{\perp}^2 \equiv B_y^2 + B_z^2$, $\rho \notin C_T$ (II-40)

But comparing this equation with the dispersion law (II-14), we recognize that the effect of finite transverse dimension upon $\sigma_p(A)$ is merely to shift the point eigenvalues from κ to $\rho = \sqrt{\kappa^2 + B_{\perp}^2}$. Note that this is what one would have expected from elementary diffusion theory.

Much of the subsequent analysis will be concerned with the theory of one-dimensional neutron wave propagation. However, as we have just shown, to adapt these results to the more realistic situation in which transverse dimensions are finite, one merely modifies $\sigma_c(A)$ and $\sigma_p(A)$ as outlined above. From time to time we shall indicate these modifications as well as their implications for experiment.

E. THE POINT SPECTRUM $\sigma_p(A)$

1. General Discussion

It has been shown that the point eigenvalue spectrum is given by an associated eigenvalue problem³

³Most of the analysis of this and subsequent sections will be given for noncrystalline media. However an effort will be made to indicate extensions and differences arising in the treatment of polycrystalline moderators.

$$f(k; \mu, \nu) = \int_{-1}^{+1} d\mu' \int_0^{\infty} d\nu' \left\{ \frac{\nu' \Sigma_s(\nu' \rightarrow \nu, \mu' \rightarrow \mu)}{[i\omega + \nu' \Sigma_t(\nu') - k\mu'\nu']} \right\} f(k; \mu', \nu')$$

$k \notin C$ (II-14)

As it stands, (II-14) is quite complicated, since it is a two-dimensional Fredholm integral equation as well as an implicit eigenvalue problem [i.e., it cannot be factored into the form $Hf_K = \kappa f_K$]. But perhaps the most severe difficulty concerns the kernel

$$K(\nu', \mu'; \nu, \mu) \equiv \frac{\nu' \Sigma_s(\nu' \rightarrow \nu, \mu' \rightarrow \mu)}{[i\omega + \nu' \Sigma_t(\nu') - k\mu'\nu']} \quad (II-41)$$

It is impossible to symmetrize this kernel into a form such that

$$\tilde{K}(\nu', \mu'; \nu, \mu) = \tilde{K}(\nu, \mu; \nu', \mu')$$

[although one can construct a kernel such that $\tilde{K}(\nu', \mu'; \nu, \mu) = \tilde{K}(\nu, \mu; \nu', \mu')$]. Thus even the associated eigenvalue problem for the discrete eigenvalues is non-self-adjoint. This was expected since the discrete eigenvalues are known to be complex. Unfortunately, the standard methods^(30, 34) used to treat the point spectrum of the infinite medium initial value problem and the static diffusion length experiment are inapplicable to such non-symmetric kernels. Hence alternative techniques are necessary. We shall first direct our attention towards developing necessary conditions for the existence of a point spectrum $\sigma_p(A)$.

2. Theorems Concerning the Existence of Discrete Eigenvalues

Of course the first question which should be answered is whether the point spectrum $\sigma_p(A)$ is ever an empty set, i.e. one must determine when discrete eigenvalues exist. Earlier work⁽³⁵⁾ has shown that when certain limits on B^2 and $\Sigma_a(v)$ are exceeded in the pulsed neutron and diffusion length problems, respectively, discrete eigenvalues cease to exist. We expect that there exist similar bounds on ω , $\Sigma_a(v)$, and B_{\perp}^2 in the wave propagation problem:

THEOREM IV: There exist certain critical bounds on the source frequency ω , the absorption $\Sigma_a(v)$, and the transverse buckling B_{\perp}^2 such that if

$$\omega > \omega^* \quad \text{or} \quad \Sigma_a > \Sigma_a^* \quad \text{or} \quad B_{\perp}^2 > B_{\perp}^{*2},$$

the point eigenvalue spectrum $\sigma_p(A)$ is empty.

Comments: Of course each of these bounds is dependent on the other two parameters, e.g. $\omega^* = \omega^*(\Sigma_a, B_{\perp}^2)$, etc. One can show in fact that increasing any two of the parameters lowers the bound on the third parameter in most cases. This theorem is of particular interest in that it indicates the interrelations between the three independent experimental parameters of the neutron wave experiment: source frequency ω , absorption or "poison" $\Sigma_a(v)$, and transverse dimension B_{\perp}^2 .

Proof: A detailed proof of this theorem is given in Appendix C. However it is enlightening to sketch this proof here. The basic idea is to demonstrate that for sufficiently high ω , $\Sigma_a(v)$, or B_{\perp}^2 , the associated

eigenvalue problem for discrete eigenvalues possesses no nontrivial solutions for $\kappa \in \sigma_c(A)$. Of course such a demonstration must be made for each model considered. By way of illustration, consider the case of noncrystalline, isotropic scattering where $B_{\perp}^2 = 0$. Then the associated eigenvalue problem can be written as

$$\Phi_{\kappa}(v) = \underbrace{\frac{1}{2K} \ln \left[\frac{i\omega + v\Sigma_t(v) + Kv}{i\omega + v\Sigma_t(v) - Kv} \right]}_{g(\kappa, \omega; v)} \underbrace{\int_0^{\infty} dv' \Sigma_s(v', v) \Phi_{\kappa}(v')}_{S_{(v)} \Phi_{\kappa}} \equiv K_{\kappa} \Phi_{\kappa} \quad (\text{II-15})$$

A necessary condition for (II-15) to possess nontrivial solutions is for $\|K_{\kappa}\| \geq 1$ for some κ . The crux of the proof is to show that for sufficiently high ω or $\Sigma_a(v)$, $\|K_{\kappa}\| < 1$ for all $\kappa \notin C$. As ω or $\Sigma_a(v)$ increases, $g(\kappa, \omega; v)$ decreases to zero for all except very high v . That is, only the high v behavior of $g(\kappa, \omega; v)S_{(v)}$ can contribute to creating a norm $\|K_{\kappa}\| \geq 1$. But this means that in an effort to sustain the eigenvalue problem, $N(\kappa, v)$ is pushed to higher v as ω or $\Sigma_a(v)$ is increased. Eventually the velocity spectrum of $N(\kappa, v)$ becomes so heated that the scattering operator assumes essentially a slowing-down (Volterra) form and the eigenvalue problem can no longer be satisfied. That is, one can show that $\lim_{\substack{\omega \\ \text{or } \Sigma_a}} \|K_{\kappa}\| = 0$, verifying the theorem.

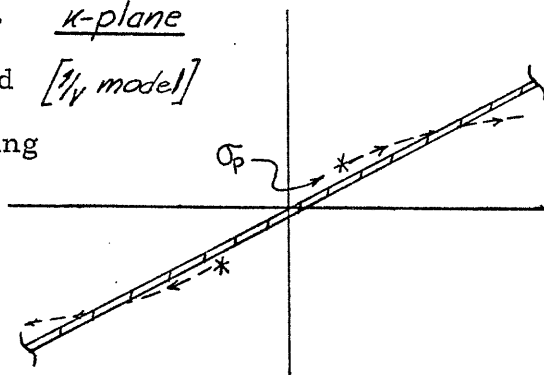
Furthermore it is possible to show that at $\omega = \omega^* [\Sigma_a(v) = \Sigma_a^*(v) \text{ or } B_{\perp}^2 = B_{\perp}^{*2}]$, the lowest discrete eigenvalue κ_0 intersects C [or in the case of polycrystalline media, it intersects the boundary of the area C_{AB}]. Thus we can visualize the last of the discrete eigenvalues disappearing into C when these critical bounds are exceeded.

The solution to wave propagation problems (II-18) will then apparently be composed entirely of continuum plane wave eigenfunctions corresponding to $\sigma_c(A)$.

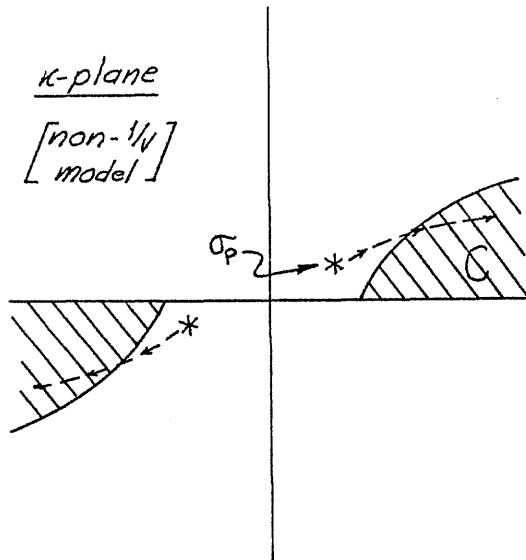
From purely physical considerations, we do not expect any abrupt change in the form of the neutron distribution as the critical limits on ω are exceeded. That is, although the mathematical representation of the solution may assume a different form, we expect that the experimenter will observe only a gradual change in the measured waves due to a change in the spectral representation, and then only at ω well past ω^* . Thus if the solution could be represented as a superposition of plane waves of wave number k_j plus a small continuum contribution for $\omega < \omega^*$, we expect these plane waves will be observable for some range of $\omega > \omega^*$ and will only gradually fade away into continuum jumble as ω is raised still higher.

This would imply that, in some sense, a "continuation" of the point spectrum into C causes corresponding peaks in the integrand of the continuum integral of (II-18), giving rise to pseudo-plane-wave behavior for $\omega > \omega^*$. That is, the continuum "remembers" the point spectrum for some range of $\omega > \omega^*$.

Such behavior has been noted ^[1/v model] for a very simple model⁽³⁶⁾ assuming a one-term separable kernel and $1/v$ total cross-sections. In this case the point spectrum $\sigma_p(A)$ can



be analytically continued across C (which is now a line continuum) for $\omega > \omega^*$. More recent work⁽³⁷⁾ has verified that for a slightly more general one-term kernel, as $\omega > \omega^*$, the point eigenvalues



become eigenvalues imbedded in $\sigma_c(A)$ --that is, for $\omega > \omega^*$, the dispersion relation can be solved for $\kappa \in C$. These two examples suggest that it is not unreasonable to expect that as the critical parameter bounds are exceeded, the $\sigma_p(A)$ merely moves into C where it now yields "imbedded" eigenvalues and corresponding

"pseudo-discrete" plane wave modes.⁴ [This must be verified by numerical calculation for each cross-section model considered.]

However it will be shown later that the continuum contribution dominates asymptotically in x so that eventually for sufficiently high ω and/or x , plane wave behavior can no longer be detected.

3. Perturbation Schemes for Low Frequency

It has been indicated that the dispersion relation for discrete eigenvalues (II-14) represents a formidable mathematical problem

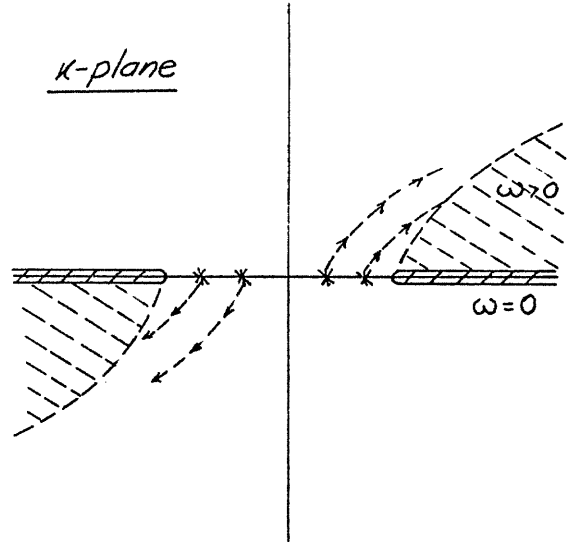
⁴It must be mentioned that these remarks, while interesting, are rather academic since the parameter bounds are quite high for all materials [e.g. $\omega^* \sim \langle v \Sigma_t(v) \rangle \sim 10$ times higher than presently obtainable source frequencies].

because it is non-self-adjoint. However some direct information can be obtained about the point spectrum for low ω by recognizing that in the limit as $\omega \rightarrow 0$, the wave propagation problem reduces to the well-known static diffusion length problem. That is, one can carry out a perturbation procedure

in powers of $(i\omega)$ for

$$AF(\kappa; \mu, \nu) = \kappa F(\kappa; \mu, \nu)$$

about the unperturbed problem which shall be taken as the exact diffusion length problem whose discrete eigenvalues χ are determined by



$$[\nu \Sigma_t(\nu) - \chi \mu \nu] F_0(\chi; \mu, \nu) = S F_0 \quad \chi \notin C \quad (\omega = 0) \quad (\text{II-42})$$

Now expand for a given eigenvalue

$$\kappa = \sum_n c_n (i\omega)^n \quad (\text{II-43})$$

$$F(\kappa; \mu, \nu) = \sum_n \mathfrak{F}_n(\kappa; \mu, \nu) (i\omega)^n$$

Following the standard procedure, substitute (II-43) into (II-5) and collect various orders in $(i\omega)$. This yields

$$(i\omega)^0: \quad [\nu \Sigma_t(\nu) - c_0 \mu \nu] \mathfrak{F}_0(\kappa; \mu, \nu) = S \mathfrak{F}_0 \quad \kappa \notin C \quad (\text{II-44})$$

But this is immediately recognized as (II-42) so that we can identify $c_0 = \chi = 1/L_\chi$, the reciprocal diffusion length, and $\mathfrak{F}_0(\chi; \mu, \nu)$ as the corresponding zero-frequency eigenfunction.

$$(i\omega)^1: \quad [v\Sigma_t(\nu) - \chi\mu\nu] \mathfrak{F}_1(k; \mu, \nu) - \mathfrak{S}\mathfrak{F}_1 = [c_1\mu\nu - 1] \mathfrak{F}_0 \quad k \notin C \quad (II-45)$$

This is just an inhomogeneous version of (II-44). By the Fredholm alternative, a necessary condition for solutions $\mathfrak{F}_1(k; \mu, \nu)$ to exist to (II-45) is that the inhomogeneous term be orthogonal to the adjoint eigenfunctions of (II-45), i. e.

$$\int_{-1}^{+1} d\mu \int_0^\infty d\nu \mu\nu \mathfrak{F}_0^\dagger(\chi; \mu, \nu) [c_1\mu\nu - 1] \mathfrak{F}_0(\chi; \mu, \nu) = 0$$

Thus we find

$$c_1 = \frac{\int_{-1}^{+1} d\mu \int_0^\infty d\nu \mu\nu \mathfrak{F}_0^\dagger(\chi; \mu, \nu) \mathfrak{F}_0(\chi; \mu, \nu)}{\int_{-1}^{+1} d\mu \int_0^\infty d\nu (\mu\nu)^2 \mathfrak{F}_0^\dagger(\chi; \mu, \nu) \mathfrak{F}_0(\chi; \mu, \nu)} \equiv \frac{1}{\langle v_x \rangle_\chi}$$

Note $1/c_1$ is equal to the particle velocity along the x-axis, v_x , averaged over the χ th mode of the static diffusion length problem.

$$(i\omega)^2: \quad [v\Sigma_t(\nu) - \chi\mu\nu] \mathfrak{F}_2(k; \mu, \nu) - \mathfrak{S}\mathfrak{F}_2 = [c_1\mu\nu - 1] \mathfrak{F}_1 + c_2\mu\nu \mathfrak{F}_0 \quad k \notin C$$

If one repeats the argument above, the restriction on the inhomogeneous term yields

$$c_2 = + \frac{\int_{-1}^{+1} d\mu \int_0^\infty d\nu \mu\nu \mathfrak{F}_0^\dagger [1 - c_1\mu\nu] \mathfrak{F}_1}{\int_{-1}^{+1} d\mu \int_0^\infty d\nu (\mu\nu)^2 \mathfrak{F}_0^\dagger \mathfrak{F}_0}$$

Now $\mathfrak{F}_1(\chi; \mu, \nu)$ must be determined by solving (II-45) or using some suitable approximation. Thus c_2 remains rather complicated. We can conclude however that

$$\alpha = \frac{1}{L} - c_2 \omega^2 + O(\omega^4)$$

$$\xi = \frac{\omega}{\langle v_x \rangle} + O(\omega^3)$$

which to second order in $(i\omega)$ is what we might have expected.

Thus far our perturbation theory has been quite consistent, developing exact expressions for the coefficients c_n without making any a priori assumption about the behavior of the eigenvalues κ . However a more naive approach, due originally to Nelkin^(38,39), can be adopted in which a perturbation scheme is developed for a certain region of eigenvalue behavior. To be more precise, return to the isotropic scattering model (II-15) and expand

$$\frac{2K\nu}{\ln \left[\frac{i\omega + \nu \Sigma_t(\nu) + K\nu}{i\omega + \nu \Sigma_t(\nu) - K\nu} \right]} = i\omega + \nu \Sigma_t(\nu) - \frac{\kappa^2 \nu^2}{3 [i\omega + \nu \Sigma_t(\nu)]} - \frac{4}{45} \frac{\kappa^4 \nu^4}{[i\omega + \nu \Sigma_t(\nu)]^3} - \dots \quad (\text{II-46})$$

$$\text{for } \left| \frac{K\nu}{i\omega + \nu \Sigma_t(\nu)} \right| \ll 1$$

If one now uses this expression in (II-15) and performs a perturbation

scheme in $(i\omega)^n$ for small $\Sigma_a(v) = \Sigma_a^0/v$, one can find

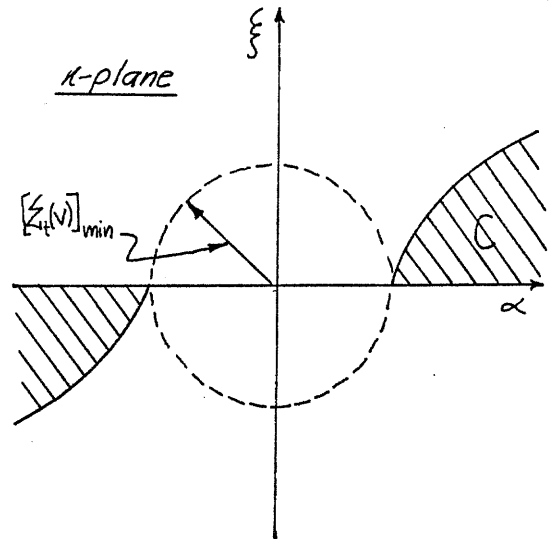
$$\begin{aligned} \text{Re}\{\kappa^2\} &= a^2 - \xi^2 = \frac{\Sigma_a^0}{D_0} - \left[\frac{C_0}{D_0^3} + \left(\frac{D_0 F - 2C_0^2}{D_0^5} \right) 3\Sigma_a^0 \right] \omega^2 + \dots \\ &\cong \frac{\Sigma_a^0}{D_0} - \frac{C_0}{D_0^3} \omega^2 + \dots \end{aligned} \tag{II-47}$$

$$\begin{aligned} \text{Im}\{\kappa^2\} &= 2\alpha\xi = \left[\frac{1}{D_0} - \frac{2C_0 \Sigma_a^0}{D_0^3} \right] \omega - \left[\frac{D_0 F - 2C_0^2}{D_0^5} \right. \\ &\quad \left. + 4 \left(\frac{5D_0 C_0 F - D_0^2 G - 5C_0^2}{D_0^7} \right) \Sigma_a^0 \right] \omega^2 + \dots \cong \frac{\omega}{D_0} + \dots \end{aligned}$$

where D_0, C_0, F, G, \dots are the usual λ vs. B^2 expansion parameters from the pulsed neutron experiment and are evaluated in Williams⁽²⁶⁾. (II-47) can also be obtained by directly reverting the λ vs. B^2 series.

Such expressions as (II-47) are quite valid provided

$\left| \frac{\kappa v}{i\omega + v\Sigma_t(v)} \right| \ll 1$. That is, the eigenvalues must remain within a circle of radius $[\Sigma_t(v)]_{\min}$ in the κ -plane. This restriction is certainly satisfied for neutron wave experiments performed in noncrystalline media. However this condition is violated in polycrystalline materials such as graphite for low ω because of



of the dip in the total cross-section below v_B . In fact, as we shall show in Chapter VI, for wave experiments performed in graphite for which $B_{\perp}^2 > 15 \times 10^{-4} \text{ cm}^{-2}$ (both of the reported experiments^(3,5) exceed this bound), even the $\omega = 0$ eigenvalue is imbedded in $\sigma_c(A)$. That is, no such perturbation expansion is valid for any source frequency! This rather surprising point will be discussed in more detail later in Chapter VI.

F. HIGH FREQUENCY BEHAVIOR

We shall now examine the behavior of $f(x, \mu, v, t)$ for large frequency (following the work of Grad⁽¹⁹⁾). If one imagines a source $S(\mu, v)e^{i\omega t}$ at $x = 0$, the Boltzmann equation (II-2) can be integrated to find two coupled integral equations⁵ for $f(x, \mu, v, t)$

$$f(x, \mu, v, t) = \frac{S(\mu, v)}{\mu v} e^{-\left[\frac{v\Sigma_t(v) + i\omega}{\mu v}\right]x + i\omega t} + \frac{1}{\mu v} \int_0^x e^{-\left[\frac{v\Sigma_t(v) + i\omega}{\mu v}\right]y + i\omega t} \mathcal{S}[f] dy \quad \mu > 0$$

$$f(x, \mu, v, t) = \frac{1}{\mu v} \int_x^{\infty} e^{-\left[\frac{v\Sigma_t(v) + i\omega}{\mu v}\right]y + i\omega t} \mathcal{S}[f] dy \quad \mu < 0$$

(II-48)

For large frequency we note that $f(x, \mu, v, t)$ becomes rapidly

⁵It is of interest to note that these equations imply that $f(x, \mu, v, t)$ approaches the boundary condition at $x = 0$ nonuniformly in μv . Refer to Grad⁽¹⁹⁾ for a further discussion of this phenomenon which results from the vanishing mean free path as $v \rightarrow 0$ as well as those neutrons moving perpendicular to the x -axis.

oscillating in μv . Since \mathcal{S} is a completely continuous operator, it will tend to smooth out these oscillations, reducing the magnitude of the integral term in (II-48). It can be shown that

$$\lim_{\omega \rightarrow \infty} f(x, \mu, v, t) = \begin{cases} \frac{S(\mu, v)}{\mu v} e^{-\left[\frac{v \Sigma_t(v) + i\omega}{\mu v} \right] x + i\omega t} & \mu > 0 \\ 0 & \mu < 0 \end{cases} \begin{cases} \left[\begin{array}{l} \text{pure} \\ \text{streaming} \\ \text{from the} \\ \text{source} \end{array} \right] \\ \left[\begin{array}{l} \text{no particles} \\ \text{reflected} \\ \text{back} \end{array} \right] \end{cases}$$

That is, for large frequency $[\omega \sim \langle v \Sigma_t(v) \rangle]$ the neutron distribution is essentially that due to source streaming alone.

Indeed such an argument could have been expected from the usual Neumann series expansion⁽⁴⁰⁾ of the Peierls' equation for neutron transport. Consider (II-48) in operator notation

$$f = S + Kf$$

We can invert and expand for $\|K\| < 1$ as

$$f = (1 - K)^{-1} S = S + KS + K^2 S + \dots$$

In the usual fashion one can interpret the first term as uncollided source neutrons, the second term as once-collided neutrons, and so on. Now, roughly speaking, $\|K\| = O\left(1 - \frac{\omega + \langle v \Sigma_a(v) \rangle}{\langle v \Sigma_t(v) \rangle}\right) = O\left(1 - \frac{\omega}{\langle v \Sigma_t(v) \rangle}\right)$ for large $\omega < \omega^*$. From this estimate one can conclude that at zero frequency in graphite, the average neutron experiences 10^3 collisions; at $f = 1400$ cps, 6 collisions; and at $f = 5000$, 2 collisions. Thus as experimenters go to higher and higher source

frequencies, they will be measuring a larger and larger percentage of virgin source neutrons.

G. PHYSICAL INTERPRETATIONS

Before continuing on to apply the spectral theory to actual boundary value problems, it is desirable to digress momentarily to discuss the physics of the wave propagation process and attempt to interpret the mathematical theory developed thus far in the light of this physics. This interpretation will be useful for the further analysis of the neutron wave experiment.

1. A Simple Model

We begin our study by using a very simple model due to Beckurts⁽⁴¹⁾ to examine the perturbations of the equilibrium neutron velocity spectrum due to the wave propagation process. The basic idea is to set up a heuristic energy balance for the neutron gas. Notice that there are actually two components--a real and imaginary energy spectrum corresponding to $\text{Re}\{\kappa^2\}$ and $\text{Im}\{\kappa^2\}$. That is, the change in the average energy due to leakage is

$$\left(\frac{\partial \bar{E}}{\partial t}\right)_{\text{leakage}} = \bar{D}\kappa^2\left(\bar{E}_D - \frac{3}{2}kT\right) = (\alpha^2 - \xi^2)\bar{D}\left(\bar{E}_D - \frac{3}{2}kT\right) + 2i\alpha\xi\bar{D}\left(\bar{E}_D - \frac{3}{2}kT\right)$$

$$\text{where } \bar{E}_D \equiv \frac{\int ED(E) dE}{\int D(E) dE}$$

If one then separates $E = E_R + iE_I$, the perturbations to the energy spectrum can be balanced as

$$\frac{dE_R}{dt} = (\alpha^2 - \xi^2) \overline{D}(\overline{E}_D - \frac{3}{2} kT) + \overline{\Sigma}_a(\overline{E}_A - \frac{3}{2} kT) - \frac{3}{2} k\gamma(T - T_a) \quad (\text{II-49})$$

leakage absorption thermalization

$$\frac{dE_I}{dt} = 2\alpha\xi \overline{D}(\overline{E}_D - \frac{3}{2} kT) \quad (\text{II-50})$$

leakage

Notice that if $(\alpha^2 - \xi^2) > 0$, leakage causes a heating of E_R , while if $(\alpha^2 - \xi^2) < 0$, a cooling occurs. It will be demonstrated in the later analysis that most neutron wave theories yield $|\alpha| > |\xi|$ and hence exhibit a frequency "heating" effect. In (II-50), $\alpha\xi > 0$ for all α and ξ , thus the imaginary component always experiences a heating effect. Also note that this effect is never balanced by a moderator effect, hence $\text{Im}\{N(\kappa;v)\}$ will never be Maxwellian.

Using our earlier perturbation work and (II-49,50), it is possible to tabulate the various frequency effects as

<u>Order in ω</u>	<u>Re $\{N(\kappa;v)\}$</u>	<u>Im $\{N(\kappa;v)\}$</u>
$\omega = 0$	absorption heating	$\text{Im}\{N(\kappa;v)\} = 0$
ω^1	absorption heating	wave heating
ω^2	absorption heating + wave heating	wave heating
ω^3	absorption heating + wave heating	wave heating + higher order wave cooling

Thus from this preliminary analysis it appears that the wave velocity spectrum is heated by increasing frequency. The more general analysis of the Boltzmann equation will now be used to provide a

physical explanation of this effect.

2. Interpretation of the General Solution

The preceding spectral analysis has indicated that the general solution to a problem in neutron wave propagation can be written as (II-18). If the explicit forms of the eigenfunctions are used, this solution can be written even more specifically as

$$\begin{aligned}
 f(x, \mu, v, t) = & \sum_{k_l \in \sigma_p} a_l \frac{f(k_l; \mu, v) e^{-k_l x + i\omega t}}{i\omega + v\Sigma_t(v) - k_l \mu v} \\
 & + \int_C \int \frac{A(k) f(k; \mu, v) e^{-kx + i\omega t}}{i\omega + v\Sigma_t(v) - k\mu v} dk + \frac{S(\mu, v)}{\mu v} e^{-\frac{\Sigma_t(v)}{\mu} x} e^{i\omega(t - \frac{x}{\mu v})}
 \end{aligned}
 \tag{II-51}$$

where the last term is due to the δ -function part of the continuum eigenfunction (II-17). We will now try to interpret each of these terms:

$f_s(x, \mu, v, t) = \frac{S(\mu, v)}{\mu v} e^{-\frac{\Sigma_t(v)}{\mu} x} e^{i\omega(t - \frac{x}{\mu v})}$: This term represents the uncollided neutrons of velocity v and angle μ emitted by the source. These particles correspond to a plane wave contribution moving along the x -axis at phase velocity $v_{ph} = \mu v$ and hence phase shift $\omega x / v_{ph}$. Since this plane wave is due only to uncollided particles of μ and v , it suffers an attenuation in the x -direction of $\exp[-\Sigma_t(v)x/\mu]$.

$f_c(x, \mu, v, t) = \int_C \int \frac{A(k) f(k; \mu, v)}{i\omega + v\Sigma_t(v) - k\mu v} e^{-kx + i\omega t} dk$: The individual continuum modes (eigenfunctions) also correspond to free streaming neutrons

since $\kappa \in C$ implies that the integrand of $f_c(x, \mu, \nu, t)$ contains plane wave terms of the form $e^{-\frac{\Sigma_t(\nu)}{\mu} x} e^{i\omega(t - \frac{x}{\mu\nu})}$ for all μ and ν . However the total continuum contribution $f_c(x, \mu, \nu, t)$ represents collided neutrons as well. One can distinguish these continuum mode neutrons from the discrete mode neutrons since whenever the former type suffers a collision, it is transferred to a different free streaming mode. As a consequence, it never remains in the same mode for more than one collision. [By way of contrast, a neutron propagating in a discrete mode will remain in that mode for several collisions.] This intermode coupling is represented by the factor $\left\{ \frac{A(\kappa) f(\kappa; \mu, \nu)}{i\omega + \nu \Sigma_t(\nu) - \kappa \mu \nu} \right\}$ in the integrand. The total contribution of continuum neutrons consists of the sum of these free streaming modes, each weighted with the appropriate intermode coupling factor. As the number of particles becomes very large, this sum passes to an integral corresponding to the term $f_c(x, \mu, \nu, t)$.

This total contribution, although composed of individual plane wave modes, usually is not a plane wave itself since each of the individual continuum modes in the integral interferes coherently with each other by phase mixing. $f_c(x, \mu, \nu, t)$ will suffer attenuation as x increases due to both randomizing collisions as well as phase interference between the individual continuum modes.

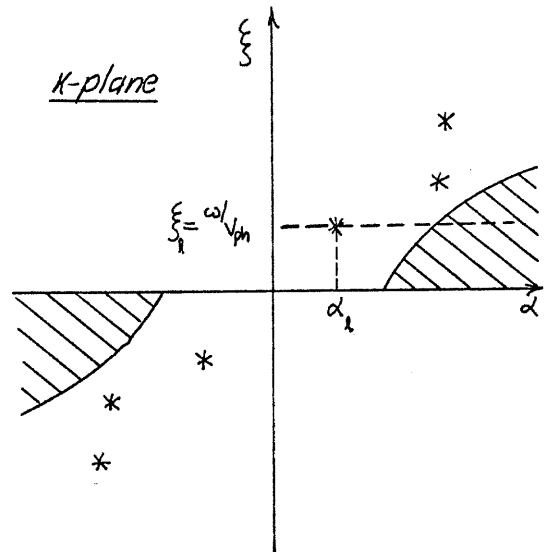
One can examine the asymptotic behavior of $f_c(x, \mu, \nu, t)$ for large x by considering the damping of these streaming modes. Far from the source the plane waves corresponding to neutrons of v_{ph} moving parallel to the x -axis will suffer less attenuation than those

moving at some angle μ . This is true for any v_{ph} . Thus one expects the continuum contribution to result in a forward angular peaking far from the source. For monotonic cross-section behavior, the neutrons of $v \rightarrow \infty$ experience the least attenuation $e^{-\Sigma_M x}$; hence we expect that sufficiently far from the source the continuum term will provide only very fast neutrons directed along the x-axis. For non-monotonic cross-sections the uncollided neutrons directed along the x-axis with speed of $v = v^*$ such that $\Sigma_t(v^*) = \Sigma_M \equiv [\Sigma_t(v)]_{min}$ will dominate, setting up a plane wave of $v_{ph} = v^*$ which decays like $e^{-\Sigma_M x}$.

$$f_D(x, \mu, v, t) = \sum_{\substack{\kappa \in \sigma_p \\ \kappa}} \frac{a_\ell \bar{f}(\kappa_\ell; \mu, v)}{i\omega + v\Sigma_t(v) - \kappa_\ell \mu v} e^{-\kappa_\ell x + i\omega t} : \text{These, of course, are}$$

the discrete or "collective" plane wave modes. To examine these

modes in more detail, return to the κ -plane diagram. Now observe that a discrete plane wave is always less damped than the continuum modes at that particular phase velocity $v_{ph} = \omega/\xi_\ell$. But since the edge of the continuum represents those modes due to uncollided neutrons streaming along the x-axis, one can only



conclude that the discrete modes must involve neutrons which have suffered collisions [otherwise the discrete wave would be damped as much as the continuum modes of the same v_{ph}].

It is instructive to consider those effects which tend to throw the particles participating in the discrete plane wave mode out of phase, i. e. tend to "disperse" the wave. Three such phenomena can be distinguished:

- i) If one considers the wave as moving at a certain phase velocity v_{ph} , the particles moving with v far from v_{ph} will tend to be more easily removed from the wave phase. Notice that this implies that since $v_{ph} = \omega/\xi_\ell$ usually increases as we increase ω , the higher velocity particles tend to have an easier time staying in phase with the wave, while the slower particles or those particles moving at large angles from the x-axis are more apt to suffer dispersion. Hence we would predict from these physical arguments that the spectrum of particles in the wave tends to become more heated as we raise ω [unless v_{ph} begins to decrease as ω increases⁶]. This explains the heating effect noticed in the earlier analysis.
- ii) If a particle suffers too many collisions, it will tend to be thrown out of phase into the random background regardless of its initial velocity or direction. Since the lower velocity neutrons suffer on the average more collisions per distance traveled than do the higher velocity neutrons, they tend to get scattered out of phase more quickly.

⁶For all of the models considered in this thesis, v_{ph} is monotonically increasing in ω . Closer examination shows that this effect corresponds to frequency heating, while a monotonic decreasing v_{ph} would correspond to a frequency cooling of the spectrum.

As ω increases, $\lambda = 2\pi/\xi$ becomes very short⁷, implying that fewer collisions are necessary to randomize the neutron; hence higher and higher velocity particles are scattered out of phase. This again contributes a spectral heating effect as frequency increases, as well as causing the attenuation α to increase with ω .

iii) Of course, the discrete waves can also be damped directly by the loss of particles due to absorption.

To gain more understanding of the discrete eigenvalues, take the inner product of (II-5) with $F^\dagger(K; \mu, \nu)$ to obtain

$$K = i\omega \frac{\langle F_K^\dagger, \frac{1}{\mu\nu} F_K \rangle}{\langle F_K^\dagger, F_K \rangle} + \frac{\langle F_K^\dagger, \frac{\Sigma_t(\nu)}{\mu} F_K \rangle}{\langle F_K^\dagger, F_K \rangle} - \frac{\langle F_K^\dagger, \frac{S}{\mu\nu} F_K \rangle}{\langle F_K^\dagger, F_K \rangle}$$

$$\equiv i\omega \langle \frac{1}{v_x} \rangle_K + \langle \frac{\Sigma_t(\nu)}{\mu} \rangle_K - \langle \frac{1}{\mu\nu} S \rangle_K \quad (\text{II-52})$$

Taking the imaginary part of this equation yields $\xi = \omega \langle \frac{1}{v_x} \rangle_K$ or $v_{ph} = \omega/\xi \cong \langle v_x \rangle_K$ where $\langle \rangle_K$ is defined as the average of a quantity over the discrete mode corresponding to the eigenvalue K . That is, the phase speed of a given discrete mode is equal to the average of the particle velocity in the x -direction weighted by the eigenfunction for that mode. Notice that as the velocity spectrum of a mode is heated with increasing ω , $v_{ph} = \langle v_x \rangle_K$ will similarly increase.

⁷Notice that if $\lambda = 2\pi/\xi$ decreases too strongly with ω , then $v_{ph} = \omega/\xi$ may also decrease. This would correspond to the mode velocity spectrum shifting towards some finite, or even zero, velocity.

A few additional comments are necessary. This analysis would predict that as the discrete waves travel along, they are spectrally heated and become angularly singular in the forward direction. This seems to contradict the H-theorem of kinetic theory⁽¹⁵⁾. However we must remember that our equations (and the experiments) are only examining that part of the neutron distribution which carries information or periodic signals from the source. The moment a neutron loses this information, i. e. by being randomized out of phase or absorbed, it disappears from our equations and falls into the random background distribution. Of course if we had attempted to describe all of the neutrons, including the background and moderator atoms, all of the usual theorems of statistical mechanics would still be in evidence. Any heating of the wave spectrum must result in a cooling of the background Maxwellian by the addition of low velocity neutrons to it.

