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SUMMER INSTITUTE
ON SPECTRAL THEORY AND STATISTICAL MECHANICS
1965

J.D. Pincus, Editor

RELEASED FOR ANNOUNCEMENT
IN NUCLEAR SCIENCE ABSTRACTS

APPLIED MATHEMATICS DEPARTMENT
BROOKHAVEN NATIONAL LABORATORY
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The Summer Institute on Spectral Theory and Statistical Mechanics was held during a five week period beginning in June, 1965.

Its purpose was to assemble a small group of mathematicians and physicists whose work contained some common elements of interest centering around recent results in spectral theory.

Besides numerous informal talks, several lectures of an expository nature were given, and most of those are recorded in the notes contained in this volume.

Professor Mark Kac served as the principal organizing force behind the Institute, and we at Brookhaven wish to record our indebtedness to him for his efforts.

Thanks are also due to Mr. Benjamin Klein who ably took notes for several of the speakers.

J. D. Pincus

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THEORY AND APPLICATIONS OF TOEPLITZ FORMS

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INTRODUCTION: It often happens that a rather specific mathematical concept finds application in quite diverse areas. Such is the case with the theory of Toeplitz matrices, as we shall attempt to show. But first we must introduce the concept itself.

Consider a real-valued function $f(\theta)$, $-\pi \leq \theta \leq \pi$, which is in $L^2(-\pi, \pi)$ [i.e. $\int_{-\pi}^{\pi} |f(\theta)|^2 d\theta < +\infty$]. Let c_k be the k^{th} Fourier coefficient of f . - i.e.

$$c_k = \frac{1}{2\pi} \int_{-\pi}^{\pi} f(\theta) e^{-ik\theta} d\theta$$

We know that $\sum_{j=-\infty}^{\infty} |c_j|^2 < +\infty$, and further that given any such square convergent sequence $\{y_k\}$, the function

$$g(\theta) = \sum_{-\infty}^{\infty} y_k e^{ik\theta}$$

is in $L^2(-\pi, \pi)$. We denote the set of all such sequences by

ℓ_2 and note finally that the correspondence between $L^2(-\pi, \pi)$ and ℓ_2 given above is one - one.

Toeplitz (1907 - 1911) investigated the behavior of the infinite matrix $c = (c_{ij})_{ij=-\infty}^{\infty}$ where $c_{ij} = c_{j-i}$ (c_k as above). Since f is a real function, we note that c is hermitian - i.e. $c_n = (c_{-n})^*$. Also, in the event that f is a(n) (essentially) bounded function, c represents a bounded operator on ℓ_2 (with respect to the usual norm for ℓ_2). In fact, c represents in ℓ_2 , under the isomorphism

mentioned above, the bounded operator F in $L^2(-\pi, \pi)$ given by the formula

$$[F(f)](x) = f(x)g(x) \text{ for } g \text{ in } L^2(-\pi, \pi)$$

We have now the following relationship between the spectrum of c and the values assumed by f , the matrix $\lambda I - c$ (where $\lambda \Delta_{ij}$) ^{∞} $i, j = -\infty$ is the identity matrix) fails to have an inverse if and only if $(\lambda - f)(x)$ fails to have an inverse as an operator on $L^2(-\pi, \pi)$. In particular, if f is continuous on $L^2(-\pi, \pi)$, then the spectrum of c coincides exactly with the range of f .

Toeplitz, Carathéodory, and others investigated matrices such as c by studying the properties of finite sections T_n of c where

$$T_n = \begin{pmatrix} c_0 & c_1 & \cdot & \cdot & c_n \\ c_{-1} & c_0 & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & c_0 & \cdot \\ c_{-n} & \cdot & \cdot & c_1 & c_0 \end{pmatrix}$$

It developed that these matrices have many applications some of which will be mentioned now.

I. Classical Function Theory

Suppose $f(z)$ is analytic in the open disc $|z| < 1$ with expansion

$\sum_{n=0}^{\infty} c_n z^n$. We define $c_{-n} = c_n^*$, and an early result of Szegő then states that

$$\min_{|z| < 1} \operatorname{Re} f(z) = \lim_{n \rightarrow \infty} \lambda_{\min}^{(n)}$$

($-\infty$ not excluded) where $\lambda_{\min}^{(n)}$ is the smallest eigenvalue of the Toeplitz matrix T_n . Furthermore, the so called Weyl-Courant lemma implies that

$$\lambda_{\min}^{(n)} \text{ decreases}$$

II) Prediction Theory

Suppose $\{X_n\}_{n=-\infty}^{\infty}$ is a normalized sequence of real-valued random variables which is stationary.

(i.e. $E(X_n, X_m) = p(n-m)$ & $p(0) = 1$). In the particular case of linear prediction, we wish to find $c_{-N}, c_{-N+1}, \dots, c_{-1}$ such that

$$E \left[\left(\sum_{k=-N}^{-1} c_k X_{n-k} - X_n \right)^2 \right] = E_n$$

is minimized. We thus are interested in whether for an appropriate choice of $\{c_n\}$, $E_n \rightarrow 0$.

According to a theorem of Wiener (Khinchin) stationarity implies that there exists some non-decreasing function σ on $[-\pi, \pi]$ such that for each n , $p(n)$ is the n^{th}

Fourier-Stieltjes coefficient of σ -i.e..

$$\rho(n) = \frac{1}{2\pi} \int_{-\pi}^{\pi} e^{-inx} d\sigma(x)$$

If it happens that σ has no singular part, then σ has a derivative, which may however, include δ functions.

This derivative σ is called the power spectrum of σ , and the δ functions correspond to the lines in this spectrum. For our purposes, we assume that σ is absolutely continuous so that σ' does exist almost everywhere and in addition

$$\sigma(w) - \sigma(-\pi) = \int_{-\pi}^w \sigma'(x) dx$$

Setting $C_n = \rho(n)$, one finds that $\min E_N = \frac{D_{N+1}}{D_N}$

where i) the min is taken over all combinations

$$\{C_n\}_{k=-N}^{-1}$$

And ii) $D_K = \det T_K [T_K \text{ defined as above}]$.

Finally, a classical theorem of Szego (1917) states that

$$\frac{D_{n+1}}{D_n} \rightarrow \exp \frac{1}{2\pi} \int_{-\pi}^{\pi} \log \sigma'(w) dw$$

From this fact, it is evident that a necessary and

sufficient condition for perfect prediction is

$$\int_{-\pi}^{\pi} \log \sigma'(w) dw = -\infty$$

III) Thermodynamics - Statistical Mechanics

Dyson's "gas".

Imagine the unit circle as a container holding N equally charged particles in some external force field. Letting $z_j = e^{i\theta_j}$ represent the position of the j^{th} particle, we have that for energy E, of the gas,

$$E = -\sum_{1 \leq i < j \leq n} \log |z_i - z_j| + \sum u(z_j)$$

where u represents the contribution of the external force field. One has that

$$\frac{1}{N!} \int_0^{2\pi} \dots \int_0^{2\pi} e^{-BE} d\theta_1 \dots d\theta_n =$$

- n -

$$\frac{(2\pi)^N}{N!} \left[\frac{1}{(2\pi)^N} \int_0^{2\pi} \dots \int_0^{2\pi} \left| e^{i\theta_i} - e^{i\theta_j} \right|^{B-B\sum_j u(z_j)} d\theta_1 \dots d\theta_n \right]$$

- n -

where $B=1/KT$; T being the absolute temperature and K being the Boltzmann constant. For the special case $B=2$, Dyson noted that the quantity in brackets above is a Toeplitz determinant.

In fact, the function

$$f(\theta) = e^{-2u(e^{i\theta})}$$

yields a matrix c whose finite sections T_N has determinant equal to the above quantity.

IV) Quantum Statistical Mechanics:

An example of Lénard (c.f. Journal of Mathematical Physics, #5, July 1964, pp. 930-943).

Consider N bosons which cannot interpenetrate contained in a one-dimensional "box" of length L . The wave function of the ground state $\psi(x_1, \dots, x_n)$ is given by the formula

$$\psi(x_1, \dots, x_n) = \left(\frac{n!}{L^n}\right)^{\frac{1}{2}} \prod_{1 \leq j < k \leq n} \left| 2 \sin \frac{\pi}{L} (x_j - x_k) \right|$$

and this quantity is a function of $x-x'$ only so that we can define $R_{n,1}$ by the formula

$$\frac{1}{L} R_{N,L} \left(\frac{2\pi}{L} (x-x') \right) = \rho_{N,L}(x, x')$$

Lénard then shows that $R_{N,L}(\alpha) = \det T_{N-1}$ where T_K

is the K^{th} Toeplitz matrix associated with the function

$$f(\theta) = |e^{i\theta} - e^{i\alpha/2}| \cdot |e^{i\theta} - e^{-i\alpha/2}|$$

One is interested in $R_{N,L}(\alpha)$ only in the so-called

"thermodynamical limit" i.e.

$$N \rightarrow +\infty, \frac{L}{N} = l$$

In this limit, Lénard shows that

$$R_{N,L}(\alpha) = O(\sqrt{n})$$

which proves that, in particular, the system does not show condensation.

V) Random Walk Problems:

We will also need a continuous analog of Toeplitz matrices.

This analog is introduced naturally in the context of integral operators. More precisely, suppose $K(x)$ is an even real-valued function in $L^2(\mathbb{R})$. Then in the usual manner $K(x-y)$ is the kernel of a self-adjoint operator K on $L^2(\mathbb{R})$. In fact

$$[K\varphi](x) = \int_{-\infty}^{\infty} K(x-y) \varphi(y) dy$$

In this context, the analog of a finite section is the operator K_a defined by the formula

$$[K_a \varphi](x) = \int_{-a}^a K(x-y) \varphi(y) dy$$

It should be noted here that $K(x-y)$ is in $L^2([-a,a] \times [-a,a])$ so that the operator K_a is completely continuous.

It will be shown that the Fredholm determinant plays the role of the Toeplitz determinant. Unfortunately, no analog in this context of Szego's orthogonal polynomials was developed until the very recent work of Achieser.

Suppose now that $K(x) \geq 0$ and that $\int_{-\infty}^{\infty} K(x) dx = 1$.

Consider a one-dimensional random walk with displacements

$X_1, X_2, \dots, X_n, \dots$ having density $K(x)$.

The probability that, starting at 0, barriers placed at $\pm a$ are not exceeded in n -steps is given by the expression

$$P\{-a < x, < a, -a < x_1 + x_2 < a, \dots, -a < x_1 + \dots + x_n < a\}$$

and this probability is given in turn by the integral

$$\int_{-a}^a \dots \int_{-a}^a K(x, -0) K(x_2 - x_1) \dots K(x_n - x_{n-1}) dx_1 \dots dx_n$$

- n -

But this integral is related to the n^{th} iterate of K and by standard theorems from the theory of integral operators we have that

$$P\{-a < x, < a, \dots, -a < x + \dots + x_n < a\} =$$

$$\sum_j \lambda_j^{(n)}(a) \psi_j^{(a)}(0) \int_{-a}^a \psi_j^{(a)}(x) dx$$

where $\lambda_j^{(n)}(a)$ and $\psi_j^{(a)}(x)$ are the j^{th} eigenvalue and eigenfunction respectively of the operator Ka .

Szego's classical work on Toeplitz matrices depended upon in part the theory of orthonormal polynomials. We shall describe here some of the relevant parts of that theory and its connections with Toeplitz matrices.

Suppose $w(\theta)$ is a positive function on $0 \leq \theta \leq 2\pi$ such that

$$\frac{1}{2\pi} \int_0^{2\pi} w(\theta) d\theta = 1$$

A system of orthonormal polynomials with respect to the weight function w is a set $\{\varphi_i(z)\}_{i=1}^{\infty}$ of polynomials in the complex variable z such that $\varphi_m(z)$ is of degree m and

$$\frac{1}{2\pi} \int_0^{2\pi} \varphi_n(e^{i\theta}) \varphi_m^*(e^{i\theta}) w(\theta) d\theta = \delta_{mn}$$

Such a system always exists, and it is possible to give an explicit representation for these polynomials. In fact, we have the formula

$$\varphi_n(z) = (D_n D_{n+1})^{-\frac{1}{2}} \det \begin{pmatrix} c_0 & c_{-1} & \dots & c_{-n} \\ c_1 & c_0 & \dots & c_{-n+1} \\ \vdots & \vdots & \ddots & \vdots \\ c_{n-1} & c_{n-2} & \dots & c_{-1} \\ 1 & z & \dots & z^{n-1} \end{pmatrix}$$

where c_n is the n^{th} Fourier coefficient of w - that is

$$c_n = \frac{1}{2\pi} \int_0^{2\pi} w(\theta) e^{-in\theta} d\theta$$

and $D_n = \det T_n$ where T_n is the n by n Toeplitz matrix associated with w .

Consider now, for some fixed integer $n \geq 0$, the set of polynomials of the form $g(z) = z^n + a_{n-1}z^{n-1} + \dots + a_0$ where $a_{n-1}, a_{n-2}, \dots, a_0$ are arbitrary complex numbers. Consider also the quadratic form

$$Q[g] = \frac{1}{2\pi} \int_0^{2\pi} |g(e^{i\theta})|^2 w(\theta) d\theta \text{ for } g \text{ as above,}$$

and the problem of minimizing this form over all such g .⁺ The answer to this problem is easy in view of the properties of the orthonormal polynomials we have already established. We write for some arbitrary $g(z)$ as above

$$(1) \quad g(e^{i\theta}) = (g_0 \varphi_0 + \dots + g_n \varphi_n)(e^{i\theta}).$$

(Then g is surely of degree n .) The orthonormality of the φ_k implies that

$$Q[g] = |g_0|^2 + \dots + |g_n|^2$$

⁺ This problem is the " L^2 - analog" of the classical problem of finding for fixed n the polynomial $f(x) = \sum_{k=0}^n a_k x^k$ where $a_n = 1$ which best approximates 0 on $[0, 1]$.

Elementary properties of determinants show that $\varphi_n(z)$ has leading coefficient $(D_n/D_{n+1})^{\frac{1}{2}}$, and it follows that

$$g_n = (D_{n+1}/D_n)^{\frac{1}{2}}$$

Since the leading coefficient of $g(z)$ is 1.

Equation (1) implies immediately that

$$Q[g] \geq |g_n|^2 = \frac{D_{n+1}}{D_n}$$

and letting $g(z) = (D_{n+1}/D_n)^{\frac{1}{2}} \varphi_n(z)$ we see that this minimum is attained. It is easy to check that

$$\frac{1}{2\pi} \int_0^{2\pi} |x_n e^{in\theta} + x_{n-1} e^{i(n-1)\theta} + \dots + x_0|^2 w(\theta) d\theta =$$

$$\sum_{k=0}^n c_{k-1} x_k \bar{x}_k$$

and also that

$$\frac{1}{2\pi} \int_0^{2\pi} |x_n e^{in\theta} + \dots + x_0|^2 w(\theta) d\theta \geq |x_n|^2 \frac{D_{n+1}}{D_n}$$

It follows from this that D_{n+1}/D_n is non-increasing, and since $D_0 = c_0 = 1$, $D_n \geq 0$. Hence

$$\lim_{n \rightarrow \infty} \frac{D_{n+1}}{D_n} = G(w) \geq 0.$$

exists, and as is well known this implies that

$$\lim_{n \rightarrow \infty} (D_n)^{1/n} = G(w).$$

It can then be shown that

$$G(w) = \exp \left\{ \frac{1}{2\pi} \int_0^{2\pi} \log w(\theta) d\theta \right\}$$

This formula can be proved by first showing that it holds for some convenient class of positive functions and then extending the result to their L - closure.

We also mention without proof that in the special case of $w(\theta) = 1/p(\theta)$ for $p(\theta)$ a positive trigonometric polynomial, D_{n+1}/D_n is constant for all sufficiently large n . The exact knowledge of this constant is very important in certain refinements of the Szego theorem.

We will have occasion to use a theorem of L. Fejér and F. Riesz concerning non-negative trigonometric polynomials (c.f. Grenander and Szego, Toeplitz Forms and their Applications, University of California Press, pp. 20-22.)

"Suppose $p(\theta)$ is a non-negative trigonometric polynomial of precise degree r . Then there exists a polynomial $d(z) = d_r z^r + d_{r-1} z^{r-1} + \dots + d_0$ ($d_r \neq 0$) such that

$$p(\theta) = |d(e^{i\theta})|^2."$$

One should not suppose that this relationship is trivially arrived at. For example, in the seemingly simple case that $p(\theta) = 2 + \cos\theta$,

$$d_0 = \sqrt{1 + \frac{\sqrt{3}}{2}} \quad \text{and} \quad d_1 = \left[2\sqrt{1 + \frac{\sqrt{3}}{2}} \right]^{-1}$$

(2) There is another approach to the study of Toeplitz matrices, however, which does not depend upon the theory of orthonormal polynomials. This second approach, based on moments of the distribution of the eigenvalues, is due primarily to the author. Already Hilbert attacked the problem of characterizing the spectra of operators such as $C = (c_{j-i})$ by studying the properties of the eigenvalues of finite sections of this infinite matrix. The theory of moments provides another approach to the problem, which has the decided advantage that some knowledge of the distribution of the eigenvalues is gained.

We begin by examining a continuous analog of a Toeplitz operator. Let $\rho(x)$ be real, even and in $L(-\infty, \infty)$. Let

$$F(\xi) = \int_{-\infty}^{\infty} \rho(x) e^{i\xi x} dx$$

Suppose that F is in $L(-\infty, \infty)$ and that $\rho(x)$ is locally of bounded variation so that the inversion formula

$$\rho(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} F(\xi) e^{-i\xi x} d\xi$$

holds. It follows from these formulae that

- i) F is real valued
- ii) ρ is continuous and bounded on $(-\infty, \infty)$.

Suppose $K(x)$ is in $L^2(-\infty, \infty)$ and $L(-\infty, \infty)$ and is continuous. Then for $\alpha > 0$, the integral operator

$$(1) \quad \int_{-\infty}^{\infty} K(\alpha x) \rho(x-y) K(\alpha y) \varphi(y) dy$$

has a Hilbert-Schmidt kernel, in particular

$$\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} |K(\alpha x) \rho(x-y) K(\alpha y)|^2 dx dy < \infty$$

Thus the operator has a discrete set of eigenvalues. We suppose that $K(0) = 1$ and that as $\alpha \rightarrow 0$ the integral operator (1) becomes "less and less Hilbert-Schmidt" - that is

$$\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} |\rho(x-y)|^2 dx dy = +\infty.$$

Thus, $\int_{-\infty}^{\infty} K(\alpha x) \rho(x-y) K(\alpha y) dy$

plays the role of a finite section of the integral operator

$$\int_{-\infty}^{\infty} \rho(x-y) \varphi(y) dy.$$

In fact, if $K(x)$ is chosen to be an appropriate characteristic function, then

$$\int_{-\infty}^{\infty} K(\alpha x) \rho(x-y) K(\alpha y) \varphi(y) dy = \int_{-a}^a \rho(x-y) \varphi(y) dy \quad (a = \alpha^{-1})$$

Suppose now that (1) has eigenvalues $\lambda_j(\alpha)$; we wish to compute the moments

$$\sum_{j=1}^{\infty} \lambda_j^k(\alpha)$$

for $k = 2, 3, \dots$

The case $k = 3$, is sufficiently general to indicate the general result. From the general theory of integral equations, we have that

$$\sum_{j=1}^{\infty} \lambda_j^3(\alpha) = \left(\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} K^2(\alpha x_1) K^2(\alpha x_2) K^2(\alpha x_3) \rho(x_2 - x_1) \rho(x_3 - x_2) \rho(x_1 - x_3) dx_1 dx_2 dx_3 \right)$$

Changing variables via the transformation

$$\begin{aligned}\alpha x_3 &= t_3 \\ \alpha x_2 &= t_3 + \alpha t_2 \\ \alpha x_1 &= t_3 + \alpha t_2 + \alpha t_1\end{aligned}$$

which has Jacobian α^{-1} , we get the formula

$$\alpha \sum_{j=1}^{\infty} \lambda_j^3 (\alpha) = \left(\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} K^2(t_3 + \alpha t_2 + \alpha t_1) K^2(t_3 + \alpha t_2) K^2(t_3) \rho(t_1) \rho(t_2) \rho(t_1 + t_2) dt_1 dt_2 dt_3 \right)$$

which as α goes to zero goes to

$$\int_{-\infty}^{\infty} K^6(t) dt \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \rho(t_1) \rho(t_2) \rho(t_1 + t_2) dt_1 dt_2$$

But, it follows easily from the inversion formula that this last is

$$\begin{aligned}\int_{-\infty}^{\infty} K^6(x) dx &\cdot \frac{1}{2\pi} \int_{-\infty}^{\infty} F^3(\xi) d\xi = \\ \frac{1}{2\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} (K^2(x) F(\xi))^3 dx d\xi\end{aligned}$$

For general k , we have the equation

$$\lim_{\alpha \rightarrow 0} \alpha \sum_{j=1}^{\infty} \lambda_j^k (\alpha) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} (K^2(x) F(\xi))^k dx d\xi$$

A slight modification of a standard theorem on moments implies that if (a, b) is an interval not containing 0 and if $N_{\alpha}(a, b)$ denotes the number of eigenvalues of (1) in (a, b) , then

$$\lim_{\alpha \rightarrow 0} \alpha N_{\alpha}(a,b) = \frac{1}{2\pi} \mu \{ (x, \xi) : a < K^2(x) F(\xi) < b \} ,$$

where μ is Lebesgue measure in the plane, provided that

$$\mu \{ (x, \xi) : K^2(x) F(\xi) \in \{a, b\} \} = 0$$

This result has an immediate application to the theory of Bessel functions. Consider the equation

$$\frac{1}{2} \int_{-\infty}^{\infty} e^{-\alpha|x|} e^{-|x-y|} e^{-\alpha|y|} \varphi(y) dy = \lambda \varphi(y)$$

It can be shown that this has eigenvalues $(\alpha r_1)^{-2}$, $(\alpha t_1)^{-2}$, $(\alpha r_2)^{-2}$, $(\alpha t_2)^{-2}$, ..., where the r_i are the roots of $J_{1/\alpha}(r) = 0$ and the t_i are the roots of $J_{1/\alpha}(t) = 0$. The theorem above implies that if $M_{\alpha}(a) = \text{number of } t\text{'s} < a^{-\frac{1}{2}}$, α^{-1} for $a < 1$ then

$$\lim_{\alpha \rightarrow 0} \alpha M_{\alpha}(a) = \frac{1}{\pi} \{ (a^{-1}-1)^{\frac{1}{2}} - \arctan (a^{-1}-1)^{\frac{1}{2}} \} .$$

Let $t_n = (\alpha \sqrt{a})^{-1}$ and $\alpha = \frac{1}{n}$, then $\sqrt{a} \sim n/t_n$ and $M_{\alpha}(a) = n$,

A little unrigorously (since $\sqrt{a} \sim n/t_n$ is not a constant) we get now

$$1 = \frac{1}{\pi} \{ (a^{-1}-1)^{\frac{1}{2}} - \arctan (a^{-1}-1)^{\frac{1}{2}} \} .$$

whence it follows that

$$a^{-1} = 1 + x_1^2$$

where x_1 is the smallest positive root of

$$\tan x = x$$

This implies that

$$\frac{t_n}{n} \sim \sqrt{1 + x_1^2}$$

a known result in the theory of Bessel functions. It is a simple matter to render our argument entirely rigorous.

We now return to the theory of Toeplitz matrices. Let

$w(\theta)$, $0 \leq \theta \leq 2\pi$, be a real function with Fourier series

$$\sum_{k=-\infty}^{\infty} c_k e^{ik\theta}, \text{ and let } T_m \text{ be the } m \times m \text{ Toeplitz matrix } (c_{j-i})_{i,j=0}^{m-1}$$

Denote its eigenvalues by $\lambda_1(m), \dots, \lambda_m(m)$, and consider the n^{th} moment $\sum_{j=1}^m \lambda_j^n(m)$. It can be shown that this moment is given by the expression

$$(2) \quad \frac{m}{2\pi} \int_0^{2\pi} w^n(\theta) d\theta = \sum_{i_1 + \dots + i_n = 0} [R(\bar{i})]_m c_{i_1} \dots c_{i_n}$$

where $\bar{i} = (i_1, \dots, i_n)$ is an n -tuple of integers,

$$(3) \quad R(\bar{i}) = \text{Max}(0, i_1, i_1 + i_2, \dots, i_1 + \dots + i_n) - \text{Min}(0, i_1, \dots, i_1 + \dots + i_n)$$

$$\text{and } [R]_m = \begin{cases} R & \text{if } R \leq m \\ m & \text{if } R > m \end{cases}$$

Suppose first that w and all its positive powers are integrable; then we get the "weak" theorem:

$$\lim_{m \rightarrow \infty} \frac{1}{m} \sum_{j=1}^m \lambda_j^n(m) = \frac{1}{2\pi} \int_0^{2\pi} w^n(\theta) d\theta$$

It can now be shown by a standard argument that if (a,b) is an interval such that

$$\mu \{x: w(x) \in (a,b)\} = 0$$

where μ is Lebesgue measure, then

$$\lim_{m \rightarrow \infty} \frac{1}{m} N_m(a,b) = \frac{1}{2\pi} \mu \{x: a < w(x) < b\}.$$

where $N_m(a,b)$ is the number of eigenvalues of T_m in (a,b) . It should be recalled here that if w is continuous, then the spectrum of (c_{j-1}) and the range of w coincide. Our last result shows that even more than this is true; in fact, the range of w and the spectrum of C are equally distributed.

One can use the "weak" result above to prove a result mentioned in section 1 - specifically, if $w(\theta)$, $0 \leq \theta \leq 2\pi$, and all its positive powers are integrable, then

$$\lim_{n \rightarrow \infty} \frac{1}{n} \log D_n = G(w)$$

where D_n is the determinant of T_n , the n by n Toeplitz matrix associated with w and

$$G(w) = \exp \left\{ \frac{1}{2\pi} \int_0^{2\pi} \log w(\theta) d\theta \right\}.$$

We will prove a refinement of this classical theorem of Szego.
We can also use the distribution theorem to prove the following:

Theorem: (R. Boas and M. Kac)

Suppose $A(w) \geq 0$ is even and is in $L(-\infty, \infty)$ with
 $\int_{-\infty}^{\infty} A(w) dw = 1$. Let $\rho(t) = \int_{-\infty}^{\infty} A(w) \cos wt dw$ be such that
 $\rho(t) = 0$ for $|t| \geq \Delta$. Then $|\rho(\frac{\Delta}{n})| \leq \cos \frac{\pi}{n+1}$ for $n \geq 2$.

Proof:

Fix $N \geq 2$ and let n be arbitrary $\geq N$. Then given arbitrary
real numbers $x_0, x_1, \dots, x_n$ we have

$$0 \leq \int_{-\infty}^{\infty} A(w) \left| \sum_{K=0}^{n-1} x_K \exp \left\{ iw \frac{K\Delta}{N} \right\} \right|^2 dw =$$

$$\sum_{K, l=0}^n \rho \left((K-l) \frac{\Delta}{N} \right) x_K x_l$$

This positive definite quadratic form arises from the n by n
Toeplitz matrix T_n associated with the function

$$w(\theta) = \sum_{K=-N+1}^{N-1} \rho \left(\frac{K\Delta}{N} \right) e^{iK\theta} = 1 + 2 \sum_{K=1}^{N-1} \rho \left(\frac{K\Delta}{N} \right) \cos K\theta$$

Since the quadratic form is positive for $n \geq N$, T_{n-1} has no
non-negative eigenvalues for $n \geq N$. Hence, since w is con-
tinuous, the distribution theorem implies that $w(\theta) \geq 0$. The
Fejer-Riesz theorem then implies that there is a polynomial of
degree $N-1$, say

$$d(Z) = d_0 + d_1 Z + \dots + d_{N-1} Z^{N-1}$$

such that

$$w(\theta) = \left| \sum_{K=0}^{N-1} d_K e^{iK\theta} \right|^2$$

Equating coefficients in the two expressions for $w(\theta)$ we have

$$\sum_{K=0}^{N-1} |d_K|^2 = 1 \quad \text{and}$$

$$\rho(\Delta/N) = \frac{1}{2} \left[\sum_{K=0}^{N-2} d_K \bar{d}_{K+1} + \sum_{K=0}^{N-2} \bar{d}_K d_{K+1} \right]$$

But then

$$\rho(\Delta/N) = (\bar{d}_0, \bar{d}_1, \dots, \bar{d}_{N-1}) \begin{pmatrix} 0 & \frac{1}{2} & 0 & 0 & \dots & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} & 0 & & \\ 0 & \frac{1}{2} & 0 & \frac{1}{2} & & \\ 0 & 0 & \frac{1}{2} & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & \dots & 0 & \frac{1}{2} & 0 \end{pmatrix} \begin{pmatrix} d_0 \\ \vdots \\ \vdots \\ d_{N-1} \end{pmatrix}$$

And this quantity on the right hand side is bounded above by

$$\lambda_{\max} \left(\sum |d_K|^2 \right)^2 = \lambda_{\max}$$

where $\lambda_{\max}$ is the largest eigenvalue of the N by N matrix above.

But it is known that

$$\lambda_{\max} = \cos(\pi/N+1)$$

In order to prove our refinement of Szego's theorem, we now suppose that

$$\sum |c_k| |k| < +\infty$$

this implies that in the limit as $m \rightarrow \infty$, the truncation of $R(\bar{v})$ by m in

$$\sum_{t_1 + \dots + t_n = 0} R(\bar{t})_m c_{t_1} \dots c_{t_n}$$

can be ignored. The symmetry in $c_{t_1} \dots c_{t_n}$ implies that when truncation can be ignored,

$$\begin{aligned} \sum_{t_1 + \dots + t_n = 0} R(\bar{t})_m c_{t_1} \dots c_{t_n} &= \\ 2 \sum_{t_1 + \dots + t_n = 0} \text{Max}(0, t_1, \dots, t_1 + \dots + t_{n-1}) c_{t_1} \dots c_{t_n} . \end{aligned}$$

This last quantity has an interesting probabilistic interpretation when $c_K \geq 0$ and $\sum c_K = 1$. Consider a game which has only integral payoffs t_1 with probability c_{t_1} . In this setting,

$$(4) \quad \sum_{t_1 + \dots + t_n = 0} \text{Max}(0, t_1, \dots, t_1 + \dots + t_{n-1}) c_{t_1} \dots c_{t_n}$$

is the expectation of maximum profit in a sequence of n independent games at the end of which there is no net profit or loss. Alternatively, let $s_1, \dots, s_n$ be the partial sums of the n independent random variables $X_1, \dots, X_n$. Then (4) is

$$E \left\{ \text{Max}(0, s_1, \dots, s_n) \mid s_n = 0 \right\} \cdot \text{Prob} \left\{ s_n = 0 \right\} .$$

The fact that the refined Szego theorem gave an explicit closed formula for this latter expression is so remarkable that these calculations were not immediately believed.

A combinational lemma of Hunt for which Dyson found a "three-line" proof permits further analysis of (4).

First, it is easy to see that

$$\sum_{i_1 + \dots + i_n = 0} \text{Max}(0, i_1 + i_2, \dots, i_1 + \dots + i_{n-1}) c_{i_1} \dots c_{i_n} =$$

$$\frac{1}{n!} \sum_{i_1 + \dots + i_n = 0} \left(\sum_{\sigma} \text{Max}(0, i_{\sigma_1}, \dots, i_{\sigma_1} + \dots + i_{\sigma_n}) \right) c_{i_1} \dots c_{i_n}$$

where the second summation is taken over all permutations σ of n letters. Hunt's result states that

$$\sum_{\sigma} \text{Max}(0, i_{\sigma_1}, \dots, i_{\sigma_1} + \dots + i_{\sigma_n}) = \sum_{\sigma} i_{\sigma_1} N(\sigma)$$

where $N(\sigma) = \sum_{K=1}^n \theta(i_{\sigma_1} + \dots + i_{\sigma_K})$ with θ defined by the

formula

$$\theta(x) = \begin{cases} 0 & \text{if } x \leq 0 \\ 1 & \text{if } x > 0 \end{cases}$$

That this purely combinational result should imply such a highly analytical result as Szego's theorem is indeed something of a mystery.

We now have the following series of equations:

$$\sum_{i_1 + \dots + i_n = 0} \text{Max}(0, i_1, i_1 + i_2, \dots, i_1 + \dots + i_{n-1}) =$$

$$\frac{1}{n!} \sum_{i_1 + \dots + i_n = 0} \left(\sum_{\sigma} i_{\sigma_1} N(\sigma) \right) c_{i_1} \dots c_{i_n} =$$

$$\sum_{i_1 + \dots + i_n = 0} \left[i_1 \sum_{k=1}^n \theta(i_1 + \dots + i_k) \right] c_{i_1} \dots c_{i_n} =$$

$$\sum_{k=1}^{n-1} \frac{1}{k} \sum_{i_1 + \dots + i_n = 0} (i_1 + \dots + i_k) \theta(i_1 + \dots + i_k) c_{i_1} \dots c_{i_n}$$

Now

$$\sum_{(i_1 + \dots + i_k) + (i_{k+1} + \dots + i_n) = 0} (i_1 + \dots + i_k) \theta(i_1 + \dots + i_k) c_{i_1} \dots c_{i_n}$$

$$= \sum_{i=1}^{\infty} \sum_{\substack{i_1 + \dots + i_k = i \\ i_{k+1} + \dots + i_n = -i}} i c_{i_1} \dots c_{i_k} c_{i_{k+1}} \dots c_{i_n}$$

$$= \sum_{i=1}^{\infty} i \sum_{\substack{i_1 + \dots + i_k = i \\ i_{k+1} + \dots + i_n = -i}} (c_{i_1} \dots c_{i_k}) (c_{i_{k+1}} \dots c_{i_n})$$

$$= \sum_{i=1}^{\infty} i \left(\sum_{i_1 + \dots + i_k = i} c_{i_1} \dots c_{i_k} \right) \left(\sum_{i_{k+1} + \dots + i_n = -i} c_{i_{k+1}} \dots c_{i_n} \right)$$

However, in the probabilistic interpretation,

$$\sum_{i_1 + \dots + i_k = i} c_{i_1} \dots c_{i_k}$$

is just the probability of ending up with a net payoff of i after k independent plays of the game, and thus equals

$$\frac{1}{2\pi} \int_0^{2\pi} w^k(\theta) e^{-i i \theta} d\theta$$

Similarly,

$$\sum_{i_{k+1} + \dots + i_n = -i} c_{i_{k+1}} \dots c_{i_n} = \frac{1}{2\pi} \int_0^{2\pi} w^{n-k} e^{i i \theta} d\theta$$

and the same equations hold in our more general case. Expression

(4) now equals

$$(5) \quad \sum_{k=1}^{n-1} \frac{1}{k} \sum_{i=1}^{\infty} \left[\frac{1}{2\pi} \int_0^{2\pi} w^k(\theta) e^{-i i \theta} d\theta \right] \left[\frac{1}{2\pi} \int_0^{2\pi} w^{n-k}(\theta) e^{i i \theta} d\theta \right].$$

To simplify the next computations, we assume also that $w(\theta) = w(-\theta)$ so that in particular

$$\int_0^{2\pi} w^k(\theta) e^{-i i \theta} d\theta = \int_0^{2\pi} w^k(\theta) e^{i i \theta} d\theta.$$

We remark, however, that this assumption is not necessary to prove our version of the refined Szego theorem.