It is also important to recognize that the "collective" modes are by no means collective in the sense that they permit interactions between the particles in the wave. Indeed any theory using a linearized Boltzmann equation (rarefied gas dynamics included) throws out these interactions with the linearization approximation. The terminology of "collective modes," used frequently in gas dynamics, seems rather misleading in this respect. Only a nonlinear theory could predict truly collective modes.

3. Explanation of the Critical Bound ω^* on Source Frequency

By considering the propagation of plane waves, one assumes

that the discrete wave modes propagate with a constant velocity spectrum in space, i.e. $f(x, \mu, v, t) = F(\kappa; \mu, v) e^{-\kappa x + i\omega t}$. However we must recognize that this can only be so when the scattering kernel can establish a spectral equilibrium for this mode, i.e. the moderator scatters enough neutrons to higher velocities to insure that $F(\kappa; \mu, v)$ is constant in x . [Of course the total number of neutrons in the mode decreases in x since only a certain fraction of the neutrons are scattered back up.]

Now it was shown earlier that as ω increases, the velocity spectrum of $F(\kappa; \mu, v)$ eventually becomes heated to such an extent that the scattering kernel is no longer capable of transferring a particle at v' to a higher velocity v such that it will remain in phase. Thus associated with each discrete κ mode is a critical frequency ω_K^* above which the mode will cease to exist. We are led to define $\omega^* \equiv \max_{\kappa \in \sigma_p(A)} [\omega_K^*]$.

One can give a very crude estimate of ω^* by returning to (II-52). We know that κ is bounded roughly by the total cross-section $\text{Re } \{\kappa\} \leq \langle \Sigma_t(v)/\mu \rangle_K$ since modes decaying with $\text{Re } \{\kappa\} > \Sigma_t(v)/\mu$ correspond to free streaming neutrons. Since in some sense $\langle \frac{1}{\mu v} S \rangle_K \sim \langle \Sigma_s(v)/\mu \rangle_K$ for $\omega \sim \langle v \Sigma_t(v) \rangle$ we find from (II-52) that $\kappa \sim \langle \Sigma_t(v)/\mu \rangle$. From this heuristic argument it appears that $\omega_K^* \sim \langle v \Sigma_t(v) \rangle_K$, i.e. the average scattering collision frequency for that mode. That is, each plane wave mode is characterized by some average collision time $\omega_K^* \sim \langle v \Sigma_t(v) \rangle_K$. When the source frequency ω exceeds ω_K^* , the mode can no longer be sustained. [The collision

process of the mode can no longer keep up with the time behavior of the source.]

III. THE SOLUTION OF FULL-RANGE BOUNDARY VALUE PROBLEMS

By definition, full-range boundary value problems involve only boundary conditions which are given at a specific position in x for all μ and ν . In particular, such problems will involve eigenfunction expansions over the full range of the eigenvalue spectrum $\sigma(A)$. The prototype problem is that of an oscillating plane source at the origin of an infinite medium, since this problem may be used to construct the infinite medium Green's function of equation (II-2).

As in all such problems, analytical procedures can be based on either integral transform techniques or the method of separation of variables (and subsequent spectral representation). These two procedures are essentially equivalent in that any problem which can be solved by one technique can also be solved with the other. However for purposes of comparison, both methods will be developed in this chapter.

A. SPECTRAL REPRESENTATION METHODS

We shall begin by developing the necessary mathematical background for the use of separation of variables and subsequent expansion of the solution in terms of the eigenfunctions (spectral representation) of the wave operator A for noncrystalline media. Before continuing further, it will be convenient to introduce a more compact notation. Notice that since $C = \{k: k = \frac{i\omega}{\mu\nu} + \frac{\Sigma_t(\nu)}{\mu}, \mu \in [-1, +1], \nu \in [0, \infty)\}$ is an area in the k -plane, the continuous spectrum can only be specified completely by two parameters. That such area

spectra arise in time-dependent transport problems has been recognized for some time^(19,42); however only recently have methods been developed to deal with such area continua. The principal work is due to C. Cercignani⁽²⁵⁾ and relies upon the theory of generalized analytic functions developed by Vekua⁽⁴³⁾ and others⁽⁵¹⁾. Much of the analysis in the next two chapters will rely heavily upon Cercignani's work, although it will be necessary to extend it somewhat to apply it to the propagation of neutron waves.

It is useful to define a new independent variable

$$z \equiv \frac{i\omega + v\Sigma_t(v)}{\mu v} \equiv \mathcal{J} + i\varphi$$

This transformation defines a one-to-one mapping of (μ, v) into the complex z -plane [for monotonic $\Sigma_t(v)$ at least]. It allows (II-5) to be rewritten as

$$(z - \kappa)F(\kappa; z) = \iint K(z', z)F(\kappa; z') dz' \equiv f(\kappa; z) \quad (\text{III-1})$$

where we have defined¹

$$F(\kappa; z) \longleftrightarrow F(\kappa; \mu(\mathcal{J}, \varphi), v(\mathcal{J}, \varphi))$$

$$K(z', z) \longleftrightarrow \frac{v \Sigma_s(v' \rightarrow v, \mu' \rightarrow \mu)}{\mu v |\partial(\mathcal{J}, \varphi)/\partial(\mu, v)|} (\mathcal{J}, \varphi)$$

$$dz' \longleftrightarrow d\mathcal{J}' d\varphi$$

Now one proceeds in the usual manner by noting that the continuum in

¹Note here that $f(z)$ is only a formal notation for $f(\mathcal{J}, \varphi)$ and is not intended to mean that $f(z) = f(\mathcal{J} + i\varphi)$.

the κ -plane is determined by those values of $\kappa = z$ for all $\mu \in [-1, +1]$, $\nu \in [0, \infty)$. But of course this is just $\kappa \in C$ as before. For $\kappa \notin C$, the discrete eigenfunctions become

$$F(\kappa_\ell; z) = \frac{f(\kappa_\ell; z)}{z - \kappa_\ell} \quad \kappa_\ell \notin C \quad (\text{III-2})$$

and the dispersion relation for discrete eigenvalues becomes

$$f(\kappa; z) = \int \int_C \left[\frac{K(z', z)}{z' - \kappa} \right] f(\kappa; z') dz' \quad (\text{III-3})$$

which, of course, is identical to (II-14).

For $\kappa \in C$, the continuum eigenfunctions become

$$F(\kappa; z) = \frac{f(\kappa; z)}{z - \kappa} + \lambda(\kappa) \delta(\kappa - z) \quad \kappa \in C \quad (\text{III-4})$$

$$\text{where } \delta(\kappa - z) \equiv \delta(\alpha - \beta) \delta(\xi - \varphi)$$

Notice that since we are working with two-dimensional integrals over C , a Cauchy principal value is not needed because the integrals exist in the ordinary sense even for $\kappa \in C$ [provided $f(\kappa; z)$ is properly behaved].

To obtain an expression for $\lambda(\kappa)$, multiply $F(\kappa; z)$ by $K(z, u)$ and integrate over z to find

$$\lambda(\kappa) = [K(\kappa, u)]^{-1} \left[f(\kappa; u) - \int \int_C \left[\frac{K(z, u)}{z - \kappa} \right] f(\kappa; z) dz \right] \quad \kappa \in C \quad (\text{III-5})$$

Notice that $f(\kappa; z)$ is still unspecified. It is found to be more convenient to use unnormalized eigenfunctions when one is concerned with

problems involving a general scattering kernel $\Sigma_s(v' \rightarrow v, \mu' \rightarrow \mu)$ in velocity-dependent transport theory⁽³¹⁾. Thus rather than normalizing $F(\kappa; z)$ and introducing some $A(\kappa)$ as the amplitude coefficient in the continuum term of (II-18), we shall treat $f(\kappa; z)$ itself as the continuum expansion coefficient. [However when a separable kernel model is adopted in Chapter IV, it will be found to be more convenient to normalize the eigenfunctions.]

One further change in notation is useful. Although most of Chapter II was concerned with "symmetrized" operators in which detailed balance had been used to symmetrize the scattering operator, we shall find it more convenient to return to the unsymmetrized form in (II-5). All of the previous theory is still applicable provided we choose as our new inner product

$$(f, g) \equiv \int_{-1}^{+1} d\mu \int_0^{\infty} dv \mu v \overline{f(\mu, v)} g(\mu, v) \quad (\text{III-6})$$

The analogue in z -notation is

$$(f, g) \equiv \iint dz \overline{f(z)} g(z) \quad (\text{III-6}')$$

Notice that under this inner product, the equation adjoint to (III-1) becomes

$$(\bar{z} - \bar{\kappa}) F^\dagger(\kappa; z) = \iint_C \overline{K(z, z')} F^\dagger(\kappa; z') dz' \quad (\text{III-7})$$

Subject to these notational changes, we shall continue on to examine the solution of full-range boundary value problems. First the usual theorems about the eigenfunctions can be given.

1. Full-Range Orthogonality

THEOREM V: The eigenfunctions $\{F(\kappa; z): \kappa \in \sigma_p(A)\}$ form a bi-orthogonal set over the full range $z \in C$.

Proof: Assume for the moment that none of the discrete eigenvalues κ_ℓ are degenerate. Then taking the inner product of (III-1) with $F^\dagger(\kappa'; z)$, then the inner product of the adjoint problem (III-7) with $F(\kappa; z)$, and subtracting, yields

$$(\kappa - \kappa')(F_{\kappa'}^\dagger, F_\kappa) = 0$$

Thus for nondegenerate eigenvalues [and even for eigenvalues of finite multiplicity provided a Gram-Schmidt procedure is used], the biorthogonality relation for discrete eigenvalues can be written as

$$(F_{\kappa_\ell}^\dagger, F_{\kappa_m}) = \int_C \overline{F^\dagger(\kappa_\ell; z)} F(\kappa_m; z) dz = \delta_{\ell m} (F_{\kappa_\ell}^\dagger, F_{\kappa_\ell})$$

$$\kappa_\ell \in \sigma_p(A) \quad (III-8)$$

Such biorthogonality can also be demonstrated for the continuum eigenfunctions corresponding to $\kappa \in \sigma_c(A)$. However such a property is of little use in the evaluation of expansion coefficients since the normalization of these eigenfunctions must still be determined from the boundary conditions. Notice that the biorthogonality relation (III-8) becomes in (μ, ν) notation

$$(F_{\kappa_\ell}^\dagger, F_{\kappa_m}) = \int_{-1}^{+1} d\mu \int_0^\infty d\nu \mu \nu \overline{F^\dagger(\kappa_\ell; \mu, \nu)} F(\kappa_m; \mu, \nu)$$

$$= \delta_{\ell m} (F_{\kappa_\ell}^\dagger, F_{\kappa_\ell}) \quad \kappa_\ell \in \sigma_p(A) \quad (III-9)$$

2. Full-Range Completeness

We shall now state and prove² a completeness theorem which justifies the eigenfunction expansion (II-18) of functions defined over all μ and ν . In the course of the proof a prescription will be given for the evaluation of the expansion coefficients.

THEOREM VI: The set of functions $\{F(\kappa; z): \kappa \in \sigma(A)\}$ is complete for the class of all functions $\psi(z) \in \mathcal{L}_1(\overline{C})$. [Here \overline{C} is the closure of C .]

Proof: The proof is constructive in nature and consists of actually evaluating the expansion coefficients in

$$\psi(z) = \sum_{\kappa_\ell \in \sigma_p(A)} a_\ell F(\kappa_\ell; z) + \int_C \int_C F(\kappa; z) dz \quad (\text{III-10})$$

and then demonstrating that such an evaluation is unique. First define

$$\psi'(z) = \psi(z) - \sum_\ell a_\ell F(\kappa_\ell; z)$$

and consider (III-10) as

$$\psi'(z) = \int_C \int_C F(\kappa; z) d\kappa = \int_C \int_C \frac{f(\kappa; z)}{z - \kappa} d\kappa + \lambda(z) \quad (\text{III-11})$$

where the explicit form of the continuum eigenfunctions (III-4) has been used. Now using equation (III-5) in (III-11), one obtains

$$K(z, u)\psi'(z) = K(z, u) \int_C \int_C \frac{f(\kappa; z)}{z - \kappa} d\kappa + f(z; u) - \int_C \int_C \left[\frac{K(\zeta, u)}{\zeta - z} \right] f(z; \zeta) d\zeta \quad (\text{III-12})$$

²This theorem is a generalization of that given by Cercignani⁽²⁵⁾ for the special case of a one-term separable kernel. The idea behind the proof is similar to that of a theorem proved by Bednarz and Mika⁽³¹⁾ for the $\omega = 0$ case.

Now (III-12) is a rather complicated two-dimensional integral equation for $f(z;u)$. Notice how both of the variables z and u are involved in the equation.

To complete the proof of the theorem we must demonstrate the existence and uniqueness of a solution to (III-12) for any $\psi'(z) \in \mathcal{L}_1(\overline{C})$. Fortunately techniques exist which will allow the construction of a formal solution to (III-12). These techniques rely upon the theory of generalized analytic functions (see Appendix D) and upon the following lemma [which gives the generalized analytic function analogue to the Plemelj formulae^(24,58)]:

Lemma: Define the operator

$$T_C[f]_z^\zeta = -\frac{1}{\pi} \int_C \int_C \frac{f(\zeta)}{\zeta - z} d\zeta \quad (\text{III-13})$$

Let $f(\zeta) \in \mathcal{L}_1(\overline{C})$. Then $T_C[f]_z^\zeta$ exists for all points z outside \overline{C} , is holomorphic in z outside C , vanishes at infinity, is continuous on ∂C except possibly at angular points, and possesses a generalized derivative with respect to \bar{z} which satisfies

$$\frac{\partial}{\partial \bar{z}} T_C[f]_z^\zeta = \begin{cases} f(z) & z \in C \\ 0 & z \notin \overline{C} \end{cases} \quad (\text{III-14})$$

If, on the contrary, $g(z)$ is holomorphic outside \overline{C} , vanishes at infinity, is continuous almost everywhere on $\partial \overline{C}$, and possesses a generalized derivative which satisfies

$$\frac{\partial g}{\partial \bar{z}} = \begin{cases} f(z) & z \in C \\ 0 & z \notin \bar{C} \end{cases} \quad (\text{III-15})$$

with $f(z) \in \mathfrak{L}_1(\bar{C})$, then $g(z)$ is determined uniquely in the entire complex plane, being given by

$$g(z) = T_C[f] \frac{\zeta}{z} \quad (\text{III-16})$$

[Note here that ∂C is symbolic for the boundary of C .]

Proof: Refer to Vekua⁽⁴³⁾.

Now rewrite (III-12) in terms of the T_C operator as

$$K(z, u)\psi'(z) = K(z, u)\pi T_C[f(\kappa; z)] \frac{\kappa}{z} + f(\kappa; u) + \pi T_C[K(\zeta, u)f(z; \zeta)] \frac{\zeta}{z} \quad z \in C \quad (\text{III-17})$$

But we can rearrange this as

$$\begin{aligned} \frac{\partial}{\partial \bar{z}} \left[\left\{ 1 + \pi T_C[K(\zeta, u) \cdot] \frac{\zeta}{z} \right\} \left\{ T_C[f(\kappa; u)] \frac{\kappa}{z} \right\} \right] &= K(z, u)\psi'(z) \quad z \in C \\ \frac{\partial}{\partial \bar{z}} \left[\left\{ 1 + \pi T_C[K(\zeta, u) \cdot] \frac{\zeta}{z} \right\} \left\{ T_C[f(\kappa; u)] \frac{\kappa}{z} \right\} \right] &= 0 \quad z \notin C \end{aligned} \quad (\text{III-18})$$

where we have defined

$$\left\{ \iint_C \frac{K(\zeta, u) \cdot d\zeta}{\zeta - z} \right\} \phi(z, u) \equiv \iint_C \frac{K(\zeta, u)\phi(z, \zeta) d\zeta}{\zeta - z}$$

Thus we can apply the lemma above to find

$$\left\{ 1 + \pi T_C [K(\zeta, u) \cdot] \frac{\zeta}{z} \right\} \left\{ T_C [f(\kappa; u)] \frac{\kappa}{z} \right\} = T_C [K(\zeta, u) \psi'(\zeta)] \frac{\zeta}{z} \quad (\text{III-19})$$

Now we must solve (III-19) for $f(z; u)$. Clearly this will involve using the inverse operator $\left\{ 1 + \pi T_C [K(\zeta, u) \cdot] \frac{\zeta}{z} \right\}^{-1} \equiv [1 - \mathfrak{L}_{(u, z)}]^{-1}$

where we have defined

$$\mathfrak{L}_{(u, z)} \phi(z, \zeta) \equiv \int_C \int_C \left[\frac{K(\zeta, u)}{\zeta - z} \right] \phi(z, \zeta) d\zeta \quad (\text{III-20})$$

Of course one must account for those values of z for which this inverse fails to exist. But we recognize from equation (III-3) that these points $z = \kappa_l$ are just the discrete spectrum $\sigma_p(A)$, and the usual application of the Fredholm alternative requires

$$\left(\varphi^\dagger(z; u), T_C [K(\zeta, u) \psi'(\zeta)] \frac{\zeta}{z} \right) = 0 \quad z \in \sigma_p(A) \quad (\text{III-21})$$

where $\varphi^\dagger(z; u)$ is the solution to the homogeneous adjoint problem

$$[1 - \mathfrak{L}_{(u, z)}^\dagger] \varphi^\dagger(z; u) = 0$$

or

$$\varphi^\dagger(z; u) = \int_C \int_C \frac{\overline{K(u, \zeta)}}{\overline{u - z}} \varphi^\dagger(z; \zeta) d\zeta \quad (\text{III-22})$$

But notice that we can identify (III-22) as just (III-7) which implies that $\varphi^\dagger(z; u) = F^\dagger(z; u)$. We can now use this fact in equation (III-21) to find, after some manipulation,

$$a_l = \frac{(F_{\kappa_l}^\dagger, \psi)}{(F_{\kappa_l}^\dagger, F_{\kappa_l})} \quad (\text{III-23})$$

which is just the expression for the discrete expansion coefficients one would have obtained by applying biorthogonality directly to (III-10). Thus subject to (III-23), we can solve (III-19) for

$$T_C[f(\kappa;u)]_z^{\kappa} = [1 - \mathfrak{L}_{(u,z)}]^{-1} T_C[K(\zeta,u)\psi'(\zeta)]_z^{\zeta}$$

or

$$f(z;u) = \frac{\partial}{\partial \bar{z}} \left\{ [1 - \mathfrak{L}_{(u,z)}]^{-1} T_C[K(\zeta,u)\psi'(\zeta)]_z^{\zeta} \right\} \quad (III-24)$$

Hence by formal construction we have demonstrated the existence of a solution $f(z;u)$ to (III-12) for arbitrary $\psi'(z) \in \mathfrak{L}_1(\overline{C})$. The converse of the lemma on p. 70 yields the uniqueness of $f(z;u)$.

Therefore by actually demonstrating how one might evaluate the expansion coefficients a_j and $f(\kappa; z)$ in (III-10), we have proven that the eigenfunctions $\{F(\kappa; z) : \kappa \in \sigma(A)\}$ are complete over the full-range of κ for the class of integrable functions defined over all μ and v .

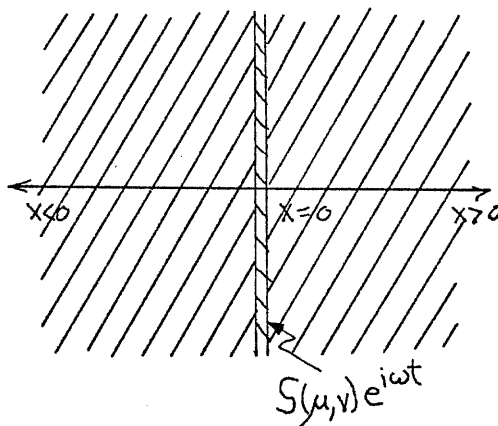
3. An Application of the Technique

Let us now consider the problem of an oscillating plane source at the origin of an infinite medium.

The Boltzmann equation of interest is (II-2) with a source term

$$S(\mu, \nu, x) = S(\mu, \nu) \delta(x)$$

We shall take the physically significant



boundary conditions at infinity

$$\lim_{|x| \rightarrow \infty} |f(x, \mu, \nu, t)| = 0 \quad (\text{III-25})$$

To obtain the boundary condition at the source, integrate (II-2) over x from $0 - \epsilon$ to $0 + \epsilon$ and then let $\epsilon \rightarrow 0$ to find

$$\mu\nu [f(0^+, \mu, \nu, t) - f(0^-, \mu, \nu, t)] = S(\mu, \nu) e^{i\omega t} \quad (\text{III-26})$$

To solve this problem by the method of spectral representation, we shall seek the solution in the form of expansions in the plane wave eigenfunctions of Chapter II. Utilizing the boundary conditions at infinity demands the expansions

$$f(x, \mu, \nu, t) = \begin{cases} \sum_{\ell^+=1}^{L/2} a_{\ell^+} F(k_{\ell^+}; \mu, \nu) e^{-k_{\ell^+} x + i\omega t} + \iint_{\Delta C^+} e^{-kx + i\omega t} F(k; \mu, \nu) dk & x > 0 \\ \sum_{\ell^-=1}^{L/2} a_{\ell^-} F(k_{\ell^-}; \mu, \nu) e^{-k_{\ell^-} x + i\omega t} + \iint_{\Delta C^-} e^{-kx + i\omega t} F(k; \mu, \nu) dk & x < 0 \end{cases} \quad (\text{III-27})$$

Then applying the source boundary condition (II-26) yields

$$\frac{S(\mu, \nu)}{\mu\nu} = \sum_{k_{\ell} \in \sigma_p(A)} a_{\ell} F(k_{\ell}; \mu, \nu) + \iint_C F(k; \mu, \nu) dk \quad (\text{III-28})$$

as the condition from which the expansion coefficients are to be determined. Since $S(\mu, \nu)$ is considered to be defined over all $\mu \in [-1, +1]$ and $\nu \in [0, \infty)$, (III-28) is just the full-range expansion (III-10). Thus from the previous completeness theorem we know that such an

expansion is possible, and indeed this theorem will actually evaluate a_ℓ and $f(k;z)$ for us as

$$a_\ell = \frac{(F_{K_\ell}^\dagger, S/\mu v)}{(F_{K_\ell}^\dagger, F_{K_\ell})} = \frac{\int_{-1}^{+1} d\mu \int_0^\infty dv \overline{F^\dagger(K_\ell; \mu, v)} S(\mu, v)}{\int_{-1}^{+1} d\mu \int_0^\infty dv \mu v \overline{F^\dagger(K_\ell; \mu, v)} F(K_\ell; \mu, v)} \quad (\text{III-30})$$

$$f(z; u) = \frac{\partial}{\partial \bar{z}} \left\{ [1 - \mathfrak{L}_{(u, z)}]^{-1} T_C [K(\zeta, u) S(z) - K(\zeta, u) \sum_\ell a_\ell F(K_\ell; z)] \right\}_{\zeta=z} \quad (\text{III-31})$$

Of course such a representation is still very formal in that one must invert the $[1 - \mathfrak{L}_{(u, z)}]$ operator which amounts to solving the associated eigenvalue problem (II-14)--a formidable task.

B. INTEGRAL TRANSFORMS

Consider once again the problem of an oscillating plane source at the origin of an infinite medium, as outlined in the previous section. An alternative approach involves the use of integral transforms in the spatial variable x . Because of the infinite geometry $x \in (-\infty, \infty)$, a Fourier transform is appropriate. Working formally then, define the transform

$$\tilde{F}(\eta; \mu, v) \equiv \int_{-\infty}^{\infty} e^{+\eta x} f(x, \mu, v) dx \quad (\text{III-52})$$

where the $e^{i\omega t}$ factor is to be understood. The existence of such a transform is insured since we assume that the boundary conditions at infinity (III-25) coupled with physical considerations imply

$f(x, \mu, \nu) \in \mathcal{L}_2(-\infty, \infty)$ in x .

Thus we can transform (II-2) into

$$[i\omega + \nu \Sigma_t(\nu) - \eta \mu \nu] \tilde{F}(\eta; \mu, \nu) = \int_{-1}^{+1} d\mu' \int_0^{\infty} d\nu' \nu' \Sigma_s(\nu' \rightarrow \nu, \mu' \rightarrow \mu) \tilde{F}(\eta; \mu', \nu') + S(\mu, \nu) \quad (\text{III-33})$$

But if we use our operator notation, this can be written as

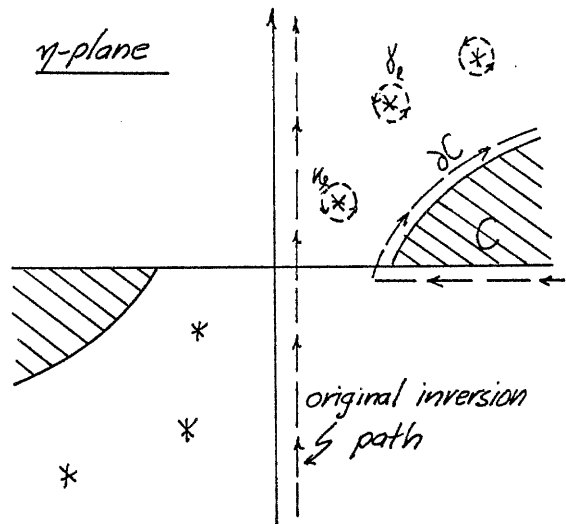
$$[A - \eta] \tilde{F}(\eta; \mu, \nu) = S(\mu, \nu) / \mu \nu \quad (\text{III-34})$$

If we introduce the resolvent operator $[A - \eta]^{-1}$, we can write the inverse transform

$$f(x, \mu, \nu, t) = \frac{1}{2\pi i} \int_{-i\infty}^{+i\infty} e^{-\eta x + i\omega t} \tilde{F}(\eta; \mu, \nu) d\eta = \frac{1}{2\pi i} \int_{-i\infty}^{+i\infty} e^{-\eta x + i\omega t} \left\{ [A - \eta]^{-1} \frac{S(\mu, \nu)}{\mu \nu} \right\} d\eta \quad (\text{III-35})$$

as a formal representation of the solution.

However such a form of the solution as (III-35) is rather awkward. A more satisfactory representation of the solution can be obtained by a suitable deformation of the inversion contour. Since we have shown that the resolvent $[A - \eta]^{-1}$ is an operator analytic in η for $\eta \notin \sigma(A)$, we can readily deform



the path into the right half plane as shown for $x > 0$, using the $e^{-\eta x}$ behavior to kill off contributions from $\text{Re} \{ \eta \} \rightarrow \infty$.

Now we know we can represent $\tilde{F}(\eta; \mu\nu)$ as

$$[A-\eta]^{-1} \frac{S(\mu, \nu)}{\mu\nu} = \sum_{\kappa \in \sigma_p(A)} \frac{(F_K^\dagger, S/\mu\nu)}{(F_K^\dagger, F_K)} \frac{F(\kappa; \mu, \nu)}{\kappa - \eta} + \int \int_{\kappa \in C} \frac{F(\kappa; \mu, \nu)}{\kappa - \eta} d\kappa \quad (\text{III-36})$$

where $f(\kappa; \mu, \nu)$ in the continuum integral is given by (III-31). Rewrite (III-35) using the path deformation above

$$f(x, \mu, \nu, t) = \sum_{\kappa_\ell \in \sigma_p(A)} \frac{1}{2\pi i} \oint_{\gamma_{\kappa_\ell}} e^{-\eta x + i\omega t} \left[[A-\eta]^{-1} \frac{S(\mu, \nu)}{\mu\nu} \right] d\eta + \frac{1}{2\pi i} \int_{\partial C} e^{-\eta x + i\omega t} \left[[A-\eta]^{-1} \frac{S(\mu, \nu)}{\mu\nu} \right] d\eta \quad (\text{III-37})$$

$x > 0$

substitute (III-36) into (III-37), and interchange the path integrations with the summation and integration over $\sigma(A)$ to find

$$f(x, \mu, \nu, t) = \sum_{\kappa_\ell \in \sigma_p(A)} \frac{(F_K^\dagger, S/\mu\nu)}{(F_K^\dagger, F_K)} F(\kappa; \mu, \nu) \frac{1}{2\pi i} \oint_{\gamma_{\kappa_\ell}} \frac{e^{-\eta x + i\omega t}}{\kappa - \eta} d\eta + \int \int_{\Delta C^+} d\kappa F(\kappa; \mu, \nu) \frac{1}{2\pi i} \oint_{\partial C} \frac{e^{-\eta x + i\omega t}}{\kappa - \eta} d\eta \quad x > 0$$

Evaluating the residues yields

$$f(x, \mu, \nu, t) = \sum_{\ell^+=1}^{L/2} \frac{(F_K^\dagger, S/\mu\nu)}{(F_K^\dagger, F_K)} F(K; \mu, \nu) e^{-Kx + i\omega t} + \int_{\Delta C^+} F(K; \mu, \nu) e^{-Kx + i\omega t} dK \quad x > 0 \quad (\text{III-38})$$

But this is identical to the expression obtained by separation of variables (III-27), hence verifying that the two methods are indeed equivalent.

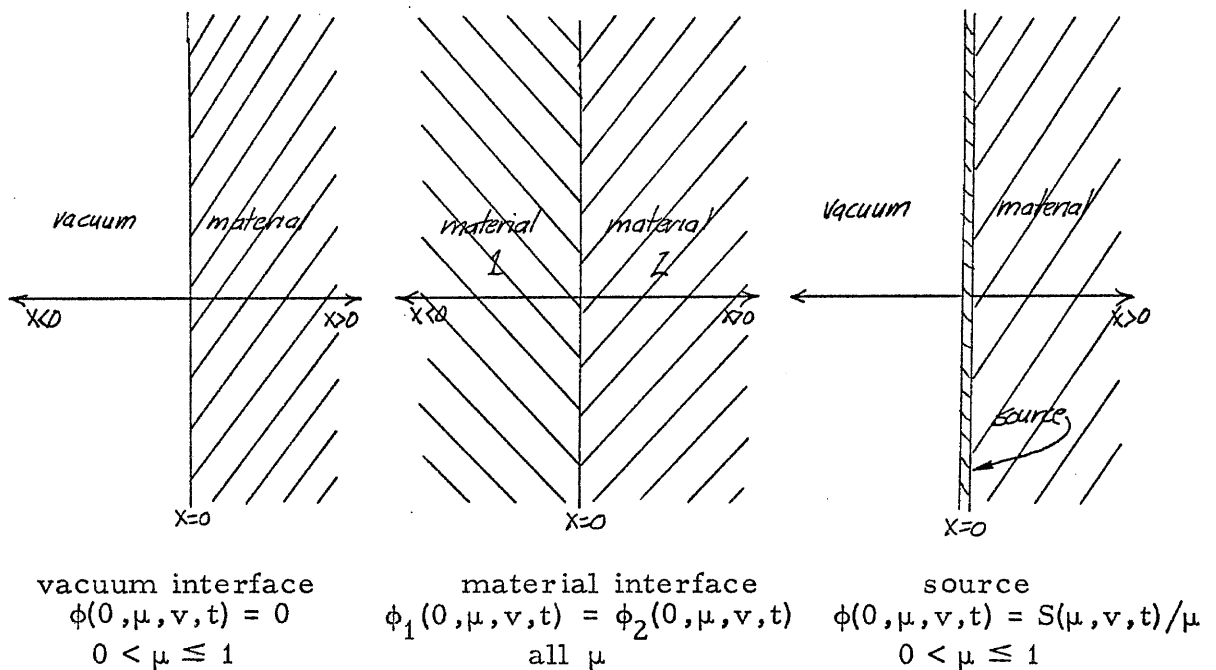
Actually once the mathematical framework of orthogonality and completeness has been developed, the spectral representation approach appears somewhat more direct for a specific problem involving wave propagation in noncrystalline media. However such a preference is largely a matter of taste, and both integral transforms and spectral representation will be used in the latter stages of this thesis.

IV. THE SOLUTION OF HALF-RANGE BOUNDARY VALUE PROBLEMS

A. INTRODUCTION

1. Half-Range Boundary Conditions

By "half-range" problems, one is referring to boundary value problems in which an eigenvalue expansion over only half of the spectrum $\sigma(A)$, $\text{Re}\{\kappa\} > 0$ or $\text{Re}\{\kappa\} < 0$, is required. These arise quite frequently when one wishes to consider one-dimensional transport in the presence of boundaries since the three typical boundary conditions placed on the neutron flux $\phi(x, \mu, v, t) = v f(x, \mu, v, t)$ are



These boundary conditions coupled with the semi-infinite geometry will necessitate eigenfunction expansions over only half of the range of κ .

Thus our immediate task from a theoretical viewpoint is two-fold: i) to verify that one can indeed expand a solution in a half-range expansion of the eigenfunctions $\{F(\kappa; \mu, \nu)\}$ and ii) to provide a prescription for calculating the expansion coefficients. As we shall demonstrate below, this task is rather futile for all but very simple models of the scattering kernel.

2. Difficulties with the General Theory

In analogy to the full-range theorem, one would like to show that the set of eigenfunctions $\{F(\kappa; z): \kappa \in \Delta\sigma_p \cup \Delta C\}$ is complete for the class of all functions defined in a simply connected subset ΔC of C and contained in $\mathcal{L}_1(\overline{\Delta C})$. [Here ΔC is that part of C such that $\text{Re}\{\kappa\} > 0$.] Now following the approach of Case⁽²⁴⁾ and Cercignani⁽²⁵⁾, one would find that the proof hinges on finding a quantity $X(z)$ such that

$$\left[1 + \pi T_C [K(\zeta, u) \cdot] \frac{\zeta}{z} \right] \frac{\partial X}{\partial \bar{z}} = K(z, u) X(z) \quad z \in \Delta C$$

$$\frac{\partial X}{\partial \bar{z}} = 0 \quad z \notin \overline{\Delta C}$$

(IV-1)

This is the analogue to the Riemann-Hilbert problem encountered in one-velocity transport theory⁽²⁴⁾. However (IV-1) is considerably more complicated in that it is a "generalized Hilbert problem" in the sense that generalized analytic functions are involved. Furthermore the unknown $X(z)$ is an operator. Such "operator Hilbert problems" have defied solution in stationary transport theory and have forced

previous authors to consider various approximations [multigroup treatments, n-term degenerate kernels⁽⁴⁴⁾, or finite polynomial expansions⁽⁴⁵⁾]. However even these approximations lead to a "matrix Hilbert problem" for the matrix $\underline{\underline{X}}(z)$ whose solution is still rather formidable.

It is important to stress that our interest in such a half-range theorem is not so much one of proving completeness [we would be surprised if the eigenfunctions did not have this property], but rather in providing some technique to evaluate the coefficients in the eigenfunction expansion. Even the more recent half-range orthogonality methods⁽⁴⁶⁾ rely upon the solution of (IV-1). Alternative techniques such as integral transform methods⁽¹⁸⁾ also appear to lead eventually to the difficulties encountered in solving (IV-1).

Thus until more basic theory is developed towards the solution of half-range boundary value problems in velocity-dependent transport theory, we appear to be limited to those very simple models of the scattering kernel for which a half-range theorem can be given. It is towards one of these models that we now direct our attention.

B. EIGENFUNCTION EXPANSION METHODS FOR A SYNTHETIC KERNEL MODEL

1. Introduction

Alerted to the difficulty of extending our general theory to half-range problems, we now retreat to a much simpler model which can be treated by existing techniques. It shall be assumed that the scattering kernel can be approximated by an isotropic one-term

separable kernel, or "synthetic kernel," of the form

$$\Sigma_s(v' \rightarrow v, \mu' \rightarrow \mu) = \frac{\beta}{2} \Sigma_s(v) v M(v) \Sigma_s(v') \quad (IV-2)$$

$$\frac{1}{\beta} \equiv \int_0^{\infty} dv v \Sigma_s(v) M(v)$$

where we further assume that $\Sigma_s(v)$ is monotonically decreasing in v . This model, due originally to Corngold, preserves detailed balance, yet integrates to give the correct total scattering cross-section.