Interchange the order of summation in (5) and note that the assumption that w is even implies that (4) equals

$$\frac{1}{2} \sum_{i=1}^{\infty} \left(\sum_{k=1}^{n-1} \frac{1}{k} f_k(i) f_{n-k}(i) + \sum_{n-k=1}^{n-1} \frac{1}{n-k} f_{n-k}(i) f_k(i) \right)$$

where

$$f_j(i) = \frac{1}{2\pi} \int_0^{2\pi} w^j(\theta) e^{i i \theta} d\theta, \quad 0 \leq j < n.$$

thus, since $\frac{1}{2} (k^{-1} + (n-k)^{-1}) = \frac{1}{2} n k^{-1} (n-k)^{-1},$

$$(4) = \frac{1}{2} \sum_{i=1}^{\infty} i \sum_{k=1}^{n-1} \frac{n}{k(n-k)} f_k(i) f_{n-k}(i)$$

Returning to our original expression (2) for the n^{th} moment and taking into account the note on pages 12-13, we see that we have

$$\lim_{m \rightarrow \infty} \sum_{j=1}^m \lambda_j^n(m) - \frac{m}{2\pi} \int_0^{2\pi} w^n(\theta) d\theta =$$

$$-n \sum_{i=1}^{\infty} i \sum_{k=1}^{n-1} \frac{1}{k(n-k)} f_k(i) f_{n-k}(i)$$

for $n = 1, 2, 3, \dots$

Hence for a suitable chosen small ξ , we have

$$\begin{aligned} & \sum_{n=1}^{\infty} \frac{1}{n} \xi^n \lim_{m \rightarrow \infty} \left\{ \sum_{j=1}^m \lambda_j^n(m) - \frac{m}{2\pi} \int_0^{2\pi} w^n(\theta) d\theta \right\} = \\ & - \sum_{n=1}^{\infty} \xi^n \sum_{i=1}^{\infty} i \sum_{k=1}^{n-1} \frac{1}{k(n-k)} f_k(i) f_{n-k}(i) \end{aligned}$$

Interchanging the order of summation on the left hand side of this equation, we get

$$\lim_{m \rightarrow \infty} \left\{ \sum_{j=1}^m \sum_{n=1}^{\infty} \left[\xi^n \frac{\lambda_j^n(m)}{n} - \frac{m}{2\pi} \int_0^{2\pi} \frac{\xi^n w^n(\theta)}{n} d\theta \right] \right\}.$$

But this equals

$$\lim_{m \rightarrow \infty} - \left\{ \sum_{j=1}^m \log(1 - \xi \lambda_j(m)) - \frac{m}{2\pi} \int_0^{2\pi} \log(1 - \xi w(\theta)) d\theta \right\}.$$

and since the determinant of an $m \times m$ matrix is the product of its eigenvalues, we have

$$\lim_{m \rightarrow \infty} \left\{ \log D_m(1 - \xi w(\theta)) - \frac{m}{2\pi} \int_0^{2\pi} \log(1 - \xi w(\theta)) d\theta \right\}.$$

Where $D_m(1 - \xi w(\theta))$ is the determinant of the m^{th} finite section of the Toeplitz matrix associated with the function $1 - \xi w(\theta)$.

Next note that

$$\begin{aligned} \sum_{n=1}^{\infty} \sum_{k=1}^{n-1} \frac{\xi^k}{k} f_k^{(1)} \frac{\xi^{n-k}}{n-k} f_{n-k}^{(1)} &= \left(\sum_{n=1}^{\infty} \frac{\xi^n}{n} f_n^{(1)} \right)^2 \\ &= \left(\frac{1}{2\pi} \int_0^{2\pi} \log(1 - \xi w(\theta)) e^{i\theta} d\theta \right)^2 \end{aligned}$$

Where the second equality follows from the definition of the $f_n^{(1)}$ and by interchanging the order of summation and integration.

Note that in the more general case (i.e. $w(\theta)$ not even), we get here

$$\left(\frac{1}{2\pi} \int_0^{2\pi} \log(1-\xi w(\theta)) e^{i\theta} d\theta \right) \left(\frac{1}{2\pi} \int_0^{2\pi} \log(1-\xi w(\theta)) e^{-i\theta} d\theta \right).$$

Exponentiating, we get finally (in our simpler case) the refined Szego theorem - i.e.

$$\lim_{m \rightarrow \infty} \frac{D_m(1-\xi w(\theta))}{\exp\left\{ \frac{m}{2\pi} \int_0^{2\pi} \log(1-\xi w(\theta)) d\theta \right\}} = \exp\left\{ \sum_{i=1}^{\infty} i K_i^2(\xi) \right\}$$

$$\text{where } K_i(\xi) = \frac{1}{2\pi} \int_0^{2\pi} \log(1-\xi w(\theta)) e^{i\theta} d\theta.$$

The reader should note what the right hand side equals in the more general case.

The extension of this result to the more general case of Toeplitz matrices whose entries are Toeplitz matrices is highly complicated by the non-commutativity of the objects involved. In fact, little is known about such situations.

Section 3. There is a continuous analog of the refined Szegő theorem which we will only describe without proof here.

Suppose $\rho(x) \in L(-\infty, \infty)$ and $\rho(x) = \rho(-x)$. Suppose also that the Fourier transform

$$F(\eta) = \int_{-\infty}^{\infty} \rho(x) e^{i\eta x} dx$$

of ρ is in L and that the inversion formula holds. Then denote by $\rho^{(n)}$ the n -fold convolution of ρ with itself - i.e.

$$\rho^{(n)}(x) = \rho * \dots * \rho(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} F^n(\eta) e^{-i\eta x} d\eta.$$

Consider the equation

$$T_a \varphi(x) = \int_{-a}^a \rho(x-y) \varphi(y) dy = \lambda \varphi(x)$$

which defines the eigenvalue λ of the integral operator T_a . Standard theorems about Hilbert-Schmidt operators imply that there exist only countably many eigenvalues of this "finite section" operator. Then ξ can be chosen so that

$$D_a(\xi) = \prod_{j=1}^{\infty} (1 - \xi \lambda_j(a))$$

exists, where $\{\lambda_j(a)\}$ is a complete set of eigenvalues for T_a .

We have, much as before, a lemma which gives the equation

$$\lim_{a \rightarrow \infty} \left\{ \sum_{j=1}^{\infty} \lambda_j^n(a) - \frac{2a}{\pi} \int_0^{\infty} F^n(\eta) d\eta \right\} =$$

$$-2 \int_{-\infty}^{\infty} \dots \int_{-\infty}^{\infty} \max(0, x_1, x_1+x_2, \dots, x_1+\dots+x_{n-1}) \rho(x_1) \dots \rho(x_n) \dots \rho(x_1+\dots+x_{n-1}) dx_1 \dots dx_{n-1}$$

and

$$\int_{-\infty}^{\infty} \dots \int_{-\infty}^{\infty} \max(0, x_1, \dots, x_1+\dots+x_{n-1}) \rho(x_1) \dots \rho(x_{n-1}) \rho(x_1+\dots+x_{n-1}) dx_1 \dots dx_n =$$

$$\frac{n}{2} \int_0^{\infty} x \sum_{k=1}^{n-1} \frac{\rho^{(k)}(x) \rho^{(n-k)}(x)}{(k)(n-k)} dx.$$

this in turn yields the analog of the refinement of Szegő's theorem - i.e.

$$\lim_{a \rightarrow \infty} D_a(\xi) \Big/ \exp \left\{ \frac{2a}{\pi} \int_0^{\infty} \log(1 - \xi F(\eta)) d\eta \right\} =$$

$$\exp \left\{ \int_0^{\infty} x \cdot \left| \frac{1}{2\pi} \int_{-\infty}^{\infty} \log(1 - \xi F(\eta)) e^{i\eta x} d\eta \right|^2 dx \right\}.$$

Section 4. Achieser in a recent paper discussed the same sort of problem using new techniques. We will present some of his techniques and results here, using his notation rather than the author's.

Suppose $H(t)$ is a real, even function such that

$$\int_{-\infty}^{\infty} |H(t)| dt < 1.$$

Define

$$h(\xi) = \int_{-\infty}^{\infty} H(t) e^{-i\xi t} dt$$

and suppose

$$\int_{-\infty}^{\infty} |h(\xi)| d\xi < \infty.$$

The theory of Neumann-Liouville series assures us that the integral equation

$$\Gamma(t) - \int_0^{\infty} H(t-s) \Gamma(s) ds = -H(t), \quad 0 \leq t < +\infty$$

has a solution $\Gamma(t)$, which is unique and in L . Then the existence of a solution in $[0, \infty)$ gives us a solution $\Gamma(t)$ on $(-\infty, +\infty)$ via the integral equation. Then we have

$$\Gamma(t) - \int_0^{\infty} H(t-s) \Gamma(s) ds = -H(t) \quad -\infty < t < \infty$$

and $\Gamma \in L$.

We now apply the technique of Wiener-Hopf to obtain an explicit representation for $\Gamma(0)$.

First note that

$$\int_{-\infty}^{\infty} \Gamma(t) e^{-itx} dt - \int_{-\infty}^{\infty} e^{-itx} \int_0^{\infty} H(t-s) \Gamma(s) ds dt = -h(x).$$

Interchanging the order of integration we find

$$\int_0^{\infty} \Gamma(t) e^{-itx} dt + \int_{-\infty}^0 \Gamma(t) e^{-itx} dt - h(x) \int_0^{\infty} \Gamma(t) e^{-itx} dt = -h(x) .$$

Letting $\rho(x) = 1-h(x)$, then

$$1 + \int_{-\infty}^0 \Gamma(t) e^{-itx} dt = \rho(x) \left\{ 1 - \int_0^{\infty} \Gamma(t) e^{-itx} dt \right\};$$

then we have

$$\rho(x) = \frac{1 + \int_{-\infty}^0 \Gamma(t) e^{-itx} dt}{1 - \int_0^{\infty} \Gamma(t) e^{-itx} dt} .$$

Define $\gamma(t)$, $\gamma \in L$ by the formula

$$\log \rho(x) = \int_{-\infty}^{\infty} \gamma(t) e^{-itx} dt$$

then

$$\rho(x) = e^{\log \rho(x)} = \exp \left\{ \int_{-\infty}^0 \gamma(t) e^{-itx} dt + \int_0^{\infty} \gamma(t) e^{-itx} dt \right\} .$$

From these two expressions for $\rho(x)$ we have

$$\begin{aligned} \left(1 - \int_0^{\infty} \Gamma(t) e^{-itx} dt \right) \exp \left(\int_0^{\infty} \gamma(t) e^{-itx} dt \right) = \\ \left(1 + \int_{-\infty}^0 \Gamma(t) e^{-itx} dt \right) \exp \left\{ - \int_{-\infty}^0 \gamma(t) e^{-itx} dt \right\} . \end{aligned}$$

Now consider where $z = x+iy$ is a complex variable

$$(1) \left(1 - \int_0^{\infty} \Gamma(t) e^{-itz} dt\right) \exp \left\{ \int_0^{\infty} \gamma(t) e^{-itz} dt \right\} \quad \text{Im } z < 0.$$

$$(2) \left(1 + \int_{-\infty}^0 \Gamma(t) e^{-itz} dt\right) \exp \left\{ -\int_{-\infty}^0 \gamma(t) e^{-itz} dt \right\} \quad \text{Im } z > 0.$$

The choice of domain for these expressions guarantees that they represent analytic functions (of z) in their respective domains. But we see that these functions agree on $\text{Im } z = 0$; thus, (1) has a unique analytic extension to the whole plane which agrees with (2) in $\text{Im } z > 0$. Hence, by Liouville's theorem, this extension is a constant, and, letting $\text{Im } z \rightarrow -\infty$, we see that this constant is 1.

Thus, we have

$$\int_0^{\infty} \Gamma(t) e^{-itz} dt = 1 - \exp \left\{ -\int_0^{\infty} \gamma(t) e^{-itx} dt \right\}$$

and

$$\int_{-\infty}^0 \Gamma(t) e^{-itx} dt = - \left[1 - \exp \int_{-\infty}^0 \gamma(t) e^{-itx} dt \right]$$

It follows, using the inversion formula, that

$$\Gamma(t) = \gamma(t) + \sum_{n=2}^{\infty} \frac{(-1)^{n+1}}{n!} \int_{s_j \geq 0} \dots \int_{s_1 + \dots + s_{n-1} \leq t} \gamma(t - \sum_{j=1}^{n-1} s_j) \gamma(s_1) \dots \gamma(s_{n-1}) ds_1 \dots ds_{n-1}$$

and in particular that

$$\Gamma(0) = \gamma(0) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \log \rho(x) dx.$$

It also can be checked, using the fact that γ is even, that

$$\rho(x) = \left| 1 - \int_0^{\infty} \Gamma(t) e^{-itx} dt \right|^{-2}$$

Now for $0 < t < \tau < r$ for fixed $r \geq 0$, define

Γ_r by the formula

$$\Gamma_r(t, \tau) - \int_0^r H(t-s) \Gamma(s, \tau) ds = -H(t-\tau)$$

and note that as before a unique solution $\Gamma_r(t, \tau)$ exists for each fixed $r \geq 0$ and τ . In fact,

$$\begin{aligned} \Gamma_r(t, \tau) = & - \left\{ H(t-\tau) + \int_0^r H(t-s_1) H(s_1-\tau) ds_1 + \right. \\ & \left. \int_0^r \int_0^r H(t-s_1) H(s_1-s_2) H(s_2-\tau) ds_1 ds_2 + \dots \right\} \end{aligned}$$

It was shown by Krein that

$$\frac{\partial}{\partial r} \Gamma_r(t, \tau) = - \Gamma_r(t, r) \Gamma_r(r, \tau)$$

and the proof though short is not trivial.

We now define $D_r(H)$, the "Fredholm determinant" of H on the finite interval $[0, r]$ by the formula

$$D_r(H) = \prod_j (1 - \lambda_j(r))$$

when $\{\lambda_j(r)\}$ is the complete set of eigenvalues of the integral operator $\int_0^r H(t-s)\Gamma(s)ds - H(t)$. Achieser shows, using a rather complicated argument, that

$$D_r(H) = \exp \left(\int_0^r \Gamma_t(0,0) dt \right).$$

This identity can be proven using much simpler arguments as follows. For $\tau = 0$, we have

$$\Gamma_t(0,0) = - \left\{ H(0) + \int_0^t H(-s_1)H(s_1)ds_1 + \int_0^t \int_0^t H(-s_1)H(s_1-s_2)H(s_2)ds_1ds_2 + \dots \right\}$$

Note that

$$\begin{aligned} D_r(H) &= \exp \left\{ - \sum_{j=1}^{\infty} \sum_{k=1}^{\infty} \frac{\lambda_j^k(r)}{k} \right\} \\ &= \exp \left\{ - \sum_{k=1}^{\infty} \sum_{j=1}^{\infty} \frac{\lambda_j^k(r)}{k} \right\} \end{aligned}$$

Now by standard theorems

$$\frac{1}{k} \sum_{j=1}^{\infty} \lambda_j^k(r) =$$

$$\frac{1}{k} \int_0^r \dots \int_0^r H(t-s_1)H(s_1-s_2) \dots H(s_{k-2}-s_{k-1})H(t-s_{k-1}) dt ds_1 \dots ds_{k-1}$$

Let $\Lambda(r)$ denote this quantity. Define $\Lambda_1(r)$

by the formula

$$\Lambda_1(r) = \int_0^r dt \int_0^t \dots \int_0^t H(-s_1) H(s_1 - s_2) \dots H(s_{k-2} - s_{k-1}) H(s_{k-1}) ds_1 \dots ds_{k-1}$$

Then, trivially $\Lambda_1(r) = \Lambda(r)$ for $r = 0$, and one can show

that $\Lambda'(r) = \Lambda_1'(r)$ so that $\Lambda_1(r) = \Lambda(r)$. But now,

$$\sum_{k=1}^{\infty} k_j^{-1} \sum_{j=1}^{\infty} \lambda_j^k(r) = - \int_0^r \Gamma_t(0,0) dt$$

since the associated series are equal term by term.

But then we have Achieser's identity.

We have that $\Gamma_s(t,0) \rightarrow \Gamma(t)$ as $s \rightarrow +\infty$, and also,

by the differentiation identity

$$\frac{d\Gamma_r(0,0)}{dr} = -\Gamma_r(0,r) \Gamma_r(r,0)$$

$$= -\Gamma_r^2(r,0)$$

since the Neumann-Liouville expansion of $\Gamma_r(t, \tau)$ makes it

clear that $\Gamma_r(t, \tau) = \Gamma_r(\tau, t)$. But now,

$$\int_t^{\infty} \frac{d\Gamma_r(0,0)}{dr} dr = \int_t^{\infty} -\Gamma_r^2(s,0) ds$$

and

$$\int_t^{\infty} \frac{d\Gamma_r(0,0)}{dr} dr = \Gamma(0) - \Gamma_t(0,0) .$$

thus,

$$\Gamma_t(0,0) - \Gamma(0) = \int_t^\infty \Gamma_s^2(s,0) ds$$

then

$$\int_0^r (\Gamma_t(0,0) - \Gamma(0)) dt = \int_0^r \int_t^\infty \Gamma_s^2(s,0) ds dt,$$

and integrating by parts, we get

$$\int_0^r (\Gamma_t(0,0) - \Gamma(0)) dt = r \int_r^\infty \Gamma_t^2(t,0) dt + \int_0^r t \Gamma_t^2(t,0) dt.$$

Exponentiating, recalling Achieser's identity and our representation for $\Gamma(0)$, we get

$$\frac{D_r(H)}{\exp \left\{ \frac{r}{2\pi} \int_{-\infty}^{\infty} \log \rho(s) ds \right\}} = \exp \left\{ r \int_t^\infty \Gamma_t^2(t,0) dt + \int_0^r t \Gamma_t^2(t,0) dt \right\}.$$

Finally, if

$$\int_{-\infty}^{\infty} |t| |H(t)| dt < \infty,$$

then the right-hand side tends to a finite limit as $r \rightarrow +\infty$.

In fact, in this case,

$$\lim_{r \rightarrow +\infty} \frac{D_r(H)}{\exp \left\{ \frac{r}{2\pi} \int_{-\infty}^{\infty} \log \rho(x) dx \right\}} = \exp \left\{ \int_0^\infty t \Gamma_t^2(t,0) dt \right\}.$$

But this is another form of the continuous analog of the refined Szegő theorem, which has the advantage that it is immediate from this form that the ratio is constant for $r \geq r_0$ if and only if $\Gamma(t, 0) = 0$ for $t \geq r_0$. If this is the case, then for $r \geq r_0$

$$\begin{aligned}\frac{\partial}{\partial r} \Gamma_r(0, t) &= -\Gamma_r(0, r) \Gamma_r(r, t) \\ &= -\Gamma_r(r, 0) \Gamma_r(r, t) = 0.\end{aligned}$$

So that for large r , $\Gamma_r(0, \tau)$ is a function $\varphi(\tau)$ of τ alone.

Hence for $r \geq r_0$, we have

$$\varphi(t) - \int_0^r H(t-s) \Gamma_r(s, 0) ds = -H(t)$$

and $\Gamma_r(s, 0) = \varphi(s)$. But for $t = 0$, we obtain

$$\varphi(0) + H(0) = \int_0^r H(0-s) \Gamma_r(s, 0) ds$$

which implies that $\Gamma_r(s, 0) = 0$ for large s (except in the trivial case $H \equiv 0$), and it follows that $\Gamma(t) = 0$ for large t .

SECTION I: In addition to the "global" theorems on the limiting distributions of the eigenvalues of Toeplitz matrices, there are theorems of a "local" nature. "Local" results have been obtained for both the continuous and discrete forms of Toeplitz operators; here we will emphasize the former setting, mentioning only one result from the matrix case, which we will need in the proof of a theorem to be presented in the next section.

Let $K(x)$, $-\infty < x < \infty$ be a positive function satisfying

$$\int_{-\infty}^{\infty} K(x) dx = 1 \quad \int_{-\infty}^{\infty} x^2 K(x) dx = \sigma^2 = 1$$

(When $\sigma^2 < +\infty$, we say that we are in the "regular" case.) Consider, as in the Introduction, a one-dimensional random walk having independent displacements $X_1, X_2, \dots$ each X having density $K(x)$. Let $S_1 = X_1$; $S = X_1 + X_2, \dots$ be the partial sums of the X_k . Then the probability P_n that, starting at ξ , barriers placed at $\pm \sqrt{n}$ are not reached (or exceeded) in n steps is given by the expression

$$P\left\{ \left| \frac{S}{\sqrt{n}} + \xi \right| < 1, \dots, \left| \frac{S_n}{\sqrt{n}} + \zeta \right| < 1 \right\}$$

which is equal to the sum

$$\sum_{j=1}^{\infty} \lambda_j^{(n)} (\sqrt{n}) \psi_j^{(\sqrt{n})} (\xi \sqrt{n}) \int_{-1}^1 \psi_j^{(\sqrt{n})} (x \sqrt{n}) dx \quad (1)$$

where $\psi_j^{(\sqrt{n})}$ is the j^{th} eigenvalue of the Hilbert - Schmidt operator

$$\int_{-n^{1/2}}^{n^{1/2}} K(x-y) \psi(y) dy$$

Define

$$F(\eta) = \int_{-\infty}^{\infty} K(x) e^{-i\eta x} dx.$$

A theorem of Erdős and the author (1946) gives a limiting value for P_n as n tends to $+\infty$.

Theorem: Let $x(\tau)$, $0 \leq \tau \leq 1$, be a Brownian motion process, and let P_n be as above; then

$$\begin{aligned} \lim_{n \rightarrow \infty} P_n &= P\{|\xi + x(\tau)| < 1: 0 \leq \tau \leq 1\} \\ &= \sum_{j=1}^{\infty} \exp\left\{-\frac{\pi^2 j^2}{8} \sigma^2\right\} \varphi_j(\xi) \int_{-1}^1 \vartheta_j(x) dx \end{aligned} \quad (2)$$

where

$$\varphi_{2k}(x) = \sin(k\pi x)$$

$$\varphi_{2k+1}(x) = \cos((k+\frac{1}{2})\pi x)$$

Note that the expression on the right hand side of (2) does not involve $K(x)$. Thus, $\lim_{n \rightarrow \infty} P_n$ exhibits an important invariance.

In fact, the theorem was proved by first showing that the limit exists and is independent of $K(x)$ and then choosing a convenient $K(x)$ to compute the limit.

It is natural to ask whether the convergence of the series

(1) to the series (2) is term by term; i.e., if

$$\lambda_j(\sqrt{n}) \rightarrow 1 - \frac{\pi^2 j^2}{8n} \sigma^2 + \dots$$

This question was answered in the affirmative by Widom¹⁾ and is the first of our "local" theorems.

As additional examples we mention two more results of Widom,²⁾³⁾

1) If $F(\xi) = o(|\xi|^{-2})$, then

$$\lambda_j(a) = 1 - \frac{\pi^2 j^2}{8a^2} (1 + c/a) a^2 + o(a^{-3})$$

where

$$c = \frac{1}{\pi} \int_{-\infty}^{\infty} \left(\frac{F'(\xi)}{F(\xi)-1} - \frac{2}{\xi} \right) \frac{d\xi}{\xi}$$

and $|c| < +\infty$

2) If $F(\xi) \sim 1 - |\xi|^{-1}$

so that, in particular, the second moment is infinite (e.g. if

$$K(x) = \frac{1}{\pi} (1+x^2)^{-1/2}),$$

then

$$\lambda_j(a) = 1 - \mu_j/a$$

where μ_j^{-1} is the j^{th} eigenvalue of the integral operator

$$\frac{1}{4} \int_{-1}^1 \log \frac{1-xy+\sqrt{(1-x^2)\sqrt{(1-y^2)}}}{1-xy-\sqrt{(1-x^2)\sqrt{(1-y^2)}}} \psi(y) dy.$$

Finally, we mention a similar result for Toeplitz matrices which will be of use in our extension of the refined Szegő theorem.

(c.f. Kac, Murdock, Szegő)

Definition: Let $f(\theta)$ be periodic with period 2π and continuous.

Let $\max f(\theta) = f(\theta_0) = M$ and let $\theta = \theta_0$ be the only value of θ (modulo 2π) for which this maximum is assumed. Moreover, suppose $f(\theta)$ has continuous second derivative $f''(\theta)$ in a certain neighborhood of θ_0 and suppose $f''(\theta) \neq 0$ (hence < 0). Then $f(\theta)$ is said to satisfy condition B' .

Theorem: Let $f(\theta)$ satisfy condition B' . Then for fixed j ,

$$\lim_{m \rightarrow \infty} m^2 (\lambda_j(m) - M) = \left(\frac{1}{2} f''(\theta_0) \right) \pi^2 j^2$$

where $\lambda_j(m)$ is the j^{th} eigenvalue of the m^{th} finite section of the Toeplitz matrix associated with $f(\theta)$. $(\lambda_1(m) \geq \lambda_2(m) \geq \dots \geq \lambda_m(m))$

Section II

In this section we are interested in certain extensions of the refined Szegő theorem. We will consider two different cases.

Let $f(\theta) = \sum_{k=-\infty}^{\infty} c_k e^{ik\theta}$ where to emphasize the probabilistic aspects of the situation we assume

$$c_k \geq 0; \quad c_k = c_{-k}; \quad \sum c_k = 1$$

We say that we are in the regular case if

$$\sum_{k=-\infty}^{\infty} k^2 c_k = \sigma^2 < +\infty.$$

We assume also that $f(\theta)$ has a unique maximum at $\theta = 0$ ($f(0)=1$) and we note that $f''(0) = -\sigma^2$.

We define as before T_n to be the n^{th} finite section of the Toeplitz matrix associated with $f(\theta)$. (i.e. $T_n = (c_{j-i})_{i,j=0}^{n-1}$); and we set

$$D_n = \det(I - T_n)$$

thus

$$D_n = D(I - \xi T_n)$$

with $\xi = 1$.

Suppose that we are in the regular case (a different situation will be treated later). Then we have

$$\begin{aligned}
\log Q_m &= \log \det(I - T_m) \\
&= \sum_{j=1}^m \log(1 - \lambda_j(m)) \\
&= \sum_{j=1}^m \left(- \sum_{n=1}^{\infty} \frac{\lambda_j^n(m)}{n} \right) \\
&= - \sum_{n=1}^{\infty} \frac{1}{n} \sum_{j=1}^m \lambda_j^n(m)
\end{aligned}$$

where $\{\lambda_j(m)\}$ are the eigenvalues of T_m arranged in non-increasing order (i.e. $\lambda_1(m) \geq \dots \geq \lambda_m(m)$).

Now, for reasons which become clear later, we split the sum on n at $m^2 \delta$ ($\delta > 0$) so that

$$\log Q_m = - \sum_{n < \delta m^2} \frac{1}{n} \sum_{j=1}^m \lambda_j^n(m) - \sum_{n \geq \delta m^2} \frac{1}{n} \sum_{j=1}^m \lambda_j^n(m) \quad (1)$$

We apply our local theorem to the second term on the right hand side in (1). We note that

$$\lambda_j(m) \sim \left| - \frac{\pi^2 j^2}{2m^2} \sigma^2 \right| \quad (2)$$

Some rather tedious computations involving the conversion of sums to integrals, Poisson summation, etc., coupled with a direct application of (2), show that

$$\begin{aligned}
\sum_{n < \delta m^2} \frac{1}{n} \sum_{j=1}^m \lambda_j^n(m) &\sim \\
\delta^{-\frac{1}{2}} \frac{\sqrt{2}}{\sqrt{\pi} \sigma} - \log \delta^{-\frac{1}{2}} - \log \frac{\sqrt{2}}{\delta} + \frac{\gamma}{2} - \log 2 + o(\delta) &\quad (3)
\end{aligned}$$

where γ is Euler's constant.

$$\gamma = \lim_{n \rightarrow \infty} \left(\sum_{k=1}^n \frac{1}{k} - \log n \right)$$

With the second term in (1) thus disposed of, we now turn our attention to the first term. We recall that for $n=1,2,\dots$

$$\sum_{\lambda} \lambda^n (m) = \frac{m}{2\pi} \int_{-\pi}^{\pi} f^n(\theta) d\theta - \sum_{\ell_1 + \ell_2 + \dots + \ell_n = 0} [R_n]_m c_{\ell_1} \dots c_{\ell_n} \quad (4)$$

where

$$R_n = \text{Max}(0, \ell_1, \dots, \ell_1 + \dots + \ell_n) - \text{Min}(0, \ell_1, \dots, \ell_1 + \dots + \ell_{n-1})$$

and $[]_m$ denotes truncation by m . In the probabilistic interpretation in terms of a random walk with independent increments $X_1, \dots, X_k, \dots$ with

$$P\{X_i = k\} = c_k,$$

we have

$$\sum_{\ell_1 + \dots + \ell_n = 0} [R_n]_m c_{\ell_1} \dots c_{\ell_n} = P\{S_n = 0\} E\{[R_n]_m | S_n = 0\}$$

where $S_k = X_1 + \dots + X_k$

Thus (4) can be written in the equivalent form

$$\sum_{j=1}^m \lambda^n (m) = \frac{m}{2\pi} \int_{-\pi}^{\pi} f^n(\theta) d\theta - P\{S_n = 0\} E\{[R_n]_m : S_n = 0\} \quad (5)$$

and we have

$$\begin{aligned}
 & - \sum_{n < \delta m^2} \frac{1}{n} \sum_{j=1}^m \lambda_j^n (m) = \\
 & - \sum_{n < \delta m^2} \frac{1}{n} \left[\frac{m}{2\pi} \int_{-\pi}^{\pi} f^n(\theta) d\theta - P\{S_n = 0\} E\{[R_n]_m | S_n = 0\} \right] \quad (6)
 \end{aligned}$$

Now, R_n is of the order of magnitude $\sqrt{n} < \sqrt{\delta} m$; hence truncation of R_n will rarely (if ever) occur, and, in fact, in the limit as $\delta \rightarrow 0$, the error resulting from ignoring the truncation will go to zero.⁴⁾ We can now apply a previously derived formula and obtain

$$\begin{aligned}
 & - \sum_{n < \delta m^2} \frac{1}{n} \sum_{j=1}^m \lambda_j^n (m) \sim \\
 & 2 \sum_{n < \delta m^2} \frac{1}{n} \cdot \frac{n}{2} \sum_{\ell=1}^{\infty} \ell \sum_{k=1}^{n-1} \frac{1}{k(n-k)} f_{n-k}(\ell) f_k(\ell) \quad (7)
 \end{aligned}$$

with an error which approaches 0 as $\delta \rightarrow 0$. The f 's are defined by the formula

$$f_j(\ell) = \frac{1}{2\pi} \int_{-\pi}^{\pi} f^j(\theta) \cos \ell \theta d\theta.$$

Let

$$u_{\ell}(\xi) = \sum_{k=1}^{\infty} \frac{\xi^k}{k} f_k(\ell)$$

That is

$$u_{\ell}(\xi) = \frac{-1}{2\pi} \int_{-\pi}^{\pi} \log(1 - \xi f(\theta)) \cos \ell \theta d\theta$$

Define a_n ($n=1,2,\dots$) by the equation

$$\sum_{l=1}^{\infty} l \lambda_l (\xi)^2 = \sum_{n=1}^{\infty} a_n \xi^n \quad (8)$$

We now find using (3) and (8) that

$$\log \mathcal{D}_m \sim \left\{ \frac{m}{2\pi} \int_{-\pi}^{\pi} \log(1-f(\theta)) d\theta + \sum_{n \leq \delta m^2} a_n + \right. \quad (9)$$

$$\left. \frac{m}{2\pi} \sum_{n \geq \delta m^2} \frac{1}{n} \int_{-\pi}^{\pi} f^n(\theta) d\theta \right\} -$$

$$\left\{ \frac{\sqrt{2}}{\sigma\sqrt{\pi}} \delta^{-\frac{1}{2}} - \log \frac{1}{\sqrt{\delta}} - \log \frac{\sqrt{2}}{\sigma} + \frac{\gamma}{2} - \log 2 \right\} + o(\delta)$$

where the first term in (9) on the right hand side corresponds to

$$\sum_{n < \delta m^2} \frac{1}{n} \sum_{j=1}^m \lambda_j^n(m)$$

and the second to

$$\sum_{n \geq \delta m^2} \frac{1}{n} \sum_{j=1}^m \lambda_j^n(m)$$

We consider now an example which will show clearly how to combine terms in (9). Let

$$f(\theta) = \cos \theta = \frac{1}{2} e^{i\theta} + \frac{1}{2} e^{-i\theta}$$

in which case $\mathcal{D}_m$ can be calculated exactly, the result being

$$\mathcal{D}_m = \left(\frac{1}{2}\right)^{m(m+1)}$$

or

$$\begin{aligned}\log \mathcal{G}_m &= -m \log 2 + \log(m+1) \\ &= -m \log 2 + \log m + o(1) + \frac{1}{m} + \frac{1}{m^2} + \dots\end{aligned}\quad (10)$$

Note that $\sigma = 1$.

Suppose $n = 2\ell$, then

$$\frac{1}{2\pi} \int_{-\pi}^{\pi} \cos^n \theta d\theta = \frac{(2\ell)!}{\ell! \ell!} \cdot \frac{1}{2^{2\ell}} \sim \pi^{-\frac{1}{2}} \ell^{-\frac{1}{2}}$$

using Stirling's formula. It follows that in (9)

$$\frac{m}{2\pi} \sum_{n \geq \delta m^2} \frac{1}{n} \int_{-\pi}^{\pi} f^n(\theta) d\theta \sim \frac{m}{2} \sum_{\ell \geq \delta m^2/2} \pi \ell^{-\frac{1}{2}} \quad (11)$$

Comparing this sum with the integral of $x^{-3/2}$ on $[\delta m^2/2, \infty)$, we find

$$\frac{m}{2\pi} \sum_{n \geq \delta m^2} \frac{1}{n} \int_{-\pi}^{\pi} f^n(\theta) d\theta \sim \frac{\sqrt{2}}{\sqrt{\pi}} \delta^{-\frac{1}{2}}$$

Now,

$$u_\ell(\xi) = \ell^{-1} \left[\frac{1 - (1 - \xi^2)^\ell}{\xi} \right]$$

Thus

$$\sum_{\ell=1}^{\infty} \ell u_\ell(\xi) = -\frac{1}{2} \log(1-\xi) - \frac{1}{2} \log(1+\xi) - \log \frac{2}{1 + \sqrt{1-\xi^2}}.$$

Hence

$$\sum_{n < \delta m^2} a_n = \frac{1}{2} \sum_{n \leq \delta m^2} n^{-1} - \frac{1}{2} \log 2 - \log 2 + o(\delta, m) \quad (12)$$

And ignoring $o(\delta, m)$ in (12) we get

$$\sum_{n < \delta m^2} a_n \sim \log \sqrt{\delta} + \log m + \frac{\gamma}{2} - \frac{3}{2} \log 2 \quad (13)$$

using the definition of γ . Inserting (11) and (13) into (9) we get

$$\log \mathcal{D}_m \sim$$

$$\frac{m}{2\pi} \int_{-\pi}^{\pi} \log (1-f(\theta)) d\theta + \frac{1}{2} \log \delta + \log m + \frac{\gamma}{2} - \frac{3}{2} \log 2 + \frac{\sqrt{2}}{\sqrt{\pi\delta}} \left\{ \frac{\sqrt{2}}{\sqrt{\pi\delta}} + \frac{1}{2} \log 2 - \frac{3}{2} \log 2 + \frac{\gamma}{2} \right\} + o(\delta)$$

Miraculously the constant term is zero, and since

$$\frac{m}{2\pi} \int_{-\pi}^{\pi} \log (1-\cos \theta) d\theta = m \log \left(\frac{1}{2}\right)$$

we get

$$\log \mathcal{D}_m \sim -m \log 2 + \log m$$

which checks with (10).

It is now clear that (9) should be rewritten in the form:

$$\begin{aligned} \log \mathcal{D}_m \sim & \frac{m}{2\pi} \int_{-\pi}^{\pi} \log (1-f(\theta)) d\theta + \left(\sum_{n < \delta m^2} a_n + \log \frac{1}{\sqrt{\delta}} \right) + \\ & \left(\frac{m}{2\pi} \sum_{n \geq \delta m^2} \frac{1}{n} \int_{-\pi}^{\pi} f^n(\theta) d\theta - \frac{\sqrt{2}}{\sigma\sqrt{\pi}} \delta^{-\frac{1}{2}} \right) + \\ & \left(\log \frac{\sqrt{2}}{\sigma} - \frac{\gamma}{2} + \log 2 \right) + o(\delta) \end{aligned}$$

and that each term in parentheses can contribute to the constant term.

We now give an alternative analysis which yields a less precise result (it fails to give the constant term in the asymptotic formula for $\log \mathcal{D}_m$) but which can be applied also to non-regular cases.

Let $\{X_i\}_{i=1}^{\infty}$ and $\{S_k\}_{k=1}^{\infty}$ have the same interpretation as before.

Then, as we have seen,

$$\log Q_m = \frac{m}{2\pi} \int_{-\pi}^{\pi} \log(1-f(\theta)) d\theta + \sum_{n=1}^{\infty} \frac{1}{n} P\{S_n = 0\} E\{[R_n]_m | S_n = 0\} \quad (14)$$

and we are, of course, interested in the asymptotic behavior of

$$\sum_{n=1}^{\infty} \frac{1}{n} P\{S_n = 0\} E\{[R_n]_m | S_n = 0\} \quad (15)$$

As before, we split the sum at δm^2 and consider the two resulting sums separately. Since

$$\sum_{n > \delta m^2} \frac{1}{n} P\{S_n = 0\} E\{[R_n]_m | S_n = 0\} < m \sum_{n > \delta m^2} \frac{1}{n} P\{S_n = 0\}$$

and since in the regular case $P\{S_n = 0\} \sim n^{-1/2}$, we see that

$$\sum_{n > \delta m^2} \frac{1}{n} P\{S_n = 0\} E\{[R_n]_m | S_n = 0\} < \frac{C}{\sqrt{\delta}} \quad (16)$$

with an appropriate constant C , independent of m .

We now turn to the sum

$$\sum_{n \leq \delta m^2} \frac{1}{n} P\{S_n = 0\} E\{[R_n]_m | S_n = 0\} \quad (17)$$

As before, we argue that truncation can be ignored for $n \leq \delta m^2$, so

that (17) is approximately

$$2 \sum_{n \leq \delta m^2} \frac{1}{n} P\{S_n = 0\} \sqrt{n} E\{\text{Max}(0, \frac{S_1}{\sqrt{n}}, \dots, \frac{S_n}{\sqrt{n}} | S_n = 0\} \quad (18)$$

where we have multiplied and divided each term by $\sqrt{n}$. Now for large n (which will "usually" be the case when m is large),

$$E\{\text{Max}(0, \frac{s_1}{\sqrt{n}}, \dots, \frac{s_n}{\sqrt{n}}) | S_n = 0\} \sim$$

$$\sigma E\{\text{Max}(0, x(\tau)) | x(1) = 0\}$$

$$0 \leq \tau \leq 1$$

where $x(\tau)$, $0 \leq \tau \leq 1$, is the Wiener process.

It is well known that

$$E\{\text{Max}(0, x(\tau)) | x(1) = 0\} = \frac{(2\pi)^{1/2}}{4}$$

$$0 \leq \tau \leq 1$$

so that (18) is asymptotic to

$$\frac{\sigma(2\pi)^{1/2}}{2} \left[\sum_{n \leq \delta m^2} n^{-1/2} P\{S_n = 0\} \right]$$

Since

$$\sum_{n \leq \delta m^2} n^{-1/2} P\{S_n = 0\}$$

can be shown to be asymptotically equal to

$$\frac{1}{\sigma\sqrt{(2\pi)}} \sum_{n \leq \delta m^2} 1/n \quad (\sim \frac{1}{(2\pi)^{1/2}} (\log \delta + 2 \log m))$$

we finally get that

$$\log Q_m \sim \frac{m}{2\pi} \int_{-\pi}^{\pi} \log(1-f(\theta)) d\theta + \log m \quad (19)$$

$$+ \{\text{terms of lower order than } \log m\}$$

We consider now a non-regular case. More specifically, we assume that $f(\theta) \sim 1 - |\theta|^2$ so that $\sigma^2 = \infty$. In this case we split the sum

(15) at m_δ , and noting that since now

$$P\{S_n=0\} \sim 1/n$$

we get (exactly as before)

$$\sum_{n \geq \delta m} \frac{1}{n} P\{S_n=0\} E\{[R_n]_m | S_n=0\} < \frac{1}{\delta} \quad (20)$$

in place of (16).

The estimation of the finite sum is now more complicated since we no longer can reduce matters to a Brownian process. We can, however, imitate the above derivation and come out with a definite result.

As before, we argue heuristically that truncation can be neglected and that we must only calculate

$$2 \sum_{n < \delta m} \frac{1}{n} P\{S_n=0\} n E\{\text{Max}(\frac{S_1}{n}, \dots, \frac{S_n}{n}) | S_n=0\} \quad (21)$$

As $n \rightarrow \infty$, we can expect that

$$\lim_{n \rightarrow \infty} E\{\text{Max}(\frac{S_1}{n}, \dots, \frac{S_n}{n}) | S_n=0\} = E\{\text{Max}(0, x(\tau)) | x(1)=0\}$$

$$0 \leq \tau \leq 1$$

where $x(\tau)$ is now the Cauchy process. To make this step rigorous we need an appropriate invariance principle and this has been provided by Skorohod. The validity of the invariance principle also allows one to calculate

$$E\{\text{Max}(0, x(\tau)) | x(1)=0\}$$

for the Cauchy process. All one needs to do is to choose a convenient sequence of X 's and this is provided by the sequence of independent X_i , each of which has the Cauchy distribution with density

$$\rho(x) = \frac{1}{\pi} \cdot \frac{1}{1+x^2}$$

so that

$$F(\xi) = \int_{-\infty}^{\infty} e^{i\xi x} \rho(x) dx = e^{-|\xi|}$$

and for small $|\xi|$

$$F(\xi) \sim 1 - |\xi|$$

corresponding to

$$f(\theta) \sim 1 - |\theta|$$

Now,

$$E\left\{\text{Max}\left(0, \frac{S_1}{n}, \dots, \frac{S_n}{n}\right) \mid \frac{S_n}{n} = 0\right\} = \frac{1}{n} \int_{-\infty}^{\infty} \frac{\int \text{Max}(0, x_1, x_1+x_2, \dots, x_1+\dots+x_{n-1}) p(x) \dots p(x_{n-1}) dx_1 \dots dx_{n-1}}{\rho^{(n)}(0)} \quad (22)$$

But for our specially chosen random variables

$$\rho^{(k)}(x) = \frac{k}{\pi} \frac{1}{k^2 + x^2}$$

so that

$$\rho^{(n)}(0) = \frac{1}{\pi n}$$

Now the right hand side of (22) can be written

$$(\pi n) \cdot \frac{1}{2} \int_0^{\infty} x \sum_{k=1}^{n-1} \frac{\frac{k}{\pi} \frac{1}{k^2 + x^2} \cdot \frac{n-k}{\pi} \frac{1}{(n-k)^2 + x^2}}{k(n-k)} dx \quad (23)$$

i.e.

$$\frac{n}{2\pi} \int_0^\infty x \sum_{k=1}^{n-1} \frac{1}{k^2 + x^2} \cdot \frac{1}{(n-k)^2 + x^2} dx$$

letting $x^2 = u$,

$$\frac{n}{2\pi} \cdot \frac{1}{2} \int_0^\infty \sum_{k=1}^{n-1} \frac{1}{k^2 + u} \cdot \frac{1}{(n-k)^2 + u} du$$

or by partial fractions

$$\frac{n}{4\pi} \int_0^\infty \sum_{k=1}^{n-1} \frac{1}{n^2 - 2kn} \left(\frac{1}{u+k^2} - \frac{1}{u+(n-k)^2} \right) du \quad (24)$$

Now some care must be taken in evaluating (24); hence, consider

$$\int_0^A \left(\frac{1}{u+k^2} - \frac{1}{u+(n-k)^2} \right) du =$$

$$\log(A+k^2) - \log k^2 - (\log(A+(n-k)^2) - \log(n-k)^2)$$

which equals

$$\log \frac{A+k^2}{A+(n-k)^2} + 2 \log \left(\frac{n-k}{k} \right)$$

and as $A \rightarrow \infty$, this goes to

$$2 \log \left(\frac{n-k}{k} \right)$$

thus (24) reduces to

$$\frac{n}{2\pi} \sum_{k=1}^{n-1} \frac{1}{n^2 - 2kn} \log \left(\frac{n}{k} - 1 \right)$$

which equals

$$\frac{1}{2\pi} \cdot \frac{1}{n} \sum_{k=1}^{n-1} \frac{1}{1-\frac{2k}{n}} \log \left(\frac{n}{k} - 1 \right) \quad (25)$$

But (25) can be considered as a Riemann sum which, for large n , closely approximates

$$\frac{1}{2\pi} \int_0^1 \frac{1}{1-2x} \log \left(\frac{1}{x} - 1 \right) dx \quad (26)$$

which equals $\pi/4$, according to the following calculations:

$$\int_0^1 \frac{1}{1-2x} \log (1/x - 1) dx = \int_{-\frac{1}{2}}^{\frac{1}{2}} \frac{1}{-2v} \log \left(\frac{1-2v}{1+2v} \right) dv$$

making the substitution $x = \frac{1}{2} + v$. Setting $2v = w$, we get

$$= \int_{-1}^1 \frac{1}{w} \log \frac{1-w}{1+w} dw$$

which equals

$$2 \int_0^1 \frac{1}{w} \log \frac{1+w}{1-w} dw \quad (27)$$

But

$$\log \frac{1+w}{1-w} = \sum_{k=0}^{\infty} \frac{2w^{2k+1}}{(2k+1)}$$

so that (27) can be written as

$$4 \int_0^1 \frac{1}{w} \sum_{k=0}^{\infty} \frac{w^{2k+1}}{2k+1} dw = 4 \left\{ \frac{1}{1^2} + \frac{1}{2^2} + \dots \right\} = 4 \frac{\pi^2}{8} = \frac{\pi^2}{2}$$

this establishes (26).

Finally,

$$P\{S_n = 0\} = \frac{1}{2\pi} \int_{-\pi}^{\pi} f^n(\theta) d\theta \sim \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-n|\theta|} d\theta = \frac{1}{\pi n}$$

and so we have that

$$\sum_{n \leq \delta m} \frac{1}{n} P\{S_n = 0\} E\{[R_n]_m | S_n = 0\} \sim 2 \cdot \frac{\pi}{4} \cdot \frac{1}{\pi} \sum_{n \leq \delta m} 1/n \quad (28)$$

$$\sim \frac{1}{2} (\log \delta + \log m) \quad (29)$$

Combining (20) and (29), we find

$$\log G_m \sim \frac{m}{2\pi} \int_{-\pi}^{\pi} \log(1-f(\theta)) d\theta + \frac{1}{2} \log m \quad (30)$$

+ { terms of order lower than $\log m$ }.

Note that the only difference between (19) and (30) is the constant which multiplies $\log m$.

Footnotes:

1. H. Widom

2. H. Widom

3. H. Widom, Trans. Am. Math. Soc., (98(3)), 1961, p.p.430-449.

4. This argument is only heuristic. A rigorous justification should not be difficult, but we are not able to supply it at the present time.

A SINGULAR RIEMANN HILBERT PROBLEM

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INTRODUCTION

Our purpose is to explore a new method for explicitly diagonalizing certain self-adjoint operators, L , in $L_2(R)$ or $L_2(R, d\omega(\cdot))$. Those operators all have an absolutely continuous spectral measure and the property that the eigenfunction equation for the generalized eigenfunction $X_\xi(\lambda)$ belonging to the spectral value ξ , $LX_\xi(\lambda) = \xi X_\xi(\lambda)$, is equivalent to a special kind of singular Hilbert barrier relation for a sectionally holomorphic function canonically related to the generalized eigenfunction.

We shall show that the geometry of the invariant subspaces of our "barrier related" operators is such that it is possible to obtain a complete orthonormal set of generalized eigenfunctions directly from the theory of the associated singular barrier problem. By this we mean first, that a complete set of generalized eigenfunctions is obtained directly without having to construct the resolvent, $(L-\ell)^{-1}$, of L in an explicit fashion, and second, the orthonormality of these generalized eigenfunctions is also obtained directly in a canonical way from the theory of the barrier relation. This latter fact is particularly useful, since there are

examples where even if a complete set of generalized eigenfunctions has been obtained by some means, the construction of an orthonormal set - or the proof that the given set is orthonormal - may be difficult because the required integrations cannot be performed explicitly and because severe singularities associated with the continuous nature of the spectrum enter decisively into the necessary calculations.

An example in which these difficulties manifest themselves is the author's theory of one dimensional singular integral operators⁽¹⁾⁽²⁾. The present work will be applied, by way of an example, to such operators and will be seen to give a much more transparent derivation of the theory previously obtained by other means.

As another example, we will derive a complete spectral theory for a class of self adjoint singular integral operators on the circle. A very special case of the theory of these operators will make it possible for us to diagonalize the much studied semi-infinite self adjoint Toeplitz matrices. These operators were first diagonalized by other means by R. S. Ismagilov⁽³⁾ and M. Rosenblum⁽⁴⁾, but our results will be seen to make the theory of Toeplitz matrices appear quite naturally and very simply in an enlarged context.

(1) ELEMENTARY GEOMETRIC STRUCTURE

Let $L = \int_{\sigma} \xi dE_{\xi}$ be a self-adjoint operator on a separable Hilbert space, H , with an absolutely continuous spectral measure. Let $H = \sum \oplus H_{k_i}$ be a minimal* direct sum decomposition of H into pairwise orthogonal invariant subspaces of L , each generated by a cyclic vector k_i . Let $\beta_i(\xi) \equiv \frac{\partial}{\partial \xi} \|E_{\xi} k_i\|^2$, and $S_i f(\xi) = [\beta_i(\xi)]^{-1} \frac{\partial}{\partial \xi} (f, E_{\xi} k_i)$ for $f \in H$.

It is easy to establish the following three theorems.

Theorem I.I

$$P_{\xi}[f, g] \equiv \frac{\partial}{\partial \xi} (f, E_{\xi} g) = \frac{1}{2\pi i} \lim_{\eta \rightarrow 0} (f, (L - \xi - i\eta)^{-1} - (L - \xi + i\eta)^{-1} g) \\ = \sum_1^{m(\xi)} S_i f(\xi) \overline{S_i g(\xi)} \beta_i(\xi), \text{ where } m(\xi) \text{ is the}$$

Von-Neumann spectral multiplicity function.

Definition

If $f(\cdot, z)$ is a vector valued analytic function for $z \in C$, a smooth arc in the complex plane with the property that finite linear combinations of the form $\sum_i a_i f(\cdot, z_i)$ are dense in the domain of a self adjoint operator A with absolutely

* in the sense of Hellinger-Hahn (11)

continuous spectrum defined on a subspace of H , we define $F_i(\xi, z) \equiv [\beta_i(\xi)]^{-1} s_i(f(\cdot, z))(\xi)$ to be the indicatrix function of A relative to the analytic generating family $f(\cdot, z)$ and the invariant subspace $\mathcal{H}_{k_i}$. (We always choose a version of $F_i(\xi, z)$ which is analytic for almost all $\xi \in \sigma(A)$ when $z \notin C$).

Let $\mathcal{H}^*$ be the Hilbert space whose elements are generated from (the equivalence classes of) those functions $g(\xi, z)$ that can be represented as finite linear combinations of the form $g(\xi, z) = \sum \alpha_j(\xi) G_j(\xi, z)$, where $G_j(\xi, z) = [\beta_j(\xi)]^{-1/2} F_j(\xi, z)$, and each $\alpha_j(\xi)$ is measurable with $\int_{\sigma} |\alpha_j(\xi)|^2 d\xi < \infty$, by imposing the scalar product $(g, g')_{\mathcal{H}^*} = \int \sum \alpha_j(\xi) \overline{\alpha_j'(\xi)} d\xi$.

Let $\mathcal{H}_{\xi}$ be the Hilbert space formed from finite linear combinations of the form $a(\xi, x) = \sum \alpha_k P_{\xi}(x, y_k)$ where α_k and y_k (with $\text{Im } y_k \neq 0$) are arbitrary, by imposing the scalar product $(a, a')_{\mathcal{H}_{\xi}} = \sum_{i,k} \alpha_i \overline{\alpha_k'} P_{\xi}(x_i, y_k)$, where $P_{\xi}(x, y) = P_{\xi}[f(\cdot, x), f(\cdot, y)]$.

Theorem 1.2

Let $f \in \mathcal{H}$, define $f(\xi, z) \in \mathcal{H}^*$ by setting $f(\xi, z) = \sum_j s_j f(\xi) F_j(\xi, z)$. Then the correspondence $f(\xi, z) \leftrightarrow f$ furnishes an isometric isomorphism between $\mathcal{H}^*$ and $\mathcal{H}$; moreover, $\mathcal{H}^*$ furnishes a spectral representation for L in the sense that $f(\xi, z) \leftrightarrow f$

implies $\xi f(\xi, z) \leftrightarrow Lf$, and $\mathcal{H}^*$ is the direct integral of the $\mathcal{H}_\xi$ with respect to Lebesgue measure so that the spectral multiplicity $m(\xi)$ of L is equal to the dimension of $\mathcal{H}_\xi$.

Theorem 1.3

A necessary and sufficient condition that L have an absolutely continuous spectrum is $\int_{\sigma} P_\xi[f, g] d\xi = (f, g)_{\mathcal{H}} \quad \forall f, g \in \mathcal{H}$.

The preceding theorems reduce the task of diagonalizing L to that of constructing a bilinear "splitting kernel" $P_\xi(x, y)$ for L .

The aim of the discussion that follows is to demonstrate that there are important cases in which such a splitting kernel can be simply identified.

For the applications which we will make here it will suffice for us to restrict our attention to two special cases; namely the case that our basic set C is a measurable set of the real line, and the case that C is a measurable set on the unit circle.

We will carry out theory through under two hypothesis.

(2) THE ANALYTIC RELATIONS

Hypothesis 1 [For the case that C lies in R]

There exists an analytic generating family $f(\cdot, z)$ for L , self adjoint, defined on $L_2(C)$, relative to which the indicatrix functions $F_i(\xi, z)$ are sectionally holomorphic with, for each $\xi \in \sigma(L)$, boundary values, $F_i(\xi, \lambda \pm i0)$, finite almost everywhere and satisfying, for each $\xi \in \sigma(L)$ and for almost all $\lambda \in C$.

$$(*) \quad F_i(\xi, \lambda + i0) = \left(1 + \int_{\sigma(L)} \frac{dM_\lambda(v)}{v - \xi - i0} \right) F_i(\xi, \lambda - i0)$$

where $dM_\lambda(v)$ is a positive purely singular measure of finite total mass such that $\int_{\Delta} dM_\lambda(v)$ is an integrable function of λ for each Borel set Δ of the real line.

lemma 2.1 To each positive purely singular measure $dM_\lambda(v)$ on R such that $\int_{\Delta} dM_\lambda(v)$ is integrable in λ for each Borel set Δ , there corresponds a set in $R \times C$ with characteristic function $g(v, \lambda)$ such that $\int g(v, \lambda) dv$ is integrable, and such that $1 + \int \frac{dM_\lambda(v)}{v - \lambda} = \exp \int g(v, \lambda) \frac{dv}{v - \lambda}$. (5) Conversely, any such $g(v, \lambda)$ gives rise to such a measure, $dM_\lambda(v)$.

Thus, there exists a measure with the above properties, $dR_v(\lambda)$, such that

$$\theta(v, z) \equiv \exp \int g(v, \lambda) \frac{d\lambda}{\lambda - z} = 1 + \int \frac{dR_v(\lambda)}{\lambda - z},$$

and we can verify that the following assertion holds:

lemma 2.2

$$\frac{1}{1 - \theta(v, z)} = A(v)z + \int \frac{dR_v(\lambda)}{\lambda - z}$$

where $A(v) \geq 0$, and $dR_v(\lambda)$ is a measure of the type above,

i.e. positive, purely singular*, and of finite total mass.

Let $P_{\xi}^{(j)}(\lambda)$ be a complete orthonormal set in $L_2(C; dR_{\xi}(\cdot))$.

Set $F(\xi, z) = E(\xi + i0, z) - E(\xi - i0, z)$, where

$$E(\ell, z) = \exp \frac{1}{2\pi i} \iint g(v, \mu) \frac{dv}{v - \ell} \frac{d\mu}{\mu - z}. \quad \text{Then define}$$

$$F_1(\xi, z) = F(\xi, z) \sqrt{A(\xi)}$$

$$F_j(\xi, z) = F(\xi, z) \int \frac{P_{\xi}^{(j)}(\mu)}{\mu - z} dR_{\xi}(\mu), \quad 1 < j \leq m(\xi)$$

where $m(\xi) = n$ if $\{\lambda \mid g(\xi, \lambda) = 1\}$ is the union of n disjoint intervals, and otherwise $m(\xi)$ is infinite.

* This fact follows immediately from well known results, but it can also be demonstrated directly from the Plemelj relations.

Theorem 2.1

The functions $F_j(\xi, z)$ are solutions of (*); furthermore the dimension of $L_2(C; dR_\xi(\cdot))$ is $m(\xi) - 1$. This result follows very simply from the fact (used twice) that

$$\int_{-\infty}^{\infty} \frac{d\tilde{M}(\tau)}{\tau - t - i0} = \int_{-\infty}^{\infty} \frac{d\tilde{M}(\tau)}{\tau - t + i0}, \text{ whenever these limits exist, for purely singular measures } d\tilde{M}(\cdot).$$

$$\text{Thus, let } G(\ell, \lambda) = 1 + \int \frac{dM_\lambda(\nu)}{\nu - \ell},$$

then $E(\ell, \lambda + i0) = G(\ell, \lambda) E(\ell, \lambda - i0)$. Set $\ell = \xi \pm i\eta$, and subtract the resulting two equations to obtain $F(\xi, \lambda + i0) = G(\xi, \lambda) F(\xi, \lambda - i0)$. Multiplication and the equality of the singular limits proves the rest.

The assertion about the dimension of $L_2(C, dR_\xi(\cdot))$ is also not very difficult to verify. The essential observation is that when the set of λ 's for which $g(\xi, \lambda) = 1$ is a union of n -disjoint intervals, the singular measure $dR_\xi(\cdot)$ consists simply of $n-1$ point masses. Thus the orthonormal family $\{P_\xi^j(\cdot)\}$ consists of functions vanishing on all but the j th point where the measure is concentrated.

In an exactly similar way we can treat the case that C is a measurable subset of the unit circle. We again have (by hypothesis) that the indicatrix functions of L , defined on $L_2(C)$, satisfy a singular barrier relation

$$(**) \quad F_i^+ (\xi, \tau) = \left(1 + \int \frac{d M_\tau(v)}{v - \xi - i0} \right) F_i^- (\xi, \tau) , \quad \tau \in C$$

where the $\pm \tau$ limits are taken along the interior and exterior normals to C respectively, and again $d M_\tau(v)$ is a positive purely singular measure.

In the case that $C \subset R$, we constructed all of the solutions of (*) from the barrier relation obtained by analytically continuing (*) in the spectral variable, taking $E(\ell, z)$ so that

$$E(\ell, \lambda + i0) = \left(1 + \int \frac{d M_\lambda(v)}{v - \ell} \right) E(\ell, \lambda - i0)$$

when $\text{Im } \ell \neq 0$.

For the case that C lies on the unit circle we again work with a solution of the analytically continued barrier problem (**). But it is convenient to choose another normalization. Thus we consider

$$A(\ell, z) = E(\ell, z) \left(e^{-\frac{1}{4\pi i} \int_{-\infty}^{\infty} \int_C g(v, \tau) \frac{dv}{v - \ell} \frac{d\tau}{\tau}} \right)$$

(where $g(v, \tau)$ is now the characteristic function of a set in $R \times C$).

The salient feature is contained in the easily verified

lemma 2.3

$$\overline{E(\ell, z)} = \frac{1}{E(\bar{\ell}, \bar{z})}$$

$$[A(\bar{\ell}, \bar{z})]^{-1} = \overline{A(\ell, \frac{1}{z})}.$$

lemma 2.4

$$\text{Let } \varphi(\xi, y) = i \exp \int_{-\pi}^{\pi} g(\xi, e^{i\theta}) \frac{e^{i\theta+y}}{e^{i\theta-y}} d\theta.$$

for $|y| < 1$.

Then there exists a one-parameter family of positive singular measures, $d\sigma_{\xi}(\cdot)$, of finite total mass, and a real function $\beta(\xi)$ such that

$$\varphi(\xi, y) = i\beta(\xi) + \int_{-\pi}^{\pi} \frac{e^{i\theta+y}}{e^{i\theta-y}} d\sigma_{\xi}(\theta)$$

Let $F(\xi, z) = A(\xi+io, z) - A(\xi-io, z)$ and let $P_{\xi}^{(j)}$ now denote a complete orthonormal set in $L_2(C, d\sigma_{\xi}(\cdot))$.

Define $F_j(\xi, z) = A(\xi, z) \int \frac{P_{\xi}^{(j)}(\theta)}{1-z e^{-i\theta}} d\sigma_{\xi}(\theta)$. $1 \leq j \leq m(\xi)$.

Where $m(\xi) = \dim[L_2(C, d\sigma_{\xi}(\cdot))]$.

Theorem 2.2

The functions $F_j(\xi, z)$ are solutions of (**); furthermore $m(\xi) = n$ when $\{e^{i\theta} \mid g(\xi, e^{i\theta}) = 1\}$ is a union of n disjoint intervals - otherwise $m(\xi) = \infty$.

Let us call the solutions to (*) and (**) constructed in the preceding paragraphs the distinguished solutions.

We will develop our spectral theory under an additional hypothesis - which we state separately for the circle and for the line.

Hypothesis 2R

Each distinguished solution of (*) is related to a generalized eigenfunction, $X_j(\xi, \lambda)$, of L through

$$F_j(\xi, z) = \frac{1}{2\pi i} \int_C \frac{k(\mu)}{\mu - z} \overline{X_j(\xi, \mu)} d\mu, \quad \text{Im } z \neq 0,$$

where $\int_{\sigma(L)} g(v, \mu) dv = |k(\mu)|^2$, $\mu \in C$.

Hypothesis 2C

Each distinguished solution of (**) is related to a generalized eigenfunction, $X_j(\xi, \tau)$, of L through

$$F_j(\xi, z) = \frac{1}{2\pi} \int_C \frac{k(e^{i\theta})}{1 - ze^{-i\theta}} \overline{X_j(\xi, e^{i\theta})} d\theta$$

where $\int_{\sigma(L)} g(v, \tau) dv = |k(\tau)|^2$, $\tau \in C$.

(3)

We will state the main theorem first for the case that $C \subset \mathbb{R}$.

Main Theorem (3.1)(R)

Under the hypothesis (1) and (2) we have

$$P_{\xi} \left[\frac{k(\mu)}{\mu-x}, \frac{k(\mu)}{\mu-y} \right] = \frac{1}{2} \frac{1}{x-y} \left(\frac{E(\xi+io, x)}{E(\xi+io, y)} - \frac{E(\xi-io, x)}{E(\xi-io, y)} \right)$$

$$= \sum_1^{m(\xi)} F_j(\xi, x) \overline{F_j(\xi, y)}.$$

Proof

Let the operator T_j be defined on the manifold of finite linear combinations of the form $\bar{X}(\mu) = \sum_P \frac{a_P k(\mu)}{\mu-x_P}$ by setting $T_j \bar{X} = \sum_P a_P F_j(\xi, x_P)$.

Lemma 3.1

T_j has a unique bounded extension defined on all of $L_2(k)$ whose range is in $L_2(\sigma)$, call this extension $\hat{T}_j$.

Proof

$$\text{Let } Q(\xi; x, y) = \frac{1}{2} \frac{1}{x-y} \left(\frac{E(\xi+io, x)}{E(\xi+io, y)} - \frac{E(\xi-io, x)}{E(\xi-io, y)} \right).$$

$$F(\xi, z) = E(\xi + i0, z) - E(\xi - i0, z), \quad \text{thus}$$

$$\begin{aligned} F(\xi, z) &= \exp \frac{1}{2\pi i} \oint \int g(v, \mu) \frac{d\mu}{\mu - z} \frac{dv}{v - \xi} \left(\exp \frac{1}{2} \int g(\xi, \mu) \frac{d\mu}{\mu - z} - \exp \frac{1}{2} \int g(\xi, \mu) \frac{d\mu}{\mu - z} \right) \\ &= E^+(\xi, z) \left(1 - \exp - \int g(\xi, \mu) \frac{d\mu}{\mu - z} \right) \end{aligned}$$

But, by lemma 2.1, there exists a positive purely singular measure $dR_\xi(\mu)$ of finite total mass such that

$$1 - \exp - \int g(\xi, \mu) \frac{d\xi}{\xi - z} = \int \frac{d\sigma_\xi(\mu)}{\mu - z}$$

Thus, noting that $\overline{E(\ell, z)} = E(\bar{\ell}, \bar{z})^{-1}$, we have

$$\begin{aligned} Q(\xi; x, y) &= \frac{1}{2} \frac{1}{x-y} \frac{F(\xi, x) \overline{F(\xi, y)}}{\int \frac{d\sigma_\xi(\mu)}{\mu - x} \int \frac{d\sigma_\xi(\mu)}{\mu - \bar{x}}} \left[\left(1 - \int \frac{d\sigma_\xi(\mu)}{\mu - x} \right) - \overline{\left(1 - \int \frac{d\sigma_\xi(\mu)}{\mu - \bar{y}} \right)} \right] \\ &= \frac{1}{2} \frac{1}{x-y} F(\xi, x) \overline{F(\xi, y)} \left[\frac{1}{\int \frac{d\sigma_\xi(\mu)}{\mu - x}} - \frac{1}{\int \frac{d\sigma_\xi(\mu)}{\mu - y}} \right] \end{aligned}$$

But, the function $\frac{1}{\int \frac{d\sigma_{\xi}(\mu)}{\mu-x}}$, has

positive imaginary part in the upper half plane, and we can assert by known theorems⁽¹¹⁾ that there exists a positive purely singular measure $d\sigma_{\xi}(\mu)$ of finite total mass and a positive function $A(\xi)$ such that

$$\frac{1}{\int \frac{d\sigma_{\xi}(\mu)}{\mu-x}} = A(\xi)x + \int \frac{dR_{\xi}(\mu)}{\mu-x}$$

Thus, by the Parseval relation

$$Q(\xi; x, y) = F(\xi, x) \overline{F(\xi, y)} \left(A(\xi) + \int \frac{dR_{\xi}(\mu)}{(\mu-x)(\mu-\bar{y})} \right)$$

$$= \sum_1^{m(\xi)} F_j(\xi, x) \overline{F_j(\xi, y)}$$

$$\text{Thus } Q(\xi; x, \bar{y}) = \sum_1^{m(\xi)} \hat{T}_j \left(\frac{k(\mu)}{\mu-x} \right) (\xi) \overline{\hat{T}_j \left(\frac{k(\mu)}{\mu-\bar{y}} \right) (\xi)}$$

lemma 3.2

$$\int_{\sigma} Q(\xi; x, y) d\xi = \int_{-\infty}^{\infty} \frac{|k(\mu)|^2}{(\mu-x)(\mu-\bar{y})} d\mu$$

We simply rewrite the integral in the form $\int_0 \frac{E(\ell, x)}{E(\ell, y)} d\ell$

where 0 is a smooth contour that encircles the spectrum of L, and evaluate the integral by extracting residues at infinity.