The eigenvalue problem (II-5) then becomes

$$[i\omega + v \Sigma_t(v) - \kappa \mu v] F(\kappa; \mu, v)$$

$$= \frac{\beta}{2} \Sigma_s(v) v M(v) \int_{-1}^{+1} d\mu' \int_0^{\infty} dv' v' \Sigma_s(v') F(\kappa; \mu', v') \quad (IV-3)$$

or in the notation of section (III-A),

$$(z - \kappa) F(\kappa; z) = g(z) \int_C \int h(z') F(\kappa; z') dz' \quad (IV-4)$$

where

$$g(z) \longleftrightarrow \frac{\beta}{2} \frac{\Sigma_s(v) v M(v)}{\mu v} \quad h(z) \longleftrightarrow v \Sigma_s(v) \left| \frac{\partial(\mathcal{L}, \varphi)}{\partial(\mu, v)} \right|$$

Thus adapting our earlier treatment, the eigenfunctions become

Discrete Eigenfunctions:

$$F(\kappa_\ell; z) = \frac{g(z)}{z - \kappa_\ell} \quad \kappa_\ell \notin C \quad (IV-5)$$

where we choose to normalize $\int \int h(z) F(\kappa; z) dz = 1$. Note that this yields the dispersion relation for the discrete eigenvalues as

$$\Lambda(\kappa) \equiv 1 - \int_C \int \frac{h(z)g(z)}{z - \kappa} dz = 1 - \frac{\beta}{2} \int_{-1}^{+1} d\mu \int_0^\infty dv \frac{v^2 M(v) [\Sigma_s(v)]^2}{[i\omega + v\Sigma_t(v) - \kappa\mu v]} = 0 \quad (\text{IV-6})$$

Continuum Eigenfunctions:

$$F(\kappa; z) = \frac{g(z)}{z - \kappa} + \lambda(\kappa) \delta(\kappa - z) \quad \kappa \in \mathbb{C} \quad (\text{IV-7})$$

and the normalization yields

$$\lambda(\kappa) = \frac{1}{h(\kappa)} \left[1 - \int_C \int \frac{h(z)g(z)}{z - \kappa} dz \right] = \Lambda(\kappa)/h(\kappa) \quad (\text{IV-8})$$

The orthogonality relations become

$$\int_C \int \frac{h(z)}{g(z)} F(\kappa_\ell; z) F(\kappa_m; z) dz = N_\ell \delta_{\ell m} \quad \kappa_\ell \in \sigma_p(A) \quad (\text{IV-9})$$

where

$$N_\ell \equiv \int_C \int \frac{h(z)g(z)}{(z - \kappa_\ell)^2} dz = \int_{-1}^{+1} d\mu \int_0^\infty dv \frac{\mu v v^2 M(v) [\Sigma_s(v)]^2}{[i\omega + v\Sigma_t(v) - \kappa_\ell \mu v]^2} \quad (\text{IV-10})$$

and

$$\int_C \int \frac{h(z)}{g(z)} F(\kappa; z) F(\kappa'; z) dz = N(\kappa) \delta(\kappa - \kappa') \quad \kappa \in \mathbb{C} \quad (\text{IV-11})$$

where

$$N(\kappa) = \frac{\Lambda^2(\kappa)}{h(\kappa)g(\kappa)} \quad (\text{IV-12})$$

2. Completeness Theorems

Of course the earlier full-range theorem applies to this model

THEOREM VIa: The set of functions $\{F(\kappa; z); \kappa \in \sigma(A)\}$ is complete for the class of all functions $\psi(z) \in \mathfrak{L}_1(\overline{\mathbb{C}})$.

Proof: This theorem is proven as a subcase of the more general Theorem VI. But of greater importance is the fact that one can now prove a half-range theorem (after Cercignani⁽²⁵⁾):

THEOREM VIb: The set of functions $\{F(\kappa; z) : \kappa \in \Delta\sigma_p \cup \Delta C\}$ is complete for the class of all functions defined on a simply connected subset ΔC and contained in $\mathfrak{L}_1(\overline{\Delta C})$.

Proof: Since it can be shown that $\Lambda(\kappa)$ possesses at most two symmetric zeros, $\pm\kappa_0$, we need only evaluate a_{0+} and $A(\kappa)$ in

$$\psi(z) = a_{0+}F(\kappa_0; z) + \iint_{\Delta C} A(\kappa)F(\kappa; z) d\kappa \quad (IV-13)$$

In the usual manner, define

$$\psi'(z) = \psi(z) - a_{0+}F(\kappa_0; z) \quad (IV-14)$$

Now substitute (IV-7), (IV-8), and (IV-14) into (IV-13) to find

$$h(z)\psi'(z) = h(z)g(z) \iint_{\Delta C} \frac{A(\kappa)}{z-\kappa} d\kappa + A(z) \left[1 - \iint_C \frac{h(z)g(z)}{z-\kappa} dz \right]$$

or (IV-15)

$$h\psi' = \pi hg T_{\Delta C} A + A [1 + \pi T_C hg] \quad (IV-16)$$

To solve this integral equation for $A(z)$, consider the associated generalized Riemann-Hilbert problem for the function $X(z)$

$$\begin{aligned} [1 + \pi T_C hg] \frac{\partial X}{\partial \bar{z}} &= \pi hg X & z \in \Delta C \\ \frac{\partial X}{\partial \bar{z}} &= 0 & z \notin \overline{\Delta C} \end{aligned} \quad (IV-17)$$

If such an $X(z)$ can be found, then (IV-16), (IV-17) and the lemma on

p. 70 can be used to find

$$T_{\Delta C} A = \frac{1}{X} T_{\Delta C} \left[\frac{Xh\psi'}{1 + \pi T_C hg} \right] \quad (IV-18)$$

again provided $X(z) \neq 0$ for $z \in \overline{\Delta C}$ and $T_{\Delta C} A \rightarrow 0$ as $z \rightarrow \infty$.

Of course in contrast to the operator or matrix version of (IV-16), we can now solve (IV-16) directly by applying Theodorescu's formula⁽⁴³⁾ to find

$$X(z) = \varphi(z) \exp \left\{ T_{\Delta C} \left[\frac{\pi hg}{1 + \pi T_C hg} \right] \right\} \quad (IV-19)$$

where $\varphi(z)$ is an analytic function for $z \notin \partial \Delta C$. On the boundary $\partial \Delta C$ we require $A(z) \in \mathcal{L}_1(\overline{\Delta C})$. To investigate this latter restriction, rewrite

$$T_{\Delta C} \left[\frac{\pi hg}{1 + \pi T_C hg} \right] = T_{\Delta C} \left\{ \frac{\partial}{\partial \bar{z}} [\log (1 + \pi T_C hg)] \right\} \equiv T_{\Delta C} \left[\frac{\partial}{\partial \bar{z}} L(z) \right] \quad (IV-20)$$

Now applying Green's theorem allows us to write

$$T_{\Delta C} \left[\frac{\pi hg}{1 + \pi T_C hg} \right] = \log (1 + \pi T_C hg) - \frac{1}{2\pi i} \int_{\partial \Delta C} \frac{\log (1 + \pi T_C hg)}{u - z} du \quad z \in \Delta C \quad (IV-21)$$

$$T_{\Delta C} \left[\frac{\pi hg}{1 + \pi T_C hg} \right] = -\frac{1}{2\pi i} \int_{\partial \Delta C} \frac{\log (1 + \pi T_C hg)}{u - z} du \quad z \notin \overline{\Delta C}$$

The branch of the log must be fixed at some point on $\partial \Delta C$. As we traverse $\partial \Delta C$, $\Delta \arg L(z) \Big|_{\partial \Delta C} = 2\pi i (\# \text{poles} - \# \text{zeros outside } \Delta C) = 2\pi i$

or 0 for the synthetic kernel model. Thus the presence of discrete spectra causes a discontinuity in $L(z)$ on $\partial\Delta C$. But from Vekua⁽⁴³⁾, the only points where $L(z)$ can be discontinuous are the angular points of $\partial\Delta C$, e.g. $z = \infty$ or $z = [\Sigma_t(v)]_{\min}$. For monotonic $\Sigma_t(v)$ one can show that the only point of discontinuity is at $z = \infty$.

Now we can use the theory of Muskhelishvili⁽⁵⁸⁾ on the line integrals in (IV-21) [since they are Cauchy integrals] to show

$$T_{\Delta C} \left[\frac{\pi h g}{1 + \pi T_C h g} \right] = \begin{array}{ll} O(1) & \text{no discrete spectrum (Case I)} \\ O(1) + \log(-z) & \text{discrete spectrum (Case II)} \end{array}$$

In case I, choose $\varphi(z) = 1$. In case II, use (IV-19) to pick

$$\frac{X}{z\varphi} = O(1) \Rightarrow \varphi(z) = \frac{1}{z} \Rightarrow A(z) \in \mathcal{L}_1(\overline{\Delta C})$$

Thus (IV-19) becomes

$$X(z) = z^{-h} \exp \left\{ T_{\Delta C} \left[\frac{\pi h g}{1 + \pi T_C h g} \right] \right\} \quad \text{(IV-22)}$$

where $h = \begin{cases} 0 & \text{case I} \\ 1 & \text{case II} \end{cases}$

Now for case II, $h = 1$ and the behavior of $X(z)$ at infinity can be used to evaluate the discrete coefficient a_{o+} . Since $X(z) = O(1/z)$ as $z \rightarrow \infty$, this requires

$$\lim_{z \rightarrow \infty} \left\{ z T_{\Delta C} \left[\frac{X\psi'h}{1 + \pi T_C h g} \right] \right\} = 0 \quad \text{(IV-23)}$$

But since

$$\begin{aligned} T_{\Delta C} \left[\frac{X\psi'h}{1+\pi T_C hg} \right] &= \left(\frac{1}{z} \right) \frac{1}{\pi} \iint_{\Delta C} \frac{X\psi'h}{1+\pi T_C hg} d\kappa \\ &+ \left(\frac{1}{z^2} \right) \frac{1}{\pi} \iint_{\Delta C} \frac{X\psi'h\kappa}{1+\pi T_C hg} d\kappa + o\left(\frac{1}{z^3}\right) \end{aligned}$$

(IV-23) implies

$$\iint_{\Delta C} \frac{X(\zeta)\psi'(\zeta)h(\zeta)}{\Lambda(\zeta)} d\zeta = 0 \quad (IV-24)$$

Now using (IV-14), we find from (IV-24)

$$\begin{aligned} a_{o+} &= \frac{\iint_{\Delta C} \frac{X(\zeta)\psi(\zeta)h(\zeta)}{\Lambda(\zeta)} d\zeta}{\iint_{\Delta C} \frac{X(\zeta)g(\zeta)h(\zeta)}{(\zeta-\kappa_o)\Lambda(\zeta)} d\zeta} = \frac{\iint_{\Delta C} \frac{X(\zeta)\psi(\zeta)h(\zeta)}{\Lambda(\zeta)} d\zeta}{-T_{\Delta C} \left[\frac{\pi Xgh}{1+\pi T_C hg} \right]_{\kappa_o}} \quad (IV-25) \end{aligned}$$

This a_{o+} is so determined for any $\psi(\zeta) \in \mathfrak{L}_1(\overline{\Delta C})$.

One can also solve for the continuum expansion coefficient $A(z)$ from (IV-18) as

$$\begin{aligned} A(z) &= \frac{\partial}{\partial z} \left\{ \frac{1}{X} T_{\Delta C} \left[\frac{Xh\psi'}{1+\pi T_C hg} \right] \right\} \\ &= \frac{h\psi'}{1+\pi T_C hg} - \frac{\pi hg}{[1+\pi T_C hg]X} T_{\Delta C} \left[\frac{Xh\psi'}{1+\pi T_C hg} \right] \quad (IV-26) \end{aligned}$$

Hence the existence of a_{o+} and $A(\kappa)$ has been demonstrated for arbitrary $\psi(z) \in \mathfrak{L}_1(\overline{\Delta C})$ by actual evaluation. Furthermore the converse statement of the lemma on p. 70 implies that such an evaluation is unique. Thus the theorem has been proved.

3. Identities for the $X(z)$ Functions

To facilitate the solution of half-range boundary value problems, one can derive several identities among the $X(z)$ functions.

These are summarized below:

$$X(z) = - T_{\Delta C} \left[\frac{\pi X g h}{\Lambda} \right] \quad h = 1 \quad (\text{IV-27})$$

$$X(z) = 1 - T_{\Delta C} \left[\frac{\pi X g h}{\Lambda} \right] \quad h = 0 \quad (\text{IV-27b})$$

$$X(z)X(-z) = \frac{\Lambda(z)}{\gamma(z^2 - \kappa_0^2)} \quad \text{where } \gamma \equiv \lim_{z \rightarrow \infty} \Lambda(z) \quad h=1 \quad (\text{IV-28a})$$

$$X(z)X(-z) = \frac{1}{\gamma} \Lambda(z) \quad h=0 \quad (\text{IV-28b})$$

$$X(z) = - T_{\Delta C} \left[\frac{\pi g h}{\gamma(\zeta^2 - \kappa_0^2)X(-\zeta)} \right] \quad h = 1 \quad (\text{IV-29a})$$

$$X(z) = 1 - T_{\Delta C} \left[\frac{\pi g h}{\gamma X(-\zeta)} \right] \quad h = 0 \quad (\text{IV-29b})$$

$$\frac{X(z_2) - X(z_1)}{z_2 - z_1} = \int \int_{\Delta C} \frac{X(\zeta)g(\zeta)h(\zeta)}{(\zeta - z_1)(\zeta - z_2)\Lambda(\zeta)} d\zeta \quad h = 0, 1 \quad (\text{IV-30})$$

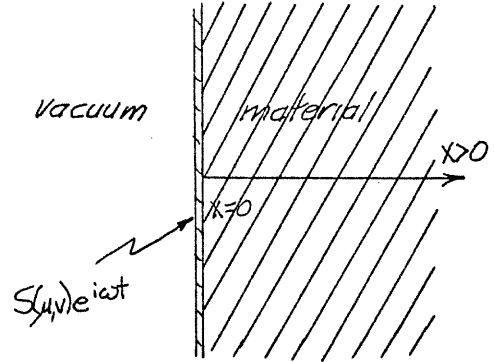
[By introducing suitable notation, these identities can be adapted to the two-adjacent half-space problem.]

4. Solution of the Wave Albedo Problem

To illustrate how the standard half-range problems of neutron transport can now be solved, we consider the problem of a modulated source $S(\mu, \nu)e^{i\omega t}$ incident upon the boundary of a half-space for

$x > 0$. From (IV-A-1), the boundary conditions are

- i) $\lim_{x \rightarrow \infty} |f(x, \mu, \nu, t)| = 0$
- ii) $f(0, \mu, \nu, t) = \frac{S(\mu, \nu)}{\mu \nu} e^{i\omega t}$
 $0 < \mu \leq 1$



The solution to the synthetic kernel modeled Boltzmann equation subject to these boundary conditions shall be sought as the eigenfunction expansion

$$f(x, \mu, \nu, t) = a_{0+} F(\kappa_0; \mu, \nu) e^{-\kappa_0 x + i\omega t} + a_{0-} F(-\kappa_0; \mu, \nu) e^{+\kappa_0 x + i\omega t} + \int_C \int A(\kappa) F(\kappa; \mu, \nu) e^{-\kappa x + i\omega t} d\kappa \quad (IV-31)$$

[where we have assumed that $\omega < \omega^*$ so that a discrete eigenvalue exists]. Applying the boundary condition as $x \rightarrow \infty$ implies $a_{0-} = A(\kappa) \equiv 0, \kappa \in \Delta C^-$. Furthermore, applying the source condition yields, in the z -notation,

$$S(z) = a_{0+} F(\kappa_0; z) + \int_{\Delta C^+} A(\kappa) F(\kappa; z) dz \quad z \in \Delta C^+ \quad (IV-32)$$

But this is identical to the form of the expansion considered in the half-range Theorem VIb, provided we take $\psi(z) = S(z)$. Hence one finds

$$a_{o+} = \frac{\int \int \frac{X(\zeta)S(\zeta)h(\zeta)}{\Lambda(\zeta)} d\zeta}{-T_{\Delta C} \left[\frac{\pi X g h}{1 + \pi T_C g h} \right]_{\kappa_o}} = - \frac{\pi T_{\Delta C} \left[\frac{X h S}{\Lambda} \right]}{X(\kappa_o)} \quad (\text{IV-33})$$

where identity (IV-27a) has been used. Furthermore from (IV-26) and identity (IV-30)

$$A(\kappa) = \frac{h(\kappa)S(\kappa)}{\Lambda(\kappa)} - \frac{\pi h(\kappa)g(\kappa)}{\Lambda(\kappa)X(\kappa)} \left\{ \left[\frac{X(\kappa_o) - X(\kappa)}{\kappa_o - \kappa} \right] + T_{\Delta C} \left[\frac{X h S}{\Lambda} \right] \left[1 - \frac{\kappa}{\kappa - \kappa_o} \frac{X(\kappa)}{X(\kappa_o)} \right] \right\} \quad (\text{IV-34})$$

PART II

APPLICATION OF THE GENERAL THEORY
TO THE NEUTRON WAVE EXPERIMENT

V. THE NEUTRON WAVE EXPERIMENT

A. DESCRIPTION OF THE EXPERIMENTS

1. Introduction

As mentioned earlier, the neutron wave experiment involves the use of a modulated neutron source to excite wave-like disturbances in the neutron distribution within a medium. In general this disturbance is composed of a superposition of plane wave modes. However sufficiently far from the source, one of these modes should dominate. The goal of the experiment is to determine the complex wave number $\kappa = \alpha + i\xi$ of this dominant mode at a fixed frequency by measuring its exponential attenuation factor α and its linear phase shift per unit length, ξ .

From the general theory of the propagation process, it is evident that each of the plane wave modes corresponds to an eigenfunction, $F(\kappa; \mu, \nu) e^{-\kappa x + i\omega t}$, of the Boltzmann wave operator A . Stated mathematically, the experimental goal is to measure the discrete eigenvalue κ_0 with least real part α_0 (damping) at a given frequency since this should correspond to the dominant mode at large distances from the source.

A series of such measurements is made at various source frequencies in order to obtain information about the behavior of $\kappa_0(\omega)$ with frequency. That is, the experiment essentially measures the "dispersion curve" of the fundamental eigenvalue $\kappa_0(\omega)$ in the κ -plane. Presumably this measurement can then be compared to theoretical calculations of the dispersion curve.

Neutron wave experiments have been performed in a variety of systems--both single and multiregion, multiplying and moderating. However for reasons of expediency, we shall only concern ourselves here with wave experiments conducted in one-region, moderating systems. To date, the only experiments of this type have been those conducted in graphite and D_2O parallelepipeds by Perez^(3,4) et al. at the University of Florida and by Takahashi and Sumita⁽⁵⁾, at the University of Osaka, Japan. It is useful to examine the experimental techniques involved in making these measurements before continuing on to their analysis.

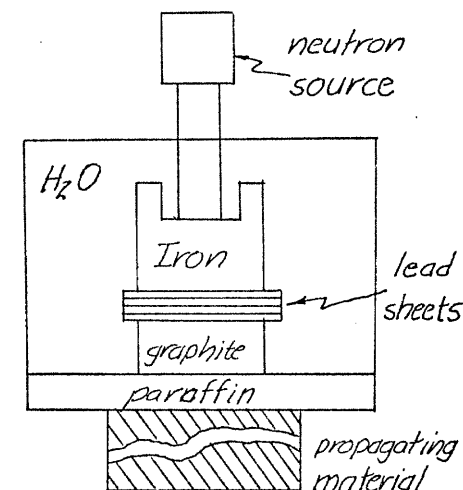
2. Experimental Techniques

There are actually two techniques available for performing the neutron wave experiment. One can either use a modulated source of fixed frequency ω , or one can use a pulsed source whose time behavior can then be analyzed into its Fourier frequency components. Both techniques have been used in performing the wave experiments in graphite and D_2O [although recent communications have indicated that the latter technique is preferable⁽⁵⁴⁾].

The actual sources have been either Crockoft-Walton or Van de Graff accelerators producing neutrons of several Mev in energy. These initial fast source neutrons are directed through a thermalizing tank to produce a thermal neutron source upon the boundary of the system of interest. A cadmium difference technique is used to subtract out any remaining epithermal flux background.

He^3 or BF_3 detectors are used to measure the resulting flux

at various locations within the propagating medium. More specifically, the phase shift and signal amplitude are measured relative to a reference detector as functions of position at a given frequency ω . Then least squares fitting is used to determine the attenuation coefficient $\alpha(\omega)$ and the linear phase shift $\xi(\omega)$ for



Experimental Schematic

this source frequency [or Fourier frequency component] . By repeating this procedure for various source frequencies [or Fourier components] , the behavior of $\kappa(\omega) = \alpha(\omega) + i\xi(\omega)$ as a function of ω is determined.

It has been customary to use these data to determine the coefficients of a power series expansion of $\kappa_0^2(\omega)$ similar to equation (II-47), and then these coefficients are compared with theoretical predictions. However the experimentally measured dispersion curve can also be directly compared to the theoretically calculated dispersion curve for the fundamental eigenvalue.

3. Goals for a Satisfactory Theory

The primary goal of the second part of this thesis is to demonstrate the validity of the general theory by applying it to understand and interpret existing experiments. Several stages of analysis are necessary. First, the solution must be obtained for a boundary

value problem which is a reasonable mathematical model of the experiments. This solution will be composed of contributions from various portions of the eigenvalue spectrum $\sigma(A)$. One must determine whether the discrete plane wave modes corresponding to $\sigma_p(A)$ dominate for any ranges of parameters, and to what degree the remaining spectrum contributions "contaminate" the measurements of the experimenters.

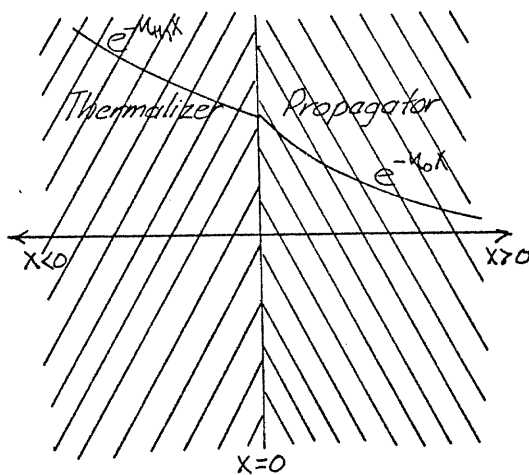
It is also of some importance to examine the manner in which experimental and theoretical results may be presented and compared. And certainly one should also study the theoretical connection between the experimental data and interesting physical parameters.

B. CONSTRUCTION OF A SUITABLE MATHEMATICAL MODEL

Of course to apply the theory in its most general and exact form is not only extremely difficult, but also of questionable value if one merely desires qualitative understanding of the experiments and not quantitative prediction of measured results. We shall therefore develop a simple mathematical model of the neutron wave experiment which retains most of the interesting physical and mathematical features of the exact description, yet allows a reasonably simple application of the theory of the first part of the thesis. In doing so, we expect only a qualitative agreement between the experimental data and numerical calculations from our modeled theory. However extensions will be indicated which should yield better quantitative agreement.

1. Choice of the Boundary Value Problem

We would now like to approximate the experimental geometry [which includes a complicated thermalizing tank in addition to the graphite or D_2O parallelepiped] by one more amenable to analysis by transport theory. As in our earlier analysis, it will be convenient to consider initially one-dimensional problems; then later the effects of transverse dimension can be introduced by appropriate modification of the spectrum $\sigma(A)$. Within this context, it appears that the most realistic problem which could be treated by transport theory would be the two-adjacent half-space problem in which one imagines a source at infinity exciting the fundamental wave mode in the thermalizing medium, and this in turn acting as the source at the boundary of the propagating medium.¹

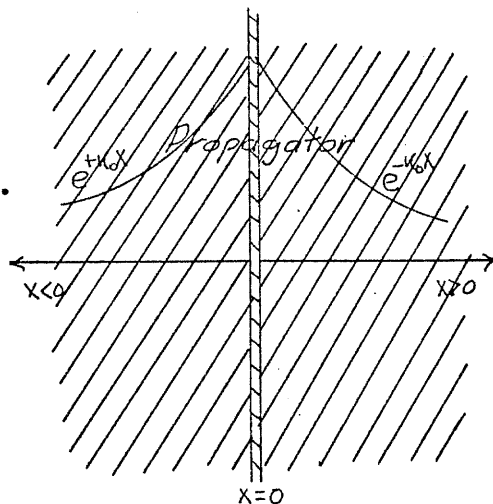


However the complications of the two adjacent half-space problem, although solvable, would tend to obscure the desired results. Since the experiment only involves measurements "far" [greater than several mean free paths] from the source, it is reasonable to

¹It is important to note that the thermalizing tank creates a thermal source distributed in all angles and speeds at the interface. It is therefore unrealistic to approximate this source by a beam source or a given source distribution on a free surface.

consider instead an oscillating plane source of given distribution $S(\mu, \nu)$ at the origin of an infinite medium of the propagating material.

Indeed this full-space problem, although mathematically much simpler, gives a better description of the true source conditions than the half-space problem with the



source at a free boundary [which has recently been considered by others in the synthetic kernel approximation⁽³⁷⁾]. And by suitably adjusting the source distribution, it is even possible to examine the wave structure near the source.

2. Modeling of the Scattering Kernel (Modified Synthetic Kernel Model)

It has been mentioned in the earlier analysis that the most direct manner by which one may simplify the general theory, and yet retain most of the interesting features of the transport process, is to approximate the form of the scattering kernel $\Sigma_s(\nu' \rightarrow \nu, \mu' \rightarrow \mu)$. However we recognize that the simple synthetic kernel approximation made in section (IV-B) is inadequate for materials such as graphite because of their crystalline structure. The complications arising in the treatment of polycrystals have been discussed in detail in section (II-C). These crystalline effects play an extremely important role in the transport of neutrons in these materials and cannot be ignored.

Therefore we shall adopt the simplest possible model of the scattering kernel which retains the features of crystalline media. This model, also due to Corngold⁽⁵⁵⁾, approximates the inelastic scattering by a one-term separable kernel while modeling the elastic scattering by a Dirac δ -function

$$\Sigma_s(v' \rightarrow v, \mu' \rightarrow \mu) = \frac{\beta}{2} \Sigma_i(v) v M(v) \Sigma_i(v') + \frac{\Sigma_e}{2} (v) \delta(v-v') \quad (V-1)$$

$$\text{where } \frac{1}{\beta} \equiv \int_0^{\infty} dv v M(v) \Sigma_i(v)$$

and where $\Sigma_i(v)$ and $\Sigma_e(v)$ are the cross-sections for inelastic and elastic scattering. Since the structure of these cross-sections is rather complicated, we chose to model them by assuming: i) $1/v$ absorption, ii) only one Bragg diffraction peak such that $\Sigma_e(v) = H(v - v_B) \Sigma_e(v)$, and iii) for $v < v_B$, $\Sigma_t(v) = \Sigma_t^0/v$ [which is reasonable to within current cross-section measurement accuracy]. Notice that the modified synthetic kernel model (V-1)

- i) exhibits the property of detailed balance
- ii) preserves the correct total cross-section [and thus insures conservation of neutrons]
- iii) gives the proper physics of elastic scattering, as well as imitates the non-compact nature of the true elastic scattering operator
- iv) will yield at most two discrete eigenvalues, $\pm K_0$, which is in agreement with more detailed calculations performed for graphite^(1,2)
- v) can be reduced to the synthetic kernel for studying non-crystalline media by setting $\Sigma_e(v) \equiv 0$, $\Sigma_i(v) \equiv \Sigma_s(v)$.

The more obvious limitations of this model can also be listed

- i) the assumption of isotropic scattering
- ii) a rather crude modeling of coherent scattering
- iii) the description of the moderator as a perfect thermalizer, i. e. only one inelastic collision is sufficient to throw the neutron into thermal equilibrium with the moderator. [Since we expect the neutron wave velocity spectrum to be frequency heated, this crude treatment of the higher velocity form of the kernel should cause some discrepancy at large ω .]
- iv) The fact that the elastic term in (V-1) is non-degenerate will greatly complicate the extension of this model to problems with half-range geometries.

We shall now use this model in the general theory to obtain an analytic solution of the boundary value problem outlined on p. 97. Most of our attention will be directed towards the study of wave propagation in polycrystalline media [i. e. graphite] because of its more interesting features. The study of noncrystalline materials such as D_2O is straightforward using this modeled theory, and only the results will be presented in Chapter VII.

VI. APPLICATION OF THE MODELED THEORY

A. ANALYSIS OF THE EIGENVALUE SPECTRUM $\sigma(A)$

First we shall examine the simplifications that follow by using the modified synthetic kernel (V-1) in the general theory for polycrystalline media (section II-C). The eigenvalue problem (II-24) now reduces to

$$[i\omega + v\Sigma_t(v) - \kappa\mu v] F(\kappa; \mu, v) = \frac{\beta}{2} \Sigma_1(v) v M(v) \bar{f}(\kappa) + \frac{v\Sigma_e(v)}{2} N(\kappa; v) \quad (\text{VI-1})$$

$$\text{where} \quad \bar{f}(\kappa) \equiv \int_{-1}^{+1} d\mu \int_0^{\infty} dv v \Sigma_1(v) F(\kappa; \mu, v) \quad (\text{VI-2})$$

$$N(\kappa; v) \equiv \int_{-1}^{+1} d\mu F(\kappa; \mu, v)$$

One can now analyze (VI-1) to determine the eigenvalue spectrum for this model.

1. The Continuous Spectrum C

Since the elastic scattering angular probability $P(\mu' \rightarrow \mu) = \frac{1}{2}$ for this model [and thus certainly $P(\mu' \rightarrow \mu) \in \mathcal{L}_2(I_1)$], the theory of section II-C indicates that $C \equiv \{ \kappa: \kappa = \frac{i\omega}{\mu v} + \frac{\Sigma_t(v)}{\mu}, \mu \in [-1, +1], v \in [0, \infty) \}$. But notice that since $\Sigma_t(v)$ has a discontinuity at $v = v_B$, the area continuum C becomes split into two disjoint sets

$$C_{BB} \equiv \{ \kappa: \kappa = \frac{i\omega + \Sigma_t^0}{\mu v}, \mu \in [-1, +1], v \in [0, v_B] \}$$

(BB - Below Bragg)

$$C_{AB} \equiv \{ \kappa: \kappa = \frac{i\omega}{\mu v} + \frac{\Sigma_t(v)}{\mu}, \mu \in [-1, +1], v \in [v_B, \infty) \}$$

(AB - Above Bragg)

where for C_{BB} we have used the specific assumption that $\Sigma_t(v) = \Sigma_t^0/v$ for $v < v_B$. Notice furthermore that while C_{AB} remains an area in the κ -plane, the $1/v$ cross-section behavior below the Bragg velocity v_B has caused C_{BB} to degenerate into a line continuum (Figure 6). This fact will be of importance to the later analysis.

2. The Elastic Continuum Γ

If we use the modified synthetic kernel (V-1) in equation (II-22), we find that the elastic continuum Γ is given as the set of all κ such that

$$\Lambda_e(\kappa;v) \equiv 1 - \frac{\Sigma_e(v)}{2\kappa} \ln \left[\frac{i\omega + v\Sigma_t(v) + \kappa v}{i\omega + v\Sigma_t(v) - \kappa v} \right] = 0 \quad v \in [0, \infty) \quad (VI-3)$$

Notice that since $\Sigma_e(v) = 0$ for $v < v_B$, (VI-3) tells one to plot the locus of the zeros $\kappa_e(v)$ of $\Lambda_e(\kappa;v)$ for all $v \in [v_B, \infty)$. These will sweep out a curve Γ in the first and third quadrants as shown on p. 104.

Actually since (VI-3) is essentially identical to the one-velocity dispersion law (A-5), much of the analysis in Appendix A can be suitably adapted to conclude:

- i) The principle of the argument can be used to show that $\Lambda_e(\kappa;v)$ has two complex zeros, $\pm \kappa_e(v)$, symmetric about the origin, for $\omega < \frac{\pi}{2} \mu_0(v)v\Sigma_e(v)$. As v varies between v_B and ∞ , these zeros trace out the two symmetric curves Γ in the κ -plane.

For $\omega > \max_{v \in [v_B, \infty)} \left[\frac{\pi}{2} \mu_0(v)v\Sigma_e(v) \right]$, these curves vanish entirely into C_{AB} .

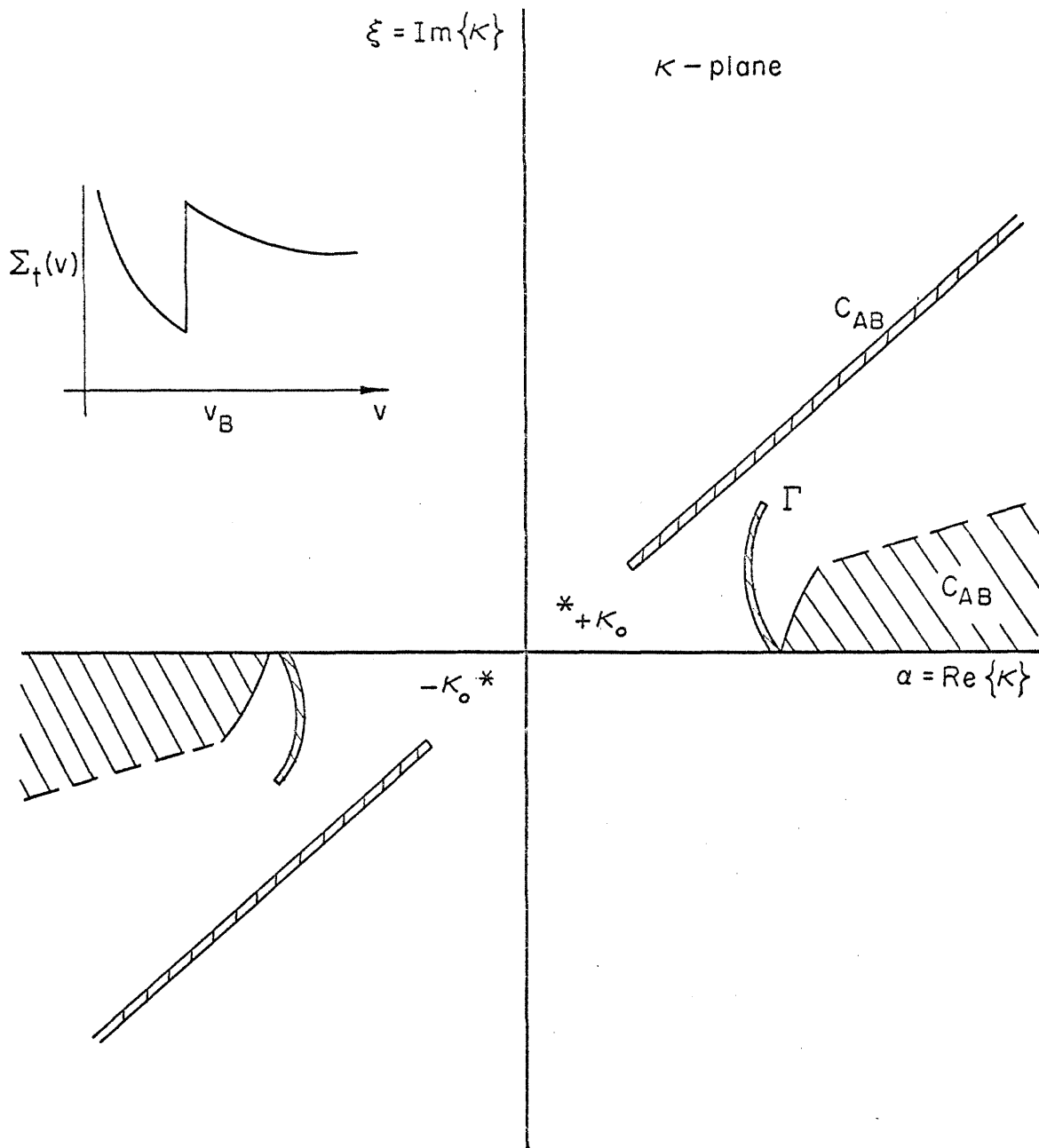


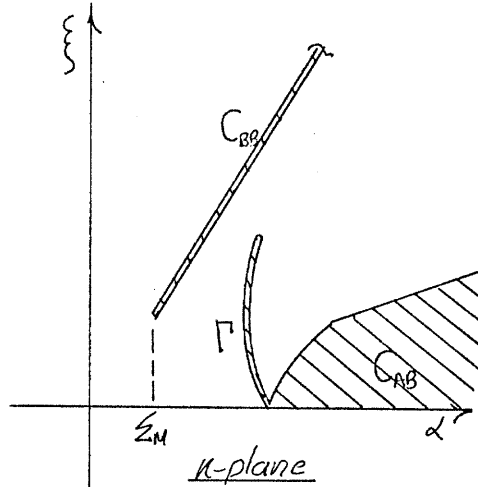
Figure 6. A Sketch of the Spectral κ -Plane for the Modified Synthetic Kernel Model

ii) Using power series expansions,

one can show that Γ lies always below C_{BB} and to the right of $\Sigma_M = \Sigma_t^0/v_B$ provided one requires

$\lim_{v \rightarrow \infty} \Sigma_e(v) = 0$. Fortunately this latter restriction is

demanding also by the physics of elastic scattering.



iii) The detailed shape and location of the Γ curves are extremely sensitive to the modeling of the cross-sections $\Sigma_e(v)$ and $\Sigma_t(v)$. Some sample plots of the Γ spectrum for various ω have been computed numerically for the cross-section modeling of graphite and are presented in Figure 7.