It follows immediately that

$$\left\| \hat{T}_j \left(\sum \frac{a_p k(\mu)}{\mu - x_p} \right) \right\|_{L_2(\sigma(L))}^2 \leq \int_{-\infty}^{\infty} \left| \sum \frac{a_p}{\mu - x_p} \right|^2 |k(\mu)|^2 d\mu$$

and thus, using the fact that finite sums of our form $\sum \frac{a_p k(\mu)}{\mu - x_p}$ are dense in $L_2(R)$, lemma 3.1 is established.

We have actually established somewhat more; namely,

lemma 3.3

$$\int_{\sigma} \sum_1^{m(\xi)} \hat{T}_j f(\xi) \overline{\hat{T}_j g(\xi)} d\xi = (f, g)_H$$

for arbitrary $f, g \in H$.

Let us therefore consider the following expression

$$\begin{aligned} & \left((L-\ell)^{-1} \frac{k(\mu)}{\mu-x}, (L-\ell)^{-1} \frac{k(\mu)}{\mu-y} \right) \\ &= \int \sum_1^{m(\xi)} \hat{T}_j \left((L-\ell)^{-1} \frac{k(\mu)}{\mu-x} \right) (\xi) \overline{\hat{T}_j \left((L-\ell)^{-1} \frac{k(\mu)}{\mu-y} \right) (\xi)} d\xi \end{aligned}$$

Now use the fact that $(l-\bar{l})(L-l)^{-1}(L-\bar{l})^{-1} = (L-l)^{-1} - (L-\bar{l})^{-1}$, together with hypothesis 2R which implies that

$$\hat{T}_j (L-l)^{-1} \frac{k(\mu)}{\mu-x} (\xi) = (\xi-l)^{-1} \hat{T}_j \frac{k(\mu)}{\mu-x} (\xi),$$

and set $l = \xi + i\eta$. The Plemelj formulae enable us to extract the limit - and conclude the proof.

The Case That C is a measurable subset of the Unit Circle

In analogy to the bilinear function formed before we now

$$\text{let } q(\xi; x, y) = i \left(\frac{A(\xi + i0, x)}{A(\xi + i0, y)} - \frac{A(\xi - i0, x)}{A(\xi - i0, y)} \right)$$

If we set

$$\theta(\xi, y) = i \exp \int_{-\pi}^{\pi} g(\xi, e^{i\theta}) \frac{e^{i\theta+y}}{e^{i\theta-y}} d\theta$$

we can show that $\theta(\xi, y)$ has a non-negative real part in $|y| < 1$; using the fact that $g(\xi, e^{i\theta})$ is a characteristic function of a set in $R \times C$, we can assert that there exists a one-parameter family of positive singular measures, $d\sigma_{\xi}(\cdot)$ of finite total mass and a real function $\beta(\xi)$ such that

$$\theta(\xi, y) = i\beta(\xi) + \int_{-\pi}^{\pi} \frac{e^{i\theta+y}}{e^{i\theta-y}} d\sigma_{\xi}(\theta)$$

Thus,

$$q(\xi; x, y) = \frac{A(\xi + i0, x)}{A(\xi - i0, x)} \int_{-\pi}^{\pi} \frac{e^{i\theta} + y}{e^{i\theta} - y} - \frac{e^{i\theta} + x}{e^{i\theta} - x} d\sigma_{\xi}(\theta)$$

or, equivalently,

$$\frac{1}{1-x\bar{w}} q(\xi, x, \frac{1}{\bar{w}}) = A(\xi + i0, x) \overline{A(\xi + i0, w)} \int_{-\pi}^{\pi} \frac{2d\sigma_{\xi}(\theta)}{(1-xe^{-i\theta})(1-\bar{w}e^{i\theta})}$$

If we take $P_{\xi}^{(j)}(\theta)$ to be a complete orthonormal set in $L_2(-\pi, \pi; d\sigma_{\xi}(\theta))$ we can use the Parseval relation to write

$$\frac{1}{1-x\bar{w}} q(\xi, x, \frac{1}{\bar{w}}) = 2 A(\xi + i0, x) \overline{A(\xi + i0, y)}$$

$$\sum_{j=1}^{m(\xi)} \int_{-\pi}^{\pi} \frac{P_{\xi}^{(j)}(\theta)}{1-xe^{-i\theta}} d\sigma_{\xi}(\theta) \overline{\int_{-\pi}^{\pi} \frac{P_{\xi}^{(j)}(\theta)}{1-\bar{w}e^{-i\theta}} d\sigma_{\xi}(\theta)}$$

where $m(\xi) = n$ if $\{\tau \mid g(\xi, \tau) = 1\}$ is a union of n disjoint arcs and is infinite otherwise.

But, we can evaluate

$$\frac{1}{2} \int_{\sigma} \frac{1}{1-x\bar{w}} q(\xi, x, \frac{1}{\bar{w}}) d\xi \text{ by residues in an}$$

exactly analogous way to the corresponding calculation of the previous section, and we obtain

$$\frac{1}{2} \int_{\sigma} \frac{1}{1-x\bar{w}} q(\xi; x, \frac{1}{w}) d\xi = \int_C \frac{|k(e^{i\theta})|^2}{(1-xe^{-i\theta})(1-\bar{w}e^{-i\theta})} d\theta$$

Thus, in the same way as before - we can assert:

Main Theorem (for the circle)

$$P_{\xi} \left[\frac{1}{1-xe^{-i\theta}}, \frac{1}{1-we^{-i\theta}} \right]_{L_2(C)} = \frac{1}{2} \frac{1}{1-x\bar{w}} q(\xi; x, \frac{1}{w})$$

(4) APPLICATIONS

Singular Integral Operators on the line.

C is assumed now to be a measurable subset of the real line.

Let $D(\lambda)$ be a real, essentially bounded, measurable function and let $k(\lambda) \in L_2(C)$. We define L on $L_2(C)$ by setting

$$Lx(\lambda) = D(\lambda)x(\lambda) + \frac{1}{\pi i} \oint_C \frac{\overline{k(\lambda)}k(\mu)}{\mu - \lambda} x(\mu) d\mu.$$

Throughout the sequel we always consider that we have made the obvious reduction so the case that $k(\lambda) \neq 0$ a.e.

Theorem 4.1

L satisfies hypothesis 1-R and hypothesis 2-R.

We will sketch an explanation of why this is so. Suppose that $x(\xi, \lambda)$ is a distribution eigenfunction of L , so that $Lx(\xi, \lambda) = \xi x(\xi, \lambda)$. Set $\phi(\xi, z) = \frac{1}{2\pi i} \int_C \frac{k(\mu)}{\mu - z} x(\xi, \mu) d\mu$.

It is not difficult to generalize the well known Plemelj formulae in such a way that we can show that $\phi(\xi, z)$ necessarily satisfies

$$\phi(\xi, \lambda + i0) = \frac{D(\lambda) - \xi - |k(\lambda)|^2}{D(\lambda) - \xi + |k(\lambda)|^2} \phi(\xi, \lambda - i0), \quad \lambda \in C, \text{ a.a. } \xi \in \sigma(L)$$

It follows that $\left\{ \frac{k(\mu)}{\mu-z} \right\}$ is an analytic generating family relative to which the indicatrix functions of L satisfy a barrier relation of our singular type. Explicitly

$$g(v, \mu) = \frac{1}{\pi} \arg \frac{D(\mu) - v - i0 - |k(\mu)|^2}{D(\mu) - v - i0 + |k(\mu)|^2}$$

The second part of hypothesis 2 is verified most easily by writing

$$E(\ell, z) = \exp \frac{1}{2\pi i} \int_{\sigma(L)} \int_C g(v, \mu) \frac{dv}{v-\ell} \frac{d\mu}{\mu-z} = \exp \frac{1}{2\pi i} \int_C \log \frac{D(\mu) - \ell - |k(\mu)|^2}{D(\mu) - \ell + |k(\mu)|^2} \frac{d\mu}{\mu-z}$$

and evaluating the contour integral $\int_0 E(\ell, z) d\ell$ and then setting $z = \lambda \pm i\eta$ - using the Plemelj formulae, where O is a smooth contour encircling the spectrum of L .

Now let us sketch the justification of the first part of hypothesis 2. It suffices to show that

$$\hat{T}_j L f = \xi \hat{T}_j f, \quad \forall f \in L_2(C).$$

$$F_j(\xi, z) = \hat{T}_j \left[\frac{k(\mu)}{\mu-z} \right], \text{ and the } L_2 \text{ version of the}$$

Plemelj formulae gives us

$$\lim_{\eta \downarrow 0} \frac{1}{2\pi i} \int_C f(\lambda) \hat{T}_j \left[\frac{k(\mu)}{\mu-\lambda+i\eta} - \frac{k(\mu)}{\mu-\lambda-i\eta} \right] d\lambda = \hat{T}_j [\overline{k(\cdot)} f(\cdot)]$$

$$\lim_{\eta \downarrow 0} \frac{1}{2\pi i} \int_C f(\lambda) \hat{T}_j \left[\frac{k(\mu)}{\mu - \lambda + i\eta} + \frac{k(\mu)}{\mu - \lambda - i\eta} \right] d\lambda = \hat{T}_j [\bar{k}(\cdot) H f(\cdot)]$$

$$\text{where } H[f(\cdot)] = \frac{1}{\pi i} \int_C \frac{f(\mu)}{\mu - \lambda} d\mu,$$

$$\text{but } \frac{D(\lambda) - \xi}{\bar{k}(\lambda)} [F_j(\xi, \lambda + i0) - F_j(\xi, \lambda - i0)]$$

$$+ k(\lambda) [\overline{F_j(\xi, \lambda + i0)} - \overline{F_j(\xi, \lambda - i0)}] = 0$$

Thus

$$\int_C d\lambda f(\lambda) \left(\frac{D(\lambda) - \xi}{\bar{k}(\lambda)} [F_j(\xi, \lambda + i0) - F_j(\xi, \lambda - i0)] + k(\lambda) [\overline{F_j(\xi, \lambda + i0)} - \overline{F_j(\xi, \lambda - i0)}] \right) = 0$$

$$\text{or } \hat{T}_j [(D(\cdot) - \xi)f(\cdot) + \bar{k}(\cdot)H k f(\cdot)] = 0,$$

$$\text{i.e. } \hat{T}_j L f = \xi \hat{T}_j f$$

By theorem (3.1) it is easy to see that the preceding construction gives the absolutely continuous part of L when C is properly included in $(-\infty, \infty)$, and in this case the whole spectrum of L is absolutely continuous.

If $C = (-\infty, \infty)$, however there may be - in addition to this absolutely continuous component - two infinitely degenerate eigenmanifolds. We will content ourselves with an informal description of the situation - which seems to involve no new ideas.

If $D(\lambda) - |k(\lambda)|^2 = \xi^-$, a constant, then (by *) $\Phi(\xi^-, \lambda + i0) = 0$. However we can show that if $y(\xi^-, \mu) \in L_2(C)$, then $\Phi(\xi, z) = \frac{1}{2\pi i} \int_C \frac{k(\mu)}{\mu - z} y(\xi^-, \mu) d\mu = 0$, $\text{Im } z \geq 0$, i.e. $y(\xi^-, \mu) = 0$. This result follows because the limit from above can be written

$$\frac{1}{2} k(\lambda) y(\xi^-, \lambda) + \frac{1}{2\pi i} \oint \frac{k(\mu) y(\xi^-, \mu)}{\mu - \lambda} d\mu = 0,$$

or $\frac{1}{2} (I + H)k y = 0$, where $H x(\lambda) \equiv \frac{1}{\pi i} \int_C \frac{x(\mu)}{\mu - \lambda} d\mu$. The

foregoing analysis can be used to show that H has a continuous spectrum $[-1, 1]$ unless $C = (-\infty, \infty)$, in which case the points $-1, 1$ are infinitely degenerate eigenvalues. Thus $k y = 0$, and so, $y = 0$ - if we assume, for simplicity that $k L_2 \subset L_2$ - which we now do.

The analogous conclusion follows if $D(\lambda) + |k(\lambda)|^2 = \xi^+$.
 However, when $C = (-\infty, \infty)$ it is possible for the operator
 to annihilate a linear subspace of $L_2(-\infty, \infty)$.

The eigenmanifolds corresponding to ξ^- and ξ^+
 will simply be all functions $y(\mu) \in L_2(-\infty, \infty)$ such that

$$\xi^\pm(\lambda) = \pm \frac{1}{2} k(\lambda) y(\lambda) + \frac{1}{2\pi i} \oint \frac{k(\mu) y(\mu)}{\mu - \lambda} d\mu = 0.$$

When both $D(\lambda) - |k(\lambda)|^2 = \text{constant}$ and $D(\lambda) + |k(\lambda)|^2 = \text{constant}$
 are satisfied, then $D(\lambda)$ and $|k(\lambda)|^2$ are constant, and the
 analysis reduces to the known case of the Hilbert transform.
 Thus, in this case there will be two infinitely degenerate
 eigenmanifolds corresponding to the eigenvalues ξ^+ and ξ^- . *

* These considerations will be taken up again in the
 final section of these notes, which is devoted to Wiener-
 Hopf operators.

Singular Integral Operators on the Circle

We will construct below a complete spectral theory of singular integral operators on the circle. C is assumed now to be some measurable subset of the unit circle, $D(\tau)$ is a real valued, essentially bounded function defined on C , and $k(\tau) \in L_2(C)$. ($k(\tau) \neq 0$ a.e. on C)

Let

$$L x(t) = D(t)x(t) + \frac{1}{\pi i} \oint_C \frac{\overline{k(t)}k(\tau)}{t-\tau} x(\tau) d\tau,$$

L is a self-adjoint operator on $L_2(C)$, and we can proceed exactly as we did for the case of operators on the real line.

$$\text{Thus, let } H(\xi, z) = \frac{1}{2\pi i} \int_C \frac{k(\tau)}{\tau - z} x(\xi, \tau) d\tau$$

$$= \frac{1}{2\pi} \int_C \frac{k(e^{i\theta})}{1 - ze^{-i\theta}} x(\xi, e^{i\theta}) d\theta$$

where $x(\xi, t)$ is a generalized eigenfunction of L so that

$$L x(\xi, t) = \xi x(\xi, t).$$

Then, just as in the previous case,

$$H^+(\xi, \tau) = \frac{D(\tau) - \xi - |k(\tau)|^2}{D(\tau) - \xi + |k(\tau)|^2} H^-(\xi, \tau)$$

Thus the indicatrix functions belonging to L relative to the analytic generating family $\frac{k(e^{i\theta})}{1-ze^{-i\theta}}$ all satisfy a singular

barrier relation of the type (**).

$$\text{Let } g(v, \tau) = \frac{1}{\pi} \arg \frac{D(\tau) - \xi - i0 - |k(\tau)|^2}{D(\tau) - \xi - i0 + |k(\tau)|^2}$$

and let

$$A(l, z) = \exp \left(\frac{1}{2\pi i} \int_{-\infty}^{\infty} \int_C g(v, \tau) \frac{dv}{v-l} \frac{d\tau}{\tau-z} \right) \exp \left(-\frac{1}{4\pi i} \int_{-\infty}^{\infty} \int_C g(v, \tau) \frac{dv}{v-l} \frac{d\tau}{\tau} \right)$$

The results and method of the preceding sections can be taken over now almost literally to show that the two hypothesis of the main theorem are satisfied, and we can therefore use the main theorem in its circular form to assert that

$$P_{\xi} \left[\frac{1}{1-xe^{-i\theta}}, \frac{1}{1-ye^{-i\theta}} \right] \\ = 2 A(\xi+i0, x) A(\xi-i0, y) \sum_{j=1}^{m(\xi)} \int_{-\pi}^{\pi} \frac{P_{\xi}^j(\theta)}{1-xe^{-i\theta}} d\sigma_{\xi}(\theta) \int \frac{P_{\xi}^j(\theta)}{1-xe^{-i\theta}} d\sigma_{\xi}(\theta)$$

so that a complete set of orthonormalized generalized eigenfunctions, for which inversion formulae of the Fourier type hold, are given by

$$x_j(\xi, \tau) = \frac{1}{2\pi i} \frac{1}{k(\tau)} \left[A(\xi + i0, \tau^+) \int \frac{P_\xi^j(\theta)}{1 - \tau^+ e^{-i\theta}} d\sigma_\xi(\theta) - A(\xi - i0, \tau^-) \int \frac{P_\xi^j(\theta)}{1 - \tau^- e^{-i\theta}} d\sigma_\xi(\theta) \right]$$

More explicitly, if we define $\mathcal{S} x(\tau) = \{g_1(\xi), \dots, g_m(\xi)(\xi)\}$

by setting $g_j(\xi) = \int x(e^{i\theta}) \overline{x_j(\xi, e^{i\theta})} d\theta$, so that

$\mathcal{S} : L_2(C) \rightarrow \mathbb{H}^*$ and $\mathcal{J} : \mathbb{H}^* \rightarrow L_2(C)$, by setting

$$\mathcal{J} g(\tau) = \int_{\sigma(L)} \sum_{l=1}^{m(\xi)} g_l(\xi) x_l(\xi, \tau) d\xi. \quad \text{Then the theorems}$$

we have demonstrated show that $\mathcal{S}\mathcal{J} = 1$, and $\mathcal{J}\mathcal{S} = 1$, and

$$\int_{\sigma} \sum_{l=1}^{m(\xi)} |g_l(\xi)|^2 d\xi = \int_C |x(e^{i\theta})|^2 d\theta.$$

Eigenmanifolds

The construction we have just carried through gives the absolutely continuous part of L whenever C is a measurable subset of the unit circle. However, just as in the case of the line there is the possibility of one or two infinitely degenerate eigenmanifold corresponding to the case that $D(\tau) = |k(\tau)|^2$ and, or, $D(\tau) + |k(\tau)|^2$ are constant almost everywhere on C in the case that C is the whole circle. The reasoning and results are exactly as in the case of the line.

TOEPLITZ FORMS

The semi-infinite Toeplitz forms have been the subject of many investigations. They are also considered in Marvin Rosenblum's lectures.

The first proof that these Toeplitz matrices have always got an absolutely continuous spectrum is due to Marvin Rosenblum⁽⁸⁾. The first calculation of the unitary invariants of these matrices is contained in a Doklady note of Ismagilov⁽²⁾. Rosenblum then achieved an explicit diagonalization using results due to Krein and Widom about the resolvents of Toeplitz matrices.⁽³⁾

The Toeplitz operator has the form⁽⁹⁾ $Tf = P k f$, where P is the orthogonal projector from $L_2(-\pi, \pi)$ to the Hardy space H^2 , and where $k(e^{i\theta})$ is positive and integrable on $(-\pi, \pi)$.

If $f \in H^2$, then $kf \in L_2$ and, in the sense of mean convergence,

$$k(e^{i\theta}) f(e^{i\theta}) = \sum_{n=-\infty}^{\infty} a_n e^{in\theta} \quad \text{where} \quad \sum_{n=-\infty}^{\infty} |a_n|^2 < \infty,$$

but

$$\sum_{n=0}^{\infty} a_n z^n = \frac{1}{2\pi i} \int_{|t|=1} \frac{k(t)f(t)}{t-z} dt, \quad |z| < 1$$

so that

$$\lim_{r \uparrow 1} \sum_{n=0}^{\infty} a_n r^n e^{in\theta} = P k(e^{i\theta}) f(e^{i\theta}).$$

But if we use the Plemelj formulae to evaluate this limit, we obtain

$$Tf = Pk(e^{i\theta})f(e^{i\theta}) = \frac{1}{2} k(e^{i\theta})f(e^{i\theta}) + \frac{1}{2\pi i} \oint_{|\tau|=1} \frac{k(\tau)f(\tau)}{\tau - e^{i\theta}} d\tau$$

This representation for the operator T makes sense on a wider domain than $\mathcal{H}^2$. In fact, T , as extended above, is a self-adjoint operator in $L_2(-\pi, \pi; k(e^{i\theta})d\theta)$. The methods we have developed in the preceding lectures will clearly work for T because the absolutely continuous part of this operator is its restriction to the completion of $\mathcal{H}^2$ with respect to the k -weighted scalar product. We call this space $\mathcal{H}_k^2$.

Thus, if $x \in (\mathcal{H}_k^2)^\perp$, then $\langle Tx, y \rangle_{L_2(k)} = \langle x, Ty \rangle_{L_2(k)} = 0$, so that $(\mathcal{H}_k^2)^\perp$ is the null eigenmanifold of the extended operator.

There is no essential difference between the theory in $L_2(-\pi, \pi, k(e^{i\theta})d\theta)$ and the theory we have developed for $L_2(-\pi, \pi)$. We simply use the same formulas as before but take

$$g(v, \tau) = \frac{1}{\pi} \arg \frac{-v - i0}{k(\tau) - v - i0}, \quad v \in \sigma(T).$$

then $\int g(v, \tau) dv = k(\tau)$, and we will have, simply substituting this characteristic function into the splitting kernel formulas of the preceding section,

$$\int_{\sigma} P_{\xi} \left[\frac{1}{1-xe^{-i\theta}}, \frac{1}{1-ye^{-i\theta}} \right] d\xi = \left(\frac{1}{1-xe^{-i\theta}}, \frac{1}{1-ye^{-i\theta}} \right)_{\mathbb{H}_k^2}$$

This result is, of course, somewhat different from Rosenblum's and Ismagilov's because the Hilbert spaces on which the diagonalization has been achieved are different. However, it is clear that our result implies Ismagilov's if $k(\tau)$ is bounded below away from zero since two self-adjoint operators which are related by a similarity transformation are known to be unitarily equivalent.

As a final example*, I wish to show that self-adjoint Wiener-Hopf integral operators can be diagonalized by means of our theorems. This example plays exactly the same role for the line that the Toeplitz operators play for the circle.

Let $k(t) = \overline{k(-t)}$, and let $k(\cdot) \in L_1 \cap L_2$, with $\hat{k}(\lambda)$, the Fourier transformation of $k(\cdot)$, non-negative.

* This example was added after the actual lectures were given.

REDUCTION TO CANONICAL FORM

Let P be the orthogonal projection from $L_2(-\infty, \infty)$ onto $L_2(0, \infty)$ such that $P x(t) = \begin{cases} x(t) & 0 \leq t < \infty \\ 0 & -\infty < t \leq 0 \end{cases}$

Let us consider the Fourier Transform, $\mathfrak{F}$, of the expression $L x(s) = P \int_0^\infty k(s-t)x(t)dt$.

Lemma $\mathfrak{F} P \mathfrak{F}^{-1} y(\lambda) = \frac{1}{2} y(\lambda) + \frac{1}{2\pi i} \int_{-\infty}^{\infty} \frac{y(\mu)}{\mu - \lambda} d\mu.$

Proof

By the Paley-Wiener theorem $\mathfrak{F} P x$ is the limit in mean and almost everywhere of an analytic function $\Phi(z)$ such that $\int_{-\infty}^{\infty} |\Phi(x+iy)|^2 dx < \text{constant}, 0 < y < \infty.$

Furthermore, we may express $\Phi(z)$ in terms of its boundary values as: $\Phi(z) = \frac{1}{2\pi i} \int_{-\infty}^{\infty} \frac{\mathfrak{F} P x(\mu)}{\mu - z} d\mu.$

But the Plemelj formulae tell us that

$$\begin{cases} \Phi(\lambda + i0) - \Phi(\lambda - i0) = \mathfrak{F} P x(\lambda) \\ \Phi(\lambda + i0) - \Phi(\lambda - i0) = \frac{1}{\pi i} \int_{-\infty}^{\infty} \frac{\mathfrak{F} P x(\mu)}{\mu - \lambda} d\mu \end{cases}$$

from which the desired conclusion follows.

It is now clear that

Lemma

$$\hat{L} y(\lambda) \equiv \mathfrak{F} L \mathfrak{F}^{-1} y(\lambda) = \frac{1}{2} \hat{k}(\lambda) y(\lambda) + \frac{1}{2\pi i} \int_{-\infty}^{\infty} \frac{\hat{k}(\mu) y(\mu)}{\mu - \lambda} d\mu$$

Let H be the Hilbert space which arises by completion out of the continuous functions on $(-\infty, \infty)$ with respect to the norm derived from the scalar product $\langle f, g \rangle = \int_{-\infty}^{\infty} \hat{k}(\mu) \mathfrak{F} f(u) \overline{\mathfrak{F} g(\mu)} d\mu \equiv (\hat{k}(\cdot) \mathfrak{F} f(\cdot), \mathfrak{F} g(\cdot))$

lemma

The operator L on H defined by setting $L x(s) = P \int_0^{\infty} k(s-t)x(t)dt$ is self-adjoint on H .

Proof

$$\langle y, Lx \rangle = (\hat{k} \mathfrak{F} y, \mathfrak{F} L \mathfrak{F}^{-1} \mathfrak{F} x) = (\hat{k} \mathfrak{F} y, \hat{L} \mathfrak{F} x) = \langle Ly, x \rangle$$

lemma

Let $\hat{H}^{\perp}$ denote the completion in H of the linear manifold of functions that vanish in $(-\infty, 0)$. $\hat{H}^{\perp}$ is annihilated by L .

Proof

Let $x \in \hat{H}^{\perp}$. $\langle Lx, y \rangle = \langle x, Ly \rangle = 0$, $\forall y$, because the range of L is $\hat{H}$.

lemma

L restricted to $\hat{H}$ has an absolutely continuous spectral measure.

We will close by examining a simple special case.

Consider the eigenvalue problem for the Lalesco equation

$$L x(\lambda) = \frac{\sqrt{2\pi}}{2} \int_0^{\infty} e^{-|\mu-\lambda|} x(\mu) d\mu = \xi x(\lambda)$$

$$\hat{k}(\lambda) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-|x|+ix\lambda} dx = \frac{1}{1+\lambda^2}$$

The standard Wiener-Hopf theory proceeds by factoring $1 - \hat{k}(\lambda)$. Let us apply our formulae instead. After an integration by parts we may write

$$E(\ell, z) = \exp \left\{ \frac{1}{2\pi i} \int_{-\infty}^{\infty} \left[\frac{1}{u+\sqrt{1/\ell-1}} + \frac{1}{u-\sqrt{1/\ell-1}} - \frac{1}{u+i} - \frac{1}{u-i} \right] \ln(u-z) du \right\}$$

Now taking $0 < \text{Re } \ell \leq 1$ and $\text{Im } \ell$ sufficiently small we can evaluate the above integral by residues, obtaining:

$$E(\ell, z) = \frac{-i-z}{-\sqrt{1/\ell-1} - z} \quad \text{Im } z > 0, \text{ Im } \ell > 0$$

$$E(\ell, z) = \frac{-i-z}{\sqrt{1/\ell-1} - z} \quad \text{Im } z > 0, \text{ Im } \ell < 0$$

$$E(\ell, z) = \frac{\sqrt{1/\ell-1} - z}{i-z} \quad \text{Im } z < 0, \text{ Im } \ell > 0$$

$$E(\ell, z) = \frac{-\sqrt{1/\ell-1} - z}{i-z} \quad \text{Im } z < 0, \text{ Im } \ell < 0.$$

from which we obtain in turn:

$$F(\xi, \lambda + i0) - F(\xi, \lambda - i0) = \frac{2\sqrt{1/\xi - 1}}{1/\xi - 1 - \lambda^2} (\lambda + i) - \frac{2\sqrt{1/\xi - 1}}{i - \lambda}$$

$$\text{or } \frac{F(\xi, \lambda + i0) - F(\xi, \lambda - i0)}{\hat{k}(\lambda)} = \frac{2}{\xi} \sqrt{\frac{1}{\xi} - 1} \frac{\lambda + i}{\frac{1}{\xi} - 1 - \lambda^2}$$

which is, except for the normalization, the standard result for the (generalized) Fourier Transform of the eigendistribution of L corresponding to the spectral point ξ . (The spectral multiplicity is of course identically equal to one in this example).

FINAL REMARK

The singular integrals have appeared in much the same form in all our examples despite the fact that the operators we have described look rather different on the surface.

The geometry of all these problems is related to the following important theorem of Xa-Dao-Xeng¹⁰⁾

Theorem

Let U and V be bounded symmetric operators on a Hilbert space H , and suppose that $UV - VU = (i/\pi)P$, where P is an orthogonal projection onto a one-dimensional subspace of H . If U is such that the smallest closed invariant subspace of it containing the range of P is H itself, then there is a unitary transformation W diagonalizing U which converts V into a singular integral operator, M , whose coefficients satisfy the hypothesis we imposed for our first example.

$$M x(\lambda) = W V W^{-1} x(\lambda) = A(\lambda) x(\lambda) + \frac{1}{\pi i} \oint \frac{\overline{k(\lambda)} k(\mu)}{\mu - \lambda} x(\mu) d\mu.$$

The author has shown that V becomes unitarily equivalent to a matrix singular integral operator when the restriction on the spectral multiplicity of U is dropped. These and related results will be reported elsewhere.

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THE REFINED SZEGÖ THEOREM AND ITS ANALOGS

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Let $c(\theta)$ be an absolutely integrable function on the interval $0 \leq \theta \leq 2\pi$, and suppose that the k^{th} Fourier coefficient of $c(\theta)$ is denoted by $c^{\wedge}(k)$ so that c has the Fourier series

$$\sum_{k=-\infty}^{\infty} c^{\wedge}(k) e^{ik\pi}.$$

Let $D_n(c)$ be defined by the formula

$$D_n(c) = \det[c^{\wedge}(k-j)] \quad k, j = 0, 1, \dots, n$$

and define $G(c)$ by

$$G(c) = \exp\left\{\frac{1}{2\pi} \int_0^{2\pi} \log c(\theta) d\theta\right\}.$$

A classical theorem of Szegő states that if c is non-negative, then

$$\lim_{n \rightarrow +\infty} [D_n(c)]^{1/n+1} = G(c).$$

We will be concerned here with a refinement of Szegő's theorem.

I) In 1952, [17], Szegő showed that if $c(\theta)$ is positive and $c'(\theta)$ is in $\text{Lip}(\epsilon)$ for some positive ϵ , then

$$(1) \quad \lim_{n \rightarrow \infty} \frac{D_n(c)}{G(c)^{n+1}} = E(c)$$

where

$$E(c) = \exp \left\{ \frac{1}{2} \sum_{k=-\infty}^{\infty} |k| \gamma(k) \gamma(-k) \right\}.$$

Here

$$\log c(\theta) = \sum_{k=-\infty}^{\infty} \gamma(k) e^{ik\theta}.$$

II) In 1954, [13], M. Kac obtained an equivalent formula under different assumptions and using quite different arguments. Modulo a certain combinatorial identity he showed that if

$$i) \quad \sum_{k=-\infty}^{\infty} |c^{\wedge}(k)| |k| < \infty$$

and

$$ii) \quad |c^{\wedge}(0)| > \sum_{k \neq 0} |c^{\wedge}(k)|$$

then (1) holds.

III) In 1961, [2], G. Baxter, using new methods from the theory of Wiener-Hopf equations, showed that (1) is true if $c(\theta)$ is an arbitrary complex-valued function on $(0, 2\pi)$ such that

- i) $\sum |c^{\wedge}(k)| |k|^{\frac{1}{2}} < \infty$, $\sum |c^{\wedge}(k)| < \infty$,
- ii) $c(\theta) \neq 0$ for any θ ,
- iii) $[\arg c(\theta)]_0^{2\pi} = 0$.

He was also able to show that no exponent less than $\frac{1}{2}$ in i) is sufficient to give (1).

IV) In 1965, [9], the author showed that Baxter's arguments could be slightly modified to prove (1) under weaker hypotheses. He showed that if $c(\theta)$ is as in III) but with i) replaced by

$$i) \quad \sum |c^{\wedge}(k)|^2 |k| < +\infty \quad \text{and} \quad \sum |c^{\wedge}(k)| < \infty$$

then (1) holds.

In order to obtain the Szegő refinement it is necessary to study Szegő polynomials. In what follows we will in fact generalize the concept of orthogonal polynomials considerably, but first we discuss this theory in the classical case. Suppose $c(\theta)$ is in $L^1(T)$ where T is the one-dimensional torus--i.e., the real numbers modulo 2π . Suppose also that $c(\theta) \geq 0$. If we apply the Gram-Schmidt orthonormalization process to the functions $\{e^{ik\theta}\}_{k=0}^{\infty}$ with respect to the weight function $c(\theta)$, we obtain a family of trigonometric polynomials, the Szegő polynomials,

$$(2) \quad \varphi(k, \theta) = \sum_{j=0}^k \varphi^{\wedge}(k, j) e^{ij\theta},$$

satisfying the orthonormality relations

$$(3) \quad \frac{1}{2\pi} \int_T \varphi(k, \theta) \varphi(n, \theta)^* c(\theta) d\theta = \delta(n, k).$$

It is evident that (2) implies

$$(4) \quad \frac{1}{2\pi} \int_T c(\theta) \varphi(k, \theta) e^{-ij\theta} d\theta = 0 \quad \text{for } j = 0, 1, \dots, k-1.$$

Let us now introduce the following notation. We write

$f(\theta) \in [a, b]$ if

$$\frac{1}{2\pi} \int_T f(\theta) e^{-ik\theta} d\theta = f^\wedge(k)$$

is zero for all k not in $[a, b]$. We shall also sometimes write $[a, b]$ for a function in $[a, b]$. This notation has the advantage of making it unnecessary to give names to irrelevant functions. In this notation, (2) and (4) read respectively,

$$\varphi(k, \theta) \in [0, k],$$

$$c(\theta) \varphi(k, \theta) = [-\infty, -1] + Oe^{i0} + Oe^{i\theta} + \dots + Oe^{i(k-1)\theta} + p(k)e^{ik\theta} + [k+1, \infty]$$

for some constant $p(k)$.

Consider the operators

$$E^+(n) f(\theta) = \sum_{k \leq n} f^\wedge(k) e^{ik\theta} \quad -\infty < n < +\infty,$$

and

$$E^-(n) f(\theta) = \sum_{k \leq n} f^\wedge(k) e^{ik\theta} \quad -\infty < n < +\infty,$$

Note that $E^+(n+1) + E^-(n) = I$. We have

$$E^+(0) E^-(k) [\varphi(k, \theta) c(\theta)] = p(k) e^{ik\theta}.$$

This motivates the following definition of $W_C^+(k)$ which is a "finite section Wiener-Hopf operator". We set

$$W_C^+(k) f(\theta) = E^+(0) E^-(k) f(\theta) c(\theta)$$

where the domain of $W_C^+(k)$ is $[0, k]$; we note that when $k = +\infty$, we have a classical Wiener-Hopf operator. Let c now be complex valued. If we suppose that $W_C^+(k)$ has inverse $W_C^+(k)^{-1}$, we can set

$$\varphi(k, \theta) = p(k) W_C^+(k)^{-1} e^{ik\theta}$$

Similarly, we define the dual operator $W_C^-(k)$ by the formula

$$W_C^-(k) f(\theta) = E^+(-k) E^-(0) f(\theta)$$

where $f(\theta) \in [-k, 0]$, and if this operator is invertible we can set

$$\psi(k, \theta) = p(k) W_C^-(k)^{-1} e^{-ik\theta}.$$

It is now easy to show that if $p(k)$ is correctly chosen

$$\frac{1}{2\pi} \int_0^{2\pi} \varphi(k, \theta) \psi(j, \theta) c(\theta) c(\theta) d\theta = \delta(k, j);$$

the $\{\varphi(k, \theta)\}$ and $\{\psi(k, \theta)\}$ are the biorthogonal Szegő polynomials introduced by Baxter.

All of the above can be extended to a more general setting--specifically a locally compact abelian group Θ with dual group Ξ on which there is a fixed linear order relation " $<$ " which is compatible with the group structure of Ξ and is such that the set $\xi > 0$ is measurable. For technical simplicity, we assume here that Θ is compact (which implies that Ξ is discrete). By assumption we are given a fixed order relation " $<$ " on Ξ such that:

- i) for each ξ_1, ξ_2 in Ξ exactly one of $\xi_1 < \xi_2$, $\xi_1 = \xi_2$, or $\xi_2 < \xi_1$ holds:
- ii) $\xi_1 < \xi_2$ and $\xi_2 < \xi_3$ implies $\xi_1 < \xi_3$;
- iii) $\xi_1 < \xi_2$ implies $\xi_1 + \xi < \xi_2 + \xi$ for all ξ in Ξ .

We assume that the Haar measure $d\theta$ of Θ has been normalized so that

$$\int_{\Theta} d\theta = 1,$$

and we assign point of Ξ measure 1. We write (ξ, θ) to denote the action of the character $\xi \in \Xi$ on θ in Θ .

Some familiar examples :

$\Theta = T$, $\Xi = Z$ (the integers) with topology, order relation, etc. as usual. It should be noted here that $d\theta$ is now the ordinary Lebesgue measure divided by 2π .

$\Theta = T + T$, $\Xi = Z + Z$ where the topology of Θ is the usual product topology and where the order on Ξ is given by specifying a Helson-Lowdenslager half-plane of positive elements. For example, one can take all the elements on one side of a line through 0 of irrational slope.

We now define several classes of algebras of functions on Θ .

Definition 1. A_0 is the algebra of functions on Θ with absolutely convergent Fourier series. We define a norm $\|\cdot\|_0$ on A_0 by the formula

$$\|f\|_0 = \sum_{\Xi} |f^\wedge(\xi)|$$

where $f^\wedge(\xi) = \int_{\Theta} f(\theta)(-\xi, \theta) d\theta$.

Note that every element of A_0 is continuous.

Definition 2. A Banach algebra of A of functions on Θ with norm $\|\cdot\|$ is said to be of type M if

- i) $A \subset A_0$ and $\|f\| \geq \|f\|_0$.
- ii) Every character (ξ, θ) is in A and the linear span of the characters is norm dense in A .
- iii) There exists a constant $M \geq 0$ such that for every $\eta \in \Xi$, the following inequalities hold:

$$\|E^+(\eta)\| \leq M, \quad \|E^-(\eta)\| \leq M,$$

$$\|E^+(\eta+)\| \leq M, \quad \|E^-(\eta-)\| \leq M,$$

where $E^+(\eta)$, etc. are operators on whose action on f in is given by:

$$E^+(\eta)f(\theta) = \sum_{\xi \geq \eta} f^\wedge(\xi)(\xi \cdot \theta),$$

$$E^+(\eta+)f(\theta) = \sum_{\xi > \eta} f^\wedge(\xi)(\xi \cdot \theta),$$

$$E^-(\eta)f(\theta) = \sum_{\xi \leq \eta} f^\wedge(\xi)(\xi \cdot \theta),$$

$$E^-(\eta-)f(\theta) = \sum_{\xi < \eta} f^\wedge(\xi)(\xi \cdot \theta).$$

We will also need certain relations of dominance.

Given a function f in A_0 with $f(\theta) = \sum f^\wedge(\xi)(\xi \cdot \theta)$ define $f^\#(\theta)$ by the equation

$$f^\#(\theta) = \sum |f^\wedge(\xi)| (\xi \cdot \theta).$$

Now define $f \prec g$ (f dominated by g) to mean that $|f^\wedge(\xi)| \leq |g^\wedge(\xi)|$ for all g in Ξ . It is clear that

$$f + g \prec f^\# + g^\# , \quad fg \prec f^\# g^\# .$$

Definition 3. A Banach algebra A of functions on Θ with norm $\|\cdot\|$ is said to be of type S if

- i) as in Definition 2.
- ii) as in Definition 2.
- iii) If f is in A_0 and g is in A and $f \prec g$ then f is in A and $\|f\| \leq \|g\|$.

Note that an algebra of type S is surely of type M, since, for example,

$$E^+(\eta) f(\theta) \prec f^\#(\theta)$$

which implies that $\|E^+(\eta) f(\theta)\| \leq \|f(\theta)\|$ so that $\|E^+(\eta)\| = 1$.

Suppose $\Theta = T$ and $\Xi = Z$. Let v be a function of the Beurling-Gelfand type on the integers (i.e., $v(n) \geq 1$ and $v(n+k) \leq v(n) \cdot v(k)$). Define the norm $\|\cdot\|$ by the formula

$$\|f\| = \sum |f^\wedge(n)| v(n).$$

This norm defines an algebra of type S. Baxter used the Beurling-Gelfand function

$$v(n) = (1 + |n|)^{\frac{1}{2}}$$

in his study of the refined Szegő theorem. Another algebra of type S is defined by setting

$$\|f\| = 3\{\sum |f^\wedge(n)| + [\sum |n| |f^\wedge(n)|^2]^{\frac{1}{2}}\}$$

This algebra also has application to the refined Szegő theorem.

Let A be a fixed algebra of type M; we now introduce the desired analogs of Wiener-Hopf operators and the analogs of finite sections of these operators. For $f(\theta)$ in $E^+(0)E^-(\eta)A$, define $W_C^+(\eta)$ by the formula

$$W_C^+(\eta)f(\theta) = E^+(0)E^-(\eta) c(\theta) f(\theta) \quad \eta \geq 0,$$

where $c(\theta)$ is some fixed function in A. Similarly, for $f(\theta) \in E^-(0)E^+(-\eta)$, we define $W_C^-(\eta)$ by the formula,

$$W_C^-(\eta)f(\theta) = E^-(0)E^+(-\eta) c(\theta) f(\theta) \quad \eta \geq 0.$$

Note that in general $E^+(0)E^-(\eta)A$ will not be finite dimensional; for example if $\Theta = T^2$, $E^+(0)E^-(\eta)A$ will have countably infinite dimension. We finally define W_C^+ and W_C^- by the formulae

$$W_C^+f(\theta) = E^+(0) c(\theta)f(\theta) \quad f \in E^+(0)A,$$

$$W_C^-f(\theta) = E^-(0) c(\theta)f(\theta) \quad f \in E^-(0)A.$$

It is evident that "uniform invertibility" of the $W_C^+(\eta)$ for large η implies that W_C^+ is invertible. Baxter's finite section norm inequality shows that this condition is also sufficient. The following definition will be convenient.

Definition 1. $c \in A$ is said to be in $WH(A)$ provided $(W_c^+)^{-1}$ and $(W_c^-)^{-1}$ exist.

There is an important theorem on Wiener-Hopf operators which in the present setting reads:

Theorem 1. $c \in WH(A)$ if and only if $c(\theta) = d^2/U(\theta)V(\theta)$

where $U(\theta), U(\theta)^{-1}$ are in $E^+(0)A$,

$V(\theta), V(\theta)^{-1}$ are in $E^-(0)A$,

$$d^2 = U^\wedge(0) = V^\wedge(0) \neq 0.$$

Proof Necessity. Choose $U(\theta)$ and $V(\theta)$ so that

$$W_c^+ U = 1 \quad \text{and} \quad W_c^- V = 1$$

with $U(\theta)$ in $E^+(0)A$ and $V(\theta)$ in $E^-(0)A$. Set

$$V_1(\theta) = U(\theta) c(\theta) \quad \text{and} \quad U_1(\theta) = V(\theta) c(\theta).$$

Then since $E^+(0) V_1(\theta) = 1$, $V_1(\theta)$ is in $E^-(0)A$ and similarly $U_1(\theta)$ is in $E^+(0)A$. But,

$$U(\theta) U_1(\theta) = U(\theta) V(\theta) c(\theta) = V(\theta) V_1(\theta)$$

and $U(\theta) U_1(\theta)$ is in $E^+(0)A$ and $V(\theta) V_1(\theta)$ is in $E^-(0)A$. Hence $U(\theta) V(\theta) c(\theta) = d^2$ for some constant d . Since $c(\theta) \neq 0$, it follows that $d^2 \neq 0$, and since $U_1^\wedge(0) = V_1^\wedge(0) = 1$, we have $U^\wedge(0) = d^2 = V^\wedge(0)$.

Sufficiency. Suppose that $W_c^+ f = g$ where $g \in E^+(0)A$, then $c(\theta) f(\theta) = g_1(\theta) + g(\theta)$ where $g_1(\theta) \in E(0-)A$ and hence $d^2 U(\theta)^{-1} f(\theta) = V(\theta) g_1(\theta) + V(\theta) g(\theta)$. Applying $E^+(0)$ we get

$$d^2 U(\theta)^{-1} f(\theta) = E^+(0) V(\theta) g(\theta)$$

so that $f(\theta) = d^{-2} U(\theta) E^+(0) V(\theta) g(\theta)$.

This explicit representation of f shows that f , if it exists, is unique. However, applying W_c^+ to f defined by this formula, shows that $W_c^+ f = g$.

In the proof of the finite section norm inequality the following identity of Shinbrot [14] is helpful. Suppose $c(\theta) = 1/u(\theta) v(\theta)$ where

$$\begin{aligned} u(\theta) & \text{ is in } E^+(0) E^-(\xi)A \\ u(\theta)^{-1} & \text{ is in } E^+(0)A \\ v(\theta) & \text{ is in } E^+(-\xi)E^-(0)A \\ v(\theta)^{-1} & \text{ is in } E^-(0)A. \end{aligned}$$

Then we have for $\eta \geq \xi$ and g in $E^+(0)E^-(\eta)A$

$$[W_c^+(\eta)]^{-1} g(\theta) = vE^-(\eta) v^{-1} uE^+(0) vg.$$

Proof. Suppose f in $E^+(0) E^-(\eta)A$ is a solution to

$$W_c^+(\eta)f = g,$$

then we have

$$cf = g_1 + g + g_2$$

where g_1 is in $E^-(0-)A$ and g_2 is in $E^+(\eta+)A$. Since $c = 1/uv$

$$\frac{1}{u} f = vg_1 + vg + vg_2.$$

Applying $E^+(0)$, we get,

$$\frac{1}{u} f = 0 + E^+(0) vg + vg_2.$$

Multiplying by $v^{-1}u$ this becomes

$$\frac{1}{v} f = v^{-1} u E^+(0) vg + ug_2.$$

Applying $E^-(\eta)$, we find that

$$E^-(\eta) v^{-1} f = E^-(\eta) v^{-1} u E^+(0) vg + 0.$$

Finally, multiplying by v , we obtain

$$v E^-(\eta) v^{-1} f = v E^-(\eta) v^{-1} u E^+(0) vg.$$

But it can easily be checked that

$$v E^-(\eta) v^{-1} f = f.$$

Thus if

$$(1) \quad f = v E^-(\eta) v^{-1} u E^+(0) vg$$

f is the unique solution of $W_C^+(\eta)f = g$ if a solution exists. A simple substitution shows f defined by (1) is indeed always a solution. We are now in position to give a simple proof of the theorem of Baxter previously referred to.

Theorem 2. Suppose A is of type M and $c \in WH(A)$. Then there exists $\xi \geq 0$ and $a \geq 0$ such that $W_C^+(\eta)$ and $W_C^-(\eta)$ are invertible for all $\eta \geq \xi$ and

$$\|f\| \leq a \|W_C^+(\eta)f\|, \quad \|f\| \leq a \|W_C^-(\eta)f\| \quad \text{for all } \eta \geq \xi.$$

Proof. We have $c(\theta) = d^2/U(\theta) V(\theta)$, as in the previous theorem. Using standard theorems about invertible elements in Banach algebras, we find that for all sufficiently large ξ , $u_1 = E^-(\xi)d^{-1}u$ and $v_1 = E^+(-\xi)d^{-1}v$ are invertible in the Banach algebras $E^+(0)A$ and $E^-(0)A$ respectively. Set $c_\xi = 1/u_1 v_1$ then, it can be easily shown that

$$\|W_C^+(\eta) - W_{c_\xi}^+(\eta)\| \leq \|c - c_\xi\|,$$

which implies

$$\lim_{\xi \rightarrow \infty} \|W_C^+(\eta) - W_{c_\xi}^+(\eta)\| = 0.$$

Hence, $W_C^+(\eta)$ can be approximated by uniformly invertible operators $W_C^+(\eta)$, and by the same argument applied to the non-commutative Banach algebra of linear endomorphisms of the Banach space $E^+(0) E^-(\eta)A$, $W_C^+(\eta)$ is seen to be invertible.

This theorem has corollaries as follows.

Corollary Suppose A is of type S . Then there are c^+ and c^- in A such that

- i) $(c^+)^{\#} = c^+$, $(c^-)^{\#} = c^-$,
- ii) $f \prec c^+ \cdot [W_C^+(\eta)f]^{\#}$, $f \prec c^- [W_C^-(\eta)f]^{\#}$,

for $f \in E^+(0) E^-(\eta)$ and $f \in E^-(0) E^+(-\eta)$ respectively.

Proof. Omitted. See [10].

Corollary Suppose A is of type M and $g(\theta)$ is in $E^+(0)A$. Choose f so that

$$W_C^+ f = g$$

and for large η choose $f(\eta, \theta)$ so that

$$W_C^+(\eta) f(\eta, \theta) = E^-(\eta) g(\theta),$$

then $\|f(\eta, \theta) - f(\theta)\| \leq a \|E^+(\eta)f\|$ for large η .

Proof. Omitted. See [10].

From now on we assume that $c(\theta)$ is in $WH(A)$. Let U and V be such that

$$W_C^+ U = 1, \quad W_C^- V = 1,$$

and for each large η choose $u(\eta, \theta)$, $v(\eta, \theta)$ so that

$$W_C^+(\eta) u(\eta, \theta) = 1, \quad W_C^-(\eta) v(\eta, \theta) = 1.$$

It follows from the second Corollary that

$$(2) \quad \|u(\eta, \theta) - U(\theta)\| \rightarrow 0 \quad \text{and} \quad \|v(\eta, \theta) - V(\theta)\| \rightarrow 0.$$

It is also easy to show that for each large enough η

$$u^\wedge(\eta, 0) = v^\wedge(\eta, 0) = \int_{\Theta} c(\theta) u(\eta, \theta) v(\eta, \theta) d\theta.$$

Define $d(\eta)^2$ as $u^\wedge(\eta, 0) = v^\wedge(\eta, 0)$. Let $U^\wedge(0) = d^2$ and then since by Corollary 2, $d(\eta)^2 \rightarrow d^2$ and $d \neq 0$, we have $d(\eta) \neq 0$ for all large η .

We now define the Szegő polynomials for "large" η .

We set

$$\varphi(\eta, \theta) = d(\eta)^{-1} v(\eta, \theta) \quad (\eta, \theta),$$

$$\psi(\eta, \theta) = d(\eta)^{-1} u(\eta, \theta) \quad (-\eta, \theta),$$

so that

$$\varphi \text{ is in } E^+(0)E^-(\eta)A,$$

$$\psi \text{ is in } E^-(0)E^+(-\eta)A .$$

It is easy to see that

$$\int_{\Theta} \varphi(\eta_1, \theta) \psi(\eta_2, \theta) c(\theta) d\theta = \delta(\eta_1, \eta_2) .$$

For all large enough η , $u(\eta, \theta)$ and $v(\eta, \theta)$ and have reciprocals in $E^+(0)A$ and $E^-(0)A$ respectively. For such an η , we define

$$c_{\eta}(\theta) = \frac{d(\eta)^2}{u(\eta, \theta)v(\eta, \theta)} .$$

Theorem 1. For all "large η "

$$c_{\eta}^{\wedge}(\xi) = c^{\wedge}(\xi)$$

for all $-\eta \leq \xi \leq \eta$.

Proof. Define on $E^+(-\eta)E^-(\eta)A$, the operator $Q(\eta)$ given by the formula

$$Q(\eta)f(\theta) = u(\eta, \theta) E^-(0-)f(\theta) + v(\eta, \theta)E^+(0)f(\theta);$$

then it is easy to see that

$$i) \int [Q(\eta)f](\theta) c(\theta) d\theta = f^{\wedge}(0) ,$$

$$ii) \int [Q(\eta)f](\theta) c_{\eta}(\theta) d\theta = f^{\wedge}(0) .$$

Therefore,

$$\text{iii)} \int [Q(\eta)f](\theta) [c(\theta) - c_\eta(\theta)] d\theta = 0.$$

Now, define $R(\eta)$ on $E^+(-\eta) E^-(\eta)A$ by the formula

$$\begin{aligned} R(\eta) f(\theta) &= E^-(\eta) u(\eta, \theta) E^+(0) u(\eta, \theta)^{-1} v(\eta, \theta)^{-1} f(\theta) \\ &\quad + E^+(-\eta) v(\eta, \theta) E^-(0) u(\eta, \theta)^{-1} v(\eta, \theta)^{-1} f(\theta). \end{aligned}$$

It is then easy to see that

$$R(\eta) Q(\eta) = Q(\eta) R(\eta) = I$$

on $E^+(-\eta) E^-(\eta)A$. Thus $Q(\eta)$ is onto, so that given ξ in $[-\eta, \eta]$, $Q(\eta) f_\xi(-\theta) = (-\xi, \theta)$ for some f_ξ . This together with iii. proves the theorem.

Corollary. Let c be an element of $WH(A)$ and let η be sufficiently large; then if

$$Y_C^+(\eta) f(\theta) = d(\eta)^{-2} v(\eta, \theta) E^-(\eta) u(\eta, \theta) v(\eta, \theta)^{-1} E^+(0) v(\eta, \theta) f(\theta)$$

then $Y_C^+(\eta)$ is an (explicit) inverse for $W_C^+(\eta)$. Similarly,

$$Y_C^-(\eta) f(\theta) = d(\eta)^{-2} u(\eta, \theta) E^+(-\eta) u(\eta, \theta)^{-1} v(\eta, \theta) E^-(0) u(\eta, \theta) f(\theta)$$

is an inverse for $W_C^-(\eta)$.

Proof. This follows from the theorem above and Shinbrot's identity

We turn now to the problem of expanding a prescribed function $f(\theta)$ in $E^+(0)A$ in terms of the $\varphi(\eta, \theta)$'s. (We assume, of course, that $c \in WH(A)$.) One would like to have

$$(1) \quad f(\theta) = \sum_{\eta \geq 0} \tilde{f}(\eta) \varphi(\eta, \theta)$$

for "appropriately chosen" coefficients $\tilde{f}(\eta)$. It is easy to see, formally at least, how to choose $\tilde{f}(\eta)$. Multiplying both sides of (1) by $\psi(\xi, \theta) c(\theta) d\theta$ and integrating gives

$$(2) \quad \int_{\Theta} f(\theta) \psi(\xi, \theta) c(\theta) d\theta = \tilde{f}(\xi).$$

One might now hope that if $\tilde{f}(\xi)$ is defined by (2) then (1) will hold. This hope is frustrated by the obvious difficulty that $\varphi(\eta, \theta)$ and $\tilde{f}(\eta)$ need not be defined for small η . The most one can show is the following:

Theorem 2. If $c \in WH(A)$ where A is of type S then exists $\xi_0 \geq 0$ such that if $f(\theta) \in E^+(0)A$, then we have

$$E^+(\xi_0+) [f(\theta) - \sum_{\eta > \xi_0} \tilde{f}(\eta) \varphi(\eta, \theta)] = 0.$$

Here the infinite series converges unconditionally.

If A is merely of type M , a slightly weaker result holds, which, however, we will not describe here.

We omit the proof of the above theorem. However, before going on, we give one inequality from the proof which is of importance later. By (2) we have

$$\begin{aligned} \tilde{f}(\xi) d(\xi) &= \int_{\Theta} f(\theta) u(\xi, \theta) c(\theta) (-\xi, \theta) d(\theta), \\ |\tilde{f}(\xi) d(\xi)| &\leq \int_{\Theta} f^{\#}(\theta) c^{+}(\theta) c^{\#}(\theta) (-\xi, \theta) d\theta, \end{aligned}$$

and thus,

$$(3) \quad |\tilde{f}(\xi) d(\xi)| \leq F^{\wedge}(\xi)$$

where

$$F(\theta) = f^{\#}(\theta) c^{+}(\theta) c^{\#}(\theta).$$

Given $g \in E^{+}(0)A$, consider the equation

$$W_C^{+} f = g \quad f \text{ in } E^{+}(0)A.$$

We know that for large enough ξ , there exists a unique $f(\xi, \theta)$ in $E^{-}(\xi) E^{+}(0)A$ such that

$$W_C^{+}(\xi) f(\xi, \theta) = E^{-}(\xi) g(\theta).$$

We assert that if it were true (which it is not), that

$$f(\theta) = \sum_{\eta \geq 0} \tilde{f}(\eta) \varphi(\eta, \theta)$$

then $f(\xi, \theta)$ would be given by the formula

$$f(\xi, \theta) = \sum_{0 \leq \eta \leq \xi} \tilde{f}(\eta) \varphi(\eta, \theta).$$

An alternative correct formulation is as follows. If ξ is large enough, then we have

$$\begin{aligned} W_C^+(\xi) [f(\theta) - \sum_{\eta > \xi} \tilde{f}(\eta) \varphi(\eta, \theta)] &= W_C^+(\xi) f(\theta) + 0, \\ &= E^-(\xi) W_C^+ f(\theta), \\ &= E^-(\xi) g(\theta). \end{aligned}$$

Also, $f(\theta) - \sum_{\eta > \xi} \tilde{f}(\eta) \varphi(\eta, \theta) \in E^+(0) E^-(\xi) A$ since

$$E^+(\xi+) [f(\theta) - \sum_{\eta > \xi} \tilde{f}(\eta) \varphi(\eta, \theta)] = 0;$$

thus $f(\xi, \theta) = f(\theta) - \sum_{\eta > \xi} \tilde{f}(\eta) \varphi(\eta, \theta)$. As a special case,

we see that for large enough ξ

$$u(\xi, \theta) = U(\theta) - \sum_{\eta > \xi} \tilde{U}(\eta) \varphi(\eta, \theta)$$

and a similar formula holds for $v(\eta, \theta)$. For $\eta_1 \leq \eta_2$ large enough, we have

$$u(\eta_2, \theta) - u(\eta_1, \theta) = \sum_{\eta_1 < \xi \leq \eta_2} \tilde{U}(\xi) \varphi(\xi, \theta),$$

so that if $\alpha(\xi) = \tilde{U}(\xi) d(\xi)^{-1}$, then

$$u(\eta_2, \theta) - u(\eta_1, \theta) = \sum_{\eta_1 < \xi \leq \eta_2} \alpha(\xi) v(\xi, \theta) (\xi, \theta),$$

and similarly if $\beta(\xi) = \tilde{V}(\xi) d(\xi)^{-1}$, then

$$v(\eta_2, \theta) - v(\eta_1, \theta) = \sum_{\eta_1 < \xi \leq \eta_2} \beta(\xi) v(\xi, \theta) (\xi, \theta).$$

We now record without proof the two interesting identities which follow from the formulae above:

$$\begin{bmatrix} u(\eta_1, \theta) \\ v(\eta_1, \theta) \end{bmatrix} = \left\{ \prod_{\eta_1 < \xi \leq \eta_2} \begin{bmatrix} 1 & -\alpha(\xi)(\xi, \theta) \\ -\beta(\xi)(-\xi, \theta) & 1 \end{bmatrix} \right\} \begin{bmatrix} u(\eta_2, \theta) \\ v(\eta_2, \theta) \end{bmatrix},$$

and

$$u^\wedge(\eta_1, 0) = \prod_{\eta_1 < \xi \leq \eta_2} [1 - \alpha(\xi)\beta(\xi)] u^\wedge(\eta_2, 0).$$

Let $\Theta = T$, $\Xi = Z$ and define $(A, \|\cdot\|)$ by letting

$$\|f\| = 3 \left\{ \sum_{-\infty}^{\infty} |f^\wedge(k)| + \left[\sum_{-\infty}^{\infty} |k| |f^\wedge(k)|^2 \right]^{\frac{1}{2}} \right\}$$

which gives an algebra of type S. Let $c(\theta)$ be in $WH(A)$. Let

$$D_n[c] = \det[c^\wedge(k-j)]_{k,j} = 0, \dots, n,$$

$$G(c) = \exp \left\{ \frac{1}{2\pi} \int_0^{2\pi} \log c(\theta) d\theta \right\} = -d^2,$$

where

$$c(\theta) = d^2 u(\theta)^{-1} v(\theta)^{-1}.$$

For sufficiently large positive n , if

$$c_n(\theta) = \frac{d(n)^2}{u(n, \theta)v(n, \theta)}$$

then by Theorem 1

$$D_n[c] = D_n[c_n].$$

also

$$G[c_n] = -d(n)^2.$$

Szegő showed in [17] that the following identity holds

$$\frac{D_n[c_n]}{G[c_n]^{n+1}} = \exp \left\{ \frac{1}{2} \sum_{-\infty}^{\infty} |k| \gamma_n(k) \gamma_n(-k) \right\}$$

where

$$\log c_n(\theta) = \sum_{-\infty}^{\infty} \gamma_n(k) e^{ik\theta}$$

by using techniques from complex variable theory. (Actually, Szegő dealt with the case $c(\theta) > 0$. However, his ideas extend to the more general case considered above.) The maximal ideal space of A is easily seen to be T . We know that $c_n(\theta) \rightarrow c(\theta)$ in A as $n \rightarrow +\infty$. By what is essentially the Gelfand-Wiener-Levy theorem, this implies that $\log c_n(\theta) \rightarrow \log c(\theta)$ in A and thus that if

$$\log c(\theta) = \sum_{-\infty}^{\infty} \gamma(k) e^{ik\theta}$$

then as $n \rightarrow \infty$

$$\sum_{-\infty}^{\infty} |\gamma_n(k) - \gamma(k)| + \sum_{-\infty}^{\infty} |\gamma_n(k) - \gamma(k)|^2 \cdot |k|^{\frac{1}{2}} \rightarrow 0.$$

It follows that

$$\frac{D_n[c_n]}{G[c_n]^{n+1}} \rightarrow \exp \left[\frac{1}{2} \sum |k| \gamma(k) \gamma(-k) \right].$$

Since $d^2 = \lim_{n \rightarrow \infty} d(n)^2$, we have

$$\frac{G[c]}{G[c_n]} = \frac{d(n)^2}{d^2} = \prod_{n+1}^{\infty} (1 - \alpha(m)\beta(m))^{-1}.$$

By (3) we know that

$$\sum m |\alpha(m)|^2 < +\infty \quad \text{and} \quad \sum m |\beta(m)|^2 < +\infty$$

which implies that

$$\sum m |\alpha(m)\beta(m)| < +\infty,$$

and from this it is apparent that

$$\lim_{n \rightarrow \infty} \frac{G[c]^{n+1}}{G[c_n]^{n+1}} = 1.$$

Combining these results we see that

$$(4) \quad \lim_{n \rightarrow \infty} \frac{D_n[c]}{G[c]^{n+1}} = \exp\left[\frac{1}{2} \sum_{-\infty}^{\infty} |k| \gamma(k) \gamma(-k)\right],$$

which is the refined Szegő limit theorem.

It is usual to write the conditions for the validity of (4) in a somewhat different form. One assumes that

$$(5) \quad \sum_{-\infty}^{\infty} |c^{\wedge}(k)| < \infty, \quad \sum_{-\infty}^{\infty} |c^{\wedge}(k)|^2 |k| < \infty,$$

and that, if $\sum_{-\infty}^{\infty} c^{\wedge}(k) e^{ik\theta} = c(\theta)$,

$$(6) \quad c(\theta) \neq 0 \quad \theta \in T, \quad [\arg c(\theta)]_{-\pi}^{\pi} = 0.$$

It follows from the Wiener-Levy theorem that under these assumptions

$$\log c(\theta) = \sum_{-\infty}^{\infty} \gamma(k) e^{ik\theta} \text{ is in } A. \text{ If we set}$$

$$U(\theta) = \exp \left[\sum_0^{\infty} \gamma(k) e^{ik\theta} \right],$$

$$V(\theta) = \exp \left[\sum_{-\infty}^0 \gamma(k) e^{ik\theta} \right],$$

$$d^2 = \exp \gamma(0),$$

then $c(\theta) = d^2/U(\theta) V(\theta)$ and $U(\theta), U(\theta)^{-1} \in E^+(0)A, V(\theta), V(\theta)^{-1} \in E^-(0)A,$

so that $c \in WH(A)$. Conversely $c \in WH(A)$ implies (5) and (6).

In this lecture we give a new and different proof of the refined Szegő theorem, which has the advantage that it can be used to prove other related results as well.

Let $c(\theta) \in C(T)$, where $C(T)$ is the class of continuous functions on T , and let $\hat{c}(k)$ be defined as usual. If $\{\lambda(n,k)\}_{k=0}^n$ are the eigenvalues of the matrix

$$[\hat{c}(k-j)]_{k,j=0,\dots,n}$$

then for $s = 1, 2, \dots$

$$\begin{aligned} \sum_{k=0}^n \lambda(n,k)^s &= \text{trace}\{[\hat{c}(k-j)]_{k,j=0,\dots,n}\}^s \\ &= \sum_{\substack{0 \leq k_v \leq n \\ v=1,\dots,s}} \hat{c}(k_1-k_2) \hat{c}(k_2-k_3) \dots \hat{c}(k_s-k_1) . \end{aligned}$$

Let $\underline{j} = (j_1, \dots, j_s)$ where we consider only s -tuples $(j_1, \dots, j_s)$ for which $j_1 + \dots + j_s = 0$. We define the range $R(s, \underline{j})$ to be

$$R(s, \underline{j}) = \max(0, j_1, j_1+j_2, \dots, j_1+\dots+j_{s-1}) - \min(0, j_1, j_1+j_2, \dots, j_1+\dots+j_{s-1})$$

and we set

$$R(s, \underline{j})_n = \min\{R(s, \underline{j}), n\} .$$

A simple calculation then shows that

$$(1) \quad \sum_{k=0}^n \lambda(n,k)^s = \frac{n+1}{2\pi} \int_T c(\theta)^s d\theta = - \sum_{\underline{j}} R(s, \underline{j})_n \hat{c}(j_1) \dots \hat{c}(j_s) .$$

Let

$$B = \sum_{-\infty}^{\infty} |c^{\wedge}(k)|$$

$$C = \left(\sum_{-\infty}^{\infty} |c^{\wedge}(k)|^2 |k| \right)^{\frac{1}{2}}.$$

It is not hard to show that

$$(2) \quad \sum_{\underline{j}} |R(s, \underline{j})_n c^{\wedge}(j_1) \dots c^{\wedge}(j_s)| \leq \begin{cases} 0 & s = 1 \\ s^2 C^2 B^{s-2} & s > 1 \end{cases}$$

Choose any complex ρ for which $B|\rho| < 1$. Multiplying (1)

by $-\rho^s s^{-1}$ and summing over s we obtain

$$\log D_n[1-\rho c] - (n+1) \log G[1-\rho c] = \sum_{s=1}^{\infty} \frac{\rho^s}{s} \sum_{\underline{j}} R(\underline{j}, s)_n c^{\wedge}(j_1) \dots c^{\wedge}(j_s).$$

Using (2) we see that

$$(3) \quad \lim_{n \rightarrow \infty} \log \left[\frac{D_n[1-\rho c]}{G[1-\rho c]^{n+1}} \right] = \sum_{s=1}^{\infty} \frac{(-1)^s \rho^s}{s} \sum_{\underline{j}} R(\underline{j}, s) c^{\wedge}(j_1) \dots c^{\wedge}(j_s).$$

It can be shown that the right-hand side can be rewritten as

$$(4) \quad \frac{1}{2} \sum_{k=-\infty}^{\infty} \gamma_{\rho}(k) \gamma_{\rho}(-k) |k|$$

where

$$\gamma_{\rho}(k) = \frac{1}{2\pi} \int_T \log[1-\rho c(\theta)] e^{-ik\theta} d\theta.$$

The above arguments are due to Kac [12] and are discussed in his lectures. In particular the difficult transition from (3) to (4) which depends upon Spitzer's combinatorial lemma is carried out in detail. The only modification from Kac's presentation lies in the estimates (2), due to Baxter and Hirschman, which are somewhat better than those originally given by Kac.

The result above implies the refined Szegö theorem holds if:

$$c \in A,$$

$$|c^{\wedge}(0)| > \sum_{k \neq 0} |c^{\wedge}(k)|.$$

Here A is as in Lecture III. In what follows we will show how the complete refined Szegö theorem can be deduced from this special case.

We will need for this purpose an alternative simpler version of the theory developed in Lectures I and II. Let

$$\|f(\theta)\|_2 = \left[\frac{1}{2\pi} \int_T |f(\theta)|^2 d\theta \right]^{\frac{1}{2}}.$$

It was shown by Reich [13], who used a modification of Baxter's argument, that if

$$(5) \quad c(\theta) = \frac{d^2}{U(\theta)V(\theta)}$$

where

$$(6) \quad \begin{aligned} U(\theta), U(\theta)^{-1} &\in E^+(0) \cap C(T) & U^\wedge(0) &= d^2, \\ V(\theta), V(\theta)^{-1} &\in E^-(0) \cap C(T) & V^\wedge(0) &= d^2, \end{aligned}$$

then there exists an integer n_0 and a constant a such that if $n \geq n_0$

$$\|f\|_2 \leq a \|W_C^+(n) f\|_2$$

for all $f \in E^+(0) \cap E^-(n) \cap C(T)$. This result, and also the dual result for $W_C^-(n)$ can also be proved using Shinbrot's identity.