3. The Dispersion Law for Discrete Eigenvalues

One can use the modified synthetic kernel (V-1) to reduce the general dispersion law (II-30) for polycrystalline media to

$$\Lambda(\kappa) \equiv 1 - \int_{-1}^{+1} d\mu \int_0^{\infty} dv \frac{\frac{\beta}{2} v^2 M(v) [\Sigma_i(v)]^2}{[i\omega + v\Sigma_t(v) - \kappa\mu v] \Lambda_e(\kappa; v)} = 0 \quad \kappa \notin \text{CUF} \quad (\text{VI-4})$$

[Notice that by setting $\Sigma_e(v) = 0$ and $\Sigma_i(v) = \Sigma_s(v)$, one can also use (VI-4) to examine the usual synthetic kernel model (IV-2). This will be useful for the analysis of noncrystalline media.]

Thus to examine the point spectrum for the modified synthetic kernel model, we must search for the zeros of $\Lambda(\kappa)$ in those regions

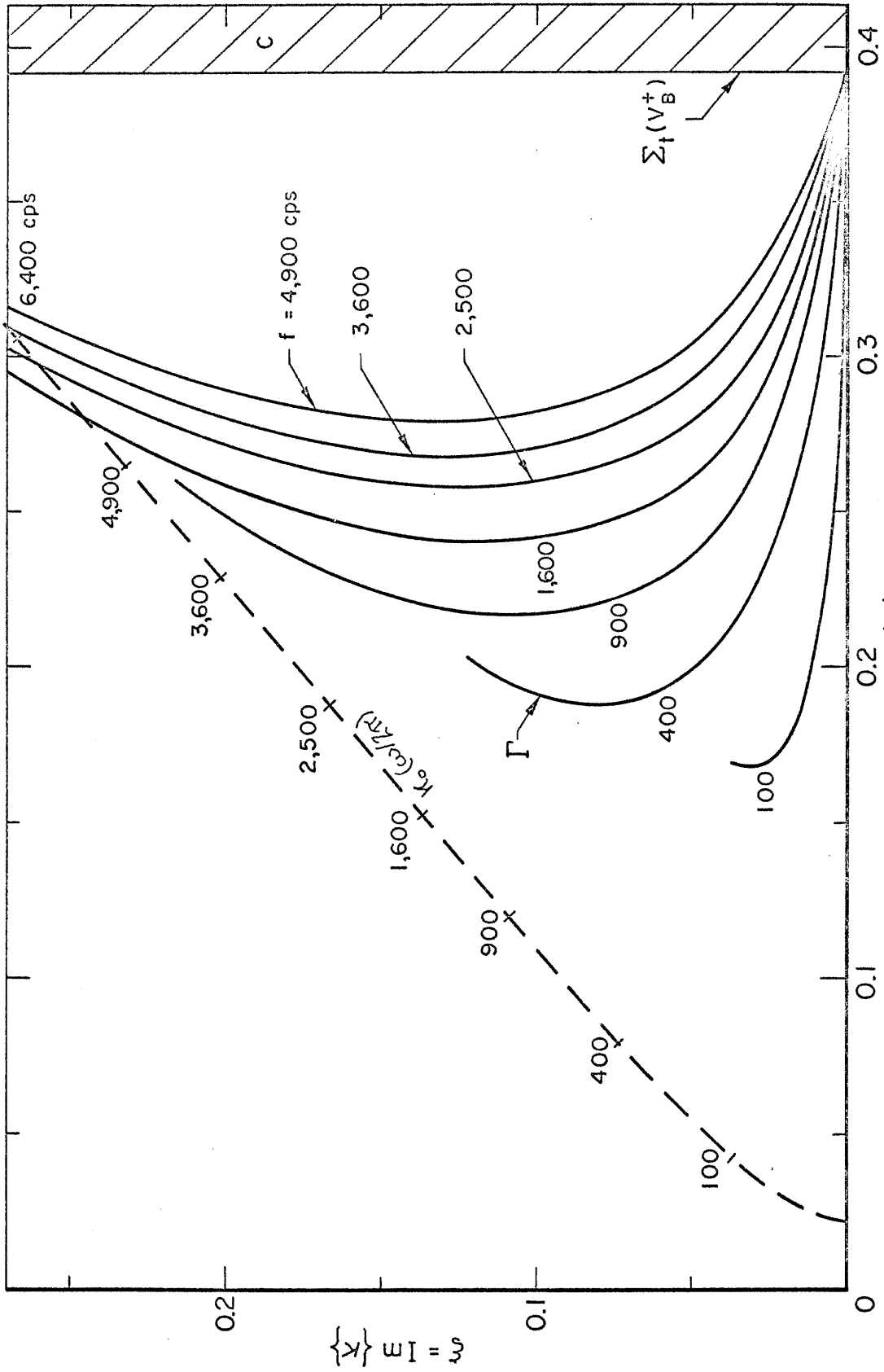


Figure 7. The Elastic Continuum for Graphite

of the κ -plane not contained in the eigenvalue continuum C or Γ . As in earlier analyses, we shall confine our discussion to the first quadrant, using the symmetry of the spectrum to infer the structure of the remaining quadrants.

a) Number of discrete eigenvalues: Because of the complicated structure of the κ -plane and the arbitrary forms of the cross-sections, it is rather difficult to apply the Principle of the Argument to determine the number of zeros of

$\Lambda(\kappa)$. However one can examine the $\omega = 0$ case rather easily.

Since this case corresponds to the diffusion length experiment, we know that any zeros of $\Lambda(\kappa)$ lie on the real axis between 0

and $\pm \Sigma_M$. One can easily show

that $\left. \frac{d\Lambda}{d\kappa} \right|_{\omega=0}$ is always negative

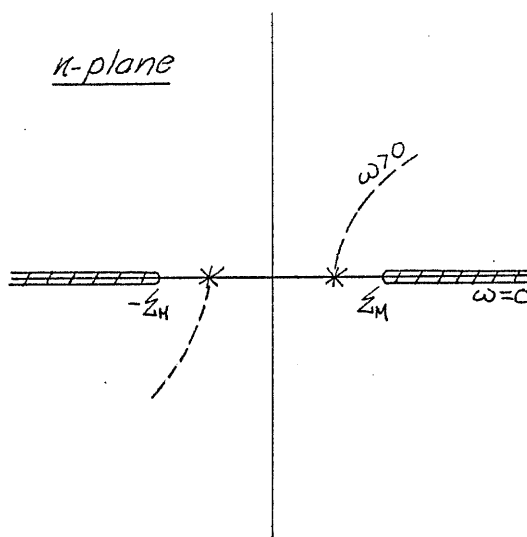
for $\kappa \in [0, \Sigma_M]$ (and $\left. \frac{d\Lambda}{d\kappa} \right|_{\omega=0} > 0$

for $\kappa \in [-\Sigma_M, 0]$). Thus since $\Lambda(\kappa)|_{\omega=0}$ must be monotonically de-

creasing on the interval, there can be at most one zero $\kappa_0 \in [0, \Sigma_M]$.

Since $\Lambda(\kappa)$ is analytic in $\kappa \notin C \cup \Gamma$ for $\omega > 0$, one can use the ideas of analytic continuation¹ to conclude that this zero moves off on the

axis into the κ -plane for $\omega > 0$. Hence we conclude that $\Lambda(\kappa)$ will possess at most one zero in the first quadrant for sufficiently low



¹ or the implicit function theorem for functions of several complex variables⁽³⁷⁾.

frequencies. That is, there are at most two discrete eigenvalues, $\pm \kappa_0$, in the point spectrum $\sigma_p(A)$ for sufficiently low ω . As ω is increased from zero, these eigenvalues move off of the real axis into the κ -plane. From the maximum ω theorem, we know that at some sufficiently high ω [or $\Sigma_a(v)$] the discrete eigenvalues will disappear into C_{AB} . However the detailed structure of the κ -plane suggests that the eigenvalues $\pm \kappa_0(\omega)$ might also encounter the line continuum C_{BB} or the elastic continuum Γ at a lower ω [or $\Sigma_a(v)$]. These questions shall be examined in more detail on p. 108.

b) Low frequency behavior: It is possible to apply the perturbation ideas of (II-E) to study the trajectory of the discrete eigenvalues as they move off of the real axis. Recall that the basic idea was to consider an expansion $\kappa_0^2(\omega) = P_0 + P_1(i\omega) + P_2(i\omega)^2 + P_3(i\omega)^3 + \dots$. If one assumes $v\Sigma_a(v) = \Sigma_a^0$ to be very small, then the work of this section yields

$$P_0 \cong \frac{3\Sigma_a^0 \int_0^\infty dv M(v)}{\int_0^\infty dv M(v) \left[\frac{v}{\Sigma_s(v)} \right]} = \frac{\Sigma_a^0}{D_0} = \frac{1}{L^2} \quad (\text{VI-5})$$

$$P_1 \cong \frac{3 \int_0^\infty dv M(v)}{\int_0^\infty dv M(v) \left[\frac{v}{\Sigma_s(v)} \right]} = \frac{1}{D_0} \quad (\text{VI-6})$$

$$P_2 \cong \frac{3 \int_0^\infty dv v M(v) \left[\frac{D_0^2}{v^2 \Sigma_i} - \frac{D_0}{3v \Sigma_s^2 \Sigma_i} (3\Sigma_i + 2\Sigma_e) + \frac{4}{45} \frac{\Sigma_e}{\Sigma_s^4} \right]}{\int_0^\infty dv M(v) \left[\frac{v}{\Sigma_s(v)} \right]} = \frac{C_0}{D_0^3} \quad (\text{VI-7})$$

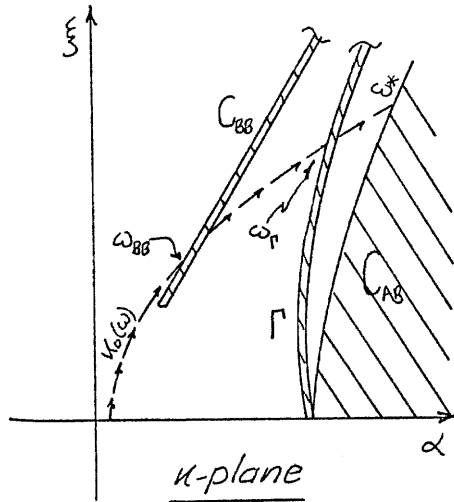
where we have also indicated expressions for the coefficients in terms of D_0 , the diffusion coefficient, and C_0 , the diffusion cooling coefficient. These latter quantities can help us to better understand the limitations of our model (V-1).

Since D_0 is dependent only upon the total scattering cross-section, we would expect it to be well described by the modified synthetic kernel model. Thus first order effects in ω should be predicted quite well by our analysis [as numerical calculations will verify later]. However since C_0 is dependent upon the more detailed form of the scattering kernel, one would not expect second order effects in ω to be well described by our models. Indeed one can easily show that the usual synthetic kernel model (IV-2) predicts a $C_0 \sim 0$. However the modified synthetic kernel model (V-1) containing an elastic scattering contribution yields a more reasonable value for C_0 [e.g. for graphite, $C_0 \sim 15 \times 10^5 \text{ cm}^4/\text{s}$ as compared to the measured value of $C_0 = 38 \times 10^5 \text{ cm}^4/\text{s}$]. Hence we should expect at least qualitative information about second order effects in ω .

c) Numerical Calculations: The above information was sufficient to allow a direct numerical evaluation of the discrete eigenvalues, $\pm \kappa_0(\omega)$, for various source frequencies. To do this, a complex arithmetic Newton-Raphson iteration scheme was used to find the zeros of $\Lambda(\kappa)$ for each fixed ω . These calculations were programmed and easily performed on an IBM 7040-7094 computer. The resulting dispersion curves of the discrete eigenvalues are shown on pp. 120, 121. Since the calculation of these dispersion curves provides the only

direct comparison with experimental data, these calculations will be discussed in some detail and compared with other theoretical calculations in Chapter VII.

d) Critical Frequencies: Specific calculations for graphite have revealed that for sufficiently high frequencies, $\omega^* \sim \langle v \Sigma_t(v) \rangle$, the discrete eigenvalue $\kappa_0(\omega)$ encounters the area continuum C_{AB} as predicted by Theorem IV. However at a much lower frequency, $\omega_{BB} \sim \Sigma_t^0$, the dispersion curve also intersects the line continuum C_{BB} , while at a frequency $\omega_{\Gamma} \sim \langle v \Sigma_e(v) \rangle$ the dispersion curve intersects the elastic continuum Γ .



It is important to recognize that all of these "critical frequencies" are dependent upon the transverse dimensions of the propagating medium. We have seen that transverse leakage, when introduced via asymptotic reactor theory, yields a new spectrum $\sigma_c(A_T)$ in which C_{BB} becomes an area similar to C_{AB} . But of even more significance is the fact that the point spectrum $\sigma_p(A_T)$ is shifted from κ to $\rho = \sqrt{\kappa^2 + B_{\perp}^2}$. That is, the presence of finite transverse dimension shifts the discrete eigenvalues closer to the continuum, thus effectively lowering the frequencies at which these eigenvalues will eventually encounter various portions of $\sigma_c(A_T)$. In

fact, detailed calculations for graphite [see Chapter VII] indicate that for $B_{\perp}^2 > 15 \times 10^{-4} \text{ cm}^{-2}$, the discrete eigenvalue $\rho_o(\omega)$ is shifted into C_{BB} even for $\omega = 0$ ⁽⁵³⁾. For transverse dimensions smaller than this critical limit [$\sim 115 \text{ cm} \times 115 \text{ cm}$], $\omega_{BB} \rightarrow 0$ implying that for even zero frequency, the discrete eigenvalue is imbedded in the continuum C_{BB} . The implications of this behavior will be discussed later in Chapter VII.

The influence of transverse dimensions upon ω^* is not so dramatic since in the neighborhood of C_{AB} , $|k^2| \gg B_{\perp}^2$ implying that $\rho \sim k$ and thus that the intersection of $\rho_o(\omega)$ with C_{AB} occurs at essentially the same frequency ω^* at which $\kappa_o(\omega)$ intersects C_{AB} . We similarly expect B_{\perp}^2 to have little effect upon ω_{Γ} since this intersection of $\kappa_o(\omega)$ with Γ also occurs in a region in which $|k^2| \gg B_{\perp}^2$.

B. CONSTRUCTION OF THE SOLUTION

The boundary value problem for an oscillating plane source in an infinite medium has been proposed as a suitable model of the neutron wave experiment. This problem has already been solved formally for a general noncrystalline scattering kernel in Chapter III. Here it was shown that either eigenfunction expansions or Fourier transforms could be used to construct the solution. It is more convenient to use the latter approach for the modified synthetic kernel $(V-1)^2$.

²Let it be mentioned that there appears to be some difficulty in demonstrating an expansion theorem such as Theorem VI for the modified synthetic kernel model.

The Fourier transformed Boltzmann equation (II-33) becomes

$$[i\omega + v\Sigma_t(v) - \eta\mu v] \tilde{F}(\eta; \mu, v) = \frac{\beta}{2} \Sigma_i(v) v M(v) \int_{-1}^{+1} d\mu' \int_0^{\infty} dv' v' \Sigma_i(v') \tilde{F}(\eta; \mu', v') \\ + \frac{v\Sigma_e(v)}{2} \int_{-1}^{+1} d\mu' \tilde{F}(\eta; \mu', v) + S(\mu, v) \quad (\text{VI-8})$$

In the usual fashion one can solve for the moments $\tilde{f}(\eta)$ and $\tilde{N}(\eta; v)$ to obtain

$$\tilde{F}(\eta; \mu, v) = \frac{\frac{\beta}{2} \Sigma_i(v) v M(v) \chi(\eta)}{[i\omega + v\Sigma_t(v) - \eta\mu v] \Lambda(\eta) \Lambda_e(\eta; v)} + \frac{Q(\eta; \mu, v)}{[i\omega + v\Sigma_t(v) - \eta\mu v] \Lambda_e(\eta; v)} \quad (\text{VI-9})$$

where $\Lambda_e(\eta; v)$ and $\Lambda(\eta)$ are the dispersion relations defined by equations (VI-3) and (VI-4). We have also defined the source moments

$$Q(\eta; \mu, v) \equiv S(\mu, v) \Lambda_e(\eta; v) + \frac{v\Sigma_e(v)}{2} \chi_e(\eta; v)$$

$$\chi_e(\eta; v) \equiv \int_{-1}^{+1} d\mu \frac{S(\mu, v)}{i\omega + v\Sigma_t(v) - \eta\mu v} \quad (\text{VI-10})$$

$$\chi(\eta) \equiv \int_{-1}^{+1} d\mu \int_0^{\infty} dv \frac{v\Sigma_i(v) Q(\eta; \mu, v)}{[i\omega + v\Sigma_t(v) - \eta\mu v] \Lambda_e(\eta; v)}$$

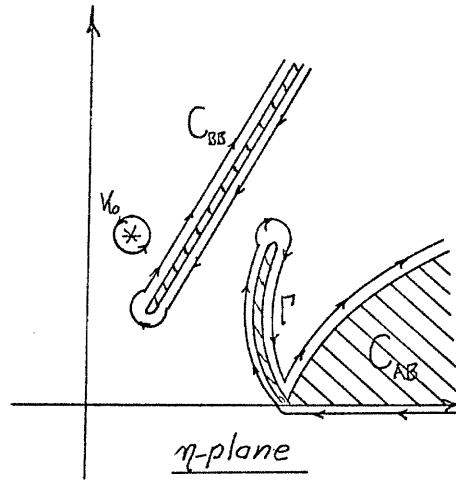
[Notice that if we assume an isotropic source $S(\mu, v) \equiv S_0(v)$, then we find that $Q(\eta; \mu, v) \rightarrow S_0(v)$.]

Now to perform the inversion

$$f(x, \mu, v, t) = \frac{1}{2\pi i} \int_{-i\infty}^{+i\infty} e^{-\eta x + i\omega t} \tilde{F}(\eta; \mu, v) d\eta$$

we can make use of our knowledge about the structure of the η -plane

which was obtained in the study of the eigenvalue spectrum of A for this model. For $x > 0$, we can deform the inversion contour into the right half plane, picking up the residues from the simple poles [zeros of $\Lambda(\eta)$, $\Lambda_e(\eta;v)$, and $[i\omega + v\Sigma_t(v) - \eta\mu v]$] and line integral contributions from around C



and Γ . The details of this calculation, although straightforward, are rather tedious, and only the final solution will be given here. It is convenient to write the solution as the superposition of a number of terms [from each of the singularities--eigenvalues--in the η -plane]

$$f(x, \mu, v, t) = f_{\text{discrete}} + f_{\text{source}} + f_{\text{elastic}} + f_{C_{BB}} + f_{\Gamma} + f_{C_{AB}} \quad (\text{VI-11})$$

The first term in this representation is

$$f_{\text{discrete}}(x, \mu, v, t) = \frac{\frac{\beta}{2} \Sigma_i(v) v M(v) \chi(\kappa_0)}{[i\omega + v\Sigma_t(v) - \kappa_0 \mu v] \Lambda_e(\kappa_0; v) \left. \frac{\partial \Lambda}{\partial \eta} \right|_{\eta=\kappa_0}} e^{-\kappa_0 x + i\omega t} \quad (\text{VI-12})$$

This term is the discrete plane wave mode corresponding to the eigenvalue κ_0 and hopefully is the quantity measured by the neutron wave experiment. For $\text{Re} \{\kappa_0\} \equiv \alpha_0 < \Sigma_M$, this mode will be less damped than any of the other terms in (VI-11) and thus should dominate for

for large x . However if ω should be raised sufficiently high, $\alpha_o(\omega) > \Sigma_M$, and $f_{C_{BB}}$ will then become less damped than $f_{discrete}$. The detection of $f_{discrete}$ then becomes more difficult. The effect of this "continuum contamination" will be discussed in more detail in section VII-A.

Notice also that if $\kappa_o(\omega)$ is small such that $\left| \frac{\kappa_o v}{i\omega + v\Sigma_t(v)} \right| \ll 1$, the neutron distribution $f_{discrete}$ becomes isotropic. However as $\kappa_o(\omega)$ becomes larger, $f_{discrete}$ becomes more anisotropically peaked in the forward direction. Its velocity spectrum is also shifted to higher velocities [see Figure 8].

The next term in (VI-11) is

$$f_{source}(x, \mu, v, t) = \frac{S(\mu, v)}{\mu v} e^{-\frac{\Sigma_t(v)x}{\mu}} e^{i\omega(t - \frac{x}{\mu v})} \quad (VI-13)$$

One finds this term to be a solution of the first flight Boltzmann equation

$$\frac{\partial f}{\partial t} + \mu v \frac{\partial f}{\partial x} + v \Sigma_t(v) f(x, \mu, v, t) = S(\mu, v) \delta(x) e^{i\omega t} \quad (VI-14)$$

Hence f_{source} represents those neutrons emitted by the source at (μ, v) which travel from source to detector without suffering any collisions.

The third term in (VI-11) is more complicated:

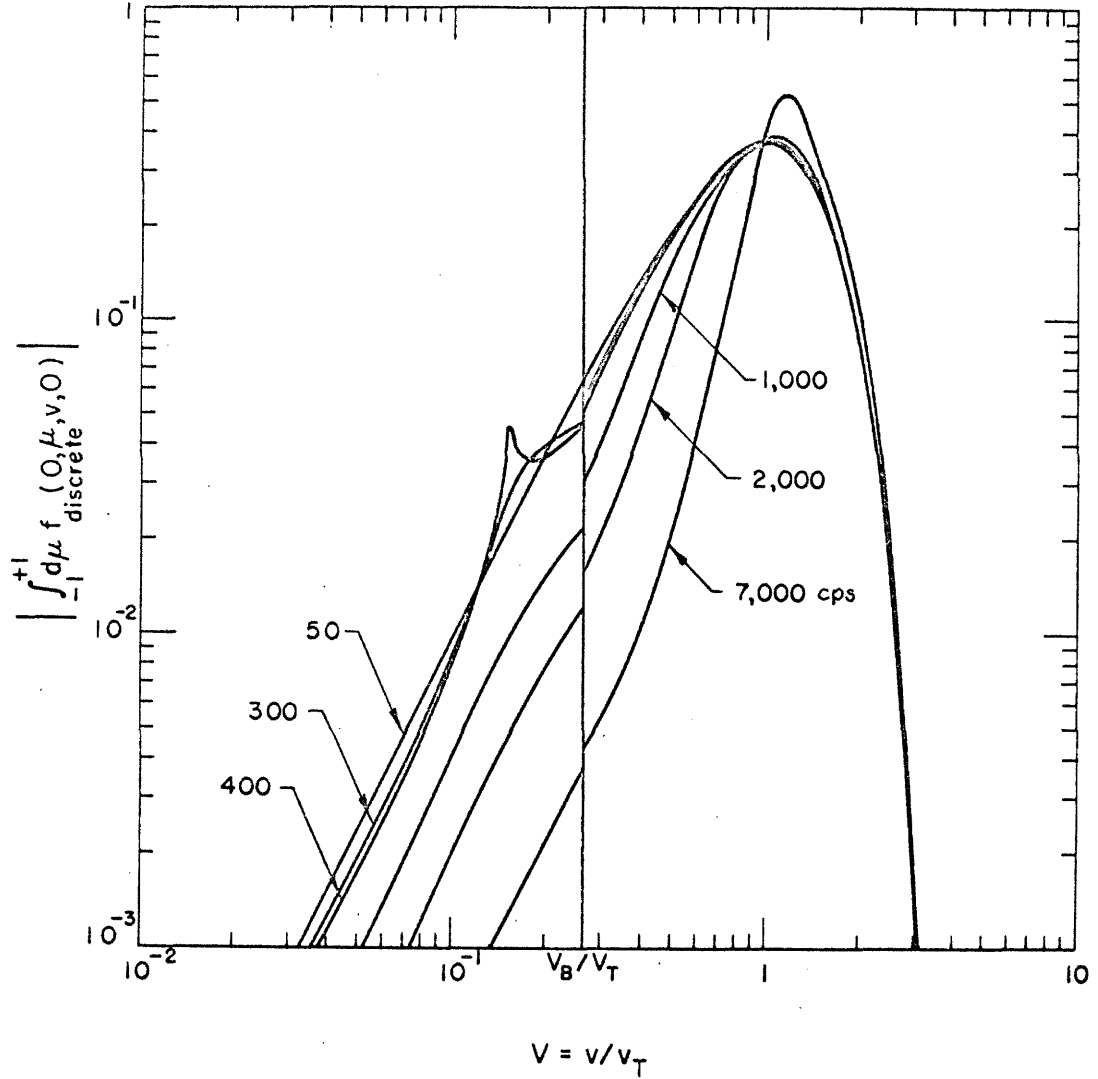


Figure 8. The velocity spectrum of the fundamental mode, $f_{\text{discrete}}(x, \mu, v, t)$.

(The "resonance" effect which appears at $V \sim 0.15$, $f = 400$ cps, is due to the intersection of $\kappa_o(\omega)$ with C_{BB} at this frequency.)

$$\begin{aligned}
 f_{\text{elastic}}(x, \mu, v, t) = & \frac{v \Sigma_e(v) \chi_e(\kappa_e; v)}{2[\ i\omega + v \Sigma_t(v) - \kappa_e \mu v]} \frac{\partial \Lambda_e}{\partial \eta} \Big|_{\eta = \kappa_e(v)} e^{-\kappa_e(v)x + i\omega t} \\
 & + \frac{1}{2\pi i} \int_{\frac{i\omega}{v} + \Sigma_t(v)}^{\left[\frac{i\omega}{v} + \Sigma_t(v)\right] + \infty} d\eta e^{-\eta x + i\omega t} \frac{v \Sigma_e(v)}{2[\ i\omega + v \Sigma_t(v) - \eta \mu v]} \left\{ \frac{\chi_e^+(\eta)}{\Lambda_e^+(\eta)} - \frac{\chi_e^-(\eta)}{\Lambda_e^-(\eta)} \right\} \\
 & - \frac{1}{4} \frac{\Sigma_e(v)}{\mu} \left\{ \frac{\chi_e^+(\eta)}{\Lambda_e^+(\eta)} + \frac{\chi_e^-(\eta)}{\Lambda_e^-(\eta)} \right\} \Big|_{\eta = \left[\frac{i\omega + v \Sigma_t(v)}{\mu v} \right]} e^{-\frac{\Sigma_t(v)}{\mu} x} e^{i\omega \left(t - \frac{x}{\mu v} \right)}
 \end{aligned}
 \tag{VI-15}$$

To interpret this term, consider the associated "one-velocity" transport equation under the assumption of isotropic scattering and an oscillating plane source at the origin

$$\frac{\partial f}{\partial t} + \mu v \frac{\partial f}{\partial x} + v \Sigma_t(v) f(x, \mu, t) = \frac{v \Sigma_e(v)}{2} \int_{-1}^{+1} d\mu' f(x, \mu', t) + S(\mu, v) \delta(x) e^{i\omega t}$$

v fixed (VI-16)

One can readily verify that (VI-15) is the solution to this equation [subject to the boundary conditions $\lim_{|x| \rightarrow \infty} |f(x, \mu, t)| = 0$]. Thus we can physically interpret f_{elastic} as representing those neutrons which are emitted by the source at speed v , suffer only elastic collisions prior to absorption by the detector, and hence obey an effective "one-velocity" transport equation at velocity v .

The final three terms in (VI-11) are due to the line integrals about the continuous eigenvalue spectrum and can be written as

$$\begin{aligned}
 f_{C_{BB}}(x, \mu, v, t) &= \frac{\beta \Sigma_i(v) v M(v)}{2\pi i} \int_{C_{BB}} \frac{d\eta e^{-\eta x + i\omega t}}{2[\ i\omega + v\Sigma_t(v) - \eta\mu v] \Lambda_e(\eta; v)} \left\{ \frac{\chi^+(\eta)}{\Lambda^+(\eta)} - \frac{\chi^-(\eta)}{\Lambda^-(\eta)} \right\} \\
 &\quad - \frac{\beta \Sigma_i(v) v M(v) H(v_B - v)}{4\mu v \Lambda_e\left(\frac{i\omega + \Sigma_t^0}{\mu v}; v\right)} \left\{ \frac{\chi^+(\eta)}{\Lambda^+(\eta)} + \frac{\chi^-(\eta)}{\Lambda^-(\eta)} \right\} \Bigg|_{\eta = \left[\frac{i\omega + \Sigma_t^0}{\mu v} \right]} e^{-\frac{\Sigma_t^0}{\mu v} x} e^{i\omega(t - \frac{x}{\mu v})} \quad (VI-17)
 \end{aligned}$$

$$f_{C_{AB}}(x, \mu, v, t) = \frac{\beta \Sigma_i(v) v M(v)}{2\pi i} \int_{\partial C_{AB}} \frac{d\eta e^{-\eta x + i\omega t} \chi(\eta)}{2[\ i\omega + v\Sigma_t(v) - \eta\mu v] \Lambda_e(\eta; v) \Lambda(\eta)} \quad (VI-18)$$

$$\begin{aligned}
 f_{\Gamma}(x, \mu, v, t) &= \frac{\beta \Sigma_i(v) v M(v)}{2\pi i} \int_{\Gamma} \frac{d\eta e^{-\eta x + i\omega t}}{2[\ i\omega + v\Sigma_t(v) - \eta\mu v] \Lambda_e(\eta; v)} \left\{ \frac{\chi^+(\eta)}{\Lambda^+(\eta)} - \frac{\chi^-(\eta)}{\Lambda^-(\eta)} \right\} \\
 &\quad - \frac{\beta \Sigma_i(v) v M(v) H(v - v_B)}{2[\ i\omega + v\Sigma_t(v) - \eta\mu v] \frac{\partial \Lambda_e}{\partial \eta}} \left\{ \frac{\chi^+(\eta)}{\Lambda^+(\eta)} + \frac{\chi^-(\eta)}{\Lambda^-(\eta)} \right\} \Bigg|_{\eta = \kappa_e(v)} e^{-\kappa_e(v) x + i\omega t} \Bigg|_{\eta = \kappa_e(v)} \quad (VI-19)
 \end{aligned}$$

The discussion of section II-G suggests that the contributions from C_{BB} and C_{AB} represent a superposition of free-streaming modes with appropriate intermode coupling factors to account for collisions. Similar arguments indicate that the term due to Γ corresponds to a superposition of elastic scattering modes such as f_{elastic} with the intermode coupling effect now due to inelastic scattering collisions.

Of course we must remember that (VI-11) is only a representation of the solution for one-dimensional geometries. However to include the effects of transverse leakage, it is a simple matter to use asymptotic reactor theory as in Chapter II and carry through the same Fourier transform analysis for $B_{\perp}^2 > 0$. Then, of course, the integral over C_{BB} becomes a line integral about an area similar to that about C_{AB} , but otherwise the general structure of the solution is left unchanged. Indeed, one can use physical arguments to assign the same interpretation to each of these terms as in the $B_{\perp}^2 = 0$ case.

VII. THEORETICAL INTERPRETATION OF EXPERIMENTS

A. GRAPHITE

The modified synthetic kernel model (V-1) was applied to analyze neutron wave experiments performed in graphite. Since the detailed cross-section behavior of this material is rather complicated, it was convenient to model only the gross structure as shown in Figure 9 [variations in such modeling actually produced little change in the calculated dispersion curve].

1. Calculations of the Discrete Eigenvalues

The dispersion curve $\kappa_0(\omega)$ was calculated numerically from (VI-4) using the graphite cross-section modeling of Figure 9. These calculations are shown on the following κ -plane diagram along with sample sketches of the continuum structure for several frequencies. An inverted spectral plane diagram is also shown.

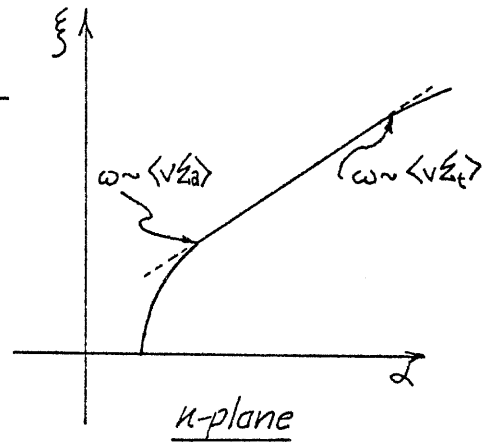
It is useful to compare these calculations with the experimentally measured $\kappa_0(\omega)$ as well as with alternative theoretical calculations of the point spectrum $\sigma_p(A)$. Several comments concerning these diagrams are necessary:

- i) Notice that one-velocity diffusion theory gives better agreement with experiment than does one-velocity transport theory. This is evidently a consequence of the fact that the diffusion approximation and one-velocity approximation tend to cancel to some degree, resulting in somewhat better agreement than expected.

- ii) P_1 theory actually gives quite poor agreement with experiment since the $\partial^2/\partial t^2$ term overcompensates for the transport effects (see Travelli⁽¹³⁾).
- iii) The κ -plane plots of the dispersion curve show that for $f > 100$ cps, one has essentially straight line behavior--i.e. $\xi = C_1 \alpha + C_2$. A closer examination of the dispersion relation reveals that in this frequency regime

$$\frac{d\kappa}{d\omega} = \kappa \frac{iC}{[i\omega + \langle v\Sigma_t(v) \rangle][i\omega + \langle v\Sigma_a(v) \rangle]}$$

Thus the dispersion curve is characterized by two "break frequencies" corresponding first to the mean absorption collision frequency $\langle v\Sigma_a(v) \rangle$ and then to the mean total collision frequency $\langle v\Sigma_t(v) \rangle$. For $\langle v\Sigma_a(v) \rangle \ll \omega \ll \langle v\Sigma_t(v) \rangle$



$$\frac{d\kappa}{d\alpha} \sim C_1 \kappa \implies \frac{d\xi}{d\alpha} \sim \frac{\xi}{\alpha}$$

which implies straight line behavior as observed numerically. Notice that in the diffusion theory models, $\langle v\Sigma_t(v) \rangle \rightarrow \infty$, thus the higher break frequency does not exist for this model. This higher break frequency is of the same order of magnitude as ω^* ; therefore it is not distinct in several of the more advanced transport models.