It now follows that

$$u(n, \theta) = W_C^+(n)^{-1} 1, \quad v(n, \theta) = W_C^-(n)^{-1} 1$$

are defined for n large and that

$$\lim_{n \rightarrow \infty} \|U(\theta) - u(n, \theta)\|_2 = \lim_{n \rightarrow \infty} \|V(\theta) - v(n, \theta)\|_2 = 0.$$

Similarly $\lim_{n \rightarrow \infty} d(n)^2 = d^2$. As before let

$$\begin{aligned} \varphi(n, \theta) &= d(n)^{-1} v(n, \theta) e^{in\theta} = \sum_{k=0}^n \varphi^\wedge(n, k) e^{ik\theta}, \\ \psi(n, \theta) &= d(n)^{-1} u(n, \theta) e^{-in\theta} = \sum_{k=-n}^0 \psi^\wedge(n, k) e^{ik\theta}. \end{aligned}$$

It follows from the above that if

$$\varphi^0(n, z) = \sum_{k=0}^n \varphi^\wedge(n, k) z^k, \quad \psi^0(n, z) = \sum_{k=-n}^0 \psi^\wedge(n, k) z^k$$

then as $n \rightarrow \infty$

$$(7) \quad \begin{aligned} \varphi^0(n, z) &\cong z^n d^{-1} V^0(z) & |z| > 1, \\ \psi^0(n, z) &\cong z^{-n} d^{-1} U^0(z) & |z| < 1. \end{aligned}$$

If $c(\theta)$ is as in (5) and (6) we say that $c(\theta) \in R$.

If $c \in R$ then it follows that $D_n(c) \neq 0$ for all large n . If $c \in R$ and if $D_n(c) \neq 0$ for $n = 0, 1, \dots$ then we say that $c \in R^*$. In this case $\varphi(n, \theta)$ and $\psi(n, \theta)$ are defined for all $n = 0, 1, \dots$.

Let $c(\theta) \in R^*$ and let $f \in L^1(T)$. We set

$$\tilde{f}(j, k) = \frac{1}{2\pi} \int_T f(\theta) \psi(j, \theta) \varphi(k, \theta) c(\theta) d\theta,$$

$$D_n[f|c] = \det[\tilde{f}(j, k)]_{j, k=0, \dots, n}.$$

$D_n[f|c]$ is the "relative" Toeplitz determinant of f with respect to c . Note that if $c = 1$ then $\psi(j, \theta) = e^{-ij\theta}$, $\varphi(k, \theta) = e^{ik\theta}$ and $D_n[f|1] = D_n[f]$. A basic step in our argument is the following.

Theorem 1. Let $c \in R^*$ and let

$$f^0(z) = \prod_{\alpha=1}^{\nu} (\xi_{\alpha} - z)$$

where $\{\xi_{\alpha}\}_1^{\nu}$ are distinct and $|\xi_{\alpha}| > 1$, $\alpha = 1, \dots, \nu$. Then

$$\lim_{n \rightarrow \infty} \frac{D_n[f|c]}{G(c)^{n+1}} = E[f|c]^2.$$

Here

$$E[f|c] = \exp\left[\frac{1}{2} \sum_{-\infty}^{\infty} |k| f_{\lambda}(k) c_{\lambda}(-k)\right],$$

$$c_{\lambda}(k) = \frac{1}{2\pi} \int_T \log c(\theta) e^{-ik\theta} d\theta, \quad f_{\lambda}(k) = \frac{1}{2\pi} \int_T \log f(\theta) e^{-ik\theta} d\theta.$$

This result is more general than the Szegő refinement in that c replaces 1 , but it is proved only for a very special class of f 's. We will only sketch the proof. Let

$$\Delta_n = \det \begin{bmatrix} \varphi^0(n, \xi_1) & \dots & \varphi^0(n + v - 1, \xi_1) \\ \vdots & & \vdots \\ \varphi^0(n, \xi_v) & \dots & \varphi^0(n + v - 1, \xi_v) \end{bmatrix}.$$

It can be shown that

$$D_n[f|c] = \Delta_{n+1} \left\{ \prod_{k=1}^v \varphi^{\wedge}(n+k, n+k)^{-1} \right\} \left\{ \Delta_0 \prod_0^{v-1} \varphi^{\wedge}(k, k)^{-1} \right\}^{-1}.$$

The argument is as follows. Compute the Szegő polynomials relative to the weight function $c(\theta)f(\theta)$ once by the Gram-Schmidt method and once using the Christoffel formula and compare the answers. An identity results which, under further manipulation, leads to the above. It is easy to see that $\Delta_0 \prod_0^{v-1} \varphi^{\wedge}(k, k)^{-1}$ is a Vandermonde determinant. Using (7) we obtain a simple asymptotic formula for Δ_{n+1} , etc.

There is of course a parallel result to Theorem 1 in which $f^0(z)$ is replaced by

$$g^0(z) = \prod_{\alpha=1}^{\mu} (\zeta_{\alpha} - z^{-1}).$$

We will regard Theorem 1 as embracing both cases.

The next fact we need is the following multiplication identity.

Theorem 2. Let $c \in R^*$ and let $f \in L^1(T)$. Then

$$D_n[fc|1] = D_n[f|c] D_n[c|1].$$

Proof. Let $h(\theta) = f(\theta)c(\theta)$. Then

$$\tilde{f}(j,k) = \frac{1}{2\pi} \int_T h(\theta) \left\{ \sum_{\alpha} \psi^{\wedge}(j, -\alpha) e^{-i\alpha\theta} \right\} \left\{ \sum_{\beta} \varphi^{\wedge}(k, \beta) e^{i\beta\theta} \right\} d\theta,$$

$$[\tilde{f}(j,k)]^{\sim} = [\psi^{\wedge}(j, -\alpha)] [h^{\wedge}(\alpha-\beta)] [\varphi^{\wedge}(k, \beta)]^t,$$

where all matrices here are $(n+1) \times (n+1)$. Taking determinants we find that

$$D_n[f|c] = \det[\psi^{\wedge}(j, -\alpha)] D_n[fc|1] \det[\varphi^{\wedge}(k, \beta)].$$

In the special case $f = 1$ we obtain

$$1 = \det[\psi^{\wedge}(j, -\alpha)] D_n[c|1] \det[\varphi^{\wedge}(k, \beta)].$$

Inserting this we obtain our desired result.

We can now prove the refined Szegö theorem. Let A be as in Lecture III and let

$$c(\theta) \in WH(A) .$$

It is easy to see that we can write $c(\theta)$ in the form

$$c(\theta) = c_1(\theta) f(\theta) g(\theta)$$

where $c_1(\theta) \in A$ and satisfies Kac's condition,

$$|c_1^\wedge(0)| > \sum_{k \neq 0} |c^\wedge(k)| ,$$

and where

$$f(z) = \prod_1^v (\xi_\alpha - z)$$

$$g(z) = \prod_1^\mu (\zeta_\beta - z^{-1}) ,$$

etc. By Theorem 2

$$D_n[c|1] = D_n[f|gc_1] D_n[g|c_1] D[c_1|1] .$$

In addition we have the elementary identities

$$G(ab) = G(a) G(b) ,$$

$$E[ab|ab] = E[a|a] E[a|b]^2 E[b|b] .$$

Combining our various results we obtain the desired formula.

Ultraspherical polynomials. For $\nu > 0$ let

$\{W_\nu(n, x)\}_{n=0}^\infty$ be orthogonal polynomials relative to the weight function $\Omega_\nu(dx) = (1-x^2)^{\nu-\frac{1}{2}} dx$ on $-1 \leq x \leq 1$ normalized by the condition

$$W_\nu(n, 1) = 1 .$$

The orthogonality conditions then are

$$\int_{-1}^1 W_\nu(n, x) W_\nu(m, x) \Omega_\nu(dx) = \frac{\delta(n, m)}{w_\nu(n)} .$$

The $W_\nu(n, x)$ are the ultraspherical polynomials of index ν with an unconventional normalization. Let

$$\int_{-1}^1 W_\nu(k, x) W_\nu(m, x) W_\nu(n, x) \Omega_\nu(dx) = c_\nu(k, m, n) ;$$

then

$$c_\nu(k, m, n) \geq 0 .$$

This remarkable fact, which implies that the $\{W_\nu(n, x)\}_0^\infty$ behave rather like characters on a compact group, makes it possible to extend to ultraspherical polynomials a number of results from harmonic analysis which cannot be extended to orthogonal polynomials in general.

Let for $f \in L^1[\Omega_\nu]$

$$\hat{f}^\wedge(j, k) = [w(j)w(k)]^{\frac{1}{2}} \int_{-1}^1 f(x) W_\nu(j, x) W_\nu(k, x) \Omega_\nu(dx) ,$$

and set

$$D_n[f] = [f^\wedge(j,k)]_{j,k=0,1,\dots,n}.$$

Further for $f(x)$ continuous and not zero on $-1 \leq x \leq 1$ let

$$G[n,f] = \exp \int_{-1}^1 \log f(x) \sum_{k=0}^n W_v(n,x)^2 \Omega_v(dx),$$

$$E[f] = \exp \frac{1}{2} \sum_{k=1}^{\infty} k f_\lambda^\wedge(k)^2.$$

Here

$$f_\lambda^\wedge(k) = \frac{1}{\pi} \int_0^\pi \log f(\cos \theta) e^{-ik\theta} d\theta$$

The arguments sketched above for the trigonometric case can now be made to yield the following result. See [5] and [12]. Note that the first of these papers was written in collaboration with Jeffrey Davis.

Theorem 3. Let $f(x) = \sum_0^\infty b(k) W_v(k,x)$ where

$$\sum |b(k)| < \infty, \quad \sum k |b(k)|^2 < \infty.$$

Assume further that

$$f(x) \neq 0 \quad -1 \leq x \leq 1.$$

Then

$$\lim_{n \rightarrow \infty} \frac{D_n(f)}{G(n,f)} = E[f].$$

Note that since $|W_\nu(n, x)| \leq 1$, $-1 \leq x \leq 1$, $n = 0, 1, \dots$, $f(x)$ is necessarily continuous. If $f(x)$ is subjected to a further mild restriction, namely,

$$\int_{-1}^1 |f(1) - f(x)| (1-x)^{-3/2} dx < \infty,$$

$$\int_{-1}^1 |f(x) - f(-1)| (x+1)^{3/2} dx < \infty,$$

one can show that if

$$G(f) = \exp \frac{1}{\pi} \int_0^\pi \log f(\cos \theta) d\theta$$

then

$$G[n, f] \cong G[f]^{n+(2\nu-1)/2} [f(1)f(-1)]^{-(2\nu-1)/4} \text{ as } n \rightarrow \infty.$$

APPENDIX

On the formulas of Kac and Achiezer

In his 1954 paper Kac after giving a new demonstration of the refined Szegő limit theorem applied his methods to the case where the underlying group is the line instead of the circle. More recently this subject has been taken up by Achiezer in 1964. A somewhat improved version of Achiezer's results is given in Professor Kac's lectures.

In this note we will describe very briefly and without proof a generalization of the formulas of Kac and Achiezer.

Let $\hat{c}_a(\xi)$ be defined for $-\infty < \xi < \infty$ satisfy

$$a. \quad \hat{c}_a(\xi) \in C(-\infty, \infty)$$

where $C(-\infty, \infty)$ is the set of all complex continuous functions on $(-\infty, \infty)$. Let

$$\hat{c}(\xi) = \delta(\xi) - \hat{c}_a(\xi)$$

where $\delta(\xi)$ is the Dirac delta functions. Consider the finite section Toeplitz operator

$$(1) \quad \hat{c} * \hat{f} \cdot (\xi) \quad 0 \leq \xi \leq r$$

where $\hat{f}(\xi) = f_s \delta(\xi) + \hat{f}_a(\xi)$. Here f_s is a constant and

$\hat{f}_a(\xi) \in L^1(0, r)$. It follows from the theory of Fredholm equations

that the operator (1) is invertible if and only if the Fredholm determinant $D(r) \neq 0$, where

$$D(r) = 1 + \sum_{n=1}^{\infty} \frac{(-1)^n}{n!} \int \dots \int \det[c_a^{\wedge}(\xi_i - \xi_j)] d\xi_1 \dots d\xi_n.$$

Let us now assume that

$$b. \quad \int_{-\infty}^{\infty} |c_a^{\wedge}(\xi)| d\xi < \infty, \quad \int_{-\infty}^{\infty} |c_a^{\wedge}(\xi)|^2 |\xi| d\xi < \infty.$$

We set

$$c(t) = \int_{-\infty}^{\infty} c_a^{\wedge}(\xi) e^{it\xi} d\xi = 1 - \int_{-\infty}^{\infty} c_a^{\wedge}(\xi) e^{it\xi} d\xi.$$

We finally assume that

$$c. \quad c(t) \neq 0, \quad -\infty < t < \infty,$$

$$[\arg c(t)]_{-\infty}^{\infty} = 0.$$

Under the assumptions a.b. and c. we show that

$$(2) \quad \lim_{r \rightarrow \infty} D(r) G^{-r} = E$$

where

$$(3) \quad G = \lim_{T \rightarrow \infty} \exp \frac{1}{2\pi} \int_{-T}^T \left(1 - \frac{t^2}{T^2}\right) \log c(t) dt,$$

and

$$(4) \quad E = \exp \int_0^{\infty} \gamma(\xi) \gamma(-\xi) \xi d\xi.$$

Here

$$\log c(t) = \int_{-\infty}^{\infty} \gamma(\xi) e^{it\xi} d\xi .$$

The arguments used in proving (2) are somewhat like those of Achiezer, except that the theory of finite section Wiener-Hopf equations on the line, taken as a special case from [11], is used to replace Achiezer's estimates. This yields (2) with a formula for E which reduces to Achiezer's if $c_a^\wedge$ is Hermitian. The passage to (4) is effected by a new identity. The analogue of this identity for the circle case is also new, and in this case it is more or less equivalent to the identity of Szegö mentioned at the end of Lecture III. The condition $c_a^\wedge(\xi) \in C(-\infty, \infty)$ can be considerably relaxed.

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SELF-ADJOINT TOEPLITZ OPERATORS

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Let $\mathcal{H}$ be an infinite dimensional separable complex Hilbert space. A bounded linear operator S on $\mathcal{H}$ is a simple shift if there exists a vector e_0 in $\mathcal{H}$ such that $\{S^j e_0\}_{j=0}^{\infty}$ is a complete orthonormal set. There is in fact a one-to-one correspondence between simple shifts S and (ordered) complete orthonormal sets $\{e_j\}_{j=0}^{\infty}$ in $\mathcal{H}$; S corresponds to $\{e_j\}_{j=0}^{\infty}$ if and only if $S e_j = e_{j+1}$ for $j = 0, 1, 2, \dots$. Simple shifts S have, in addition, the following properties:

- i) $S^* S = I$, that is, S is an isometry.
- ii) $S S^*$ is the orthogonal projection on $\{e_0\}^{\perp}$.
- iii) $S^* e_0 = 0$.

Examples.

i) Let ℓ^2 be sequential Hilbert space, set $e_j = (\delta_{0j}, \delta_{1j}, \delta_{2j}, \dots)$, $j = 0, 1, 2, \dots$, where δ is the Kronecker delta symbol. Clearly $\{e_j\}_{j=0}^{\infty}$ is a complete orthonormal set in ℓ^2 ; we define S by $S e_j = e_{j+1}$, $j = 0, 1, 2, \dots$. Then S can be represented by the infinite matrix

$$\begin{pmatrix} 0 & 0 & 0 & \dots \\ 1 & 0 & 0 & \dots \\ 0 & 1 & 0 & \dots \\ & 0 & 1 & \dots \\ \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots \end{pmatrix}$$

Clearly $S^* e_j = e_{j-1}$, where $e_{-1} = 0$, so S^* can be represented by the infinite matrix

$$\begin{pmatrix} 0 & 1 & 0 & 0 & \dots \\ 0 & 0 & 1 & 0 & \dots \\ 0 & 0 & 0 & 1 & \dots \\ \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots \end{pmatrix}$$

S is the "creation" and S^* the "annihilation" operator of Quantum Mechanics.

ii) Let H^2 be the Hardy space of L^2 functions on the unit circle of the form

$$f(e^{i\theta}) \sim \sum_{j=0}^{\infty} f_j e^{ij\theta}, \text{ with}$$

$$\|f\|^2 = \left[\frac{1}{2\pi} \int_{-\pi}^{\pi} |f(e^{i\theta})|^2 d\theta \right]^{\frac{1}{2}}.$$

Set $e_j(e^{i\theta}) = e^{ij\theta}$, so $\{e_j\}_{j=0}^{\infty}$ is a complete orthonormal set in H^2 and $S: f(e^{i\theta}) \rightarrow e^{i\theta} f(e^{i\theta})$ is the simple shift corresponding to $\{e_j\}_{j=0}^{\infty}$.

It is easily checked that $S^*: f(e^{i\theta}) \rightarrow e^{-i\theta}(f(e^{i\theta}) - f_0)$.

iii) Let $H = L^2(0, \infty)$ and define the Laguerre functions $\{\Phi_j\}_{j=0}^{\infty}$ by $\Phi_j(t) = e^{-t/2} L_j(t)$, $j = 0, 1, \dots$ where L_j is the j -th Laguerre polynomial. Thus we have the generating function relation

$$\sum_{j=0}^{\infty} \Phi_j(t) u^j = (1-u)^{-1} \exp \left[-\frac{1}{2} \left(\frac{1+u}{1-u} \right) t \right],$$

$$|u| < 1, 0 \leq t < \infty.$$

Then $\{\Phi_j\}_{j=0}^{\infty}$ is a complete orthonormal set in $L^2(0, \infty)$ with, say,

associated shift S . We will derive a concrete representation for S .

We introduce the Fourier-Plancherel operator F on $L^2(-\infty, \infty)$, defined by

$$Ff(x) = \lim_{T \rightarrow \infty} (2\pi)^{-\frac{1}{2}} \int_{-T}^T e^{-ixt} f(t) dt,$$

so the adjoint $F^* = F^{-1}$ is given by

$$F^*f(x) = \lim_{T \rightarrow \infty} (2\pi)^{-\frac{1}{2}} \int_{-T}^T e^{ixt} f(t) dt.$$

Define the projection operator P_+ on $L^2(-\infty, \infty)$ to $L^2(0, \infty)$ by $P_+ : f(x) \rightarrow \chi(x)f(x)$, where χ is the characteristic function of $(0, \infty)$. From the generating function relation it follows that

$$(F^*P_+\Phi_j)(x) = (2\pi)^{-\frac{1}{2}} \frac{1}{(\frac{1}{2} - ix)} \left(\frac{ix + \frac{1}{2}}{ix - \frac{1}{2}} \right)^j$$

$j = 0, 1, 2, \dots$

Thus

$$(F^*P_+S\Phi_j)(x) = \frac{ix + \frac{1}{2}}{ix - \frac{1}{2}} (F^*P_+\Phi_j)(x)$$

$j = 0, 1, 2, \dots$ and so

$$(1) \quad (F^*P_+Sf)(x) = \frac{ix + \frac{1}{2}}{ix - \frac{1}{2}} (F^*P_+f)(x), \quad -\infty < x < \infty,$$

for all $f \in L^2(0, \infty)$.

Finally, this implies that

$$SF(x) = f(x) - \int_0^\infty e^{\frac{t-x}{2}} \chi(x-t)f(t) dt,$$

$f \in L^2(0, \infty)$.

We define Toeplitz and Hankel operators (relative to a simple shift) in such a way that the operators have matrix representations that are infinite Toeplitz or Hankel matrices respectively. This definition of Toeplitz operator is due to Halmos.

Definition 1. Suppose S is a simple shift on H .

- i) A bounded operator T on H is S -Toeplitz if $S^*TS = T$.
- ii) A bounded operator H on H is S -Hankel if $S^*H = HS$.

Examples i) If p and q are polynomials then $p(S) + q(S^*)$ and

$[p(S)]^*q(S)$ are S-Toeplitz. This is so since

$$S^*(S^j S^k)S = S^*j(S^*S)S^k = S^*j S^k,$$

so $S^*j S^k$ is S-Toeplitz for $j, k = 0, 1, 2, \dots$.

ii) Fix an L^2 function w on the unit circle and define T_w and H_w on polynomials in H^2 by

$$\langle T_w f, g \rangle = \frac{1}{2\pi} \int_{-\pi}^{\pi} w(e^{i\theta}) f(e^{i\theta}) g^*(e^{i\theta}) d\theta$$

and

$$\langle H_w f, g \rangle = \frac{1}{2\pi} \int_{-\pi}^{\pi} w(e^{i\theta}) f(e^{-i\theta}) g^*(e^{i\theta}) d\theta$$

for all polynomials f and all g in H^2 . Let S be as described in example ii) above.

Suppose T_w is a bounded operator and thus has a continuous extension to all of H^2 . For all polynomials f, g , $\langle S^* T_w S f, g \rangle = \langle T_w S f, S g \rangle = \langle H_w f, g \rangle$ so $S^* T_w S = T_w$ and T_w is S-Toeplitz.

Similarly, suppose H_w is a bounded operator and thus can be extended to all of H^2 . For all polynomials f, g , $\langle S^* H_w f, g \rangle = \langle H_w f, S g \rangle = \langle H_w S f, g \rangle$, so $S^* H_w = H_w S$, and H_w is S-Hankel.

We shall use T_w and H_w (for suitable choices of w) as our "standard" representations for Toeplitz and Hankel operators. Note that, with $e_j(e^{i\theta}) = e^{ij\theta}$, $w(e^{i\theta}) \sim \sum_{-\infty}^{\infty} w_j e^{ij\theta}$, we have $\langle T_w e_j, e_k \rangle = w_{k-j}$ and $\langle H_w e_j, e_k \rangle = w_{k+j}$, $j, k = 0, 1, 2, \dots$. It is clear that H_w does not depend on w_{-j} $j=1$.

Thus T_w and H_w have matrix representations of the form $[w_{k-j}]_{j,k=0}^{\infty}$ and $[w_{k+j}]_{j,k=0}^{\infty}$ respectively; that is they have matrix representations that are of infinite Toeplitz and infinite Hankel type respectively.

Note. We associate an L^2 function $w(e^{i\theta}) \sim \sum_{-\infty}^{\infty} w_j e^{ij\theta}$ with any S-Toeplitz operator T by specifying

$$w_j = \begin{cases} \langle T e_0, S^j e_0 \rangle & j = 0, 1, 2, \dots \\ \langle T S^j e_0, e_0 \rangle & j = -1, -2, \dots \end{cases}$$

With any S-Hankel operator H we associate an H^2 function $w(e^{i\theta}) \sim \sum_0^\infty w_j e^{ij\theta}$, where

$$w_j = \langle H e_0, S^j e_0 \rangle \quad j = 0, 1, 2, \dots$$

(Bessel's inequality guarantees that $\sum |w_j|^2$ is finite in both cases).

Theorem 1. Suppose S is a simple shift on the Hilbert space $\mathcal{H}$ and that T is S-Toeplitz and H is S-Hankel on $\mathcal{H}$. Let U be the unitary transformation of $\mathcal{H}$ onto H^2 given by

$$\begin{aligned} U: f &\sim \sum_{j=0}^\infty \langle f, S^j e_0 \rangle S^j e_0 \\ &\rightarrow (Uf)(e^{i\theta}) \sim \sum_{j=0}^\infty \langle f, S^j e_0 \rangle e^{ij\theta}. \end{aligned}$$

Then $UTU^{-1} = T_w$ and $UHU^{-1} = H_w$ where w is associated with T in the first statement and with H in the second.

Proof. Suppose T is S-Toeplitz. Then $\langle TS^j e_0, S^k e_0 \rangle = \langle TS^{j-k} e_0, e_0 \rangle = w_{k-j}$ if $j \geq k$. Similarly $\langle TS^j e_0, S^k e_0 \rangle = w_{k-j}$ if $j < k$. Thus

$$\langle Tf, g \rangle = \frac{1}{2\pi} \int_{-\pi}^{\pi} w(e^{i\theta}) \bar{f}(e^{i\theta}) g(e^{i\theta}) d\theta$$

for all polynomials f and g, and $UTU^{-1} = T_w$.

The proof that $UHU^{-1} = H_w$ follows similarly.

It is clear from theorem 1 that any S-Toeplitz (or S-Hankel) operator is unitarily equivalent to a T_w operator (or H_w operator) on H^2 . We shall next show that there are interesting examples of S-Toeplitz and S-Hankel operators other than those that are obviously related to $[w_{k-j}]_{j,k=0}^\infty$ or $[w_{k+j}]_{j,k=0}^\infty$.

An operator $\mathcal{J}$ on $L^2(0, \infty)$ to $L^2(0, \infty)$ of the form

$$(\mathcal{J}f)(x) = \int_0^\infty K(x-y)f(y) dy,$$

where $K \in L^1(-\infty, \infty)$ is a Wiener-Hopf integral operator. More generally we shall be interested in operators on $L^2(0, \infty)$ to $L^2(0, \infty)$ of the form $\mathcal{J} = P_+ F M_W F^* P_+$, where F, P_+ are as before, W is in $L^\infty(-\infty, \infty)$, and

$$M_W: f(x) \in L^2(-\infty, \infty) \rightarrow W(x)f(x) \in L^2(-\infty, \infty).$$

These are generalized Wiener-Hopf operators. For example, the operator

$$f(x) \in L^2(0, \infty) \rightarrow \frac{1}{\pi i} \text{P.V.} \int_0^\infty \frac{f(t)}{x-t} dt \in L^2(0, \infty)$$

is of this type. We will also consider operators on $L^2(0, \infty)$ to $L^2(0, \infty)$ of the form $\mathcal{H} = P_+ F M_W F P_+$, which generalizes integral operators of the form

$$f(x) \in L^2(0, \infty) \rightarrow \int_0^\infty K(x+y)f(y) dy \in L^2(0, \infty),$$

where $K \in L^1(-\infty, \infty)$.

Since $(F^2 f)(x) = f(-x)$, we note that $\mathcal{H} = 0$ if W is a constant.

Theorem 2. Suppose $\mathcal{J}$ and $\mathcal{H}$ are as above, let $\{\Phi_j\}_{j=0}^\infty$ be the Laguerre functions and define the shift S by $S\Phi_j = \Phi_{j+1}$, $j = 0, 1, 2, \dots$. Define the unitary operator U on $L^2(0, \infty)$ to H^2 by

$$U: f \sim \sum_{j=0}^\infty \langle f, \Phi_j \rangle \Phi_j \rightarrow (Uf)(e^{i\theta}) \sim \sum_{j=0}^\infty \langle f, \Phi_j \rangle e^{ij\theta}.$$

Then

i) $\mathcal{J}$ is S-Toeplitz and $U\mathcal{J}U^{-1} = T_W$, where

$$w\left(\frac{ix + \frac{1}{2}}{ix - \frac{1}{2}}\right) = W(x).$$

ii) $\mathcal{H}$ is S-Hankel and $U\mathcal{H}U^{-1} = H_W$, where

$$\frac{\frac{1}{2} + ix}{\frac{1}{2} - ix} w\left(\frac{ix + \frac{1}{2}}{ix - \frac{1}{2}}\right) = W(x).$$

Proof. $\langle \mathcal{J} \Phi_k, \Phi_j \rangle = \langle P_+ F M_W F^* P_+ \Phi_k, \Phi_j \rangle$

$$= \langle M_W F^* P_+ \Phi_k, F^* P_+ \Phi_j \rangle, \text{ which by (1)}$$

$$= \frac{1}{2\pi} \int_{-\infty}^{\infty} W(x) \left(\frac{ix + \frac{1}{2}}{ix - \frac{1}{2}} \right)^k \left[\left(\frac{ix + \frac{1}{2}}{ix - \frac{1}{2}} \right)^j \right]^* \frac{dx}{x^2 + \frac{1}{4}}.$$

We set $e^{i\theta} = \frac{ix + \frac{1}{2}}{ix - \frac{1}{2}}$, so $d\theta = \frac{dx}{x^2 + \frac{1}{4}}$.

Then $\langle \mathcal{J} \Phi_k, \Phi_j \rangle =$

$$\frac{1}{2\pi} \int_{-\pi}^{\pi} w(e^{i\theta}) e^{i\theta k} e^{-i\theta j} d\theta \text{ for } j, k = 0, 1, 2, \dots,$$

so $U \mathcal{J} U^{-1} = I_W$.

Similarly, $\langle \mathcal{H} \Phi_k, \Phi_j \rangle =$

$$\begin{aligned} \langle P_+ F M_W F^* P_+ \Phi_k, \Phi_j \rangle &= \langle M_k F^* P_+ \Phi_k, F^* P_+ \Phi_j \rangle \\ &= \frac{1}{2\pi} \int_{-\infty}^{\infty} W(x) \left[\frac{1}{\frac{1}{2} - ix} \left(\frac{ix + \frac{1}{2}}{ix - \frac{1}{2}} \right)^k \right]^* \\ &\quad \left[\frac{1}{\frac{1}{2} - ix} \left(\frac{ix + \frac{1}{2}}{ix - \frac{1}{2}} \right)^j \right]^* dx \\ &= \frac{1}{2\pi} \int_{-\infty}^{\infty} W(x) \frac{\frac{1}{2} - ix}{\frac{1}{2} + ix} \left[\left(\frac{ix + \frac{1}{2}}{ix - \frac{1}{2}} \right)^{j+k} \right]^* \frac{dx}{x^2 + \frac{1}{4}} \\ &= \frac{1}{2\pi} \int_{-\pi}^{\pi} w(e^{i\theta}) e^{-i\theta j} e^{-i\theta k} d\theta \text{ for} \end{aligned}$$

$j, k = 0, 1, 2, \dots$, so $U \mathcal{H} U^{-1} = H_W$.

Examples i) Let $W(x) = (x^2 + \frac{1}{4})^{-1}$. Then

$$(\mathcal{J} f)(x) = \int_0^{\infty} e^{-\frac{1}{2}|x-t|} f(t) dt \text{ and}$$

$$(\mathcal{H} f)(x) = \int_0^{\infty} e^{-\frac{1}{2}(x+t)} f(t) dt$$

for all $f \in L^2(0, \infty)$.

Put $e^{i\vartheta} = \frac{ix + \frac{1}{2}}{ix - \frac{1}{2}}$. Then $W(x) = 2(1 - \cos \vartheta)$. Thus $\mathcal{J}$ is unitarily equivalent to T_w , where $w(e^{i\vartheta}) = 2 - 2 \cos \vartheta$. Also $\mathcal{H}$ is unitarily equivalent to H_w , with (now) $w(e^{i\vartheta}) = -2e^{-i\vartheta}(1 - \cos \vartheta)$, is unitarily equivalent to the Hankel matrix

$$\begin{pmatrix} 1 & 0 & 0 & \dots \\ 0 & 0 & \dots & \\ 0 & \dots & \dots & \\ \dots & \dots & \dots & \dots \end{pmatrix}.$$

ii) Consider $\mathcal{H}$ defined by $(\mathcal{H}f)(x) = \int_0^\infty \frac{e^{-\frac{1}{2}(x+y)}}{x+y} f(y) dy$, $f \in L^2(0, \infty)$.

Then

$$\begin{aligned} \langle \mathcal{H} \Phi_k, \Phi_j \rangle &= \int_0^\infty \int_0^\infty \frac{e^{-\frac{1}{2}(x+y)}}{x+y} \Phi_k(y) \Phi_j(x) dx dy \\ &= \int_{\frac{1}{2}}^\infty \int_0^\infty \int_0^\infty e^{-(x+y)t} \Phi_k(y) \Phi_j(x) dx dy dt \\ &= \int_{\frac{1}{2}}^\infty \frac{(t - \frac{1}{2})^{j+k}}{(t + \frac{1}{2})^{j+k+2}} dt \end{aligned}$$

Upon setting $x = \frac{t - \frac{1}{2}}{t + \frac{1}{2}}$ we find that

$$\langle \mathcal{H} \Phi_k, \Phi_j \rangle = \int_0^1 s^{j+k} ds = \frac{1}{j+k+1},$$

$j, k = 0, 1, 2, \dots$

Thus the operator $\mathcal{H}$ is unitarily equivalent to the Hilbert matrix $[\frac{1}{j+k+1}]_{j,k=0}^\infty$. I used this equivalence in a fundamental way in my papers on the Hilbert matrix. It turns out that $\mathcal{H}$ is a monotone function of a tractable second order differential operator. Upon diagonalizing this differential operator, it is possible to diagonalize $\mathcal{H}$ and the Hilbert matrix.

We shall be mainly concerned with Toeplitz operators here and shall

not go into Nehari's and Hartman's results on the boundedness and complete continuity of Hankel operators. We content ourselves here with a quick proof of a result of Hartman and Wintner's:

Theorem 3. Suppose H is S -Hankel. Then 0 is in the spectrum of H .

Proof. Suppose H^{-1} exists as a bounded operator on all of $\mathcal{H}$. H is onto so there exists $x \in \mathcal{H}$, $x \neq 0$, $Hx = e_0$. But now $HSx = SHx = S^*e_0 = 0$. H is one to one, so $Sx = 0$. But then $x = S^*Sx = 0$, a contradiction.

We fix attention on a simple shift S in H , with $S^*e_0 = 0$. Suppose h is an H^∞ function, that is, h is in H^2 and is essentially bounded. Then $h(S)$ is a well-defined bounded operator in $\mathcal{H}$ since $f(e^{i\theta}) \rightarrow h(e^{i\theta})f(e^{i\theta})$ is well-defined and bounded in H^2 .

Theorem 4. Suppose h is an H^∞ function that is not a.e. constant.

Then

i) $h(S)$ has no eigenvalues.

ii) $[h(s)]^*[(I - uS)^{-1}e_0] = h^*(u^*)[(I - uS)^{-1}e_0]$ for all complex u with $|u| < 1$. e.g. If $h(z) = z$, the spectrum of S^* is the closed unit disk.

Proof. Since S is an isometry, $(I - uS)$ is invertible if $|u| < 1$.