- iv) In Table I we have found it convenient to list the critical

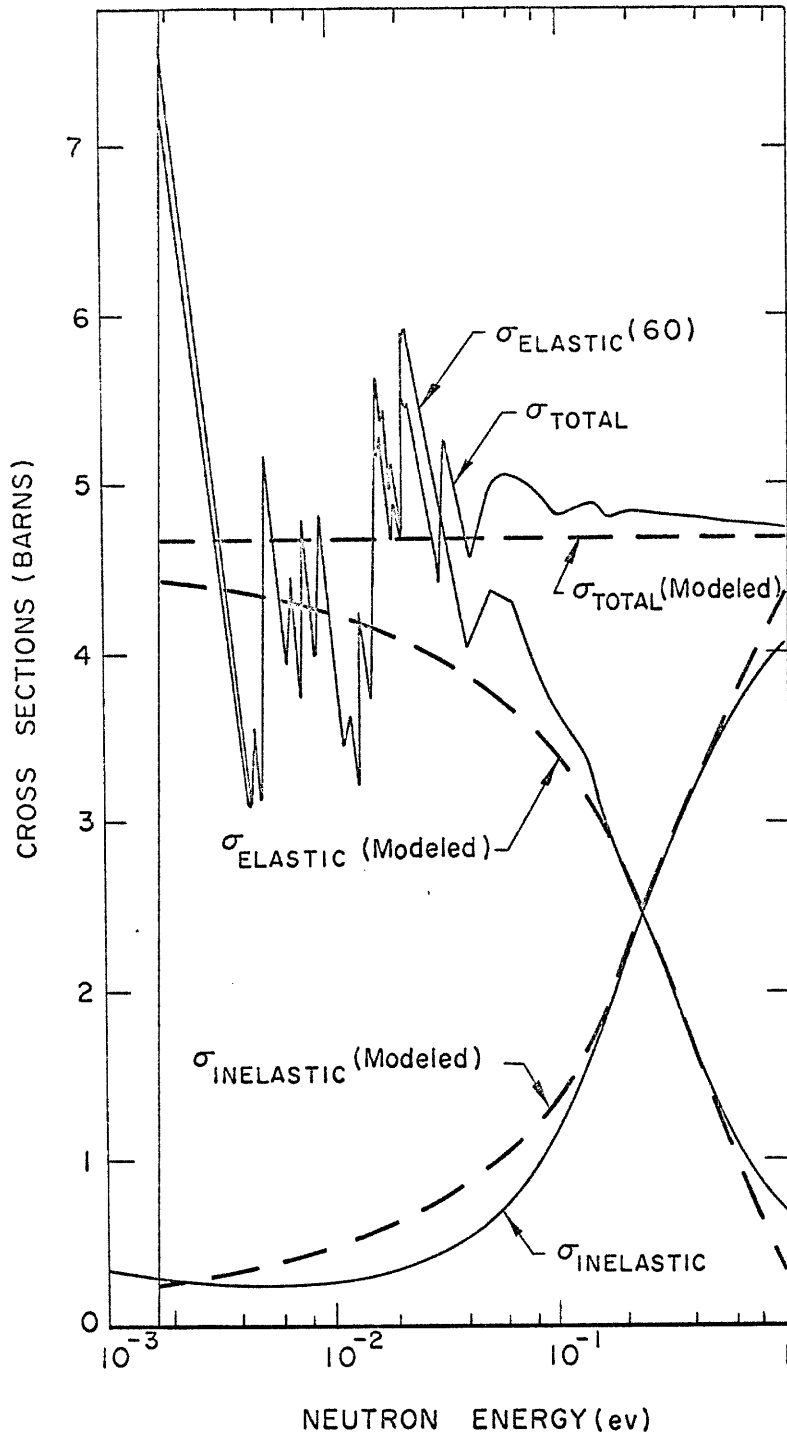


Figure 9. Cross-Section Modeling for Graphite

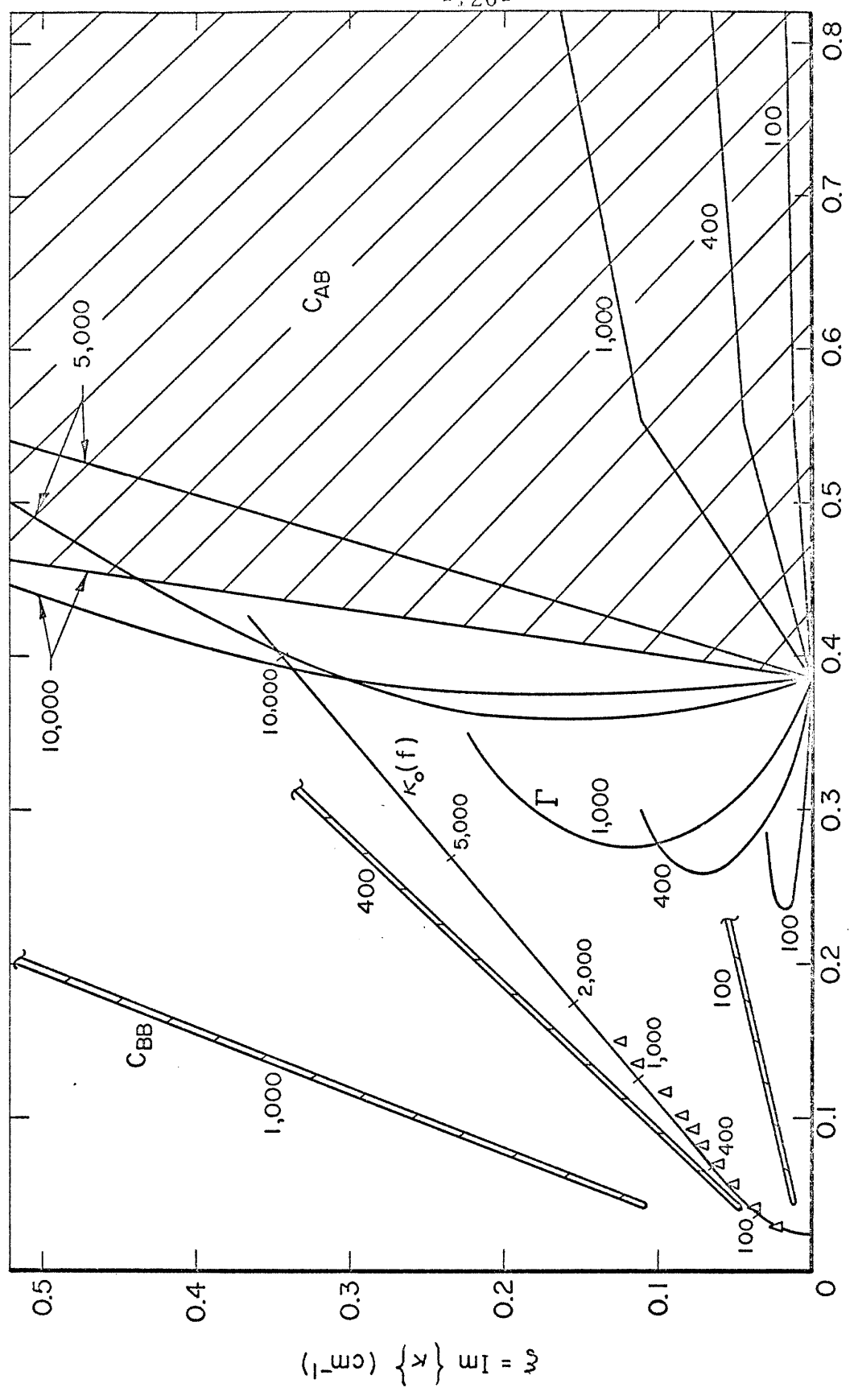


Figure 10. Eigenvalue Spectrum for Graphite

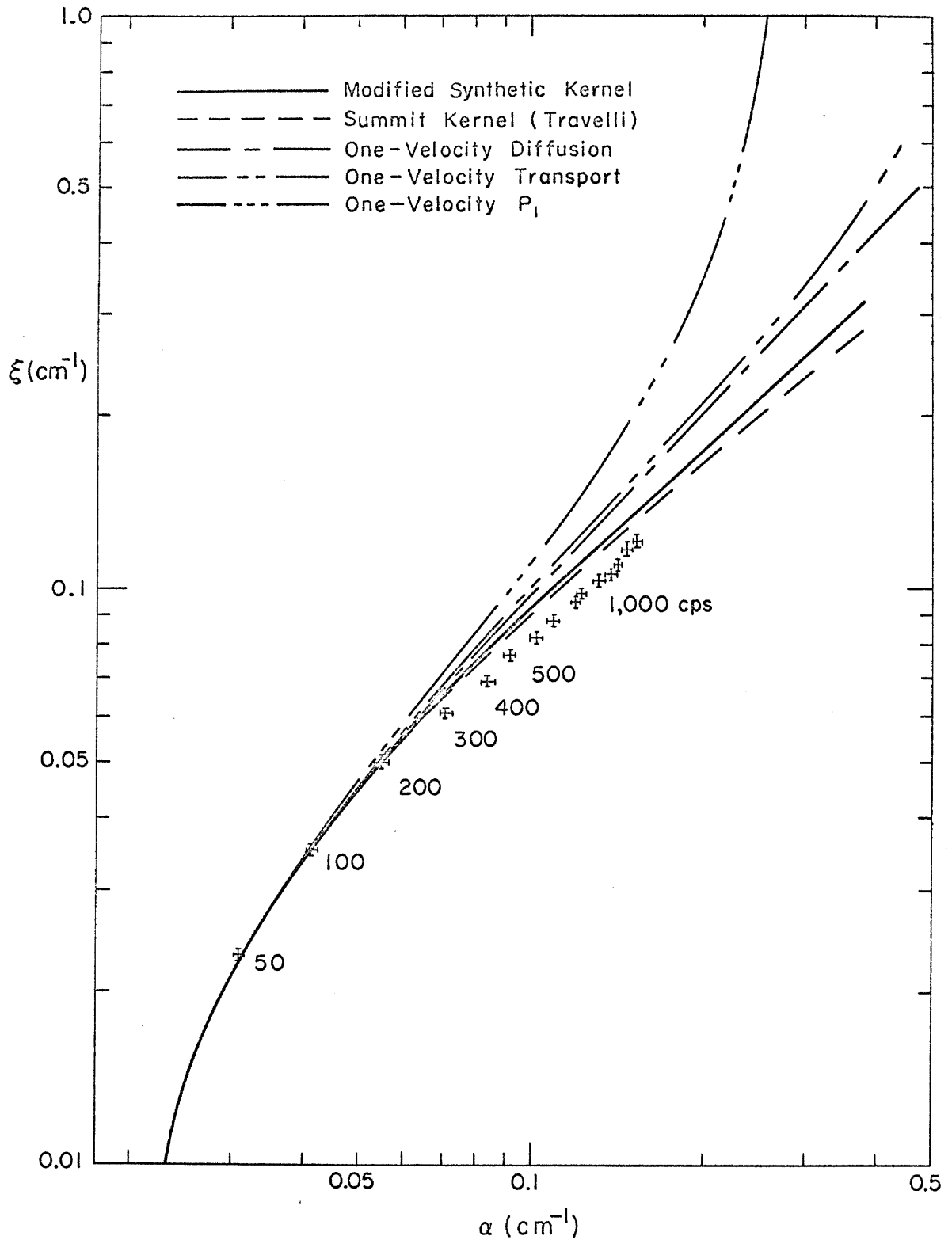


Figure 11. The Dispersion Curve of the Discrete Eigenvalue $\kappa_0(\omega)$ for Graphite

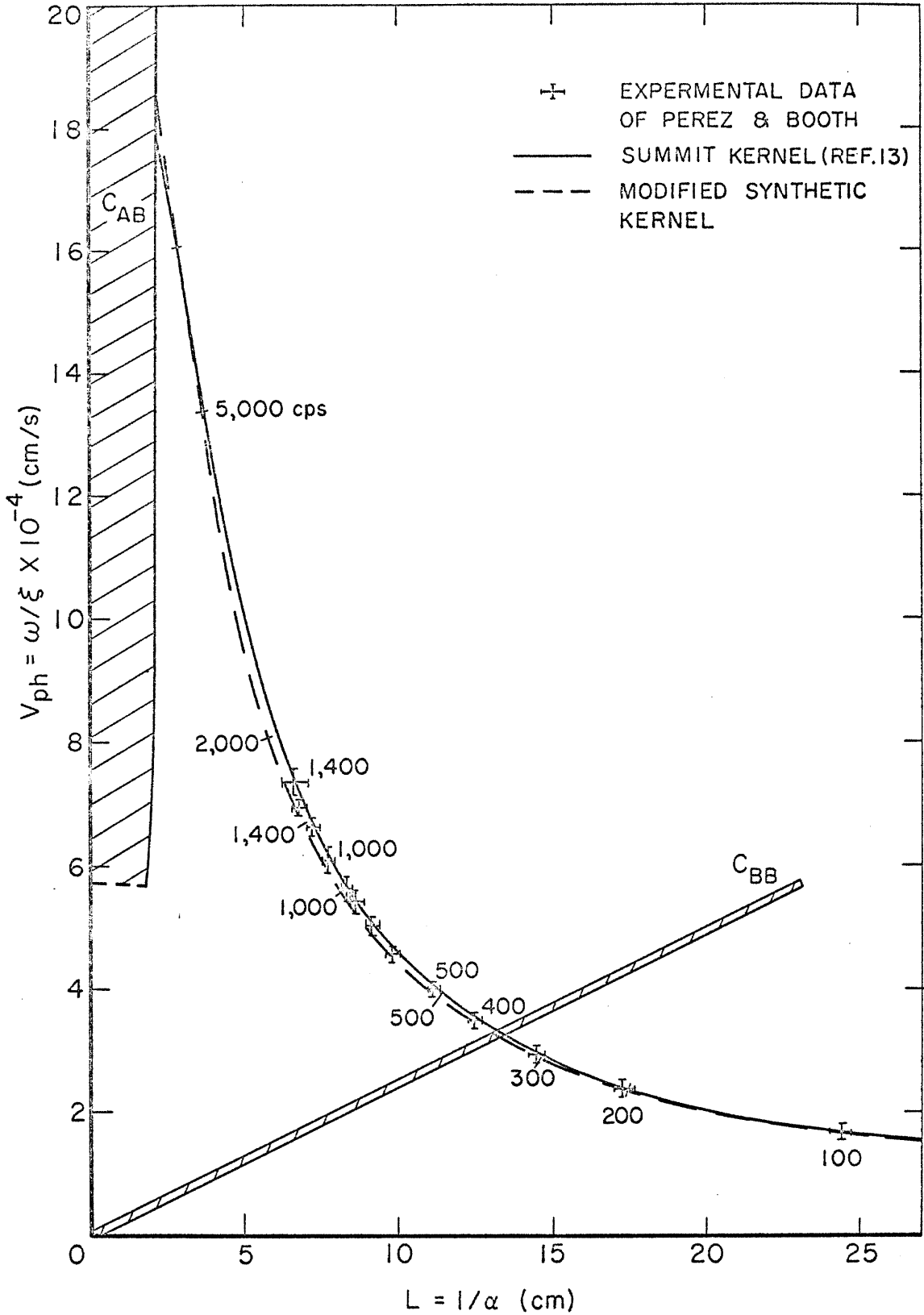


Figure 12. The Inverted Spectral Plane Diagram for Graphite

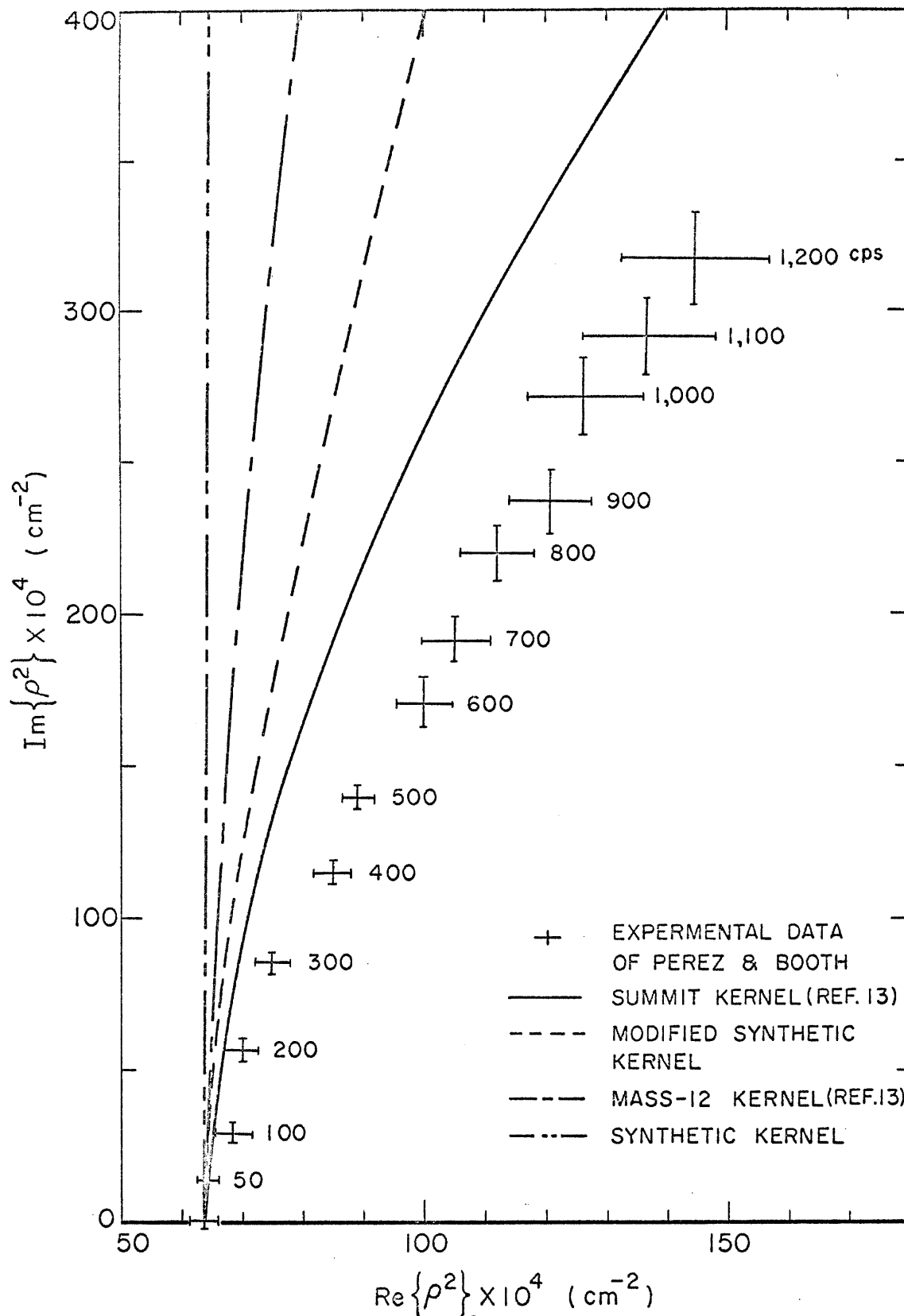


Figure 13. The ρ^2 -Plane for Graphite

TABLE I: CRITICAL FREQUENCIES (graphite)

<u>Theoretical Model</u>	<u>Critical Frequencies</u>
One-velocity diffusion theory	none
P_1 theory	none
One-velocity, isotropic transport theory	$f^* = 15,000$ cps
Velocity-dependent diffusion theory	$f_C = 400$ cps
Multi-group transport theory	$f^* = 14,000$ cps
Velocity-dependent transport theory (synthetic kernel)	$f^* = 12,000$ cps
Velocity-dependent transport theory ($B_{\perp}^2 = 0$) (modified synthetic kernel)	$f_C = 150$ cps $f_{BB} = 390$ cps $f_{\Gamma} = 7,000$ cps $f^* = 11,000$ cps
Velocity-dependent transport theory ($B_{\perp}^2 = 59.6 \times 10^{-4} \text{ cm}^{-2}$) (modified synthetic kernel)	$f_C = 0$ cps $f_{BB} = 0$ cps $f^* = 11,000$ cps

Here we are defining

f_C = frequency at which continuum is less damped than discrete mode

f_{BB} = frequency at which dispersion curve of discrete eigenvalue intersects the sub-Bragg continuum C_{BB}

f_{Γ} = frequency at which dispersion curve of discrete eigenvalue intersects the elastic continuum Γ

f^* = frequency at which discrete eigenvalues encounter C_{AB} and cease to exist (at least in the usual sense)

frequencies predicted by each of the theoretical models.

- v) It was found that the detailed modeling of the cross-sections used in the modified synthetic kernel had little effect upon the dispersion curve. The effect of changing the density of the propagating graphite was also investigated. Although this had little effect upon the location and shape of the dispersion curve, it did slightly affect the frequency parameterization [e.g. if $\kappa_o = \kappa_o(\omega)$ for $\rho = 1.60 \text{ g/cm}^3$, then $\kappa_o = \kappa_o\left(\frac{1.60}{1.67}\omega\right)$ for $\rho = 1.67 \text{ g/cm}^3$].
- vi) It is noted that the Parks' kernel-diffusion theory calculations of Perez, Booth, and Ohanian⁽¹²⁾ and the multigroup transport theory calculations of Travelli⁽¹³⁾ give the best agreement with the experimentally measured dispersion curve. However the modeled transport theory of Chapter VI gives a dispersion curve which is almost as good--and certainly better than the MASS-12 calculations and less sophisticated theories. It is rather surprising, in fact, that such a crude model of the kernel as (V-1) gives results which are even comparable to the Parks' kernel calculations.
- vii) Of course the modified synthetic kernel calculations give results which are much better than those obtained with a synthetic kernel model such as (IV-2). This was expected since we have seen that the high frequency behavior of the curve is determined by the higher terms in the expansion $\kappa_o^2(\omega) = \frac{1}{L^2} + \frac{1}{D_o}(i\omega) + \frac{C_o}{D_o^3}(i\omega)^2 + \dots$ and the synthetic kernel

model predicts $C_o \sim 0$ as compared to the modified synthetic kernel model's prediction of $C_o = 15 \times 10^5 \text{ cm}^4/\text{s}$.

viii) Noting that

$$\text{Re} \{ \rho^2 \} = \frac{1}{L^2} + B_1^2 - \frac{C}{D_o^3} \omega^2 + O(\omega^4)$$

$$\text{Im} \{ \rho^2 \} = \frac{1}{D_o} \omega + O(\omega^3)$$

one can plot the dispersion curve in the ρ^2 -plane (see Figure 13) to study the second order effects in ω . Since all of the models accurately predict D_o [i.e. the total mean free path], the agreement of $\text{Im} \{ \rho^2 \}$ vs. ω with the experimental data is quite good.

However the $\text{Re} \{ \rho^2 \}$ behavior is more sensitive to the scattering kernel through the C_o dependence. It is observed that even the Parks' modeling of the kernel gives a rather bad prediction of this curve. This appears to explain why none of the theories gave a really good quantitative agreement with the experimental data. [A similarly bad agreement is noted in the calculations of the time decay constants of the pulsed neutron experiment in graphite.] One must conclude that until a more accurate model of the scattering kernel for crystalline media is developed, quantitative calculations of the discrete eigenvalue spectrum are not possible.

ix) For purposes of comparison, we have estimated D_o , C_o , etc. for each of these models and compared these quantities with experimental estimates in Table II.

TABLE II: EVALUATION OF EXPANSION PARAMETERS IN

$$\rho^2(\omega) = P^{(0)} + P^{(1)}(i\omega) + P^{(2)}(i\omega)^2 + \dots$$

<u>Theoretical Model</u>	$P^{(0)} \times 10^4$ <u>cm⁻²</u>	$P^{(1)} \times 10^6$ <u>s cm⁻²</u>	$P^{(2)} \times 10^{10}$ <u>s² cm⁻²</u>
Experimental (Perez & Booth)	63.86 ± 0.09	4.64 ± 0.01	3.92 ± 0.09
Energy-Dependent Diffusion Theory (SUMMIT kernel)	63.88	4.74	2.11
Multi-group Transport Theory (SUMMIT)	63.8	4.70	2.60
Velocity-Dependent Transport Theory (Synthetic kernel)	63.8	5.08	0.023
Velocity-Dependent Transport Theory (Modified Synthetic kernel)	63.8	4.73	1.60

<u>Theoretical Model</u>	$D_o (10^5 \text{ cm}^2/\text{s})$	$C_o (10^5 \text{ cm}^4/\text{s})$
Experimental (Perez & Booth)	2.16 ± 0.01	39.0 ± 2
Energy-Dependent Diffusion Theory (SUMMIT kernel)	2.11	20.15
Multi-group Transport Theory (SUMMIT)	2.13	25
Velocity-Dependent Transport Theory (Synthetic kernel)	1.97	0.18
Velocity-Dependent Transport Theory (Modified Synthetic kernel)	2.11	15

x) To indicate the effects of transverse leakage, we have sketched the ρ -plane spectrum $\sigma(A_T)$ for $B_1^2 = 59.6 \times 10^{-4} \text{ cm}^{-2}$ in Figure 14 [corresponding to the transverse dimensions of the Perez & Booth experiment]. One notes that even for $\omega = 0$, the discrete eigenvalue $\rho_o(\omega)$ is imbedded in C_{BB} [at least in the approximation of asymptotic reactor theory]. As the frequency is increased, the discrete eigenvalue is eventually "left behind" by C_{BB} and emerges into the resolvent set $\rho(A_T)$. The implications of this behavior will be discussed in section (VII-A-3).

2. Resolution of the Discrete Mode

We must now determine whether the neutron wave experiment in graphite actually is measuring the complex wave number $\kappa_o(\omega)$ of a dominating discrete plane wave mode, and whether there are any ranges of experimental parameters, $[\omega, \Sigma_a(v), B_1^2, x]$ in which such a measurement cannot be performed. The theory of neutron wave propagation in polycrystalline materials has shown that the neutron distribution can be written as a superposition of terms (VI-11), each corresponding to a portion of the eigenvalue spectrum $\sigma(A)$. Hence the detector response $R(x,t) = \int_{-1}^{+1} d\mu \int_0^\infty dv v \Sigma_d(v) f(x,\mu,v,t)$ can also be written as a sum of terms

$$R(x,t) = R_{\text{discrete}}(x,t) + R_{C_{BB}}(x,t) + R_{\Gamma}(x,t) + R_{C_{AB}}(x,t)$$

where we have combined the elastic term of (VI-11) with the term due to Γ , and the source term with the C_{AB} term. By studying $\sigma(A)$

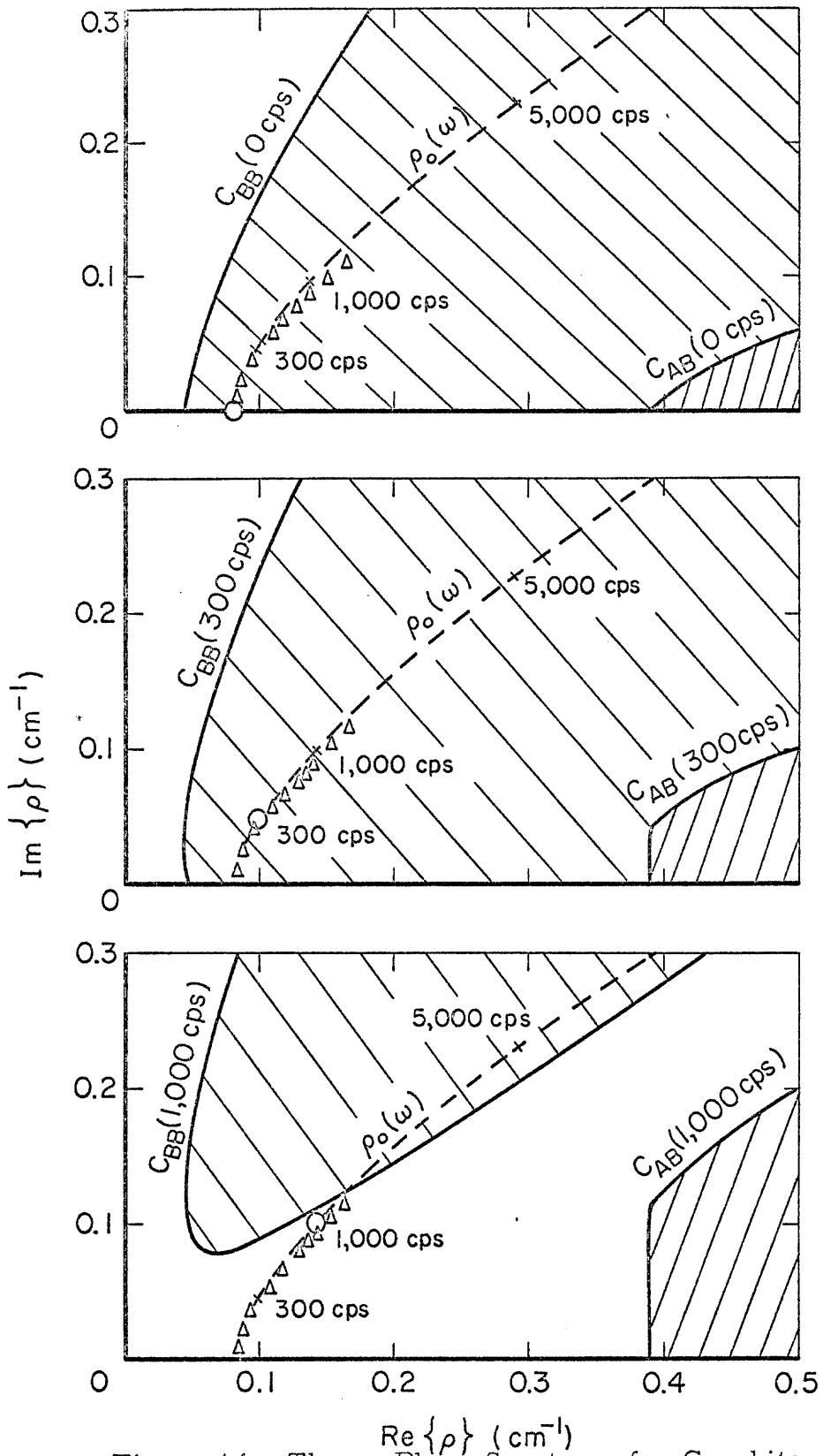


Figure 14. The ρ -Plane Spectrum for Graphite

we can see that for all frequencies below ω^* , the eigenvalues corresponding to C_{AB} and Γ are considerably more damped than the discrete eigenvalue. Hence it is evident that for sufficiently large x , R_{Γ} and $R_{C_{AB}}$ can be neglected in comparison to R_{discrete} . To estimate how far from the source one must go to insure that these "source transients" are negligible, we need to estimate the relative magnitude of each of the components of $R(x,t)$ as well as their respective attenuation in x . In general these relative magnitudes depend upon the source distribution $S(\mu, \nu)$ as well as the frequency ω . However one can use physical arguments to estimate the relative magnitudes of these source transients crudely as

$$\left| \frac{R_{C_{AB}}(0,0)}{R_{\text{discrete}}(0,0)} \right| = O(1) ; \quad \left| \frac{R_{\Gamma}(0,0)}{R_{\text{discrete}}(0,0)} \right| = O \left(\frac{\langle \Sigma_e(\nu) \rangle}{\langle \Sigma_t(\nu) \rangle} \right)$$

Such estimates indicate that these terms decay so rapidly that for x greater than 20 cm from the source and frequencies less than 5,000 cps, they comprise less than 3% of the total solution.

There are other possible sources of contamination such as higher discrete modes [higher discrete eigenvalues] which are not predicted by our model. Actually it appears that these modes can be ruled out for the case of graphite since all calculations with more detailed kernels⁽¹²⁾ seem to indicate only one discrete mode. In addition, diffusion theory analyses of higher transverse modes indicate that these can safely be ignored, as can reflections from boundaries.

Notice however that the eigenvalues $\kappa \in C_{BB}$ can actually be less damped than the discrete eigenvalue κ_0 even for low ω . Indeed, if $B_{\perp}^2 > 15 \times 10^{-4} \text{ cm}^{-2}$, such behavior will be present for all ω since $\rho_0(\omega)$ is imbedded in C_{BB} even for $\omega = 0$. Hence we do not expect the discrete mode to dominate asymptotically in x for experiments performed in graphite. To determine the influence of this continuum contamination upon experimental measurements, we must estimate not only the relative magnitude of $R_{C_{BB}}$, but as well its behavior in x [which is certainly not exponential].

Numerical calculations [such as Figure 15] as well as a two-group diffusion theory analysis [Appendix E] have shown that for $S(\mu, v) = M(v)$, the relative magnitude of this term is initially

$|R_{C_{BB}}(0,0)/R_{\text{discrete}}(0,0)| \sim 0.6\%$. The attenuation is roughly exponential only for intermediate x , although for very large x ($x \gg 50$ cm), $R_{C_{BB}}(x,t)$ behaves asymptotically as

$$R_{C_{BB}}(x,t) = o \left[\frac{1}{x} e^{-\left(\frac{i\omega + \Sigma_0^0}{v_B} t\right) x + i\omega t} \right]$$

These calculations show that for intermediate distances and source frequencies ($x < 50$ cm and $f < 1000$ cps), one can indeed expect

$R_{C_{BB}}$ to be negligible.

However one might be interested in the alternative problem of trying to observe these continuum effects experimentally. In Figure 16 a diagram is given which indicates the distance from the source, $x_c(\omega)$, which the magnitude of $R_{C_{BB}}(x,t)$ will be 10%, 50%, or 100% of the discrete mode magnitude. Since this distance $x_c(\omega)$ decreases

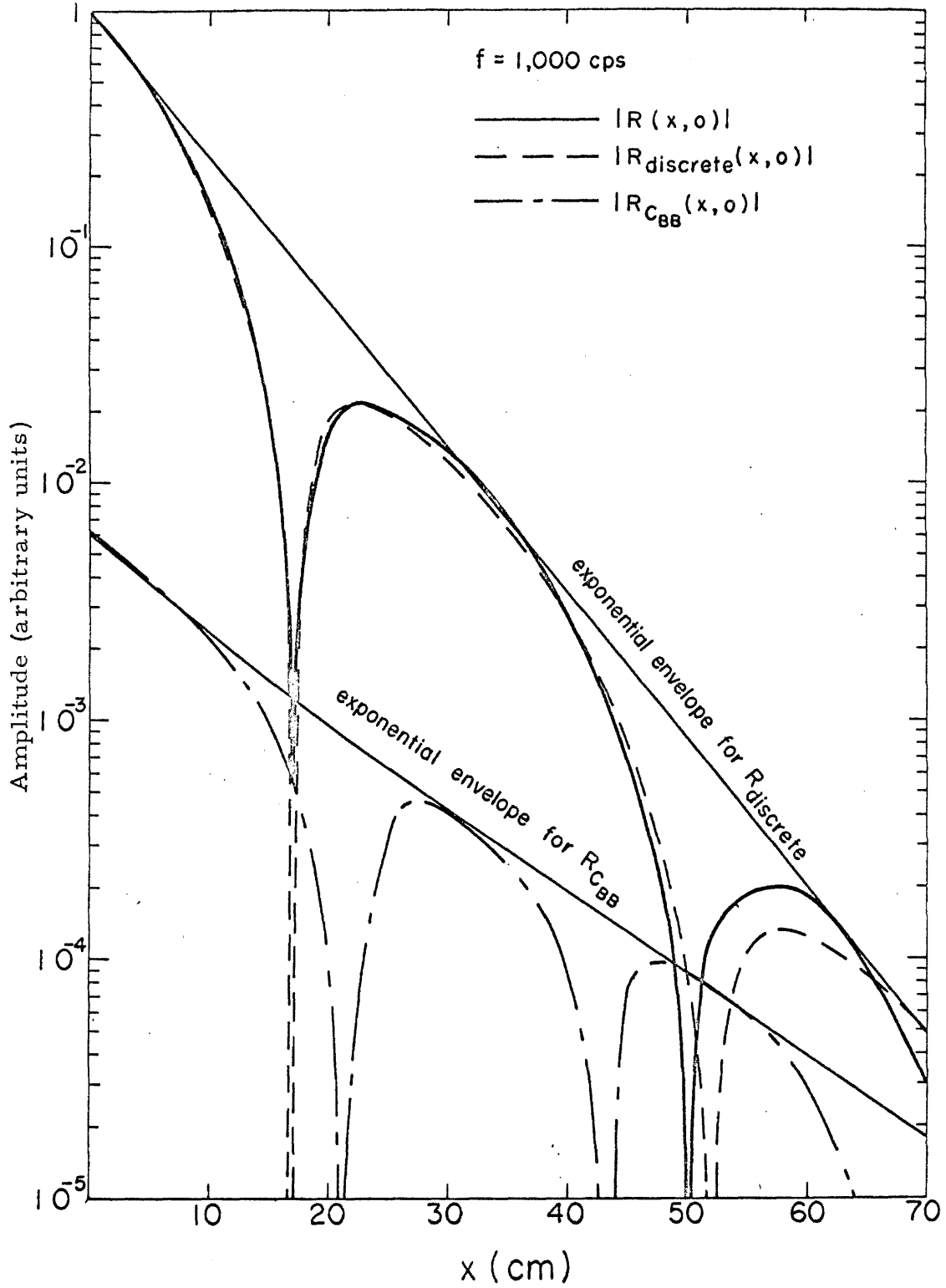


Figure 15. The Detector Response $R(x, 0)$ at $f = 1000$ cps in Graphite.

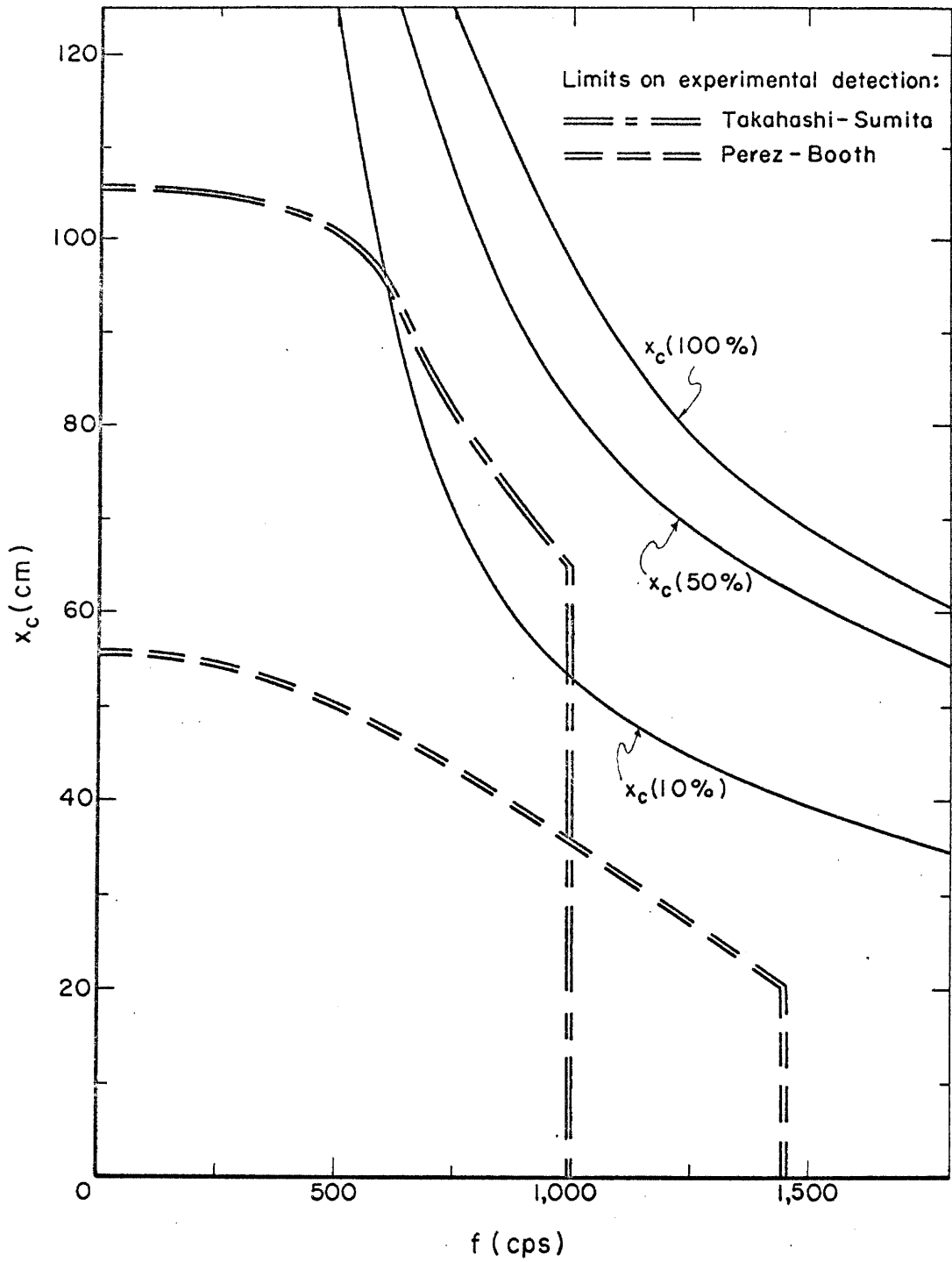
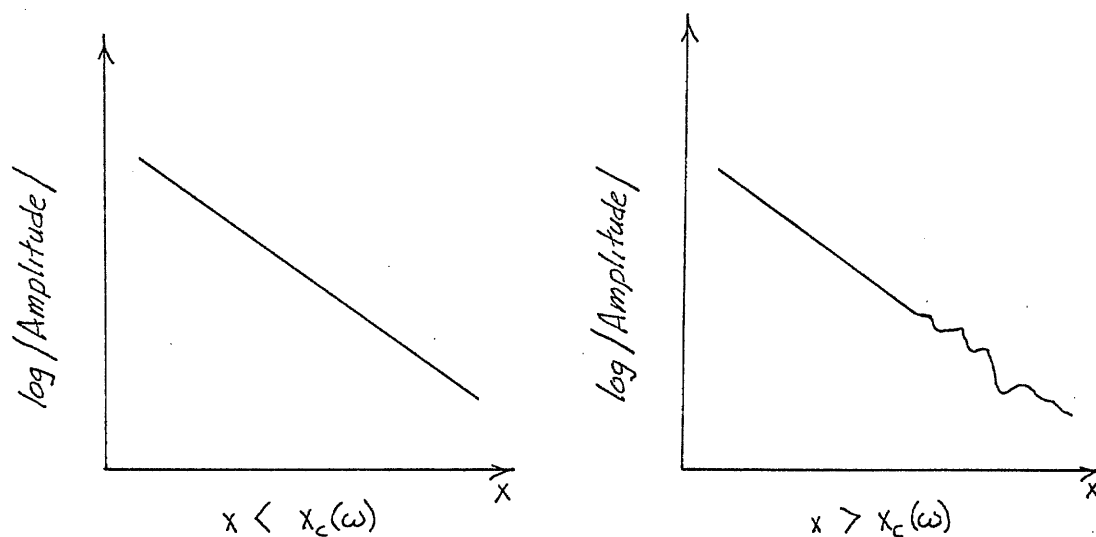


Figure 16. $x_c(f)$ vs. f for Graphite

as ω increases, a very convenient technique would be to perform measurements of the attenuation of the total response at a fixed distance x for various ω . For ω such that $x_c(\omega) > x$, one should observe an exponential attenuation in space since the discrete plane wave mode is dominant. However for ω such that $x_c(\omega) < x$, the continuum contamination should be apparent in the form of a non-exponential behavior. Since the phase shifts of $R_{C_{BB}}$ and R_{discrete} will differ, one expects an interference effect to cause oscillations in the amplitude as a function of x . Recent experiments by Takahashi



and Sumita⁽⁵⁾ appear to have found this effect. Although the counting statistics seem rather poor, oscillations in the data appear roughly where the theory would predict.

Additional experiments of this type with more intense sources or better counting statistics would be interesting. Since $R_{C_{BB}}(x,t)$ is sensitive to the source neutrons emitted below v_B , it should be possible to magnify this effect by using cold neutron sources.

In summary then, the discrete mode will dominate the source transients from C_{AB} and Γ as well as higher transverse modes for $x > 20$ cm, $f < 5000$ cps. The sub-Bragg continuum C_{BB} is actually less damped than the discrete eigenvalue κ_0 and will dominate¹ asymptotically in x . However the relative magnitude of this term still allows one to resolve the discrete mode provided the detector is sufficiently close to the source ($x < 50$ cm, for $f < 1000$ cps).

The experimenters appear to have made most of their measurements in regions in which the continuum contamination should be minimal, and thus should indeed be measuring a discrete plane wave mode. The one exception has been the above mentioned data taken by the Japanese group which appears to demonstrate the effect of continuum contamination by C_{BB} .

3. Further Comments

We have seen that the dip in the cross-section below the Bragg cutoff introduces a portion of $\sigma_c(A)$ which has less damping than the discrete eigenvalue for most experimental situations. Indeed for $B_{\perp}^2 > 15 \times 10^{-4} \text{ cm}^{-2}$, the discrete eigenvalue ρ_0 ($\omega = 0$) is actually imbedded in C_{BB} . This appears disturbing at first. However it is useful to keep in mind that C_{BB} represents sub-Bragg neutrons. A measure of the importance of these sub-Bragg effects is given by the

¹Indeed this phenomena is quite well known in wave propagation experiments in rarefied gases and plasmas in which there are continuum modes present with zero damping [corresponding to $\Sigma_t(v) \rightarrow 0$ as $v \rightarrow \infty$].

parameter

$$\epsilon \equiv \frac{\# \text{ of sub-Bragg neutrons}}{\text{total } \# \text{ of neutrons}}$$

For graphite, $\epsilon = 0.6\%$ for Maxwellian sources, and thus all of these effects are rather small.

Similar phenomena arise in any problem involving neutron transport in polycrystalline media [e.g. the pulsed neutron experiment]⁽⁴⁹⁾. Although the effects of sub-Bragg structure do certainly have a qualitative influence upon the mathematical structure of the solution, the fact that they cause only an $O(\epsilon)$ effect in most cases means that one should be able to ignore C_{BB} without making any major quantitative error [such as in the calculation of the dispersion law].

However the presence of C_{BB} does seem to invalidate the usual series expansions of $\kappa_o^2(\omega)$ such as equation (II-47). Indeed for $B_1^2 > 15 \times 10^{-4} \text{ cm}^{-2}$, $\rho_o(\omega)$ is imbedded in the continuum, and the radius of convergence of the power series in $(i\omega)^n$ is zero. One might be tempted to try an alternative type of expansion about the singularity. However we feel that such expansions are of little use in presenting data in any case, and that a direct comparison of data and theory in the κ -plane [or better yet, the ρ^2 -plane] is usually preferable.

B. D_2O

Since D_2O is noncrystalline, one would suspect that the synthetic kernel model (IV-2) would be adequate to study this type of

experiment. However due to the rather large coherent scattering cross-section, it was decided to use once again a modified synthetic kernel with cross-section modeling as shown in Figure 17. Of course there is no Bragg cutoff and thus no sub-Bragg continuum structure to worry about for this model. In addition, since $\frac{\Sigma_e(v)}{\Sigma_t(v)} \ll 1$ for all v , one can easily show that Γ lies very close to the boundary ∂C and thus can also safely be ignored.

1. Calculation of the Discrete Eigenvalues

The κ -plane structure for D_2O is presented on p. 140 along with an inverted spectral plane and the ρ^2 -plane. Again the agreement appears to be reasonably good for the κ -plane. However the ρ^2 -plane exhibits considerable deviation since it magnifies second order effects in ω .

2. Resolution of the Discrete Mode

For $x > 20$ cm there is no difficulty in resolving the discrete mode for all $\omega < \omega^* = 2\pi$ (10,000 cps). Of course since there is no C_{BB} , this discrete mode dominates asymptotically in x .

C.. OTHER MATERIALS

In principle, we have shown that the above models are capable of analyzing neutron wave experiments in both noncrystalline and polycrystalline materials. Since graphite and D_2O have been the only materials upon which simple experiments have been performed, no further calculations will be presented for additional media. However these calculations are straightforward and can easily be per-

formed when the need arises.

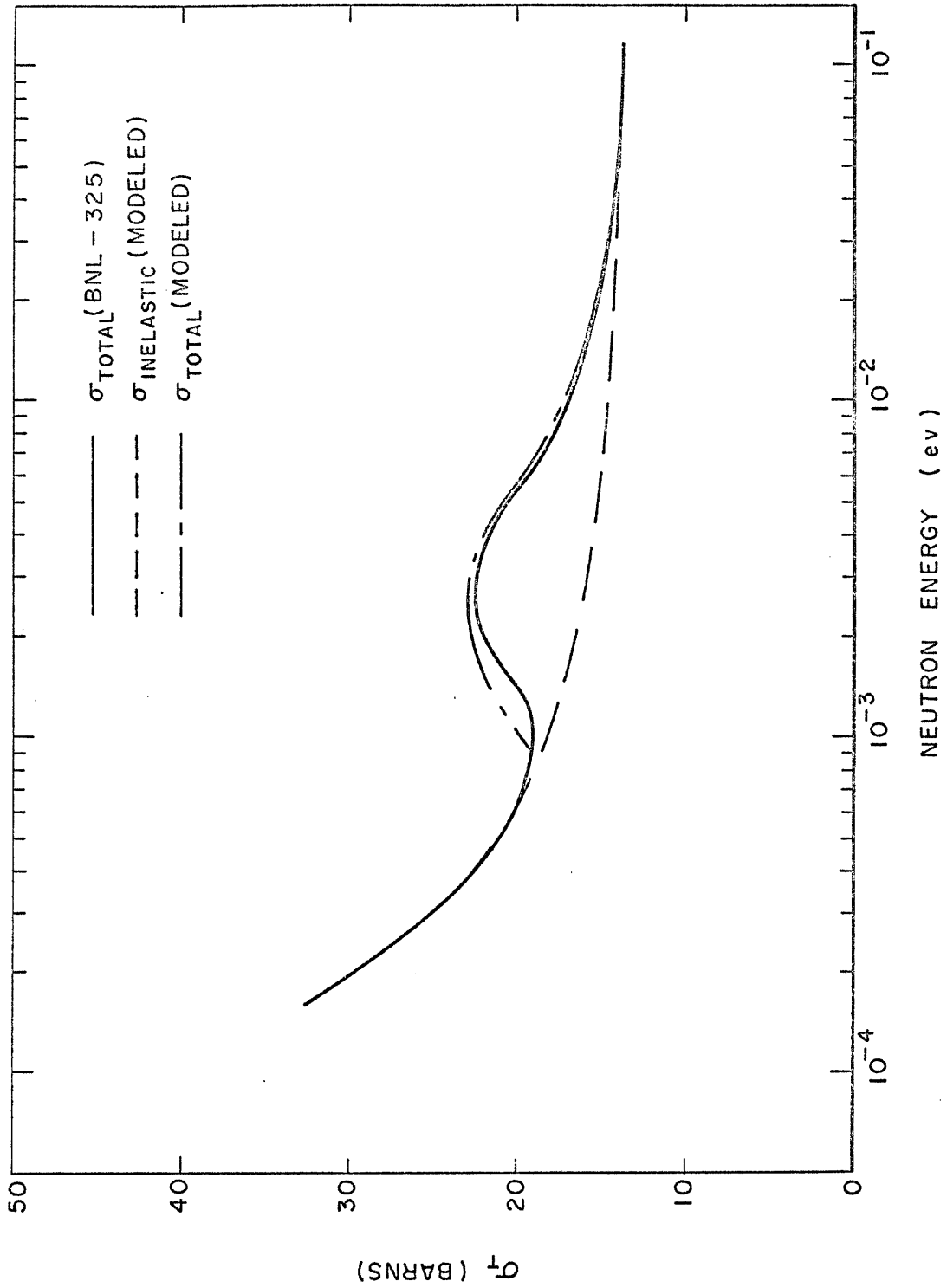


Figure 17. Cross-Section Modeling for D₂O

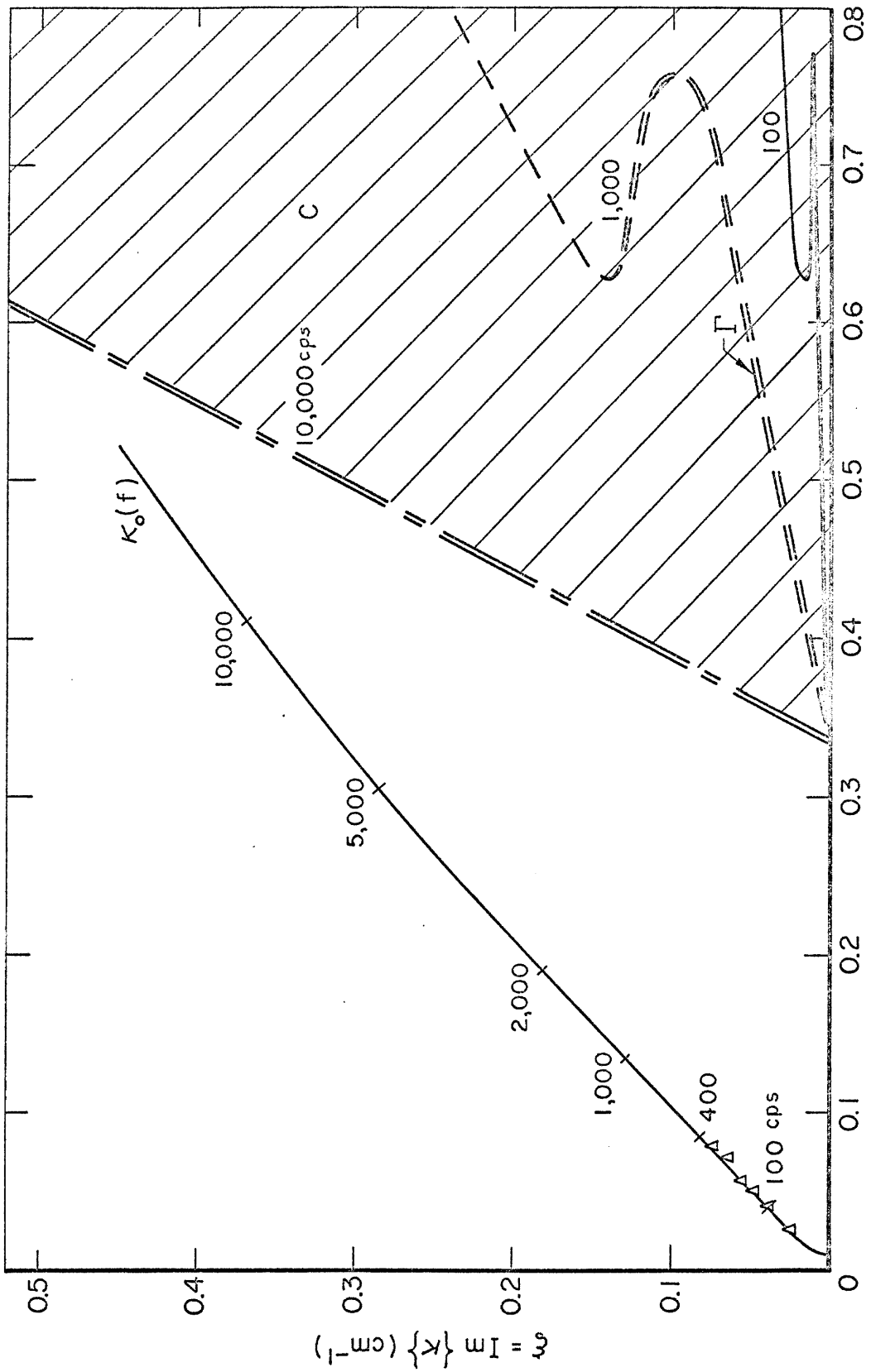


Figure 18. Eigenvalue Spectrum for D_2O

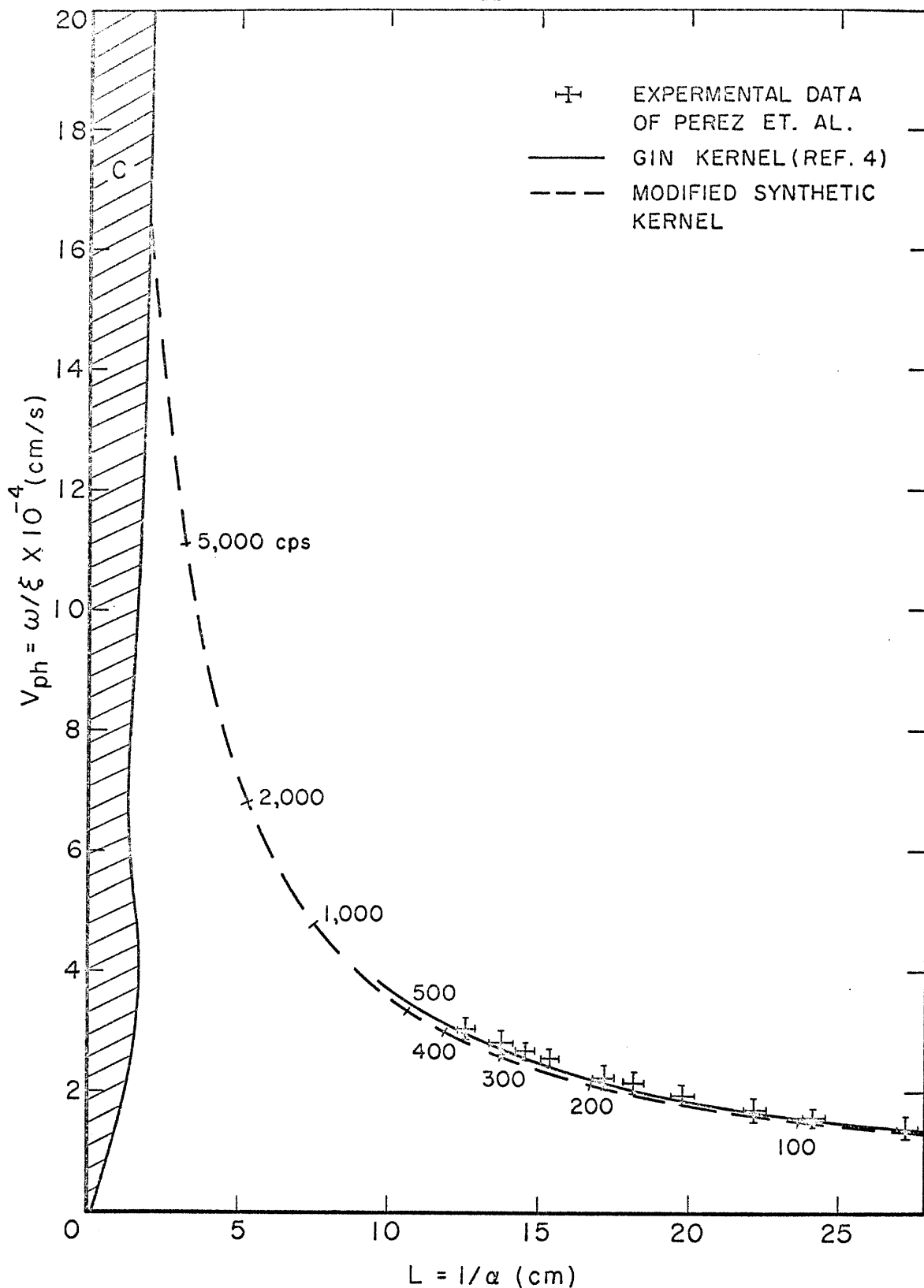


Figure 19. The Inverted Spectral Plane Diagram for D_2O

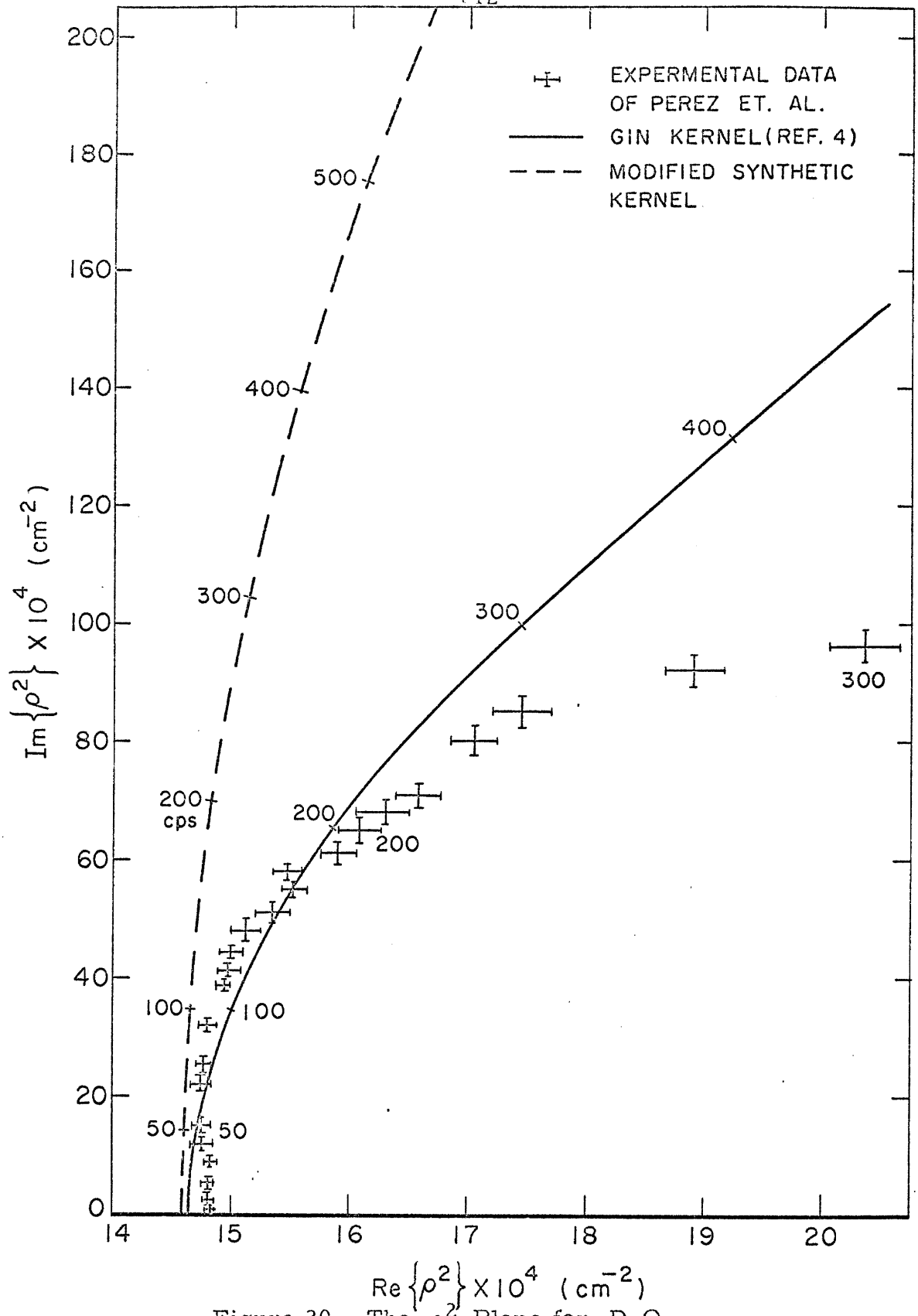


Figure 20. The ρ^2 -Plane for D_2O

VIII. CONCLUSIONS

A. SUMMARY OF RESULTS

This thesis has attempted to develop a comprehensive and exact transport theory of neutron wave propagation in homogeneous, non-multiplying media. Of course much of this theory is of a formal nature in that explicit solutions cannot be obtained without first specifying the detailed form of the cross-sections appearing in the Boltzmann equation, and then solving rather complicated Fredholm integral equations. Moreover, portions of this theory are speculative and incomplete from a mathematical point of view. But this was to be expected since the general mathematical theory of such non-self-adjoint, unbounded operators is itself rather primitive at this time. By augmenting much of the analysis with physical arguments, we have sought to bypass mathematical rigor in an attempt to obtain some general qualitative information about the propagation of such wave-like disturbances in a neutron distribution.

It was possible to give a rather general study of the eigenvalue spectrum of the Boltzmann transport operator for plane wave propagation in both noncrystalline and polycrystalline moderators. An extension of this analysis to systems of finite transverse dimension was indicated. A general solution to the problem of neutron wave propagation in an infinite medium was given for noncrystalline media. Unfortunately, at the present time no general theory appears possible for constructing the solution of partial range expansion problems involving such general scattering kernels. Nevertheless it was possible

to develop a theory utilizing a one-term separable kernel which can be used, in principle, to solve any problem with one dimensional symmetry and sectionally homogeneous media (e. g. wave reflection from an interface or slab). By way of demonstration, the problem for an oscillating source at a free boundary of a half-space was considered.

In the second phase of the thesis, simple models of the scattering kernel were used to illustrate how the general theory could be applied to analyze the neutron wave experiments performed in graphite and D_2O . The modeling of the graphite kernel was designed to exhibit those features characteristic of polycrystalline media, and led to several interesting qualitative and quantitative results. A suitable model of D_2O was also studied.

It was not expected that such crude modeling of the scattering kernel would give accurate estimates of the discrete eigenvalues. However numerical calculations revealed that the theory was surprisingly good in predicting the dispersion curves of the discrete eigenvalues. Indeed, the modeled transport theory gave better results than the MASS-12 kernel calculations of Perez and Booth⁽¹²⁾, and yielded results comparable to the SUMMIT calculations based upon the Parks' model of the graphite scattering kernel. Similarly, agreement with the GIN kernel calculations for D_2O was somewhat better than expected.

B. IMPLICATIONS FOR EXPERIMENTAL TECHNIQUES

The theory has proven useful in helping us to understand the neutron wave experiment. Of perhaps most immediate interest and

significance was the conclusion that while a discrete plane wave mode is certainly dominant asymptotically in noncrystalline media such as D_2O , the asymptotic behavior for large distances from the source in polycrystalline media such as graphite is frequently not plane-wave in nature. It was demonstrated that even for low source frequencies, the continuum contribution due to the sub-Bragg neutrons actually has less spatial damping than the discrete mode, and thus will dominate the solution for sufficiently large x . Consequently measurements in polycrystalline media must not be performed at too great a distance from the source since otherwise this non-plane wave component will be detected.

It was possible to verify in general that plane wave behavior can be observed for most moderating systems providing certain critical bounds on experimental parameters such as source frequency, absorption, and transverse dimensions are not exceeded. In most cases, existing experiments have remained well within these limitations.

The analysis has indicated that transport effects upon the dispersion law for discrete eigenvalues are rather small in most cases. Even the phenomena introduced by the Bragg cutoff in polycrystalline materials are only of order 0.5% [although it does appear that properly designed experiments can detect these effects].

Of course such a transport theory analysis is mandatory if one wishes more information than merely the trajectory of discrete eigenvalues [such as the form of the neutron distribution $f(x, \mu, v, t)$].

In particular, the Bragg cutoff behavior of $\Sigma_s(v)$ seems to invalidate the customary power series expansion in $(i\omega)^n$ as a means of data presentation and comparison with theory [although such a technique still appears to be valid for noncrystalline media].

It is certainly true that a direct comparison of the measured dispersion curve with theoretical calculations in the ρ^2 -plane provides a very sensitive test of second order effects in frequency [and hence considerable sensitivity to higher moments of the scattering kernel]. However it remains to be seen whether these defects in the modeling of the scattering kernel which are responsible for this disagreement with the wave data are of any significance to the original purposes for which these kernels were designed--i.e. reactors. And although it is of interest to present such ρ^2 -plane plots, they should always be supplemented with a κ -plane plot of the actual eigenvalue spectrum since these latter eigenvalues are the quantities of true physical significance [the "observables" of both experiment and theory].

Notice also that even though such comparisons as the ρ^2 -plane provide very sensitive tests of the scattering kernel model, they do not provide direct measurement of any physical parameters of interest. Of course for those systems in which an $(i\omega)^n$ expansion is valid, the neutron wave experiment can be used to measure the same quantities as the pulsed neutron experiment (Σ_a , L , D_0 , C_0 , etc.) by appropriate power series fitting. Our analysis has also indicated that quantities such as $\langle v_x \rangle$ can be measured, but these are of questionable interest. Thus it appears that the role of the neutron wave experiment to measure "parameters of physical interest" in

single-region, non-multiplying media is open to some challenge. Of course such experiments are still of considerable use as a test of theoretical models of neutron transport. They also provide an experimental and theoretical background for wave experiments in more complicated systems.

It is convenient at this point to make a brief comparison of the wave propagation experiment (WPE) with the two other classic experiments of neutron physics, the pulsed neutron experiment (PNE) and the diffusion length experiment (DLE). All three experiments are similar in that they seek to measure a fundamental discrete eigenvalue as a function of some experimental parameter: in the WPE, one measures the complex wave number κ vs. the source frequency ω ; in the PNE, the time decay constant λ is measured as a function of system size, B^2 ; and in the DLE, the inverse relaxation length κ is measured as a function of absorption concentration $\Sigma_a(v)$. One can roughly order the experimental difficulty of these experiments in solid moderators as $PNE < WPE < DLE$. [The DLE has been considered the most difficult experiment to perform since it is extremely difficult to vary the amount of poison in solid materials.]

However consideration of the theoretical analysis of these experiments prompts a different conclusion. The PNE is effectively a non-separable problem in space \underline{r} , time t , and velocity \underline{v} and must be treated as such. The assumption of a separable distribution $\varphi(\underline{v}, t)R(\underline{r})$ which is made in "e $\frac{iB \cdot R}{R}$ transport theory" is clearly inadequate for many experimental situations. That is, λ must be

calculated theoretically as a function of system dimensions rather than some mythical parameter such as B^2 [whose mere existence is a matter of some doubt]. However by using a source of fixed time dependence and waiting long enough for starting transients to decay, one can regard the WPE and DLE as separable in $(\underline{r}, \underline{v})$ and t since the steady state response of the neutron distribution will then have the same time behavior as the source. This considerably simplifies the theory of such experiments, essentially allowing the exact mathematical treatment of these latter problems [as in the first portion of this thesis]. Thus if one were to order the three experiments according to level of theoretical complexity, the order would be inverted from before: DLE < WPE < PNE.

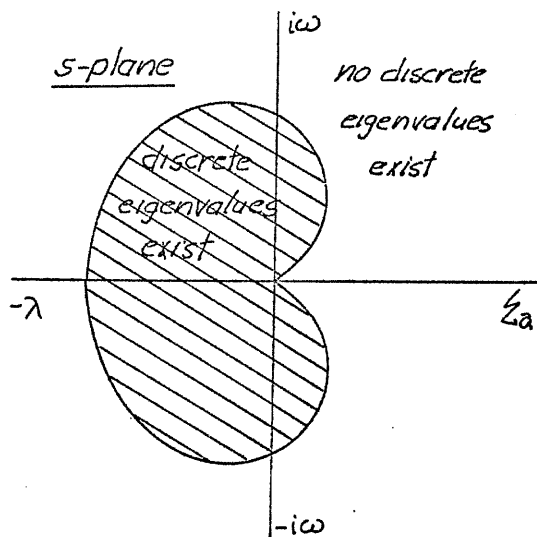
It is important here to make one further comment about the comparison of the WPE to the PNE frequently encountered in the literature. The statement is occasionally made that the WPE is complementary to the PNE since the former possesses no inherent limitation such as material size. However our analysis has shown that there exist not only limitations on system size (B_1^2), but in addition, limitations on source frequency and absorption necessary for the performance of meaningful experiments. These limitations are no more or less restrictive than similar limitations on the pulsed neutron experiment.

To understand this in more detail, one can use the dispersion laws $\Lambda(\kappa)$ discussed earlier in this thesis to study all three problems (PNE, DLE, & WPE) simultaneously if it is recognized that $\kappa \rightarrow -iB$,

$i\omega \rightarrow \lambda$ in the PNE, and $\kappa \rightarrow \kappa$, $i\omega/v \rightarrow \Sigma_a(v)$ in the DLE. That is, one can regard $\Lambda(\kappa, s) = 0$ in general as a relation between two complex variables, s and κ . In the s -plane there will be a region in which $\Lambda(\kappa, s)$ may have zeros--i.e. in which discrete eigenvalues exist.

Outside of this region, the discrete eigenvalues vanish. The existence theorems such as Theorem IV occur when the bounding curve R

dividing these regions intersects the axes. It is evident that the limiting values of various parameters for each type of experiment can be compared by examining the shape of the curve R . Our models suggest that R will be roughly circular in shape, thus implying that all three experiments are



equally restricted by their respective limitations.

Hence it appears that the major advantage of the wave experiment over the other traditional experiments of neutron physics is in the exact knowledge of the independent experimental variable ω it allows, as opposed to the use of a fictitious parameter such as B^2 . It is also true that by appropriate variation of ω , $\Sigma_a(v)$, and B_1^2 one can use the wave experiment to study the entire spectral κ -plane (dispersion law) rather than just the real axis. However it remains to be seen whether this can provide any additional information of interest.

C. SUGGESTIONS FOR FURTHER EXPERIMENTATION

This thesis has prompted several suggestions for future experimentation as well as data analysis in existing types of experimentation:

i) One should always plot the κ -plane spectrum $\sigma_c(A)$ for the material of interest before experimentation or analysis in order to determine how close the measurements will be to the continuum eigenvalue structure. [Such a diagram can be sketched by using the BNL-325 cross-section data to calculate C.]

ii) For noncrystalline media, transport effects play a minor role, and existing methods of analysis are adequate for $\omega \ll \omega^* \sim \langle v \Sigma_t(v) \rangle$. Both a direct comparison of data in the κ -plane or ρ^2 -plane as well as an evaluation of the coefficients in an $(i\omega)^n$ expansion appear useful.

iii) In polycrystalline materials more care must be taken to account for the sub-Bragg neutron effects. In particular, the customary power series expansions in $(i\omega)^n$ should be abandoned in favor of a direct comparison of measured and calculated dispersion curves in either the κ -plane or the ρ^2 -plane. Although it appears that existing experiments have experienced very little continuum contamination, one should be aware that such effects will occur for sufficiently large ω and/or x .

iv) To date most attention has been directed toward the measurement

of the dispersion curve of the fundamental eigenvalue $\kappa_0(\omega)$. However it appears that for sufficiently large ω , $\Sigma_a(v)$, or B^2 one should be able to observe the sub-Bragg continuum contribution due to C_{BB} in polycrystalline media such as graphite. Cold neutron sources such as those used by DeJuren and Swanson⁽⁵⁷⁾ might be used to enhance the magnitude of this continuum term. One would then attempt to observe C_{BB} by looking for oscillations in the measured wave amplitude vs. distance x due to phase interference between the continuum and discrete wave modes. It would be quite interesting if one could measure the period of these oscillations and then theoretically relate this period to some physical parameter (perhaps characteristic of the sub-Bragg cross-section structure of the medium).