Suppose f is in $\mathcal{H}$ and let U be as in theorem 1. Then

$$\begin{aligned} \langle h(S)f, (I - uS)^{-1}e_0 \rangle &= \frac{1}{2\pi} \int_{-\pi}^{\pi} h(e^{i\theta})(Uf)(e^{i\theta})(1 - u^*e^{-i\theta})^{-1} d\theta \\ &= h(u^*)(Uf)(u^*) \text{ for all } u, |u| < 1. \end{aligned}$$

Assume $h(S)f = 0$. Then by the above $h(u^*)Uf(u^*) = 0$ for all u , $|u| < 1$, so $Uf = 0$ and $f = 0$. This proves i).

We turn to the proof of ii). Let u, v satisfy $|u| < 1, |v| < 1$. Then, again by the above,

$$\langle [h(S)]^*(I - uS)^{-1}e_0, (I - vS)^{-1}e_0 \rangle =$$

$$\begin{aligned}
\langle (I - uS)^{-1} e_0, h(S)(I - vS)^{-1} e_0 \rangle &= \\
h^*(u^*)(I - v^*u)^{-1} & \\
= h^*(u^*) \langle (I - uS)^{-1} e_0, (I - vS)^{-1} e_0 \rangle.
\end{aligned}$$

Also, $0 = \langle f, (I - vS)^{-1} e_0 \rangle = f(v^*)$ for all $|v| < 1$ implies $f = 0$, so the linear span of $\{(I - vS)^{-1} e_0 : |v| < 1\}$ is dense in H . Thus

$$[h(S)]^*(I - uS)^{-1} e_0 = h^*(u^*)(I - uS)^{-1} e_0, \quad |u| < 1,$$

which proves ii). ii) will be used later to derive a generating function formula for the resolvent of an S -Toeplitz operator.

We will need the following result, which is a weak form of theorem of Szegő and F. Riesz (see Grenander and Szegő's book, "Toeplitz Forms and their Applications," page 24):

Lemma. Suppose w is a positive L^∞ function on the unit circle that is bounded away from 0, i.e. there exists $\delta > 0$ such that $\delta \leq w$.

Define h in the unit disk by

$$h(u) = \exp \frac{1}{4\pi} \int_{-\pi}^{\pi} \log w(e^{i\theta}) \frac{e^{i\theta} + u}{e^{i\theta} - u} d\theta.$$

Then

$$i) \quad h(e^{i\theta}) = \lim_{r \rightarrow 1^-} h(re^{i\theta}) \text{ exists a.e.}$$

and defines an H^2 function h ,

$$ii) \quad w(e^{i\theta}) = |h(e^{i\theta})|^2 \text{ a.e.,}$$

$$iii) \quad h \text{ and } 1/h \text{ are in } H^\infty.$$

We will not prove the lemma, but indicate the plausibility of ii), given i) as follows:

$$|h(re^{i\psi})|^2 = \exp \frac{1}{2\pi} \int_{-\pi}^{\pi} \log w(e^{i\vartheta}) \frac{1-r^2}{1-2r \cos(\vartheta-\psi) + r^2} d\vartheta$$

tends to $\exp \log w(e^{i\psi}) = w(e^{i\psi})$ a.e. as $r \rightarrow 1$.

Previously we have shown that if p, q are polynomials, then $T = [p(S)]^* q(S)$ is S -Toeplitz. If p, q are H^∞ the same conclusion holds. We prove a converse statement, under the assumption that T is a positive S -Toeplitz operator.

Theorem 5. Suppose T is S -Toeplitz and suppose that there exists $\delta > 0$ such that $\langle Tf, f \rangle \geq \delta \langle f, f \rangle$ for all f in $\mathcal{K}$ (so in particular T is self-adjoint). Let w be associated with T as in the note preceding theorem 1 and let $w = |h|^2$ as in the above lemma.

Then $T = [h(S)]^* h(S)$. $h(S)$ and $[h(S)]^*$ have bounded inverses, and $T^{-1} = [h(S)]^{-1} [h(S)^*]^{-1}$.

Proof. The $\mathcal{K}$ -inequality $\|T\| \langle f, f \rangle \geq \langle Tf, f \rangle \geq \delta \langle f, f \rangle$ for all f in $\mathcal{K}$ is carried by U into the H^2 -inequality

$$\|T\| \frac{1}{2\pi} \int_{-\pi}^{\pi} |f(e^{i\vartheta})|^2 d\vartheta \geq \frac{1}{2\pi} \int_{-\pi}^{\pi} w(e^{i\vartheta}) |f(e^{i\vartheta})|^2 d\vartheta \geq \delta \frac{1}{2\pi} \int_{-\pi}^{\pi} |f(e^{i\vartheta})|^2 d\vartheta.$$

for all H^∞ functions f . Let $f(e^{i\vartheta}) = (1 - re^{i(\vartheta-\psi)})^{-1}$, where $0 \leq r < 1$.

Then

$$\|T\| \geq \frac{1}{2\pi} \int_{-\pi}^{\pi} w(e^{i\vartheta}) \frac{1-r^2}{1-2r \cos(\vartheta-\psi) + r^2} d\vartheta \geq \delta.$$

Upon letting $r \rightarrow 1^-$ we see that $\|T\| \geq w(e^{i\psi}) \geq \delta$ a.e., so w satisfies the hypotheses of the lemma, and $w = |h|^2$ a.e., where $h, \frac{1}{h}$ are in H^∞ .

For all f, g in H^2

$$\langle Tf, g \rangle = \frac{1}{2\pi} \int_{-\pi}^{\pi} w(e^{i\vartheta}) f(e^{i\vartheta}) g^*(e^{i\vartheta}) d\vartheta$$

$$\begin{aligned}
&= \frac{1}{2\pi} \int_{-\pi}^{\pi} h(e^{i\theta}) f(e^{i\theta}) \left[h(e^{i\theta}) g(e^{i\theta}) \right]^* d\theta \\
&= \langle h(S)f, h(S)g \rangle = \langle [h(S)]^* h(S)f, g \rangle,
\end{aligned}$$

so $T = [h(S)]^* h(S)$. The remaining assertions of the theorem follow easily from the fact that h and $1/h$ are in H^∞ .

The next theorem was first proved (in greater generality) by Calderon-Spitzer-Widom and M. Krein. Our proof combines the result of theorem 4 on the eigenvalues of $[h(s)]^*$ with the factorization theorem 5 to derive a generating function for the resolvent of a positive S-Toeplitz T .

Theorem 6. Let T, w, h be as in theorem 5. Then

$$\begin{aligned}
\langle T^{-1}(I - uS)^{-1}e_0, (I - vS)^{-1}e_0 \rangle = \\
\left[(1 - uv^*)h^*(u^*)h(v^*) \right]^{-1}
\end{aligned}$$

for all u, v satisfying $|u| < 1, |v| < 1$.

Proof. From theorem 5 we have that

$$\begin{aligned}
\langle T^{-1}(I - uS)^{-1}e_0, (I - vS)^{-1}e_0 \rangle = \\
\langle [h(S)]^* \rangle^{-1} (I - uS)^{-1}e_0, [h(S)]^* \rangle^{-1} (I - vS)^{-1}e_0 \rangle,
\end{aligned}$$

which by theorem 4 ii)

$$\begin{aligned}
&= [h^*(u^*)h(v^*)]^{-1} \langle (I - uS)^{-1}e_0, (I - vS)^{-1}e_0 \rangle \\
&= \left[(1 - uv^*)h^*(u^*)h(v^*) \right]^{-1}.
\end{aligned}$$

We note for later reference the following:

Corollary. Suppose T is S-Toeplitz and self-adjoint on a Hilbert space $\mathcal{H}$. Define w on the unit circle as in the note preceding theorem 1.

Then for any z in the complex plane cut along the real semi-infinite interval $[\text{ess inf } w, \infty)$ and all u, v with $|u| < 1$, $|v| < 1$,

$$(2) \quad \langle (T - zI)^{-1} (I - uS)^{-1} e_0, (I - vS)^{-1} e_0 \rangle = \left[(1 - uv^*) h_z^*(u^*) h_z(v^*) \right]^{-1},$$

where

$$h_z(u) = \exp \frac{1}{4\pi} \int_{-\pi}^{\pi} \log (w(e^{i\theta}) - z) \frac{e^{i\theta} + u}{e^{i\theta} - u} d\theta$$

Proof. The result follows directly from theorem 6 if z , real, is less than $\text{ess inf } w$. The conclusion for z in the cut plane then follows from an analytic continuation argument.

The linear span of $\{(I - uS)^{-1} e_0 : |u| < 1\}$ is dense in $\mathcal{H}$ so (2) gives us an effective grab on the resolvent of the self-adjoint operator T . We shall devote the remainder of these talks indicating how to proceed from (2) to a diagonalization of T . First we say what we mean by diagonalization.

Von Neumann Spectral theorem.

Let A be a bounded self-adjoint operator on a separable complex Hilbert space $\mathcal{H}$. Then there exists a finite Borel measure μ on $(-\infty, \infty)$, a μ -measurable function n on $(-\infty, \infty)$ to $\{j\}_{j=1}^{\infty} \cup \{\infty\}$ and a unitary operator W on $\mathcal{H}$ onto $\int_{-\infty}^{\infty} \mathcal{H}_{n(\lambda)}^2 d\mu(\lambda)$, where for each λ , $\mathcal{H}_{n(\lambda)}^2$ is sequential Hilbert space of dimension $n(\lambda)$.

$$\begin{aligned} W: f &\rightarrow \{f_j(\lambda)\}_{j=1}^{n(\lambda)} \\ g &\rightarrow \{g_j(\lambda)\}_{j=1}^{n(\lambda)} \end{aligned}$$

where the f_j and g_j are Borel functions such that

$$(3) \quad \langle b(A)f, g \rangle = \int_{-\infty}^{\infty} b(\lambda) \sum_{j=1}^{n(\lambda)} f_j(\lambda) g_j^*(\lambda) d\mu(\lambda)$$

for all bounded Baire functions b and all f, g in $\mathcal{H}$.

The pair (μ, n) is associated with A through the representation (3). μ is a spectral measure for A and n is the multiplicity function of A . n is clearly only determined μ -a.e. Suppose B is a bounded self-adjoint operator on a separable complex Hilbert space $\mathcal{H}$ and B has a spectral measure ν and multiplicity function m . Then A and B are unitarily equivalent if and only if μ and ν are mutually absolutely continuous and n and m are equal μ - (or ν -) almost everywhere. Thus (μ, n) is a complete set of unitary invariants of A . We list a few examples to convince one that (3) is a "diagonalization."

Examples i) Let $\mathcal{H}$ be 3-dimensional Hilbert space and suppose A is self-adjoint on $\mathcal{H}$. Then there exists a unitary operator T on $\mathcal{H}$ diagonalizing A , so

$$Tb(A)T^{-1}f = b(\lambda_1) \langle f, \phi_1 \rangle \phi_1 + b(\lambda_2) \langle f, \phi_2 \rangle \phi_2 + b(\lambda_3) \langle f, \phi_3 \rangle \phi_3$$

for all f in $\mathcal{H}$ and continuous functions b . $\lambda_1, \lambda_2, \lambda_3$ are the eigenvalues of A corresponding to the eigenvectors ϕ_1, ϕ_2, ϕ_3 respectively. Suppose $\lambda_1 = \lambda_2 \neq \lambda_3$. Then for all f, g in $\mathcal{H}$ and all continuous functions b on $(-\infty, \infty)$

$$\begin{aligned} \langle b(A)f, g \rangle &= \\ &= b(\lambda_1) [\langle Tf, \phi_1 \rangle \langle \phi_1, Tg \rangle \\ &\quad + \langle Tf, \phi_2 \rangle \langle \phi_2, Tg \rangle] \\ &\quad + b(\lambda_2) \langle Tf, \phi_3 \rangle \langle \phi_3, Tg \rangle \\ &= \int b(\lambda) \sum_{j=1}^{n(\lambda)} f_j(\lambda) g_j^*(\lambda) d\mu(\lambda), \end{aligned}$$

where μ consists of 2 unit point masses, one at λ_1 and one at λ_2 . The multiplicity function n is defined by

$$n(\lambda) = \begin{cases} 2 & \text{if } \lambda = \lambda_1 \\ 1 & \text{if } \lambda = \lambda_2 \\ 0 & \text{otherwise.} \end{cases}$$

ii) Let $A: f(t) \rightarrow tf(t)$ on $L^2(-1,1)$. Then

$$\langle b(A)f, g \rangle = \int_{-1}^1 b(t)f(t)g^*(t) dt$$

for all f, g in $L^2(-1,1)$. μ is Lebesgue measure on $[-1,1]$ and $n(\lambda) = 1$ a.e.. A is in diagonal form.

iii) Let $A: f(t) \rightarrow t^2 f(t)$ on $L^2(-1,1)$. Then

$$\begin{aligned} \langle b(A)f, g \rangle &= \int_{-1}^1 b(t^2)f(t)g^*(t) dt \\ &= \int_0^1 b(\lambda) \left[(2\lambda)^{-\frac{1}{2}} f(\lambda^{\frac{1}{2}}) g^*(\lambda^{\frac{1}{2}}) \right. \\ &\quad \left. + (2\lambda)^{-\frac{1}{2}} f(-\lambda^{\frac{1}{2}}) g^*(-\lambda^{\frac{1}{2}}) \right] d\lambda \end{aligned}$$

for all f, g in $\mathcal{K}$ and all continuous b . Thus μ is Lebesgue measure on $[0,1]$ and $n(\lambda) = 2$ a.e..

It is easy to see that A , when restricted to $L^2(0,1)$ has $n(\lambda) = 1$ a.e. on $[0,1]$.

We consider a self-adjoint Toeplitz operator T , with notation as in (2).

In 1954, Hartman and Wintner showed that the spectral measure μ of T has no point masses and the support of μ is the closed interval $[\text{ess inf } w, \text{ess sup } w]$. In 1959 Putnam showed that μ can be taken to be Lebesgue measure on $[\text{ess inf } w, \text{ess sup } w]$ provided certain subsidiary conditions are placed on w . The subsidiary conditions were shown to be superfluous by me in 1960, using the following result of Aronszajn and Donoghue:

Let $\mathcal{P}$ be the class of not identically zero functions Φ holomorphic and having non-negative imaginary part in the upper half-plane. Such Φ

have the following two representations:

i) There exists a unique triple $(\sigma[\infty], \beta, \sigma)$ consisting of a non-negative number $\sigma[\infty]$, a real number β and a Borel measure σ on $(-\infty, \infty)$ with $\int (1+t^2)^{-1} d\sigma(t) < \infty$ such that $\mu[\infty]$, β , and σ are not all null and with

$$(4) \quad \Phi(z) = \sigma[\infty]z + \beta + \int \left(\frac{1}{t-z} - \frac{1}{t^2+1} \right) d\sigma(t),$$

$$\text{Im } z > 0;$$

ii) There exists a unique pair $(\alpha, \{f\})$ consisting of a real number α and the class of all functions equal a.e. to a measurable function f satisfying $0 \leq f \leq 1$ with

$$(5) \quad \Phi(z) = \exp \left[\alpha + \int \left(\frac{1}{\xi-z} - \frac{\xi}{\xi^2+1} \right) f(\xi) d\xi \right],$$

$$\text{Im } z > 0.$$

Fix $\Phi \in P$. Suppose there is an f in $\{f\}$ that is of bounded variation on an open interval (a,b) with $f(\xi+0) - f(\xi-0) < 1$ for all ξ in (a,b) . Then σ is absolutely continuous on (r,s) .

Theorem 7. Suppose T is S-Toeplitz and T is not a multiple of the identity operator. Then the spectral measure of T is absolutely continuous. Sketch of proof: Fix u , $|u| < 1$. Then

$$\Phi(z) = \langle (T - zI)^{-1} (I - uS)^{-1} e_0, (I - uS)^{-1} e_0 \rangle,$$

$$\text{Im } z > 0,$$

defines Φ in P . Equation (3), with $b(\lambda) = (\lambda - z)^{-1}$, $f = g = (I - uS)^{-1} e_0$ gives an expression for $\Phi(z)$ of the form (4). Upon manipulation one can put the representation (2) (with $v = u$) for $\Phi(z)$ in the form (5). One can then invoke the Aronsjahn-Donoghue result to show that the measure σ defined on real Borel sets Δ by

$$\sigma(A) = \int_E \sum_{j=1}^{n(\lambda)} |f_j(\lambda)|^2 d\mu(\lambda),$$

where $W(I - uS)^{-1}e_0 = \{f_j(\lambda)\}$, is absolutely continuous. From this one can argue that μ is absolutely continuous. (See M. Rosenblum, The absolute continuity of Toeplitz's matrices, Pacific Journal Math. 10 (1960), pp. 987-996 for details.)

The information that the spectral measure μ of T is absolutely continuous with respect to Lebesgue measure together with the concrete expression (2) for the resolvent of T gives us a promising start towards diagonalizing T . By the von Neumann spectral theorem,

$$(6) \quad \langle (T - zI)^{-1}f, g \rangle = \int_E \frac{1}{\lambda - z} \sum_{j=1}^{n(\lambda)} f_j(\lambda) g_j^*(\lambda) d\lambda,$$

for all f, g in $\mathcal{H}$ and $\text{Im } z \neq 0$. E is the support of the spectral measure of T . The problem now is to find n and the mapping W , where

$$W: f \rightarrow \{f_j(\lambda)\}_{j=1}^{n(\lambda)}.$$

Now by (6),

$$\begin{aligned} & \lim_{\epsilon \downarrow 0} \frac{1}{2\pi i} \left[\langle (T - \lambda - i\epsilon)^{-1}f, g \rangle - \langle (T - \lambda + i\epsilon)^{-1}f, g \rangle \right] \\ &= \lim_{\epsilon \downarrow 0} \frac{1}{\pi} \int_E \frac{\epsilon}{(x - \lambda)^2 + \epsilon^2} \sum_{j=1}^{n(x)} f_j(x) g_j^*(x) dx \\ (7) \quad &= \text{a.e.} \begin{cases} \sum_{j=1}^{n(\lambda)} f_j(\lambda) g_j^*(\lambda) & \text{for } \lambda \in E \\ 0 & \text{for } \lambda \notin E \end{cases} \end{aligned}$$

Suppose $f = (I - uS)^{-1}e_0$ and $g = (I - vS)^{-1}e_0$, where $|u| < 1$ and $|v| < 1$. Then by (2),

$$\lim_{\epsilon \downarrow 0} \frac{1}{2\pi i} \left[\langle (T - \lambda - i\epsilon)^{-1}f, g \rangle - \langle (T - \lambda + i\epsilon)^{-1}f, g \rangle \right]$$

$$\begin{aligned}
&= \frac{1}{2\pi i} \frac{1}{1-uv^*} \lim_{\varepsilon \downarrow 0} \left[\frac{1}{h^*_{\lambda - i\varepsilon}(u^*)} \frac{1}{h_{\lambda + i\varepsilon}(v^*)} - \right. \\
&\quad \left. \frac{1}{h^*_{\lambda + i\varepsilon}(u^*)} \frac{1}{h_{\lambda - i\varepsilon}(v^*)} \right] \\
(8) &= \frac{1}{2\pi i} \frac{1}{1-uv^*} \lim_{\varepsilon \downarrow 0} \left\{ \frac{1}{h^*_{\lambda + i\varepsilon}(u^*)} \frac{1}{h_{\lambda + i\varepsilon}(v^*)} - \right. \\
&\quad \left. \left[\frac{h^*_{\lambda + i\varepsilon}(u^*)}{h^*_{\lambda - i\varepsilon}(u^*)} - \frac{h_{\lambda + i\varepsilon}(v^*)}{h_{\lambda - i\varepsilon}(v^*)} \right] \right\}.
\end{aligned}$$

This last expression equals (7). At this juncture, however, it is not clear how to untangle (8) so as to find n and W . Ismagilov in a 1964 Doklady note gave a description of n , but without complete proof. n is defined as the "index" of $\lambda - w$. The index of a real Lebesgue measurable function f on the unit circle is as follows:

Definition 2. Let $\Gamma = \{e^{i\theta} : f(e^{i\theta}) \geq 0\}$. Necessarily Γ satisfies exactly one of the following alternatives almost everywhere:

$A(0)$; Γ is empty or Γ is the unit circle; or

$A(n)$, Γ is the union of n disjoint closed arcs but is not the union of $n-1$ disjoint closed arcs. Here n is a positive integer; or

$A(\infty)$; none of the above hold.

The index $I(f)$ of f is x in case $A(x)$ holds.

We shall analytically implement the geometric idea of index by associating a holomorphic function F and then a singular measure μ with Γ . Define F by

$$\begin{aligned}
(9) \quad i\pi F(z) &= \exp \left(\frac{1}{2} i \int_{\Gamma} \frac{1 + ze^{i\theta}}{1 - ze^{i\theta}} d\theta \right) \\
&\quad - \cos \left(\frac{1}{2} \int_{\Gamma} d\theta \right), \quad |z| < 1.
\end{aligned}$$

The additive constant normalizes F so that $\text{Im } F(0) = 0$. F has non-negative real part in the unit disk, so there exists a measure μ on

the unit circle such that

$$(10) \quad F(z) = \int \frac{1 + ze^{i\alpha}}{1 - ze^{i\alpha}} d\mu(\alpha), \quad |z| < 1$$

Direct computation shows that $\lim_{r \rightarrow 1} \operatorname{Re} F(re^{i\theta}) = 0$ a.e., so μ is a singular measure, that is, it has null absolutely continuous part.

Furthermore μ is related to $I(f)$ as follows:

Theorem 8 i) $I(f)$ is equal to the dimension of $L^2(d\mu)$.

ii) Put $e_j = \int e^{-ij\alpha} d\mu(\alpha)$ for all integers j and define the $(m+1) \times (m+1)$ Toeplitz matrix M_m as $[e_{j-k}]_{j,k=0}^m$. $I(f)$ is equal to the smallest integer n such that $\det M_n = 0$; or if no such integer exists, then $I(f) = \infty$.

See M. Rosenblum, "A concrete spectral theory for self-adjoint Toeplitz operators" which shall appear in the American Journal of Mathematics for a proof of the above theorem and for details on the diagonalization we are now discussing. (9) enters into the picture since for almost all real

$$\begin{aligned} \frac{h^*_{\lambda + i0}(u^*)}{h^*_{\lambda - i0}(u^*)} &= \lim_{\varepsilon \downarrow 0} \frac{h^*_{\lambda + i\varepsilon}(u^*)}{h^*_{\lambda - i\varepsilon}(u^*)} \\ &= \lim_{\varepsilon \downarrow 0} \exp \frac{1}{4\pi} \int_{-\pi}^{\pi} [\log(w(e^{i\theta}) - \lambda + i\varepsilon) \\ &\quad - \log(w(e^{i\theta}) - \lambda - i\varepsilon)] \frac{1 + ue^{i\theta}}{1 - ue^{i\theta}} d\theta \\ &= \exp \frac{i}{2} \int_{\Gamma_\lambda} \frac{1 + ue^{i\theta}}{1 - ue^{i\theta}}, \text{ where} \\ \Gamma_\lambda &= \{e^{i\theta}: \lambda - w(e^{i\theta}) \geq 0\}. \end{aligned}$$

Thus by (9) and (10) there exists a singular measure μ_λ on the unit circle such that

$$(11) \quad \frac{1}{\pi i} \frac{h^* \lambda + i0(u^*)}{h^* \lambda - i0(u^*)} = i \theta_\lambda + \int \frac{1 + u e^{i\theta}}{1 - u e^{i\theta}} d\mu_\lambda(\theta)$$

where θ_λ is a real number.

Next we introduce the orthonormal polynomials

$\{p_j(e^{i\theta}, \lambda)\}_{j=0}^{n(\lambda)-1}$ obtained by applying the Gram-Schmidt process to $1, e^{i\theta}, e^{2i\theta}, \dots$ in $L^2(d\mu_\lambda)$. By theorem 8i) there are $n(\lambda)$ such $p_j(\cdot, \lambda)$. We are now in a position to diagonalize S-Toeplitz T.

Theorem 9. Suppose T is S-Toeplitz and not a multiple of the identity operator. Then $b(T)$ has a Von Neumann spectral representation as in (3) with μ Lebesgue measure on $[\text{ess inf } w, \text{ess sup } w]$ and $n(\lambda) = I(\lambda - w)$. W is defined by

$$W: (I - uS)^{-1} e_0 \rightarrow \left\{ \frac{\xi_j(u, \lambda)}{h^* \lambda + i0(u^*)} \right\}_{j=1}^{n(\lambda)}, \quad |u| < 1,$$

$$\xi_j(u, \lambda) = \int \frac{1}{1 - u e^{i\theta}} p_{j-1}^*(e^{i\theta}, \lambda) d\mu_\lambda(\theta),$$

where, of course, the closed linear span of $\{(I - uS)^{-1} e_0 : |u| < 1\}$ is $\mathcal{H}$.

Sketch of Proof. Suppose λ is in the support E of the spectral measure μ of T. Let $f = (I - uS)^{-1} e_0$ and $g = (I - vS)^{-1} e_0$, where $|u| < 1$, $|v| < 1$. Then by (7) and (8),

$$\sum_{j=1}^{n(\lambda)} f_j(\lambda) g_j^*(\lambda) =$$

$$\frac{1}{2\pi i} \frac{1}{1 - uv^*} \frac{1}{h^* \lambda + i0(u^*)} \frac{1}{h \lambda + i0(v^*)}$$

$$\left[\frac{h^* \lambda + i0(u^*)}{h^* \lambda - i0(u^*)} - \frac{h \lambda + i0(v^*)}{h \lambda - i0(v^*)} \right]$$

which by (11)

$$= \frac{1}{h^* \lambda + i0(u^*)} \frac{1}{h \lambda + i0(v^*)} \int \frac{1}{1 - u e^{i\theta}} \left(\frac{1}{1 - v e^{i\theta}} \right)^* d\mu_\lambda(\theta).$$

By the Parseval equality this

$$= \sum_{j=1}^{n(\lambda)} \frac{\xi_j(u, \lambda)}{h^*_{\lambda + i0}(u^*)} \left[\frac{\xi_j(v, \lambda)}{h^*_{\lambda + i0}(v^*)} \right]^*.$$

We can conclude that $f_j(\lambda) = \frac{\xi_j(u, \lambda)}{h^*_{\lambda + i0}(u^*)}$ for all j and thus conclude the proof.

Corollary. An S-Toeplitz operator T has multiplicity one if and only if

$$\Gamma_\lambda = \{e^{i\theta} : \lambda - w(e^{i\theta}) \geq 0\} \text{ is a.e. an arc } (e^{ia(\lambda)}, e^{ib(\lambda)}),$$

$b(\lambda) - a(\lambda) < 2\pi$ on the unit circle for each λ in $[\text{ess inf } w, \text{ess sup } w]$.

Define for such T

$$Y: (I - uS)^{-1} e_0 \rightarrow \left[(1 - ue^{ib(\lambda)}) h^*_{\lambda + i0}(u^*) \right]^{-1}$$

and

$$\rho(\lambda) = \frac{1}{\pi} \sin \left[\frac{1}{2} (b(\lambda) - a(\lambda)) \right]. \text{ Then}$$

$$\begin{aligned} \langle b(T)(I - uS)^{-1} e_0, (I - vS)^{-1} e_0 \rangle = \\ \int b(\lambda) \left[Y(I - uS)^{-1} e_0 \right](\lambda) \left[Y(I - vS)^{-1} e_0 \right]^*(\lambda) \\ \rho(\lambda) d\lambda \end{aligned}$$

for all bounded Baire functions b and u, v with $|u| < 1, |v| < 1$.

Proof.

$$\begin{aligned} & \frac{1}{\pi i} \exp \left[\frac{i}{2} \int_{\Gamma_\lambda} \frac{1 + ze^{i\theta}}{1 - ze^{i\theta}} d\theta \right] - \frac{1}{\pi i} \cos \left[\frac{1}{2} \int_{\Gamma_\lambda} d\theta \right] \\ &= \frac{1}{\pi i} \exp \left[\frac{i}{2} (b(\lambda) - a(\lambda)) \right] \frac{1 - ze^{ia(\lambda)}}{1 - ze^{ib(\lambda)}} \\ & \quad - \frac{1}{\pi i} \cos \left[\frac{1}{2} (b(\lambda) - a(\lambda)) \right] \\ &= \frac{1}{\pi} \sin \left[\frac{1}{2} (b(\lambda) - a(\lambda)) \right] \frac{1 + ze^{ib(\lambda)}}{1 - ze^{ib(\lambda)}}, \quad |z| < 1 \end{aligned}$$

so μ_λ consists of a point mass at $e^{ib(\lambda)}$ of total mass $\sin \left[\frac{1}{2} (b(\lambda) - a(\lambda)) \right]$. Thus

$$\mathfrak{Z}_1(u, \lambda) = \frac{1}{\pi} \frac{1}{1 - ue^{ib(\lambda)}} \sin \left[\frac{1}{2} (b(\lambda) - a(\lambda)) \right].$$

Now apply theorem 9.

Example. $w(e^{i\theta}) = \cos \theta$.

Here

$$\rho(\lambda) = \begin{cases} \frac{1}{\pi} (1 - \lambda^2) & \text{if } -1 \leq \lambda \leq 1 \\ 0 & \text{otherwise} \end{cases}$$

$$Y: (1 - uS)^{-1} e_o \rightarrow \frac{2^{\frac{1}{2}}}{(1 - 2\lambda u + u^2)^{\frac{1}{2}}}.$$

Thus

$$(YS^j e_o)(\lambda) = 2^{\frac{1}{2}} C_n^{(1)}(\lambda),$$

where $C_n^{(1)}$ is the n -th Gegenbauer polynomial of order 1.

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A MATHEMATICAL SURVEY OF A CLASS OF
APPROXIMATIONS TO THE BOLTZMANN EQUATION

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A survey of some basic results obtained in collaboration with L. Sirovich, for a class of approximations to the Linearized Boltzmann Equation, is presented. This class of approximations was first presented by Kac (ref. 12) and Gross and Jackson (ref. 11).

They are called model equations and are generalizations of the well known Bhatnager-Gross-Krook-Welander model (see refs. 3, 4).

INTRODUCTION

This lecture is divided into three main parts. The first part consists of a general discussion of Kinetic Model approximations to the linearized Boltzmann Equation for a simple monatomic gas and which have been described in the lectures of G. Ford and L. Sirovich (see ref. 14) in this volume. In the second section a simple model (the isosteric) is developed in detail. This is because it illustrates certain essential features of all these model equations, it is easy to deal with analytically and it serves to motivate the considerations of the second section. The third part consists of an outline of a proof of the asymptotic approach to hydrodynamics of solutions of linearizations of these model equations (for more complete details see refs. 13, 20).

PART I

In a previous lecture Bill Ford discussed one of these models called the isothermal (also see refs. 12, 13, 16). For this model mass and momentum are conserved but not energy. The isothermal model gives a good qualitative description of sound propagation and is relatively easy to deal with analytically. However for quantitative purposes it is inadequate. In particular I refer to the well known experiments of Greenspan and Meyer and Sessler (see refs. 6, 7, 17, 19). For a description of these model equations see Sirovich, section 6 of these lecture series. We consider only the linearized version of these model equations (i.e. with the distribution function linearized about an absolute Maxwellian distribution).

The linearized model equations made dimensionless, take the following form:

$$(1) \quad \frac{\partial g}{\partial t} + \xi_1 \frac{\partial g}{\partial X} + g = \omega \sum_{n=0}^N a_n \lambda_n \phi_n, \text{ where}$$

$$(2) \quad \delta_{m,n} = \int_{-\infty}^{\infty} \omega \phi_n \phi_m d\xi$$

$$(3) \quad a_n = \int_{-\infty}^{\infty} g \phi_n d\xi.$$

The λ_n are constants and the $\phi_n = \phi_n(\xi)$ are Hermite polynomials in ξ (see ref. 1).

$$(4) \quad \omega = \frac{e^{-\xi^2/2}}{(2\pi)^{3/2}}$$

The a_n (see 3) are functions of t (time) and X (space) only. On the other hand g is a function of t , X and ξ (velocity in phase space).

It is important to observe that the normalization giving the dimensionless form (1) varies with the model (i.e. N) equation (see Sirovich (6.1)).

The particular equations with which we will be concerned are the following.

$$(5) \quad \frac{\partial g}{\partial t} + \xi \cdot \frac{\partial g}{\partial X} = 0 \text{ (The free flow or Knudsen gas)}$$

$$(6) \quad \frac{\partial g}{\partial t} + \xi \cdot \frac{\partial g}{\partial X} + g = 0 \text{ (The high frequency model)}$$

$$(7) \quad \frac{\partial g}{\partial t} + \xi \cdot \frac{\partial g}{\partial X} + g = \omega \rho \text{ (The isosteric model) see (12) for def. of } \rho$$

$$(8) \quad \frac{\partial g}{\partial t} + \xi \cdot \frac{\partial g}{\partial X} + g = \omega(\rho + \xi \cdot u) \text{ (The isothermal model)}$$

see (12) for def. of u

$$(9) \quad \frac{\partial g}{\partial t} + \xi \cdot \frac{\partial g}{\partial X} + g = \omega(\rho + \xi \cdot u + \left(\frac{\xi^2 - 3}{2}\right) T) \quad (\text{BGKW Equation})$$

(see (12) for def. of T)

$$(10) \quad \frac{\partial g}{\partial t} + \xi \cdot \frac{\partial g}{\partial X} + g = \omega \sum_{n=0}^N a_n \lambda_n \phi_n, \text{ with}$$

$N = 5, 8, 11$, which we call the five, eight and eleven moment models.

$$(11) \quad \frac{\partial g}{\partial t} + \xi \cdot \frac{\partial g}{\partial X} + g = \omega \sum_{m,n=0}^N a_m \mu_{m,n} \phi_n$$

which we refer to as the hard sphere models. (see refs 17, 18).

$$(12) \quad \rho = \int g \, d\xi \quad (\text{perturbed mass density})$$

$$u = \int \xi g \, d\xi \quad (\text{perturbed mean velocity})$$

$$T = \int \left(\frac{\xi^2 - 1}{3} \right) d\xi \quad (\text{perturbed temperature density})$$

Some of the assets and liabilities of the different models are tabulated below

MODEL	ASSETS	LIABILITIES
Free Flow (5) Knudsen gas	Correct for a collisionless gas. Has proper characteristics	Neglect of collisions
High frequency model (6)	Qualitatively correct behavior for very high frequency. (i.e. much higher than the collision frequency)	Poor approximation for intermediate and low frequencies. None of the conservation laws are satisfied.