D. SUGGESTIONS FOR FURTHER THEORY

There appear to be a number of useful and significant extensions of the work contained in this thesis. Of perhaps most direct interest to the experimenter would be a more thorough determination of precisely what physical parameters of the propagating media can be measured by neutron wave techniques. The measurement of Σ_a , D_0 , C_0 , etc. does not in itself justify such experiments (just as it does not justify similar work with pulsed neutron sources). There is some possibility that one might be able to obtain information directly from the continuum contributions in polycrystalline material. Certainly a more detailed investigation into these questions is needed.

Considerable work remains on the extension of this theory to both multiple region systems (wave reflection experiments) and wave

propagation in multiplying media. A significant amount of work also remains on the analysis of neutron pulse propagation--that is, the analysis of true waves with finite wave-front speed rather than "wave-like" disturbances (merely characterized by periodic behavior in x and t) such as considered in this thesis. Such work will involve an integration of our solutions over all ω in order to synthesize such pulses.

Of more mathematical interest is an adequate treatment of wave propagation in geometries of finite transverse dimensions. Asymptotic reactor theory is inadequate to provide a detailed description of transverse leakage effects, and a full transport theory analysis is needed. Of course such work has been long overdue even for the static diffusion length problem. (33, 56)

It is also of some importance to study the point eigenvalues imbedded in the continuous spectrum, and the effect of these eigenvalues upon the representation of the total solution. This of course will involve generalized analytic function theory, but should be straightforward. Of related interest is a general study of the dispersion law for neutron transport as a function of two complex variables s and k .

It was mentioned in the introductory chapter that the analysis of neutron wave propagation is mathematically quite similar to the study of plane wave disturbances in rarefied gases and low density plasmas. We suspect that much of the analysis of this thesis is similarly adaptable to these fields.

APPENDIX A: ELEMENTARY THEORIES OF
NEUTRON WAVE PROPAGATION

I. ONE-VELOCITY DIFFUSION THEORY

The diffusion equation of interest is

$$\frac{\partial n}{\partial t} - Dv \frac{\partial^2 n}{\partial x^2} + v\Sigma_a n(x,t) = S(x)e^{i\omega t} \quad (\text{A-1})$$

If one considers separable solutions of the form $n(x,t) = n_0 e^{-\kappa x + i\omega t}$, then the condition for κ becomes

$$\kappa^2 = \frac{i\omega}{Dv} + \frac{1}{L^2} \quad \text{where } L = \sqrt{\frac{D}{\Sigma_a}}$$

Hence there are two discrete plane wave modes characterized by

$$\kappa = \pm \left[\frac{i\omega}{Dv} + \frac{1}{L^2} \right]^{\frac{1}{2}} \quad (\text{A-2})$$

II. ONE-VELOCITY, ISOTROPIC TRANSPORT THEORY

Consider the one-velocity Boltzmann equation within the isotropic scattering approximation

$$\begin{aligned} \frac{\partial f}{\partial t} + \mu v \frac{\partial f}{\partial x} + v\Sigma_t f(x,\mu,t) \\ = \frac{1}{2} v\Sigma_s \int_{-1}^{+1} d\mu' f(x,\mu',t) + S(x,\mu)e^{i\omega t} \end{aligned} \quad (\text{A-3})$$

Substituting the plane wave ansatz $f(x,\mu,t) = F(\kappa;\mu)e^{-\kappa x + i\omega t}$ into the homogeneous version of (A-3) yields

$$[i\omega + v\Sigma_t - \kappa\mu v] F(\kappa;\mu) = \frac{v\Sigma_s}{2} \int_{-1}^{+1} d\mu' F(\kappa;\mu') = \frac{v\Sigma_s}{2} \quad (\text{A-4})$$

where we have normalized $\int_{-1}^{+1} d\mu' F(\kappa; \mu') \equiv 1$

Point Spectrum P: Let $\kappa \notin C$ where $C \equiv \{ \kappa: \kappa = \frac{i\omega}{\mu v} + \frac{\Sigma_t}{\mu}, \mu \in [-1, +1] \}$.

To find the conditions on the eigenvalues $\kappa \notin C$, divide through in (A-4) by $[i\omega + v\Sigma_t - \kappa\mu v]$ and integrate over μ to find the dispersion law

$$\Lambda(\kappa) = 1 - \frac{\Sigma_s}{2\kappa} \ln \left[\frac{i\omega + v\Sigma_t + \kappa v}{i\omega + v\Sigma_t - \kappa v} \right] = 0 \quad \kappa \notin C \quad (A-5)$$

The corresponding eigenfunctions are then found from (A-4) as

$$F(\kappa_\ell; \mu) = \frac{v\Sigma_s/2}{i\omega + v\Sigma_t - \kappa_\ell \mu v} \quad \kappa_\ell \in P \quad (A-6)$$

Continuous Spectrum C: Now the continuum eigenfunctions are found as

$$F(\kappa; \mu) = \frac{v\Sigma_s/2}{i\omega + v\Sigma_t - \kappa\mu v} + \lambda(\kappa) \delta \left(\mu - \frac{i\omega + v\Sigma_t}{\kappa v} \right) \quad \kappa \in C \quad (A-7)$$

To evaluate $\lambda(\kappa)$, use the normalization of $F(\kappa; \mu)$ to find

$$\lambda(\kappa) = 1 - \frac{\Sigma_s}{2\kappa} \ln \left[\frac{\kappa v + i\omega + v\Sigma_t}{\kappa v - i\omega - v\Sigma_t} \right] \equiv \Lambda(\kappa) \quad (A-8)$$

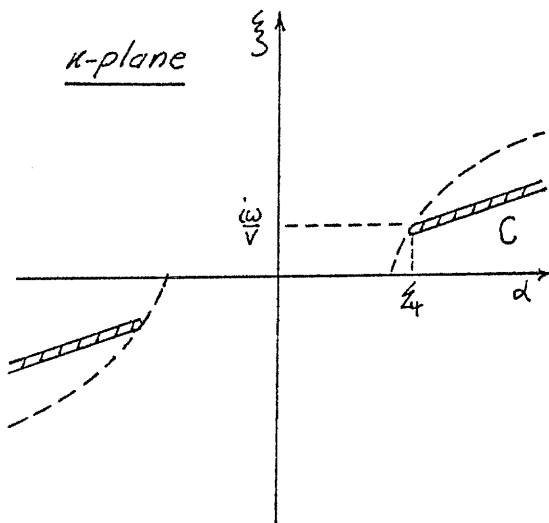
where explicit use of the Cauchy principal value has been used in the integration.

Thus one can express general solutions to (A-3) as

$$f(x, \mu, t) = \sum_{\ell} a_{\ell} F(\kappa_{\ell}; \mu) e^{-\kappa_{\ell} x + i\omega t} + \int_C d\kappa A(\kappa) F(\kappa; \mu) e^{-\kappa x + i\omega t} \quad (A-9)$$

One can show that the eigenfunctions $\{F(\kappa;\mu): \kappa \in \text{CUP}\}$ form an orthogonal set over the full-range $\mu \in [-1, +1]$ [with weighting factor μ] and are complete over both full and partial ranges of κ for any function $\psi(\mu) \in H^*[-1, +1]$ (24,58).

To obtain more information about the eigenvalue spectrum, first note that the continuum C is a cut in the κ -plane. [It is also useful to sketch in the exact area continuum for the velocity-dependent problem treated in the thesis.]



By applying the Principle of the Argument around a suitable contour in the κ -plane, one can show that $\Lambda(\kappa)$ has two zeros, $\pm\kappa_0$,

for $\omega < \omega^* = \frac{\kappa}{2} \mu_0 v \Sigma_s$ where μ_0 is determined by $1 - \frac{\Sigma_s}{\Sigma_t} \mu_0 \tanh^{-1} \mu_0 = 0$. Furthermore one can show that

$$\kappa_0(\omega) \sim \sqrt{3\Sigma_t \Sigma_a} \left[1 + i \left(\frac{\omega}{2v\Sigma_a} \right) \right], \frac{\omega}{v\Sigma_t} \ll 1, \frac{\Sigma_a}{\Sigma_t} \ll 1$$

which agrees with the diffusion theory expression (A-2).

III. CURRENT METHODS OF ANALYSIS

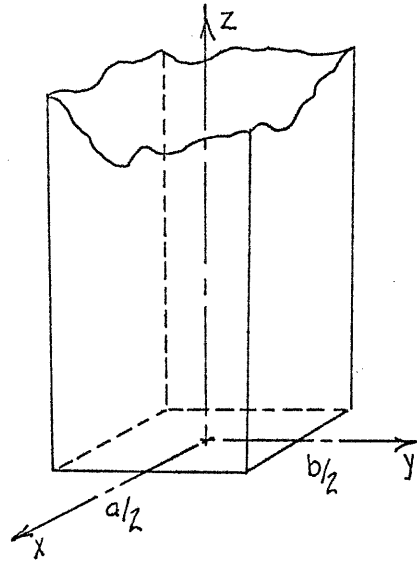
To date, the neutron wave experiments have been analyzed using an energy-dependent diffusion theory which allows a rather accurate modeling of the scattering kernel. This theory, due to

Ohanian, Booth, and Perez⁽¹²⁾, shall be outlined below.

Consider the Boltzmann equation in the diffusion approximation

$$\begin{aligned} \frac{1}{v} \frac{\partial \Psi}{\partial t} - D(E) \nabla^2 \Psi + \Sigma_t(E) \Psi(\underline{r}, E, t) \\ = \int_0^\infty dE' \Sigma_s(E', E) \Psi(\underline{r}, E', t) \end{aligned} \quad (A-10)$$

with boundary conditions for a



parallelepiped assembly with a thermal source at its base

$$\Psi(\pm \frac{a}{2}, y, z, E, t) = \Psi(x, \pm \frac{b}{2}, y, z, E, t) = \Psi(x, y, z \rightarrow \infty, E, t) = 0$$

[Here we neglect end effects and consider only the sinusoidal component of the source.]

$$D(E) \frac{\partial \Psi}{\partial z} = \frac{S(x, y, E)}{2} e^{i\omega t} \quad , \quad z = 0$$

To consider the quasi-steady-state response of the flux, assume

$\Psi(\underline{r}, E, t) = \psi(\underline{r}, E) e^{i\omega t}$, in which case (A-10) becomes

$$\left[\frac{i\omega}{v} + \Sigma_t(E) - D(E) \nabla^2 \right] \psi(\underline{r}, E) = \int_0^\infty dE' \Sigma_s(E', E) \psi(\underline{r}, E') \quad (A-11)$$

It is convenient to symmetrize the scattering kernel using detailed balance, by defining

$$\chi(\underline{r}, E) \equiv \left[\frac{D(E)}{vM(E)} \right]^{1/2} \psi(\underline{r}, E)$$

$$P(E', E) \equiv \left[\frac{v' M(E')}{D(E') D(E) v M(E)} \right]^{\frac{1}{2}} \Sigma_s(E', E) - \frac{1}{D(E')} \Sigma_t(E') \delta(E-E')$$

to rewrite (A-11) as

$$\left[\nabla^2 - i \frac{\omega}{vD(E)} \right] \chi(\underline{r}, E) = \int_0^\infty dE' P(E', E) \chi(\underline{r}, E') \quad (A-12)$$

Now expand solutions to equation (A-12) in terms of the space eigenfunctions defined by the Helmholtz equation

$$\left\{ \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + B_{lm}^2 \right\} \varphi_{lm}(x, y) = 0$$

and the energy eigenfunctions defined by

$$-\rho_{\alpha\alpha}^2 \mathcal{J}_\alpha(E) = \int_0^\infty dE' P(E', E) \mathcal{J}_\alpha(E')$$

These latter eigenfunctions are evaluated numerically using the procedure of Ohanian and Daitch⁽¹²⁾.

The solution is then approximated by a finite expansion in the eigenfunctions

$$\chi(\underline{r}, E) = \sum_{l, m, \alpha}^N A_{lm\alpha} \varphi_{lm}(x, y) \mathcal{J}_\alpha(E) e^{-Kz} \quad (A-13)$$

If (A-13) is now substituted into (A-12) and orthogonality is used, a system of algebraic equations arises

$$\sum_{\alpha} \left[(k^2 - \rho_{\alpha\alpha}^2 - B_{lm}^2) \delta_{\alpha\beta} - i\omega L_{\alpha\beta} \right] A_{lm\alpha} = 0$$

$$\text{where } L_{\alpha\beta} \equiv \int_0^\infty dE' \mathcal{J}_\alpha(E') \left[\frac{1}{vD(E')} \right] \mathcal{J}_\beta(E')$$

Thus for non-trivial solutions, we require the usual condition

$$\det \left[(\kappa^2 - \rho_{0\alpha}^2 - B_{\perp \ell m}^2) \delta_{\alpha\beta} - i\omega L_{\alpha\beta} \right] = 0 \quad (\text{A-14})$$

This condition will determine a set of eigenvalues $\kappa = \alpha + i\xi$ for each transverse ℓm mode, and thus constitutes the dispersion law for this model. The final solution to the original problem is then

$$\Psi(\underline{r}, E, t) = \left[\frac{vM(E)}{D(E)} \right]^{\frac{1}{2}} \sum_{\ell, m}^M \sum_{\alpha}^N A_{\ell m \alpha} \varphi_{\ell m}(\underline{x}, y) \mathcal{J}_{\alpha}(E) e^{-\alpha_{\ell m \alpha} z} e^{i(\omega t - \xi_{\ell m \alpha} z)}$$

Now it is hoped that one of these modes will dominate asymptotically in space far from the source and boundaries. If this is true, then the experiment should measure the lowest $\kappa_{110} = \alpha_{110} + \xi_{110}$ for each source frequency.

The dispersion relation (A-14) has been solved numerically for an expansion (A-13) of $N = 33$ terms, and the first few eigenvalues have been evaluated for various ω . For graphite, both the MASS-12 heavy gas kernel code and the SUMMIT code were used in the calculation of the energy eigenfunctions $\mathcal{J}_{\alpha}(E)$. The more accurate SUMMIT code was also used in the multigroup transport theory calculations of Travelli⁽¹³⁾. This code is based upon a model of the graphite scattering kernel due to Parks⁽⁶¹⁾ which uses the incoherent approximation to calculate the inelastic differential scattering cross-section, assuming that the vibrations of atoms perpendicular to the basal planes of the lattice are uncoupled from vibrations in the plane. The elastic scattering is modeled separately and then added on to

obtain the total scattering cross-section $\sigma_s(E)$. (It must be noted that this model fails to account in any way for coherent inelastic scattering. This latter component is of considerable importance for neutron energies below the first Bragg peak. This defect probably explains why the SUMMIT code calculations fail to give good quantitative agreement with experiment.)

For calculations in D_2O , the GIN (Goldman Improved Nelkin) kernel was used with the D_2O parameters introduced by Honeck⁽⁶²⁾. This model also uses the incoherent approximation (hence assuming that all energy transfer is due to incoherent scattering) and treats the D_2O molecule as a combination of translation, hindered rotation, and 3 vibrational states.

These calculations are shown in Figures 12 and 20 where they are compared with the results of experiment as well as the calculations using the modeled transport theory in Part II.

APPENDIX B: THE BOLTZMANN WAVE OPERATOR

I. THE BOLTZMANN WAVE OPERATOR A FOR NONCRYSTALLINE MEDIA

Recall that we wish to consider the linear operator

$$A = \left[\frac{i\omega}{\mu\nu} + \frac{\Sigma_t(\nu)}{\mu} \right] \cdot + \left[- \int_{-1}^{+1} d\mu' \int_0^\infty d\nu' \frac{\widetilde{\Sigma}_s(\nu' \rightarrow \nu, \mu' \rightarrow \mu)}{\sqrt{\mu'\mu}} \cdot \right] \quad (B-1)$$

which operates on functions contained in the Hilbert space $\mathfrak{L}_2(G)$. Also recall that our inner product was chosen as

$$(f, g) \equiv \int_{-1}^{+1} d\mu \int_0^\infty d\nu \overline{f(\mu, \nu)} g(\mu, \nu) \quad (B-2)$$

A. Classification of A

The Streaming Operator: $A_1 = \left[\frac{i\omega}{\mu\nu} + \frac{\Sigma_t(\nu)}{\mu} \right]$

Under the inner product (B-2) it is easy to show that

$$A_1^\dagger = - \frac{i\omega}{\mu\nu} + \frac{\Sigma_t(\nu)}{\mu} \neq A_1, \text{ that is, } A_1 \text{ is not self-adjoint. However}$$

$$\begin{aligned} A_1^\dagger A_1 &= \left[- \frac{i\omega}{\mu\nu} + \frac{\Sigma_t(\nu)}{\mu} \right] \left[\frac{i\omega}{\mu\nu} + \frac{\Sigma_t(\nu)}{\mu} \right] = \left[\frac{i\omega}{\mu\nu} + \frac{\Sigma_t(\nu)}{\mu} \right] \left[- \frac{i\omega}{\mu\nu} + \frac{\Sigma_t(\nu)}{\mu} \right] \\ &= A_1 A_1^\dagger \end{aligned}$$

Hence A_1 is a normal operator. Since A_1 is a multiplicative operator, it is not completely continuous. [Here we are using the definition of a completely continuous operator A as one for which $\varphi_n \rightarrow \varphi \implies A\varphi_n \rightarrow A\varphi$.] Furthermore note that

$$\|A_1 f\|^2 = \int_{-1}^{+1} d\mu \int_0^\infty d\nu \left[- \frac{i\omega}{\mu\nu} + \frac{\Sigma_t(\nu)}{\mu} \right] \left[\frac{i\omega}{\mu\nu} + \frac{\Sigma_t(\nu)}{\mu} \right] \overline{f(\mu, \nu)} f(\mu, \nu)$$

and since $\Sigma_t(v) \rightarrow \infty$ as $v \rightarrow 0$, $\|A_1 f\| \neq M \|f\|$ for some $f(\mu, v) \in \mathfrak{L}_2(G)$. Thus by definition, A_1 is an unbounded operator.

The domain of this unbounded normal operator is

$$\mathfrak{D}_{A_1} \equiv \left\{ \varphi: \varphi \in \mathfrak{L}_2(G), \frac{\varphi}{\mu v} \in \mathfrak{L}_2(G), \frac{\Sigma_t(v)}{\mu} \varphi \in \mathfrak{L}_2(G) \right\}$$

The Scattering Operator:
$$A_2 \equiv - \int_{-1}^{+1} d\mu' \int_0^\infty dv' \frac{\tilde{\Sigma}_s(v' \rightarrow v, \mu' \rightarrow \mu)}{\sqrt{\mu' \mu}}$$

This operator is hopefully bounded and is certainly self-adjoint under (B-2). However we would like to go one step further and conclude that it is completely continuous. That is, we would like to show that $\varphi_n \rightarrow \varphi \implies A_2 \varphi_n \rightarrow A_2 \varphi$. To do this, we must demonstrate that the kernel of A_2 or one of its iterates is square-integrable.

However this demonstration is a rather difficult task. Observe that for isotropic scattering kernels

$$\|A_2\|^2 = \int_{-1}^{+1} d\mu \int_0^\infty dv \int_{-1}^{+1} d\mu' \int_0^\infty dv' \left[\frac{\tilde{\Sigma}_s(v'v)}{\sqrt{\mu' \mu}} \right]^2 = \left[\int_{-1}^{+1} \frac{d\mu}{\mu} \right]^2 \|\tilde{\Sigma}_s(v', v)\|^2$$

We note a logarithmic divergence due to the $1/\mu$ term. This divergence is in addition to the divergence at high (v, v') of the free-gas kernel⁽²⁹⁾. Thus we conclude that $\|A_2\| = \infty$. Now it may happen that a higher iterate of A_2 is square-integrable. Certainly the $[\mu' \mu]^{-1/2}$ will not affect the customary divergences of $\tilde{\Sigma}_s(v' \rightarrow v, \mu' \rightarrow \mu)$ which are square-integrable in higher iterates.

However it may happen that A_2 is not compact in an $\mathfrak{L}_2(G)$ sense since the $1/\mu$ divergence occurs because of neutron streaming

perpendicular to the x-axis. This is a definite "physical" singularity in the problem. Perhaps one should actually work in the function space of Bareiss⁽⁴⁸⁾ which allows for principal value interpretation of integrals. In this case, $1/\mu$ is integrable. This latter approach was adopted in an attempt to rigorize a spectral theory approach to the Case method⁽²⁴⁾, which of course involves principal value integrations as well as the treatment of functions obeying Hölder conditions.

However as physicists rather than mathematicians, we are reluctant to cast aside the more familiar Hilbert space $\mathcal{L}_2(G)$. Thus we shall assume that A_2 can be regarded as completely continuous operator. [Additional motivation for this assumption is two-fold:

- (1) We know the Case approach involving similar operators is correct.
- (2) We can show that the $1/\sqrt{\mu'\mu}$ term in A_2 does not appear to add additional continuous spectra to $\sigma(A)$ --see p. 166.]

In summary then, A_2 is a self-adjoint, "completely continuous" operator whose domain of definition $\mathcal{D}_{A_2} \equiv \mathcal{L}_2(G)$.

It is evident that $\mathcal{D}_{A_1} \subset \mathcal{L}_2(G)$. Hence we can conclude that the domain of our original operator A is $\mathcal{D}_A \equiv \mathcal{D}_{A_1}$.

B. The Spectrum $\sigma(A)$ of A

We shall now indicate a sequence of theorems about the spectrum $\sigma(A)$ which culminate in the summary theorem presented on p. 18.

1. The Continuous Spectrum $\sigma_c(A)$:

Recall that by definition $\sigma_c(A)$ is composed of those values of κ for which $R(A - \kappa) \equiv \mathcal{L}_2(G)$, and $(A - \kappa)^{-1}$ exists but is an unbounded

operator. We shall first indicate two useful preliminary theorems:

LEMMA (Extended Weyl Criterion): A necessary and sufficient condition that κ be a limit point of the spectrum [and thus in $\sigma_c(B)$] of a normal operator B is that there exist a sequence of elements $\varphi_n \in \mathcal{D}_B$ such that

$$\|\varphi_n\| = 1, \quad \varphi_n \rightarrow 0, \quad (B - \kappa)\varphi_n \rightarrow 0 .$$

Proof: The proof of this lemma is given for self-adjoint operators in Riesz-Sz. Nagy⁽²⁷⁾, p. 363. However the only place where the assumption of a self-adjoint operator entered into this proof was in the application of the spectral decomposition theorem

$$A = \int_{-\infty}^{+\infty} \lambda dE_\lambda .$$

Since such a theorem can also be proven for a more general unbounded, normal operator [see footnote, Riesz-Sz. Nagy, p. 363]

$$B = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \kappa d^2 E_{\kappa} ,$$

the Weyl criterion appears true in addition for unbounded normal operators such as A_1 .

THEOREM (Extended Weyl-von Neumann Theorem): If A is a normal operator and B is a self-adjoint, completely continuous operator, then

$$\sigma_c(A + B) = \sigma_c(A) .$$

Proof: Suppose $\kappa \in \sigma_c(A)$ and let φ_n be a sequence such that

$$\|\varphi_n\| = 1, \varphi_n \rightarrow 0. \text{ Of course}$$

$$(A + B - \kappa)\varphi_n = (A - \kappa)\varphi_n + B\varphi_n$$

But $(A - \kappa)\varphi_n \rightarrow 0$ by the extended Weyl criterion. Furthermore by the definition of a completely continuous operator, $B\varphi_n \rightarrow 0$.

Thus

$$(A + B - \kappa)\varphi_n \rightarrow 0 \implies \kappa \in \sigma_c(A + B) \quad \text{Q.E.D.}$$

We shall now use these theorems to locate $\sigma_c(A)$ for (B-1).

THEOREM: Let $C \equiv \left\{ \kappa: \kappa = \frac{i\omega}{\mu\nu} + \frac{\Sigma_t(v)}{\mu}, \mu \in [-1, +1], \nu \in [0, \infty) \right\}$.

Then $\sigma_c(A) \equiv C$.

Proof: We first show $C \subset \sigma_c(A)$. Choose values of $\kappa \in C$ and μ_K, ν_K such that $\kappa = \frac{i\omega}{\mu_K \nu_K} + \frac{\Sigma_t(\nu_K)}{\mu_K}$. Now take for the φ_n any sequence of unit vectors which as functions approximate $\delta(\mu - \mu_K)\delta(\nu - \nu_K)$,

e. g.

$$\varphi_\delta(\mu, \nu) = \begin{cases} \left[\frac{M(\nu)}{\delta^2} \right]^{\frac{1}{2}} & \nu_K \leq \nu < \nu_K + \delta, \mu_K \leq \mu < \mu_K + \delta \\ 0 & \text{otherwise} \end{cases}$$

Clearly $\|\varphi_\delta\| = 1$ while $\varphi_\delta \rightarrow 0$. But $\|(A_1 - \kappa)\varphi_\delta\| \rightarrow 0 \implies \kappa \in \sigma_c(A_1)$. Thus we have shown by the Weyl Criterion that $C \subset \sigma_c(A_1)$.

Now to prove $C \supset \sigma_c(A_1)$ [i. e. $\kappa \notin C \rightarrow \kappa \notin \sigma_c(A_1)$], we

consider $\kappa_0 \neq \frac{i\omega}{\mu\nu} + \frac{\Sigma_t(\nu)}{\mu}$ for any $\nu \in [0, \infty)$, $\mu \in [-1, +1]$. Then

$(A_1 - \kappa_0)^{-1} = \left[\frac{i\omega}{\mu\nu} + \frac{\Sigma_t(\nu)}{\mu} - \kappa_0 \right]^{-1}$ is certainly a bounded operator.

Thus by definition $\kappa_0 \notin \sigma_c(A_1)$, implying that $C \supset \sigma_c(A_1)$.

Hence we have shown that $C \equiv \sigma_c(A_1)$. Now since A_1 is normal while A_2 is completely continuous and self-adjoint, we can apply the Weyl-von Neumann theorem to find

$$C \equiv \sigma_c(A_1) = \sigma_c(A_1 + A_2) = \sigma_c(A) \quad \text{Q.E.D.}$$

Notice that this proof has relied upon the fact that A_2 is completely continuous. It is possible to establish several facts without this assumption by referring to a theorem by Šmul'yan⁽⁵⁰⁾:

THEOREM: (Šmul'yan): Let $P(\kappa)$ be an operator which is analytic in κ for κ contained in some region G of the complex plane. Furthermore let $P(\kappa)$ be compact for each value $\kappa \in G$. Let κ_0 be a non-zero complex number and $\{\kappa_0\}$ the set of those values of $\kappa \in G$ for which κ_0 is an eigenvalue of $P(\kappa)$. Then either

i) $\{\kappa_0\} \equiv G$

or

ii) $\{\kappa_0\}$ has no limit point in G

Proof: See Šmul'yan⁽⁵⁰⁾.

Now we shall use this to show

THEOREM: $\sigma_c(A) \subset C$

Proof: Consider $P(\kappa) \equiv \int_{-1}^{+1} d\nu' \int_0^\infty d\nu \left[\frac{\nu' \Sigma_s(\nu' \rightarrow \nu, \mu' \rightarrow \mu)}{i\omega + \nu' \Sigma_t(\nu') - \kappa \mu' \nu'} \right]$. This is clearly analytic for $\kappa \notin C$. Furthermore

$$\|\tilde{P}(\kappa)\|^2 = \int_{-1}^{+1} d\mu \int_0^\infty d\nu \int_{-1}^{+1} d\mu' \int_0^\infty d\nu' \left\{ \frac{\nu \nu' \tilde{\Sigma}_s^2(\nu' \rightarrow \nu, \mu' \rightarrow \mu)}{[i\omega + \nu' \Sigma_t(\nu') - \kappa \mu' \nu'] [i\omega + \nu \Sigma_t(\nu) - \kappa \mu \nu]} \right\}$$

Now we know that since $\lim_{\nu \rightarrow 0} [i\omega + \nu \Sigma_t(\nu) - \kappa \mu \nu]^{-1} = [i\omega + \lambda^*]^{-1}$,

$\lim_{\nu \rightarrow \infty} [i\omega + \nu \Sigma_t(\nu) - \kappa \mu \nu]^{-1} = 0$ for $\kappa \notin C$, we can bound

$[i\omega + \nu \Sigma_t(\nu) - \kappa \mu \nu]^{-1} < M$ and hence bound

$$\begin{aligned} \|\tilde{P}(\kappa)\|^2 &< M^2 \int_{-1}^{+1} d\mu \int_0^\infty d\nu \int_{-1}^{+1} d\mu' \int_0^\infty d\nu' \nu' \nu \tilde{\Sigma}_s^2(\nu' \rightarrow \nu, \mu' \rightarrow \mu) \\ &= M^2 \|\nu \tilde{\Sigma}_s(\nu' \rightarrow \nu, \mu' \rightarrow \mu)\|^2 \end{aligned}$$

Now if we can assume $\mathfrak{S} = \int_{-1}^{+1} d\mu' \int_0^\infty d\nu' \nu' \Sigma_s(\nu' \rightarrow \nu, \mu' \rightarrow \mu)$ is completely continuous, as it appears to be for noncrystalline media, then we can conclude that $P(\kappa)$ is compact for $\kappa \notin C$.

Therefore we can apply Smul'yan's theorem to $P(\kappa)$ to conclude that either $\sigma(A) \equiv \{\kappa: \kappa \notin C\}$ or $\{\kappa: \kappa \notin C\}$ contains no limit points of $\sigma(A)$. But since the first alternative is clearly impossible, we can conclude that the set $\{\kappa: \kappa \notin C\}$ contains no continuous spectrum $\sigma_c(A)$. That is, $\sigma_c(A) \subset C$.

2. The Residual Spectrum $\sigma_r(A)$

The residual spectrum is defined as those values of κ for

which $(A - \kappa)^{-1}$ exists, but for which $R(A - \kappa)$ is a proper subset of $\mathfrak{L}_2(G)$. We shall demonstrate that the residual spectrum $\sigma_r(A)$ is empty for our class of operators. We first prove a lemma:

LEMMA: If $\bar{\kappa} \in \sigma_p(A^\dagger) \implies \kappa \in \sigma_p(A)$, then $\sigma_r(A)$ is empty.

Proof: We shall show that if $(A - \kappa)\mathfrak{L}_2$ is not dense in \mathfrak{L}_2 , then κ must be contained in the point spectrum $\sigma_p(A)$ [thus implying that $\sigma_r(A)$ is empty]. To see this, notice that if $(A - \kappa)\mathfrak{L}_2$ is a proper subset of \mathfrak{L}_2 , then for any $\varphi \in \mathfrak{L}_2$ there exists a vector ψ orthogonal to $(A - \kappa)\varphi$ [by the projection theorem⁽²⁸⁾]. That is,

$$(\psi, [A - \kappa]\varphi) = 0 \quad \text{for all } \varphi \in \mathfrak{L}_2$$

But we can rewrite this as

$$([A^\dagger - \bar{\kappa}]\psi, \varphi) = 0$$

Since $(A^\dagger - \bar{\kappa})\psi \in \mathfrak{L}_2$ and φ is arbitrary, this implies that

$$(A^\dagger - \bar{\kappa})\psi = 0 \implies \bar{\kappa} \in \sigma_p(A)$$

But by assumption, $\bar{\kappa} \in \sigma_p(A^\dagger) \implies \kappa \in \sigma_p(A)$. Thus if $(A - \kappa)\mathfrak{L}_2$ is a proper subset of \mathfrak{L}_2 , then $\kappa \in \sigma_p(A)$. But since $\sigma_r(A)$ and $\sigma_p(A)$ are disjoint sets, this implies that $\sigma_r(A)$ is empty. Q.E.D.

We shall now use this lemma to prove the following theorem:

THEOREM: The residual spectrum of A , $\sigma_r(A)$, is an empty set.

Proof: Consider $\sigma_p(A)$ defined by

$$A^\dagger \bar{\psi}_K = \left\{ \left[-\frac{i\omega}{\mu\nu} + \frac{\Sigma_t(v)}{\mu} \right] + A_2 \right\} \bar{\psi}_K = \bar{\kappa} \bar{\psi}_K$$

Taking the complex conjugate

$$\overline{A^\dagger \bar{\psi}_K} = \left\{ \left[\frac{i\omega}{\mu\nu} + \frac{\Sigma_t(v)}{\mu} \right] + A_2 \right\} \psi_K = \kappa \psi_K$$

or, identifying $\overline{A^\dagger} = A$, we can conclude that if $\bar{\psi}_K$ is an eigenfunction of A^\dagger with eigenvalue $\bar{\kappa}$, then ψ_K is an eigenfunction of A with eigenvalue κ . That is $\bar{\kappa} \in \sigma_p(A^\dagger) \Rightarrow \kappa \in \sigma_p(A)$.

Hence, using our lemma, we conclude that $\sigma_r(A)$ must be empty.

3. The Point Spectrum $\sigma_p(A)$

The point spectrum of A is defined as the set of those isolated values of κ for which $(A - \kappa)^{-1}$ does not exist. We have already shown that $\sigma_p(A)$ is contained in the complement of C . We can either consider $\sigma_p(A)$ as the set of values for which

$$\left[\frac{i\omega}{\mu\nu} + \frac{\Sigma_t(v)}{\mu} \right] \psi_K(\mu, \nu) - \int_{-1}^{+1} d\mu' \int_0^\infty dv' \frac{\tilde{\Sigma}_s(v' \rightarrow \nu, \mu' \rightarrow \mu)}{\sqrt{\mu'\mu}} \psi_K(\mu', \nu') = \kappa \psi_K(\mu, \nu)$$

$\kappa \notin C$ (B-3)

has nontrivial solutions, or consider the auxiliary eigenvalue problem

$$f(\kappa; \mu, \nu) = \int_{-1}^{+1} d\mu' \int_0^\infty dv' \left\{ \frac{v' \Sigma_s(v' \rightarrow \nu, \mu' \rightarrow \mu)}{[i\omega + v' \Sigma_t(v') - \kappa \mu' \nu']} \right\} f(\kappa; \mu', \nu')$$

$\kappa \notin C$ (II-14)

Since (B-3) and (II-14) are non-self-adjoint eigenvalue problems, there is little that can be said

about $\sigma_p(A)$. However we can use equation (II-5) to show that if $F(\kappa; \mu, \nu)e^{-\kappa x + i\omega t}$ is a solution to (II-2), then both

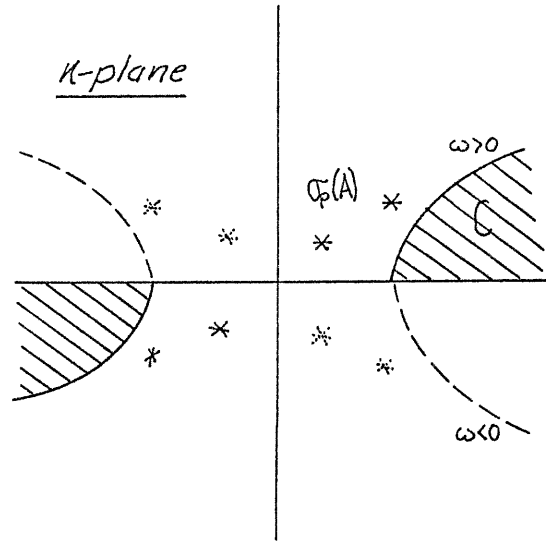
$$i) \bar{F}(\kappa; \mu, \nu)e^{-\bar{\kappa}x - i\omega t}$$

and

$$ii) F(\kappa; -\mu, \nu)e^{+\kappa x + i\omega t}$$

are also solutions. These sym-

metries arise from the irreversibility of the Boltzmann equation and detailed balance, respectively. They allow us to depict the symmetry in the κ -plane as shown, and to conclude that $\sigma_p(A)$ is confined to those regions of the first and third quadrants of the κ -plane for which $\kappa \notin \mathbb{C}$.



4. The Resolvent Set $\rho(A)$

The resolvent set of A contains those values of κ for which $(A - \kappa)^{-1}$ exists and is bounded and $R(A - \kappa) \equiv \mathfrak{L}_2(G)$. $\rho(A)$ is the complement of $\sigma(A)$ in the complex κ -plane. Hence we can conclude that $\rho(A)$ is the set of those values of κ such that $\kappa \notin \mathbb{C} \cup \sigma_p(A)$.



We have now completed the proof of the summary theorem presented on p. 18 for noncrystalline media.

II. THE BOLTZMANN WAVE OPERATOR A FOR NONCRYSTAL-LINE MEDIA

The scattering kernel now becomes

$$\Sigma_s(v' \rightarrow v, \mu' \rightarrow \mu) = \Sigma_i(v' \rightarrow v, \mu' \rightarrow \mu) + \Sigma_e(v)P(\mu' \rightarrow \mu)\delta(v' - v) \quad (B-4)$$

We shall assume

- i) $\Sigma_i(v' \rightarrow v, \mu' \rightarrow \mu)$ or one of its iterates is square-integrable over G
- ii) $P(\mu' \rightarrow \mu)$ or one of its iterates is square-integrable over I_μ
- iii) $\Sigma_e(v)$ is bounded and piecewise continuous

Our linear operator is

$$A = \underbrace{\left[\frac{i\omega}{\mu v} + \frac{\Sigma_t(v)}{\mu} \right]}_{A_1} + \underbrace{- \int_{-1}^{+1} d\mu' \int_0^\infty dv' \left[\frac{\tilde{\Sigma}_i(v' \rightarrow v, \mu' \rightarrow \mu)}{\sqrt{\mu' \mu}} \right]}_{A_2} + \underbrace{\left[- \Sigma_e(v) \int_{-1}^{+1} d\mu' \frac{\tilde{P}(\mu' \rightarrow \mu)}{\sqrt{\mu' \mu}} \right]}_{A_3} \quad (B-5)$$

A. Classification of A

As before, A_1 is an unbounded, non-self-adjoint, but normal operator with domain $\mathcal{D}_{A_1} \equiv \{ \varphi; \varphi \in \mathcal{L}_2(G), \frac{\varphi}{\mu v} \in \mathcal{L}_2(G), \frac{\Sigma_t(v)}{\mu} \varphi \in \mathcal{L}_2(G) \}$. We shall assume A_2 to be self-adjoint, completely continuous integral operator with $\mathcal{D}_{A_2} \equiv \mathcal{L}_2(G)$.

The operator A_3 is bounded and self-adjoint. It is not compact, however, because of the $\delta(v' - v)$ term which yields a multi-

plicative operator in v . [If $\varphi_n \rightarrow \varphi$, $\sum_e(v)\varphi_n \rightarrow \sum_e(v)\varphi$.] However,

$$\mathfrak{D}_{A_3} \equiv \mathfrak{L}_2(G).$$

Again the domain of $A = A_1 + A_2 + A_3$ is $\mathfrak{D}_A \equiv \mathfrak{D}_{A_1}$.

B. The Spectrum of A

Unfortunately the Weyl criterion does not apply to operators such as $A_1 + A_3$ which are not normal. Hence the Weyl-von Neumann theorem cannot be used to imply $\sigma_c(A) = \sigma_c(A_1 + A_3)$. We need a different approach.

1. The Continuous Spectrum $\sigma_c(A)$

We shall use a definition of the spectrum $\sigma(A)$ due to Hille and Phillips⁽⁵⁹⁾

Definition: If there exists a sequence $u_\delta \in \mathfrak{D}_A$ such that

$$\|u_\delta\| \geq c > 0, \quad \|(A - \kappa)u_\delta\| \rightarrow 0 \text{ as } \delta \rightarrow 0 \text{ then } \kappa \in \sigma(A).$$

Now our procedure will be to show $(C \cup \Gamma) \subset \sigma(A)$ and then show that if $\kappa \notin C \cup \Gamma$ then $\kappa \notin \sigma_c(A)$. That is, while we will be unable to determine precisely what kind of spectrum $C \cup \Gamma$ is, we will show that it is contained in $\sigma(A)$ and furthermore contains all of $\sigma_c(A)$. Then since we can show $\sigma_r(A)$ is empty, the only other possible spectrum present in $C \cup \Gamma$ is $\sigma_p(A)$. But if the set $C \cup \Gamma$ is dense-- as we shall assume it is--then $\sigma_p(A)$ cannot be contained in $C \cup \Gamma$ by definition, thus implying $\sigma_c(A) \equiv C \cup \Gamma$.

THEOREM: Let $C \equiv \left\{ \kappa: \kappa = \frac{i\omega}{\mu\nu} + \frac{\Sigma_t(\nu)}{\mu}, \mu \in [-1, +1], \nu \in [0, \infty) \right\}$.

Then $C \subset \sigma(A)$.

Proof: Again pick values of $\kappa \in C$ and $\mu_K, \nu_K \ni \kappa = \frac{i\omega}{\mu_K \nu_K} + \frac{\Sigma_t(\nu_K)}{\mu_K}$.

Now take

$$\varphi_\delta(\mu, \nu) = \begin{cases} \left[\frac{M(\nu)}{\delta^2} \right]^{\frac{1}{2}} & \nu_K \leq \nu < \nu_K + \delta, \quad \mu_K \leq \mu < \mu_K + \delta \\ 0 & \text{otherwise} \end{cases}$$

Now $\|\varphi_\delta\| \geq C > 0$ and $\|(A - \kappa)\varphi_\delta\| \rightarrow (\kappa + M\delta - \kappa) \rightarrow 0$.

Thus by the definition above, $C \subset \sigma(A)$. Q. E. D.

THEOREM: Let $\Gamma \equiv \left\{ \kappa: h_\kappa(\mu) = \nu \Sigma_e(\nu) \int_{-1}^{+1} d\mu' \left[\frac{P(\mu' \rightarrow \mu)}{i\omega + \nu \Sigma_t(\nu) - \kappa \mu' \nu} \right] h_\kappa(\mu'), \nu \in [0, \infty) \right\}$

Then $\Gamma \subset \sigma(A)$.

Proof: Similar to the above proof.

THEOREM: If $\kappa \notin C \cup \Gamma$, then $\kappa \notin \sigma_c(A)$.

Proof: Consider the associated operator

$$P(\kappa) \equiv \int_{-1}^{+1} d\mu' \int_0^\infty d\nu' \left\{ \frac{\nu' \Sigma_i(\nu' \rightarrow \nu, \mu' \rightarrow \mu)}{i\omega + \nu' \Sigma_t(\nu') - \kappa \mu' \nu'} \right\} \mathcal{L}_e^{-1} \{ \cdot \} \quad (B-5)$$

where

$$\mathcal{L}_e \varphi \equiv \varphi - \nu \Sigma_e(\nu) \int_{-1}^{+1} d\mu' \left\{ \frac{P(\mu' \rightarrow \mu)}{i\omega + \nu \Sigma_t(\nu) - \kappa \mu' \nu} \right\} \varphi(\mu')$$

It is obvious by construction that $P(\kappa)$ is analytic in κ for $\kappa \notin C \cup \Gamma$. Furthermore it should be straightforward to demonstrate that $P(\kappa)$ is compact for $\kappa \notin C \cup \Gamma$. Hence applying Smul'yan's theorem implies that $\kappa \notin \sigma_c(A)$ for $\kappa \notin C \cup \Gamma$.

Therefore we have shown that

i) $(C \cup \Gamma) \subset \sigma(A)$

ii) $\sigma_c(A) \subset C \cup \Gamma$

2. The Residual Spectrum $\sigma_r(A)$

Since the symmetry of A is not disturbed by the addition of A_3 , we can again conclude that $\sigma_r(A)$ is empty.

3. The Point Spectrum $\sigma_p(A)$

We have shown that the point spectrum $\sigma_p(A)$ is determined by those values of κ such that

$$f_i(\kappa; \mu, \nu) = \int_{-1}^{+1} d\mu' \int_0^\infty d\nu' \left\{ \frac{\nu' \Sigma_i(\nu' \rightarrow \nu, \mu' \rightarrow \mu)}{i\omega + \nu' \Sigma_t(\nu') - \kappa \mu' \nu'} \right\} \mathcal{L}_e^{-1} \{f_i(\kappa; \mu', \nu')\}$$

possesses non-trivial solutions. Since $C \cup \Gamma$ are dense sets and $\sigma_p(A)$ can contain no limit points, $\sigma_p(A)$ must lie in those regions of the first and third quadrants for which $\kappa \notin C \cup \Gamma$.

4. The Resolvent Set $\rho(A)$

Again $\rho(A)$ is the set of all points not contained in $\sigma(A)$, i.e. all κ such that $\kappa \notin C \cup \Gamma \cup \sigma_p(A)$.

Thus we have now proven the summary theorem given on p. 26 and completed the analysis of A for polycrystalline media.

APPENDIX C: NECESSARY CONDITIONS FOR THE
EXISTENCE OF $\sigma_p(A)$

A proof of Theorem IV shall now be given. Since this proof is somewhat different for each model considered, a sequence of theorems is necessary.

I. ISOTROPIC, NONCRYSTALLINE MEDIA

THEOREM A1: There exists a frequency ω^* such that for $\omega > \omega^*$, the point eigenvalue spectrum $\sigma_p(A)$ is empty.

Proof: Our task is to demonstrate that for sufficiently large ω , equation (II-15) has no non-trivial solutions for any $k \notin C$. Rather than treating this equation directly, it is convenient to multiply by $\Sigma_s(v', v)$ and integrate over v' , defining

$$\psi_K(v) \equiv \int_0^\infty dv' \Sigma_s(v', v) \Phi_K(v')$$

to arrive at an alternative formulation of the dispersion relation

$$\psi_K(v) = \int_0^\infty dv' \Sigma_s(v', v) g(k, \omega; v) \psi_K(v') \equiv K_K \psi_K \quad k \notin C \quad (C-1)$$

Now a necessary condition for (C-1) to possess a non-trivial solution is for

$$\|K_K\| = \left[\int_0^\infty dv' \int_0^\infty dv \Sigma_s^2(v', v) |g(k, \omega; v')|^2 \right]^{\frac{1}{2}} \geq 1 \text{ for some } k \notin C$$

We will show that this condition can never be satisfied for sufficiently large ω .

Consider first

$$g(k, \omega; v) = \frac{1}{2k} \ln \left[\frac{i\omega + v\Sigma_t(v) + kv}{i\omega + v\Sigma_t(v) - kv} \right]$$

We need some information about $k(\omega)$ for large ω .

From the k -plane diagram it is evident that the continuum area C fans out as shown. Thus for $k \notin C$,

$\alpha = \text{Re} \{k\}$ must certainly

be bounded by $[\Sigma_t(v)]_{\min} \equiv \Sigma_M$ as $\omega \rightarrow \infty$. However the form of $k(\omega)$ will remain otherwise arbitrary. Consider then

$$g(k, \omega; v) = \frac{1}{2[\alpha(\omega) + i\xi(\omega)]} \ln \left[\frac{v(\Sigma_t(v) + \alpha(i\omega)) + i(\omega + v\xi(\omega))}{v(\Sigma_t(v) - \alpha(\omega)) + i(\omega - v\xi(\omega))} \right] \quad (C-2)$$

for three separate cases:

i) $\xi(\omega)$ strictly increasing for large ω . Then

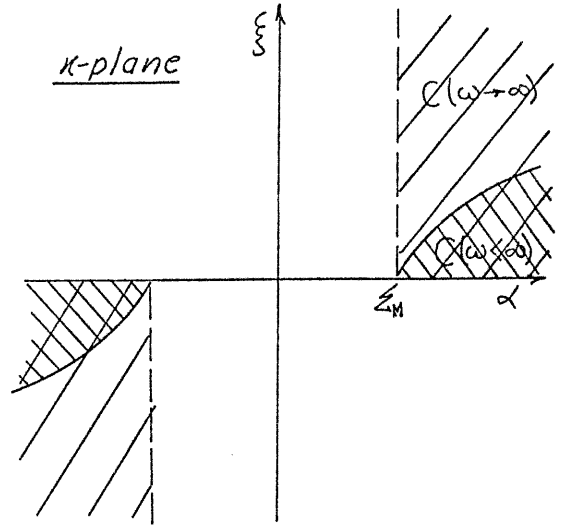
$$g(k, \omega; v) \sim \frac{1}{2i\xi(\omega)} \ln \left[\frac{\omega + v\xi(\omega)}{\omega - v\xi(\omega)} \right]$$

and the $1/\xi(\omega)$ factor will force $g(k, \omega; v)$ to zero as $\omega \rightarrow \infty$.

ii) $\xi(\omega)$ strictly decreasing in ω . For the moment, assume that v is bounded. Then as $\omega \rightarrow \infty$,

$$g(k, \omega; v) \sim \frac{1}{2\alpha(\omega)} \ln \left[\frac{\omega + v\xi(\omega)}{\omega - v\xi(\omega)} \right] \rightarrow 0$$

as the argument of the log goes to 1.



iii) $\xi(\omega)$ approaches a constant ξ_∞ as $\omega \rightarrow \infty$. If we again assume that v is bounded, the argument of the log again goes to 1 forcing $g(k, \omega; v)$ to zero as $\omega \rightarrow \infty$.

In conclusion then, $g(k, \omega; v) \rightarrow 0$ as $\omega \rightarrow \infty$ for bounded v . Thus certainly for sufficiently well-behaved $\Sigma_s(v', v)$ [which we have for noncrystalline media]

$$\lim_{\omega \rightarrow \infty} \int_0^{v^*} dv' \int_0^\infty dv \Sigma_s^2(v', v) |g(k, \omega; v')|^2 \rightarrow 0 \quad \text{for any } v^* < \infty$$

Now consider the remainder

$$\mathcal{J} \equiv \int_{v^*}^\infty dv' \int_0^\infty dv \Sigma_s^2(v', v) |g(k, \omega; v')|^2$$

Recognize that $g(k, \omega; v)$ does not approach zero uniformly in v as $\omega \rightarrow \infty$ since there is a singular behavior in case ii) and iii) when

$$v[\Sigma_t(v) - \alpha(\omega)] + i[\omega - v\xi(\omega)] = 0$$

But this can only occur as $\omega \rightarrow \infty$ for $v \rightarrow \infty$. Thus it is necessary to examine the effect of any divergences in $g(k, \omega; v)$ as $v \rightarrow \infty$.

To be more specific, let $\Sigma_t(v) = \Sigma_M + q\phi(v)$ where $\phi(v)$ is monotonically decreasing and is usually assumed⁽⁵²⁾ to go down slower than $\exp(-bv^2)$. To examine $g(k, \omega; v)$, notice that $[\frac{\omega}{v} - \xi(\omega)] \rightarrow 0$ as $v \rightarrow \infty$ like c/v . Thus we can write

$$g(k, \omega; v) \sim \frac{1}{2K_\infty} \ln \left[\frac{q\phi(v) + i\frac{c_1}{v} + c_2}{q\phi(v) + ic_1/v} \right] \quad \text{as } v \rightarrow \infty$$

Now for cases ii) or iii), the denominator $q\phi(v) + ic_1/v$ will certainly go to zero as $1/v$ or slower. Thus the divergence in $g(\kappa, \omega; v)$ can certainly be bounded as

$$g(\kappa, \omega; v) = \frac{1}{2\kappa_\infty} \ln [c_3 v^\gamma] \quad \gamma < 1 \quad (\text{C-3})$$

We now use the behavior of the scattering kernel $\Sigma_s(v', v)$ for $v > v^*$ to force $\mathcal{J} \rightarrow 0$ by noting that for large v , $\Sigma_s(v', v)$ assumes its slowing-down form

$$\Sigma_s(v', v) = \begin{cases} c_1 v/v'^2 & v \in [\sqrt{\alpha} v', v'] \\ 0 & \text{otherwise} \end{cases}$$

hence

$$\mathcal{J} = \int_{v^*}^{\infty} dv' \int_{\sqrt{\alpha} v'}^{v'} dv c_1 \frac{v^2}{v'^4} |g(\kappa, \omega; v')|^2 = c_2 \int_{v^*}^{\infty} \frac{dv'}{v'} |g(\kappa, \omega; v')|^2 \quad (\text{C-4})$$

If one now uses (C-3) in (C-4)

$$\mathcal{J} = c_4 \int_{v^*}^{\infty} \frac{dv'}{v'} 2 \ln^2 [c_3 v^\gamma]$$

Now since $\frac{\ln^2 c v^\gamma}{v} \rightarrow c'/v$, one can conclude that $\lim_{v^* \rightarrow \infty} \mathcal{J} = 0$.

Hence we have shown that \mathcal{J} can be made arbitrarily small by moving v^* to infinity. Thus we have shown that

$$\lim_{\omega \rightarrow \infty} \|K_\kappa\| = \lim_{\omega \rightarrow \infty} \left[\int_0^\infty dv' \int_0^\infty dv \Sigma_s^2(v', v) |g(\kappa, \omega; v')|^2 \right]^{\frac{1}{2}} = 0$$

In particular for some $\omega^* < \infty$, $\omega > \omega^*$ will imply $\|K_\kappa\| < 1$ for any $\kappa \notin \mathbb{C}$. Thus we can conclude that there exists a frequency

ω^* such that for $\omega > \omega^*$, $\sigma_p(A)$ is an empty set. Our proof is complete.

THEOREM A2: There exists a critical absorption $\Sigma_a^*(v) \equiv q^* \phi(v)$ such that for $\Sigma_a(v) = q\phi(v) > \Sigma_a^*$, the point spectrum $\sigma_p(A)$ is empty.

Proof: This theorem was originally presented by Corngold⁽⁵²⁾ for the $\omega = 0$ case. Its proof follows immediately from Theorem A1 by noting that

$$\lim_{q \rightarrow \infty} \int_0^{v^*} dv' \int_0^\infty dv \Sigma_s^2(v', v) |g(k, \omega; v')|^2 \rightarrow 0 \quad \text{for any } v^* < \infty,$$

and for $\phi(v)$ decreasing more slowly than e^{-bv^2} , the remainder \mathcal{J} can be shown to approach zero as $q \rightarrow \infty$. Q.E.D.

THEOREM A3: There exists a critical transverse dimension yielding a B_\perp^{*2} such that for $B_\perp^2 > B_\perp^{*2}$, the point spectrum $\sigma_p(A)$ is empty.

Proof: This theorem was first presented by Williams⁽⁵³⁾, again for the $\omega = 0$ case. His proof can be extended immediately to the $\omega > 0$ case. However a more intuitive proof is merely to recognize that if one increases B_\perp^2 sufficiently, $\rho = \kappa^2 + B_\perp^2$ will be forced into C for any $\kappa \notin C$. Q.E.D.

II. ISOTROPIC, POLYCRYSTALLINE MEDIA

THEOREM B: There exist critical bounds on ω , $\Sigma_a(v)$, and B_{\perp}^2 such that if $\omega > \omega^*$ or $\Sigma_a(v) > \Sigma_a^*(v)$ or $B_{\perp}^2 > B_{\perp}^{*2}$, the point spectrum $\sigma_p(A)$ is empty.

Proof: The dispersion law analogous to (C-1) is now

$$\psi_K(k) = \int_0^{\infty} dv' \Sigma_s(v', v) \frac{g(k, \omega; v')}{\Lambda_e(k, v')} \psi_K(v') \equiv \hat{K}_K \psi_K$$

But notice that since $\Lambda_e(k; v) = 1 - \Sigma_e(v)g(k, \omega; v)$, we can examine the influence of $\Lambda_e(k; v)$ on $\|\hat{K}_K\|$ directly. First we restrict ourselves away from $\omega \ni \Lambda_e(k; v) = 0$ --that is, $k \notin \Gamma$. Now we know that for v bounded, $|g(k, \omega; v)| \rightarrow 0$ as $\omega \rightarrow \infty$. But as $v \rightarrow \infty$, $\Lambda_e(v) \rightarrow c/v^2$ for all reasonable cross-section models. Thus it is evident that as $\omega \rightarrow \infty$, $\Lambda_e(k; v) \rightarrow 1$ for all v . This of course implies that

$$\lim_{\omega \rightarrow \infty} \|\hat{K}_K\| = \|K_K\| = 0$$

hence implying that for $\omega > \omega^*$, $\sigma_p(A)$ is empty. A similar argument can be given for $\Sigma_a > \Sigma_a^*$, or $B_{\perp}^2 > B_{\perp}^{*2}$. Q.E.D.

III. GENERAL KERNELS

Now consider the more general dispersion relation for non-crystalline media

$$f(k; \mu, v) = \int_{-1}^{+1} d\mu' \int_0^{\infty} dv' \left\{ \frac{v' \Sigma_s(v' \rightarrow v, \mu' \rightarrow \mu)}{[i\omega + v' \Sigma_t(v') - k\mu' v']} \right\} f(k; \mu', v') \quad k \notin C \quad (II-14)$$

We would like to demonstrate that the above theorems hold even for this more general model. That is, we would like to show that for sufficiently high ω (Σ_a or B_{\perp}^2),

$$\|G_K\| = \left[\int_{-1}^{+1} d\mu \int_0^{\infty} dv \int_{-1}^{+1} d\mu' \int_0^{\infty} dv' \frac{\Sigma_s^2(v' \rightarrow v, \mu' \rightarrow \mu)}{\left| \frac{i\omega}{v} + \Sigma_t(v) - K\mu \right| \left| \frac{i\omega}{v'} + \Sigma_t(v') - K\mu' \right|} \right]^{\frac{1}{2}} < 1$$

for all $K \notin C$

This, of course, is a rather difficult task since $\Sigma_s(v' \rightarrow v, \mu' \rightarrow \mu)$ is arbitrary. However a very crude argument is as follows: We know that since $\Sigma_s(v' \rightarrow v, \mu' \rightarrow \mu)$ is a relatively scattering probability, it must be finite for all (μ, μ', v', v) . Furthermore it seems evident that since the probability to scatter into any angle is always greater than the probability to scatter from a specific μ' to a specific μ , one should be able to bound.

$$|\Sigma_s(v' \rightarrow v, \mu' \rightarrow \mu)| < M |\Sigma_s(v', v)|$$

where M is a finite (perhaps large) constant. But then

$$\begin{aligned} \|G_K\| &< M' \left[\int_{-1}^{+1} d\mu \int_0^{\infty} dv \int_{-1}^{+1} d\mu' \int_0^{\infty} dv' \frac{\Sigma_s^2(v', v)}{\left| \frac{i\omega}{v} + \Sigma_t(v) - K\mu \right| \left| \frac{i\omega}{v'} + \Sigma_t(v') - K\mu' \right|} \right]^{\frac{1}{2}} \\ &= M' \left[\int_0^{\infty} dv' \int_0^{\infty} dv \Sigma_s^2(v', v) |g(K, \omega; v')|^2 \right]^{\frac{1}{2}} = M' \|K_K\| \end{aligned}$$

From Theorem A1, we know $\lim_{\omega \rightarrow \infty} \|K_K\| = 0$. Thus we can conclude

that $\|G_K\| \rightarrow 0$ as $\omega \rightarrow \infty$. Hence there exists an ω^* such that for $\omega > \omega^*$, $\|G_K\| < 1$ for all $K \notin C$. Q.E.D.

A similar idea can be used for the maximum absorption and transverse buckling theorems, as well as for polycrystalline media.

APPENDIX D: GENERALIZED ANALYTIC FUNCTIONS

In the theory of functions of a complex variable, an analytic function $w(z) = u(z) + iv(z)$ is one which satisfies the Cauchy-Riemann equations

$$\frac{\partial u}{\partial x} - \frac{\partial v}{\partial y} = 0 \quad \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} = 0 \quad (D-1)$$

where $z = x + iy$

Suppose we consider a more general form of these equations

$$\frac{\partial u}{\partial x} - \frac{\partial v}{\partial y} + au + bv = f \quad \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} + cu + dv = g \quad (D-2)$$

Then we can define a "generalized analytic function"⁽⁴³⁾ [or "pseudo-analytic function"⁽⁵¹⁾] as one which satisfies this more general form of the Cauchy-Riemann equations (D-2). A convenient notation is

$$\frac{\partial w}{\partial \bar{z}} \equiv \frac{1}{2} \left(\frac{\partial w}{\partial x} + i \frac{\partial w}{\partial y} \right) \quad \frac{\partial w}{\partial z} \equiv \frac{1}{2} \left(\frac{\partial w}{\partial x} - i \frac{\partial w}{\partial y} \right) \quad (D-3)$$

Using this notation, the Cauchy-Riemann equations (D-1) become

$$\frac{\partial w}{\partial \bar{z}} = 0 \quad (D-4)$$

and the generalized Cauchy-Riemann equations (D-2) become

$$\frac{\partial w}{\partial \bar{z}} + Aw + B\bar{w} = F \quad (D-5)$$

Then to test whether a function $\Phi(z)$ is analytic, one can merely evaluate $\frac{\partial \Phi}{\partial \bar{z}}$. If this derivative is zero, then $\Phi(z)$ is an analytic

function. However if $\frac{\partial \Phi}{\partial \bar{z}} \neq 0$, then $\Phi(z)$ must be regarded as a generalized analytic function of z .

A very useful class of generalized analytic functions are those which satisfy a simplified form of (D-5)

$$\frac{\partial w}{\partial \bar{z}} = f \tag{D-6}$$

Using a form of Green's theorem, one can actually "solve" (D-6) for some domain G as

$$w(z) = \underbrace{\frac{1}{2\pi i} \int_{\partial G} \frac{w(\zeta) d\zeta}{\zeta - z}}_{\Phi(z)} - \underbrace{\frac{1}{\pi} \iint_G \frac{f(\zeta) d\xi d\eta}{\zeta - z}}_{T_G f} \quad \zeta \equiv \xi + i\eta \tag{D-7}$$

The T_G operator defined by (D-7) plays a major role in the theory of generalized analytic functions, as evidenced by the Lemma of section (III-A).

Much of this theory can be developed in analogy to the theory of analytic functions. Many of the important theorems of the latter possess analogues for generalized analytic functions [Cauchy's theorem, identity theorem, etc.]. An extensive treatment of this theory is given in Vekua⁽⁴³⁾.

APPENDIX E: SUB-BRAGG CONTINUUM CONTAMINATION

I. INTRODUCTION

We wish to examine the role of the sub-Bragg continuum contribution in the total solution for the modified synthetic kernel model. Actually the experimenter will measure the neutron distribution integrated over a detector response $v\Sigma_d(v)$. The analysis becomes particularly transparent for a detector response of $v\Sigma_i(v)$ [detailed numerical calculations for a $1/v$ detector exhibit no significant differences]. Then the measured detector response becomes

$$\begin{aligned} R(x,t) &= \int_{-1}^{+1} d\mu \int_0^{\infty} dv v \Sigma_i(v) f(x,\mu,v,t) \\ &= \int_{-1}^{+1} d\mu \int_0^{\infty} dv v \Sigma_i(v) \left\{ \frac{1}{2\pi i} \int_{+i\infty}^{-i\infty} e^{-\eta x + i\omega t} F(\eta; \mu, v) d\eta \right\} \quad (E-1) \end{aligned}$$

Interchanging orders of integration, one can show this reduces to

$$\begin{aligned} R(x,t) &= \frac{1}{2\pi i} \int_{+i\infty}^{-i\infty} e^{-\eta x + i\omega t} \frac{\chi(k)}{\Lambda(k)} dk = R_{\text{discrete}}(x,t) + R_{C_{BB}}(x,t) \\ &\quad + R_{\Gamma}(x,t) + R_{C_{AB}}(x,t) \quad (E-2) \end{aligned}$$

where we have denoted the various terms corresponding to the contour deformation indicated on p. 111. Now for $x > 20$ cm. we have shown that we can neglect the source transients due to C_{AB} and Γ . Therefore the total solution can be written as

$$R(x,t) = R_{\text{discrete}}(x,t) + R_{C_{BB}}(x,t) =$$

$$= \frac{\chi(\kappa_0)}{\frac{\partial \Lambda}{\partial \eta} \Big|_{\kappa_0}} e^{-\kappa_0 x + i\omega t} + \int_{C_{BB}} e^{-\eta x + i\omega t} \left[\frac{\chi_R(\eta)\Lambda(\eta) + \chi(\eta)\Lambda_R(\eta)}{\Lambda^+(\eta)\Lambda^-(\eta)} \right] d\eta \quad (\text{E-3})$$

Before continuing, it is useful to regress to a simple diffusion theory model for a preliminary analysis.

II. A TWO-GROUP DIFFUSION THEORY ANALYSIS

If we identify those neutrons in $R_{C_{BB}}(x,t)$ as sub-Bragg neutrons, while those in $R_{\text{discrete}}(x,t)$ are predominately neutrons with $v > v_B$, we can use a two group diffusion theory to estimate

$$R(x,t) = R_{\text{discrete}}(x,t) + R_{C_{BB}}(x,t) = r_d e^{-\kappa_0 x + i\omega t} + r_c e^{-\kappa_c x + i\omega t}$$

We recognize two sources of sub-Bragg neutrons

- i) those due directly to the source [corresponding to $\chi_R(\eta)\Lambda(\eta)$ in (E-3)]
- ii) those due to neutrons scattering below v_B [term $\chi(\eta)\Lambda_R(\eta)$ in (E-3)].

Considering a plane source with a Maxwellian distribution yields for the first type of contribution [using as a boundary condition

$$\frac{1}{3\Sigma_t} \frac{\partial n}{\partial x} = v^2 e^{-v^2}]$$

$$C_s = \left| \frac{r_c}{r_d} \right| = \frac{\# \text{ source neutrons below } v_B}{\# \text{ source neutrons above } v_B}$$

$$= \left| \frac{\kappa_0}{\kappa_c} \right| \frac{\int_0^{v_B} dv \Sigma_i(v) v^2 e^{-v^2}}{\int_{v_B}^{\infty} dv \Sigma_s(v) v^2 e^{-v^2}} \sim 0.4\% \quad \text{for graphite}$$

and for the second type, using as a measure of downscattering the inelastic collision term in (VI-1)

$$C_{ds} = \frac{r_c}{r_d} = \frac{\# \text{ neutrons scattered below } v_B}{\# \text{ neutrons scattered above } v_B}$$

$$= \frac{\int_0^{v_B} dv \Sigma_i(v) v^3 e^{-v^2}}{\int_{v_B}^{\infty} dv \Sigma_i(v) v^3 e^{-v^2}} \sim 0.2\% \quad \text{for graphite}$$

Hence we expect from these analyses that the initial magnitude of the sub-Bragg contribution will be about 0.6% that of the magnitude of the discrete mode. [From this analysis it is also clear how one might use cold neutron sources to build up the relative contribution from C_{BB} .]

III. ASYMPTOTIC ESTIMATES

If we assume a Maxwellian source, then it is possible to rewrite $R_{C_{BB}}(x,t)$ as

$$R_{C_{BB}}(x,t) = \int_{C_{BB}} d\eta e^{-\eta x + i\omega t} \frac{\beta \Sigma_i^0}{4\eta} \underbrace{\left[e^{-\left(\frac{i\omega + \Sigma_t^0}{\eta}\right) - v_B^2} \right]}_{\varphi} \underbrace{\left[\frac{\Sigma_i^0 \chi(\eta) + \frac{1}{\beta} \Lambda(\eta)}{\Lambda^+(\eta) \Lambda^-(\eta)} \right]}_{\psi}$$

$$= \int_{1/v_B}^{\infty} \frac{du}{u} e^{-\alpha u + i\omega t} \varphi(u) \psi(u) \quad (E-4)$$

where $\alpha \equiv (i\omega + \Sigma_t^0)x$

$u \equiv \eta/\alpha$

Integrate (E-4) by parts to obtain

$$e^{-i\omega t} R_{C_{BB}}(x,t) = - \frac{e^{-\alpha u}}{\alpha} \varphi(u)\psi(u) \Big|_{1/v_B}^{\infty} - \int_{1/v_B}^{\infty} du \frac{e^{-\alpha u}}{\alpha} \frac{\partial}{\partial u} (\varphi\psi)$$

But the first term in (E-5) is identically zero; hence we must integrate by parts once more. It is possible to show that $\partial\psi/\partial u$ has a first order pole at $u = 1/v_B$. Thus we can only find

$$e^{-i\omega t} R_{C_{BB}}(x,t) = \frac{e^{-\alpha/v_B}}{\alpha^2} \frac{\partial}{\partial u} (\varphi\psi) \Big|_{1/v_B} + \int_{1/v_B}^{\infty} du e^{-\alpha u} \varphi \frac{\partial\psi}{\partial u} + \frac{1}{\alpha^2} \int_{1/v_B}^{\infty} du e^{-\alpha u} \frac{\partial}{\partial u} (\psi \frac{\partial\varphi}{\partial u}) \quad (E-5)$$

Thus, provided we can bound the integrals, (E-5) implies that

$$R_{C_{BB}}(x,t) = o \left(\frac{1}{x} e^{-(i\omega + \Sigma_t^0/v_B)x + i\omega t} \right) \text{ as } x \rightarrow \infty \quad (E-6)$$

This estimate is only useful for $x \gg \left| \frac{i\omega + \Sigma_t^0}{v_B} \right| \sim 20$ cm however.

Numerical calculations of $R_{C_{BB}}(x,t)$ have been performed which indicate that for intermediate distances at least,

$$R_{C_{BB}}(x,t) \sim e^{-\kappa^* x + i\omega t}$$

where $\text{Re} \{ \kappa^*(\omega) \}$ is given in Figure 21. Hence it appears that a reasonable form for the structure of the solution in the regime $20 \text{ cm} < x < 100 \text{ cm}$ can be written as

$$R(x,t) = e^{-\kappa_0 x + i\omega t} + 0.5\% e^{-\kappa^* x + i\omega t} \quad (E-7)$$

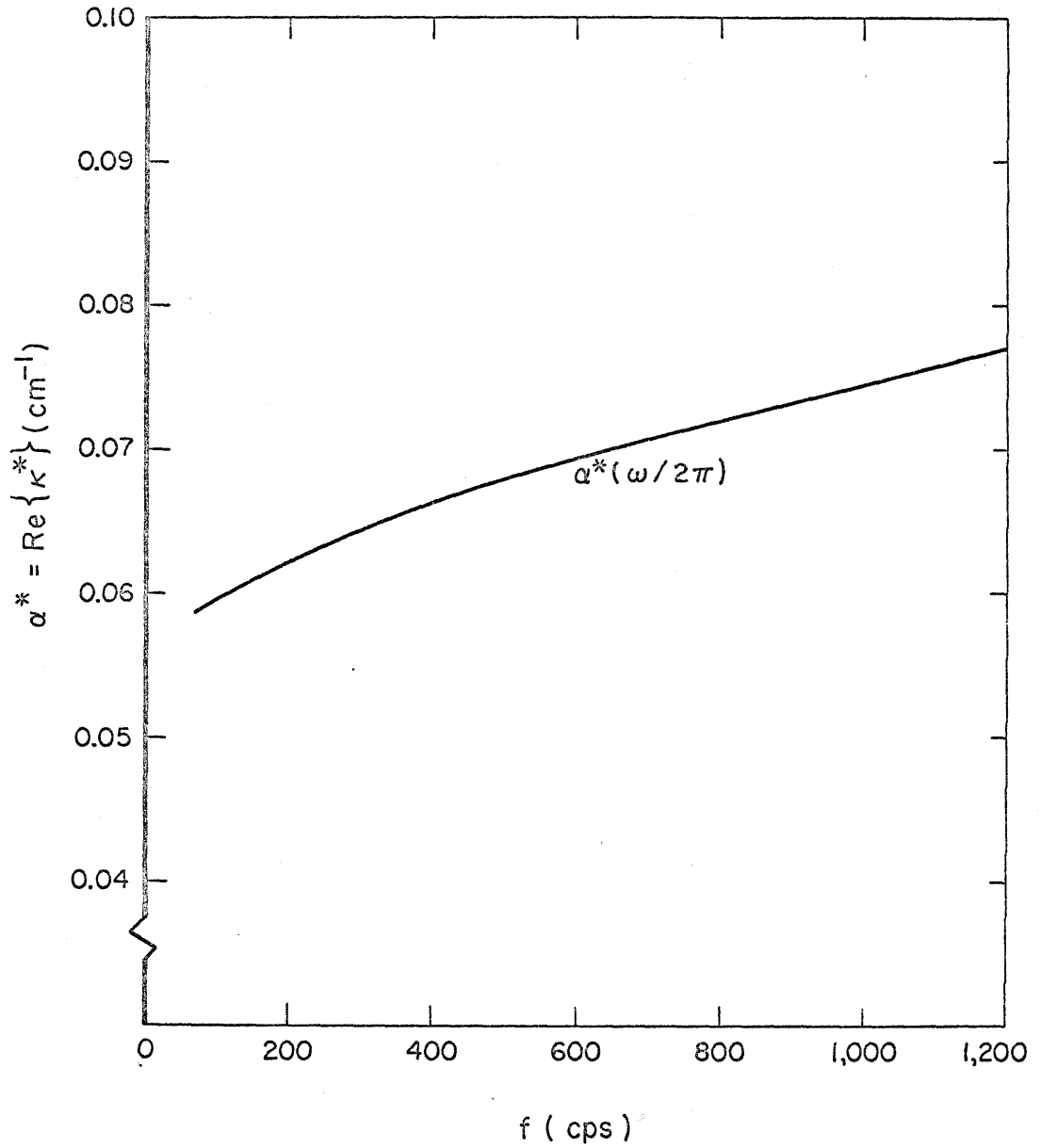


Figure 21. $\alpha^*(f)$ vs. f

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