MODEL	ASSETS	LIABILITIES
Isosteric Model (7)	Qualitatively correct for high frequency. Conservation of mass. Analytically simple and illustrates certain essential features of the physically more realistic model equations. A diffusion mode exists.	Momentum and Energy conservation laws are violated. Sound propagation mode is missing.
Isothermal Model (8)	Relatively simple analytically. Conservation of mass Conservation of momentum. Sound Propagation mode.	Energy conservation is violated. No diffusion mode. Incorrect sound speed (isothermal rather than adiabatic).
BGKW or Adiabatic Model (9)	All conservation laws are satisfied. Adiabatic sound propagation. A diffusion mode. Asymptotic approach to continuum mechanics for large time and sufficiently smooth initial data.	Incorrect value of the ratio of heat conductivity to viscosity. (roughly 3/2 of correct value)
5,8 and 11 moment models	Same as BGKW model. In addition the correct ratio of heat conductivity to viscosity is given and fairly good quantitative results for the full range of experimental values is obtained.	The collision frequency is incorrectly taken to be a constant, for hard sphere gases such as helium and argon. The incorrect force law (inverse fifth power) is taken.
Hard sphere 5,8 and 11 moment models	Same as 5,8 and 11 moment models, except that excellent agreement with the full range of experimental values is obtained.	The collision frequency is still incorrectly treated as a constant.

In order to obtain good agreement with experiment we have been forced to go to higher Mark number (i.e. higher order moment equations, such as the 5,8 and 11 order moment equations). The above table clearly indicates this necessity. Attempts have been made to describe high frequency experiments as a pressure wave and to use the free flow equation (5) for the distribution function (see refs. 6, 7, 19). Calculations which we have made (see ref. 19) both for Maxwell and hard sphere gases give the result that the percentage of molecules undergoing a collision in traveling from an emitting plate to a receiving plate a distance $1/10$ th of a mean free path away is 24% and 10% for a distance $1/20$ th of a mean free path. These plate distances are for the above mentioned experiments (6, 7) for which free flow calculations were made. Although theoretical calculations based on a free flow analysis are in qualitative agreement with experiment, the attenuation is roughly 20% below the experimentally predicted values. This is certainly due in part to a premature neglect of the effect of intermolecular collisions.

A further deficit of Equation (5) is that even for high frequency oscillations it does not correspond to the correct asymptotic behavior for large time for the initial value problem. The correct behavior is given by (6) or what we call the high frequency model.

For purposes of illustration and as an aid in developing some insight into all model equations, (7) or the isosteric model (mass conserving) will be investigated.

PART II

The Isosteric Model for one dimensional space dependence, time dependence and three velocity components is given as follows.

$$(13) \quad \frac{\partial g}{\partial t} + \xi_1 \frac{\partial g}{\partial X} + g = \omega \rho$$

$$\text{where } \rho = \int g \, d\xi \text{ and } \omega = \frac{e^{-\xi^2/2}}{(2\pi)^{3/2}} \quad (\text{see 4})$$

ρ is the density of mass per unit volume, and depends only on X and t .

(14) g_0 denotes the initial distribution at time $t = 0$.

First we apply Fourier transforms in the variable X , the new variable being k and then we apply Laplace transforms in t , the new variable being σ . Using an asterisk to denote the transformed variables we have:

$$(15) \quad (1 + \sigma - ik\xi_1)g^* = \omega\rho^* + g_0^*$$

where $\rho^* = \int g^* d\xi$ and g_0^* is a function of k and $\xi = (\xi_1, \xi_2, \xi_3)$ only.

Upon dividing by the coefficient of g^* we obtain

$$(16) \quad g^* = \frac{\omega p^* + g_0^*}{1 + \sigma - ik\xi_1} + A\delta(1 + \sigma - ik\xi_1)$$

where δ is the Dirac delta function.

In a normal mode analysis we would keep the delta function contribution on the right-hand side of (16) (see G. Ford's discussion of the isothermal problem).^{*} However for our purposes this is not necessary, although the dominance of the continuous spectrum for high frequency will reassert itself in another form. The reason that the delta function contribution can be neglected is simply that k is real and $\text{Re } \sigma > 0$, in contrast to a normal mode analysis where one looks for σ and k so related that for some ξ_1 , $1 + \sigma - ik\xi_1 = 0$. In this discussion of the initial value problem g^* will be continued analytically in the complex σ -plane, but it is still inappropriate to introduce the delta function, even if $1 + \sigma - ik\xi_1$ should equal zero in the process of analytic continuation. Thus we consider

$$(17) \quad g^* = \frac{\omega p^* + g_0^*}{1 + \sigma - ik\xi_1}.$$

^{*} The essential part of the spectrum was discussed by G. Ford in this series of lectures although this lecture does not appear in this volume. This part of the spectrum has also been discussed in lectures by H. Grad.

Upon integrating both sides of (17) w.r.t. ξ
we obtain:

$$(18) \quad \rho^* = \frac{M\rho^*}{\lambda k} + \int_{-\infty}^{\infty} \frac{g_0^* d\xi}{1+\sigma-ik\xi_1}$$

where

$$(19) \quad \lambda = \frac{1+\sigma}{k} \quad \text{and}$$

$$(20) \quad M = \lambda \int_{-\infty}^{\infty} \frac{\omega d\xi}{\lambda - i\xi_1}$$

The function $M(\lambda)$ (see 20) is for $\text{Re } \lambda > 0$
equivalent to the entire function

$$(21) \quad M(\lambda) = \sqrt{\pi/2} \lambda e^{\lambda^2/2} (1 - \Phi(\lambda/\sqrt{2})) \quad \text{for } \text{Re } \lambda > 0$$

and for $\text{Re } \lambda < 0$ we have

$$(22) \quad M(\lambda) = -\sqrt{\pi/2} \lambda e^{\lambda^2/2} (1 + \Phi(\lambda/\sqrt{2})) \quad \text{for } \text{Re } \lambda < 0$$

where

$$(23) \quad \Phi(X) = \sqrt{2/\pi} \int_0^{\sqrt{2}X} e^{-t^2/2} dt \quad (\text{error function})$$

For the initial value problem we have

$$(24) \quad \text{Re } \lambda > 0 \quad \text{for } k > 0 \quad \text{and}$$

$$\text{Re } \lambda < 0 \quad \text{for } k < 0.$$

Thus for a fixed $k \neq 0$ and its analytic continuation constitute an entire analytic function of σ and the usual techniques of shifting contours can be used to obtain the asymptotic behavior of g for large t (see refs. 13, 16, 20).

In particular we will consider here the plane wave initial value problem for g .

(25) $g_0 = a \omega e^{ik_0 X}$, where a is a constant different from zero, and k_0 is taken to be a positive constant.

Immediately we have

$$(26) \quad g_0^* = (2\pi)^{\frac{1}{2}} a \omega \delta(k+k_0) = \frac{a\omega}{(2\pi)^{\frac{1}{2}}} \int_{-\infty}^{\infty} e^{+ikX + ik_0 X} dX$$

From (18), (20) and (26) we have

$$(27) \quad \rho^* = \frac{(2\pi)^{\frac{1}{2}} a \delta(k+k_0) M}{(\lambda k - M)}$$

In order to be able to invert transforms we must know the roots of the dispersion relation

$$(28) \quad \lambda k - M = 0.$$

The asymptotic behavior of M for large λ is given as follows (see refs. 5, 13)

$$(29) \quad M \sim 1 - \frac{1}{\lambda^2} + \frac{3}{\lambda^4} - \frac{3 \cdot 5}{\lambda^6} + \frac{3 \cdot 5 \cdot 7}{\lambda^8} \dots$$

$$\text{for } -\frac{3\pi}{4} < \arg \lambda < \frac{3\pi}{4}$$

$$M \sim (2\pi)^{\frac{1}{2}} e^{\lambda^2/2} + 1 - \frac{1}{\lambda^2} + \frac{3}{\lambda^4} - \frac{3 \cdot 5}{\lambda^6} \dots$$

$$\text{for } \pi/4 < |\arg \lambda| < \frac{7\pi}{4}$$

This is the behavior for that part of M which arises from initial data with k or $\operatorname{Re} \lambda > 0$. For initial data with k or $\operatorname{Re} \lambda < 0$ we have

$$(30) \quad M \sim 1 - \frac{1}{\lambda^2} + \frac{3}{\lambda^4} - \frac{3 \cdot 5}{\lambda^6} + \frac{3 \cdot 5 \cdot 7}{\lambda^8} \dots$$

$$\text{for } -\frac{3\pi}{4} < \arg \lambda < \frac{3\pi}{4}$$

$$M \sim -(2\pi)^{\frac{1}{2}} e^{\lambda^2/2} + 1 - \frac{1}{\lambda^2} + \frac{3}{\lambda^4} - \frac{3 \cdot 5}{\lambda^6} \dots$$

$$\text{for } \pi/4 < |\arg \lambda| < \frac{7\pi}{4}$$

For the particular initial data which we have chosen $k = -k_0 < 0$ and thus we will only be concerned with (30).

FIGURE 1 - Isosteric Model

The dispersion relation (28) has infinitely many roots. All of the roots lie on or to the left of the line $\text{Re } \sigma = 0$ in the complex σ -plane. Only one root occurs on the line $\text{Re } \sigma = 0$ and this is only for $k = 0$ and it is located at $\sigma = 0$. For small k this root is given asymptotically by

$$(31) \quad \sigma = -k^2 + k^4 + O(k^6)$$

The general term of this expansion has been determined in collaboration with L. Sirovich and has been shown to be semiconvergent. This has as an interesting consequence that the Chapman-Enskog (ref. 2, 9, 15) procedure for the Isosteric Model is divergent. Although we do not have a rigorous proof we conjecture that the Chapman-Enskog procedure is divergent for all Maxwell Model equations.

For the above root (31) σ is real for all real k and $\sigma \rightarrow -\infty$ as $k \rightarrow -\infty$. For this root

$$(32) \quad \sigma = -1 \quad \text{for } k = -(\pi/2)^{\frac{1}{2}} \quad \text{and}$$

$$(33) \quad \sigma \sim -1 - |k| \sqrt{2 \ln |k|} \quad \text{as } |k| \rightarrow \infty$$

This mode is called the diffusion mode, the reason for this will shortly be made clear. The line $\text{Re } \sigma = -1$ corresponds to the continuous spectrum and is not part of the dispersion relation. At the point $\sigma = -1$ there are infinitely many roots of the dispersion relation. At this point the dispersion relation has an essential singularity.

For all modes other than the diffusion mode, $k = 0$ at $\sigma = -1$. For any fixed circle with center at $\sigma = -1$ there are only a finite number of roots for a fixed $k \neq 0$. The point $\sigma = -1$ is the only essential singularity of the dispersion relation.

Relation (33) shows that if we try to approximate the Isosteric Model equation by a finite system of partial differential equations that the approximation can only be valid for a limited range of wavenumbers, since such a system would give rise to an algebraic dispersion relation which could not give a good approximation to (33) for large enough k . This comment applies to all Model equations. It follows that if the model equations are good overall (low and high frequency) approximations to the Boltzmann equation, then the Navier Stokes, Burnett, etc. approximations must be bad at high wave-number. The experimental and analytical evidence gives exactly this result.

The other roots of the dispersion relation (i.e. $k = 0$ at $\sigma = -1$) take the form

$$(34) \quad \sigma_N \sim -1 - |k| \left\{ \begin{array}{l} \sqrt{(\ln|k|) + \sqrt{(\ln|k|)^2 + 4\pi^2 N^2}} \\ + i \operatorname{sgn} N \sqrt{-\ln|k| + \sqrt{(\ln|k|)^2 + 4\pi^2 N^2}} \end{array} \right\}$$

For each positive and negative integer N we get a distinct root. The above (34) is an asymptotic expansion for large k .

From (34) we see that all the non-diffusion modes are exponentially damped at a rate at least equal to the collision frequency (i.e. $\text{Re } \sigma = -1$). By the use of winding numbers it can be shown that our count on the number of roots given by (34) is correct (see ref. 13). For a fixed k and large index N relation (34) reduces to

$$(35) \quad \sigma_N \sim -|k| \sqrt{2\pi|N|} (1 + i \text{sgn } N)$$

In the following we will use the index 0 to denote the diffusion mode.

We now proceed to the inversion of the transforms. The inversion of the Fourier transform is trivial due to the presence of the factor $\delta(k+k_0)$. Thus from (27)

$$(36) \quad \rho = \frac{a e^{ik_0 X}}{2\pi i} \int_{B_{r_1}} \frac{e^{\sigma t} M d\sigma}{(1+\sigma-M)}$$

and from (17) and (26) we have

$$(37) \quad g = \frac{a \omega e^{ik_0 X}}{2\pi i} \int_{B_{r_1}} \frac{e^{\sigma t} M d\sigma}{(1+\sigma-M)(1+\sigma+ik_0 \xi_1)} + a \omega e^{-t+ik_0(X-\xi_1 t)}$$

where $M = M\left(-\left(\frac{1+\sigma}{k_0}\right)\right)$ and the paths of the integrals are Bromwich paths to the right of the roots of the dispersion relation (see ref. 13). The evaluation of the above integrals by residues is expedited by making use of the fact that $M(\lambda)$ satisfies a first order ordinary differential equation.

$$(38) \quad \frac{dM}{d\lambda} = \left(\frac{1}{\lambda} + \lambda\right) M - \lambda$$

Thus we obtain

$$(39) \quad \rho = -ak_0^2 e^{ik_0 X} \sum_{N=-\infty}^{\infty} \frac{e^{\sigma_N t}}{\sigma_N}$$

and

$$(40) \quad g = -ak_0^2 \omega e^{ik_0 X} \sum_{N=-\infty}^{\infty} \frac{e^{\sigma_N t}}{\sigma_N (1 + \sigma_N + ik_0 \xi_1)}$$

$$- \frac{aM(+i\xi_1) \omega e^{-t+ik_0(X-\xi_1 t)}}{ik_0 \xi_1 + M(+i\xi_1)} + a \omega e^{-t+ik_0(X-\xi_1 t)}$$

For large t the dominant contributor comes from the diffusion root or its analytic continuation. Thus for large t we have

$$(41) \quad \rho \sim \frac{-ak_0^2 e^{ik_0 X + \sigma_0 t}}{\sigma_0}$$

and

$$(42) \quad g \sim \frac{-ak_0^2 \omega e^{ik_0 X + \sigma_0 t}}{\sigma_0(1 + \sigma_0 + ik_0 \xi_1)}$$

$$- \frac{aM(i\xi_1)\omega e^{-t + ik_0(X - \xi_1 t)}}{ik_0 \xi_1 + M(i\xi_1)} + a \omega e^{-t + ik_0(X - \xi_1 t)}$$

Next we examine the two extremes $k_0 \ll 1$ and $k_0 \gg 1$.

First the case where $k_0 \ll 1$.

From (41) and (31) we have:

$$(43) \quad \rho \sim a e^{ik_0 X - k_0^2 t}, \text{ from which it follows that } \rho$$

satisfies the diffusion equation.

$$(44) \quad \frac{\partial \rho}{\partial t} = \frac{\partial^2 \rho}{\partial x^2} + O(k_0^4). \text{ This is the reason for}$$

the name diffusion mode.

When $k_0 \gg 1$ we have from (42) and (33):

$$(45) \quad g \sim a \omega \left(1 - \frac{M(i\xi_1)}{M(i\xi_1) + ik_0 \xi_1} \right) e^{-t + ik_0(X - \xi_1 t)} \\ - \frac{a \omega e^{ik_0 X - t - k_0 \sqrt{2 \ln k_0} t}}{2 \ln k_0}$$

Or keeping only the leading contribution we have:

$$(46) \quad g \sim a \omega \left(1 - \frac{M(i\xi_1)}{M(i\xi_1) + ik_0 \xi_1} \right) e^{-t + ik_0(X - \xi_1 t)}$$

To within the approximation given by (46) we see that g satisfies the high frequency equation (6). The presence of the factor

$$(47) \quad F = 1 - \frac{M(i\xi_1)}{M(i\xi_1) + ik_0 \xi_1} \text{ in (46) apparently implies}$$

equation (6) can be used only to give a qualitatively correct asymptotic solution. However

for all ξ_1 , $M(i\xi_1) = O(\xi_1)$ and thus

$$(48) \quad F \sim 1 + O(1/k_0)$$

Thus for all velocities (6) can be considered quantitatively accurate. It should be noted that the solution given by (46) arises from the analytic continuation of the diffusion mode of (43). That the low wavenumber asymptotics leads to a diffusion mode can be also seen formally as follows:

Using (12) and (13) we obtain

$$(49) \quad \frac{\partial \rho}{\partial t} + \frac{\partial u}{\partial X} = 0$$

Next expanding (17) regarding σ and k as small quantities (see refs. 10, 13, 15)

$$(50) \quad g^* \sim \omega \rho^* - (\sigma - ik\xi_1)\omega \rho^* + \frac{g_0^*}{1 + \sigma - ik\xi_1}$$

The term involving g_0^* decays exponentially the order of the collision frequency, hence

$$(51) \quad g^* \sim \omega \rho^* - (\sigma - ik\xi_1)\omega \rho^* \text{ for large time.}$$

Upon taking moments we have

$$(52) \quad u^* = \int \xi_1 g d\xi \sim ik \rho^*$$

Inverting transforms we have

$$(53) \quad u \sim - \frac{\partial \rho}{\partial X} \text{ and substituting in (49)}$$

$$(54) \quad \frac{\partial \rho}{\partial t} \sim \frac{\partial^2 \rho}{\partial X^2} \quad (\text{compare with 44})$$

The discussion of the isosteric model has been formal rather than rigorous. Before proceeding to a rigorous analysis of model equations in general, let us summarize some of the insights that we have attained. It has been plausibly demonstrated that for low initial wave number (i.e. smooth initial data) that we have a continuum mechanics corresponding to the conservation of mass. This continuum mechanics is to lowest order described by the diffusion equation which the density satisfies (see 44 and 54). For rough initial data (i.e. high wave number) the distribution function approximately satisfies the high frequency equation (see 6).

For large k_0 (see 45) the error is of order $1/\ln k_0$. For t bounded away from 0 the error is

$$O\left(\frac{e^{-k_0\sqrt{2\ln k_0}t}}{\ln k_0}\right).$$

Thus we can estimate the rate at which the use of the high frequency equation is valid. Just as for the low wave number limit the original initial data can be used in the first approximation (see 46 and 47). In the low wave number limit we have a strictly asymptotic (non-convergent expansion) which mimics the Chapman-Enskog expansion for the Boltzmann equation. On the other hand we have for $t > 0$ a convergent expansion

see (40) that reminds one of the well known Willis iteration scheme (see ref. 8) which is known to be convergent. For high frequency or large wave number we see that the leading term in the expansion for g satisfies (see 6 and 45).

These general comments hold for all Model equations. That is we obtain continuum mechanics for the low wavenumber limit (Navier Stokes, Burnett etc.) and a solution of the high frequency equation (corresponding to the essential spectrum of the Boltzmann equation) for the leading term of the large wavenumber limit. The semi-convergence of the Chapman-Enskog process for all the Maxwell Model equations is an as yet unproved though plausible assertion.

PART III

We will now consider a more rigorous approach to one aspect of the discussion in part II. Namely we demonstrate the asymptotic approach to hydrodynamics for smooth initial data for the linearized model equations (by hydrodynamics we mean the continuum mechanics appropriate to each model equation).

We will limit ourselves to an outline and motivation of the proof, since the details appear elsewhere (see refs. 13, 16, 20). The following system is investigated:

$$(55) \quad \frac{\partial G}{\partial t} + \xi \cdot \frac{\partial G}{\partial X} = \sum_{m,n=0}^N A_m \mu_{m,n} \phi_n \quad (\text{see 11, 12})$$

$$(56) \quad A_m = \int_{-\infty}^{\infty} \omega G \phi_m d\xi \quad 0 \leq m \leq N$$

The $\mu_{m,n}$ are the same constants as in (11), and the ϕ_n are Hermite polynomials (see 2, 4 and ref. 1). The relation between G and g and A_m and a_m (see 3) is given by

$$(57) \quad G = e^t g \omega^{-1}$$

$$(58) \quad A_m = e^t a_m.$$

The initial data for (11) and (55) are related as follows:

$$(59) \quad G(X, \xi, t=0) = G_0(X, \xi) = g(X, \xi, t=0) \omega^{-1}$$

In order to be able to demonstrate the asymptotic approach to hydrodynamics we were forced into investigating the questions of existence, uniqueness, continuous dependence on initial data and the validity of applying Fourier and Laplace transforms. The more direct approach of formally applying transforms, solving the transformed system and then showing that the inverse transform satisfies the original problem

was found to be unfeasible due to the complicated nature of the expressions involved.

As an aid to further analysis additional notation must be introduced.

$$(60) \quad (F, H) = \int_{-\infty}^{\infty} F \bar{H} \omega d\xi, \text{ where}$$

$$(61) \quad \bar{H} = \text{complex conjugate of } H, \text{ and } \omega \text{ is given by (4).}$$

The $\mu_{m,n}$ of (55) are real constants which are derived from the exact linear collision operator. They depend on the intermolecular force law of the gas. Until necessary they will not be further specified.

The basic idea behind the existence and uniqueness proof is the use of the contracted mapping principle (see ref. 13, 20). In order to construct the mapping and define the space in which the mapping occurs, we reformulate the system of integrodifferential equations as a system of integral equations.

$$(62) \quad G = G_0(X - \xi t, \xi) + \int_0^t \left\{ \sum_{m,n=0}^N A_m(X^*, S) \mu_{m,n} \phi_n \right\} ds$$

where

$$(63) \quad A_m(X, t) = (G, \phi_m)$$

and

$$(64) \quad X^* = X - \xi(t-s)$$

We define S (see ref. 20) to be the space of all functions $F = F(x, t)$ such that $\frac{\partial F}{\partial X_j}$ $j = 1, 2, 3$, exist and are continuous functions of t and $X = (X_1, X_2, X_3)$ for all X , and for all $t \geq 0$. S is further specified by requiring that for each F there exists a continuous function $M(t)$, such that

$$|F|, \left| \frac{\partial F}{\partial X_j} \right| \leq M(t) \text{ for all } t \geq 0 \text{ and } j = 1, 2, 3. \text{ Next we}$$

introduce the spaces S^{N+1} which is the N -fold direct product of S with itself. Let $G_0(X, \xi) \in C^1$ in X and C^0 in ξ , be such that G_0 and $\frac{\partial G_0}{\partial X_j} = O(e|\xi|^\alpha)$ uniformly in X for some $\alpha < 2$.

The following relations then define a mapping L of S^{N+1} into S^{N+1} .

$$(65a) \quad \tilde{G} = G_0(X - \xi t, \xi) + \int_0^t \left\{ \sum_{m,n=0}^N F_m(X^*, S) \mu_{m,n} \phi_n \right\} ds$$

$$(65b) \quad \tilde{F}_m = (\tilde{G}, \phi_m) \text{ for } 0 \leq m \leq N$$

$$(65c) \quad \frac{\partial \tilde{F}_m}{\partial X_j} = \left(\frac{\partial \tilde{G}}{\partial X_j}, \phi_m \right) \text{ for } 0 \leq m \leq N \text{ and } j = 1, 2, 3.$$

Although 65c is a consequence of 65b we regard it as part of the mapping. It is convenient to write

$$(66) \quad \tilde{F} = \left(F_0, \frac{\partial F_0}{\partial X_1}, \frac{\partial F_0}{\partial X_2}, \frac{\partial F_0}{\partial X_3}, \dots, F_N, \frac{\partial F_N}{\partial X_1}, \frac{\partial F_N}{\partial X_2}, \frac{\partial F_N}{\partial X_3} \right)$$

and define

$$(67) \quad |\tilde{F}|_X = \sum_{n=0}^N \left\{ \max_X |F_n| + \sum_{j=1}^3 \max_X \left| \frac{\partial F_N}{\partial X_j} \right| \right\}$$

We refer to

$$(68) \quad \left(F_{m-1}, \frac{\partial F_{m-1}}{\partial X_1}, \frac{\partial F_{m-1}}{\partial X_2}, \frac{\partial F_{m-1}}{\partial X_3} \right) \text{ as the}$$

mth component of $\tilde{F}$. The mapping L defined by 65a, 65b and 65c is written

$$(69) \quad \tilde{F} = L(\tilde{F}).$$

Also we define

$$(70) \quad ||F||_{t_0} = \max_{0 \leq t \leq t_0} |F|_X \text{ as a norm in } S^{N+1}.$$

We show (see refs. 13, 20) that there exists a positive constant P which depends only on the constants $\mu_{m,n}$ and the index N such that

$$(71) \quad ||L(\tilde{F}) - L(\tilde{F}')||_t \leq tP ||\tilde{F} - \tilde{F}'||_t.$$

It is immediate that there exists a positive T such that $0 < C = PT < 1$ and for $t \leq T$ we therefore have a contracting mapping. By the contracting mapping principle we know that there exists a unique fixed point of the mapping for the interval $0 \leq t \leq T$. We will denote this fixed point by F^0 .

Next we use F^0 to define

$$(72) \quad G_0^* = G_0(X, \xi, t) + \int_0^t \left\{ \sum_{m,n=0}^N F_n^0(X^*, S) \mu_{m,n} \phi_n \right\} ds$$

for $0 \leq t < T$. An immediate calculation shows that G_0^* satisfies (55) through (59). The F_n^0 are to be identified with the A_n and the corresponding moments of G_0^* give the appropriate F_n^0 . Further the correct initial condition is clearly satisfied. Thus we have the existence and uniqueness of G for the interval $0 \leq t < T$.

Taking $G_0^*(X, \xi, T/2)$ as our initial value at $t = T/2$ we repeat the above process and obtain existence and uniqueness of G for the interval $T \leq t < 3T/2$. This is possible since the same constant C will play the same role and depends only on P , a fixed constant, and the time interval T . Clearly this result can be extended to all $(t | 0 \leq t < \infty)$. We will not repeat the argument here but it is also possible to show continuous dependence on initial data (see ref. 20).

Next we find it necessary to investigate the validity of applying Fourier and Laplace transforms.

At this point it is not clear that we can interchange the order of taking and inverting the Fourier and Laplace transforms. This is due to the existence of functions which are such that no multiplier of the form $e^{-\sigma t}$ ($\text{Re } \sigma > 0$) will make the resulting

product absolutely integrable in both X and t , whereas for each t they may be absolutely integrable in X and vice versa.

For example let

$$(73) \quad \Phi = e^{-|X|} e^{-t^2}$$

$$(74) \quad \Phi' = e^{-\sigma t - |X|} e^{-t^2} \quad (\text{Re } \sigma > 0).$$

Then for $t \geq 0$ and $-\infty < X < \infty$ (73) is such a function as can be seen by integrating (74) in t holding X fixed and vice versa.

By restricting ourselves to the subspace $|S|^{N+1}$ of S^{N+1} consisting of all members of S^{N+1} whose components are absolutely integrable, we can by an analysis similar to the above contracted mapping argument demonstrate the validity of applying Fourier transforms.

Next it is demonstrated that the Fourier transform of G grows at most exponentially in time and thus the legitimacy of applying the Laplace transform to the Fourier transform can be validated.

In order to carry the analysis further more information on the coefficients will be necessary. We assume that

$$(75) \quad \left(G, \left\{ \sum_{m,n=0}^N A_m \mu_{m,n} \phi_n - G \right\} \right) \leq 0$$

(see 55, 56, 60)

Assumption (75) is merely a reflection of the fact that the linearized collision operator of the Boltzmann equation is a negative semi-definite operator. For the model equations based on a Maxwell gas, the coefficients $\mu_{m,n} = \lambda_m \delta_{m,n}$ where $0 \leq \lambda_m \leq 1$ and relation (75) is easily verified (see ref. 20).

In addition the equality in (75) is satisfied only if G is of the form

$$(76) \quad G = \sum_{r=0}^4 A_r \phi_r \quad \text{where}$$

$$(77) \quad \phi_0 = 1, \phi_1 = \xi_1, \phi_2 = \xi_2 + i\xi_3, \phi_3 = \xi_2 - i\xi_3$$

and $\phi_4 = \xi^2 - 3$, are the five Hermite polynomials which correspond to the conservation laws (mass, momentum and energy).

Next the dispersion relation for the Fourier and Laplace transformed version of system (55) and (56) is investigated. The dispersion relation is gotten by setting to zero the determinant obtained by solving for the transform of the moments A_m . The essential step here is the rewriting

of the dispersion relation in an equivalent form which involves the transform of G and not just the moments (see ref. 20). From this equivalent form we are able to deduce that

$$(78) \quad -1 \leq \operatorname{Re} \sigma \leq 0 \quad (\text{see ref. 20})$$

For the analytic continuation of the dispersion relation we have

$$(79) \quad \operatorname{Re} \sigma < -1.$$

Further we show that if $\operatorname{Re} \sigma = 0$ then $k = 0$. Hence from continuity $\operatorname{Re} \sigma$ is bounded away from zero (thus $\operatorname{Re} \sigma < 0$ by 78) for $k \neq 0$. Note that $k = 0$ does not imply that $\operatorname{Re} \sigma = 0$. In general for $k = 0$, $\sigma = 0$ is a five-fold root (i.e. from the BGKW (9) and higher Mark number models). The isosteric (7) (one-fold) and the isothermal (8) (four-fold) being exceptions.

Finally we prove that one-dimensional motions behave asymptotically "like hydrodynamics". In this connection for the full linearized Boltzmann equation, the Chapman-Enskog procedure and hydrodynamics has been discussed in a formal manner by Sirovich (see ref. 15) also via transform methods.

In the proof the assumption is made that the initial distribution at time $t = 0$ is of compact support in wave number space (see refs. 13, 20). This is a strong assumption which can clearly be weakened. We decided however to keep the proof as simple and convincing as we could. The solution of the initial value problem is written as the inverse Fourier transform of the inverse Laplace transform of the solution to the transformed problem. An essential part of the proof involves the decomposition of the inverse Fourier transform into two parts, for $|k| \leq \epsilon$ and $|k| \geq \epsilon$ where ϵ is an appropriately chosen function of t . This decomposition is important because it enables us to avoid the complications involved in trying to use saddle-point techniques for multiple integrals. Simple estimates on each of the terms leads us to the desired conclusion that the solution of the initial value problem for smooth initial data, tends asymptotically to the solution of a corresponding hydrodynamical equation, having to lowest order the same initial data.

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SOUND PROPAGATION

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INTRODUCTION

The purpose of these lectures is to introduce and survey the theory of sound propagation. Special emphasis will be placed on propagation in a rarefied gas*. Hence, the effect of a non-zero mean-free-path will be considered.

We make this somewhat more precise. Denote the diameter of a molecule by σ and the number density of particles by n . Simple arguments then suggest that the mean-free-path, ℓ , is given by

$$\ell = \frac{c}{n\sigma^2}$$

where c is a constant $O(1)$. It is more convenient to represent ℓ in terms of more familiar quantities. Denoting the adiabatic speed of sound by a_0 and kinematic viscosity by $\bar{\mu}$, one has

$$\ell = \frac{c' \bar{\mu}}{a_0}$$

where $c' = O(1)$.

* Actually we will be concerned with unsteady problems. A proper understanding of sound propagation can only come through such an approach.

Therefore if we denote the sound wave length by λ , we can say that our main interest will be in situations when $\ell/\lambda \neq 0$ and in fact when this ratio is $O(1)$ and large. We note in passing that we can alternately phrase our remarks in terms of

$$\frac{\frac{\ell}{a_0}}{\frac{\lambda}{a_0}} = \frac{\omega}{\nu}$$

where ω is the sound frequency and ν the mean-collision-frequency.

Ratios of length scales involving the mean-free-path are generally called Knudsen numbers, and we write

$$K_\lambda = \frac{\ell}{\lambda}.$$

This is by no means the only Knudsen number of the problem. For in any physical observation of sound the size of the apparatus, L , plays a role. This defines a second Knudsen number

$$K_L = \frac{\ell}{L}.$$

In speaking of rarefied flows a rule of thumb is;

$K \rightarrow 0 \Rightarrow$ continuum, $K \rightarrow \infty \Rightarrow$ free-flow, and $K = O(1) \Rightarrow$ transition.

This must be modified in our case due to the presence of two Knudsen numbers. If for example the pressure disturbance, p , at

a distance L from a sound emitter is considered we expect

$$p = p(K_\lambda, K_L)$$

A plausible division of the various regimes is given by the following self-explanatory diagram,

For the present ϵ only denotes a small quantity.

VARIOUS SOUND PROBLEMS

As a first step in specifying the sound problem, we classify the various geometries that are of interest. We once and for all restrict attention to one-dimensional problems.

I.V.1 Pure initial value problem. Given dependent variables at zero time to find the solution in ∞ -space for all time.

I.V.2 Possible plane wave solutions. Solutions with x - t dependence

$$\sim e^{ikx + \sigma t}, \quad \text{Im } k = 0$$

are sought. The view is that for pure sinusoidal initial data only the wave with l.u.b. $\text{Re}(\sigma)$ persists ($\text{Re} \sigma \leq 0$ can be shown in all cases) and hence only this part of the solution is sound. (One can seek to superpose solutions of I.V.2 to

gain a solution of I.V.2, but this problem must be carefully considered). Note that wave speed $v_s = \frac{\text{Im } \sigma}{k}$ and attenuation rate $\beta = \text{Re } \sigma$.

B.V.1 Infinite half-space with sinesoidally oscillating bounding plane.

B.V.2 Possible plane solutions $e^{i\omega t + sx}$ for ω real.

Note $\frac{1}{v_s} = \frac{\text{Re } s}{\omega}$, $\beta = \text{Im } s$

B.V.3 Infinite space bounded by two parallel planes, one of which is sinesoidally oscillating.

Problems IV1 and IV2 are relatively simple from the mathematical viewpoint (IV2 is simple by comparison with IV1) but relatively sterile from the physical point of view. Solutions to these problems cannot be tested in the laboratory. It has been tacitly assumed that whatever equations we use they will be linearized. This being the case only steady state solutions to B.V.1, B.V.2 are sought, i.e. $\frac{\partial}{\partial t}$ is replaced by $i\omega$ so that transients are neglected. B.V.1 is the situation which is often studied but it is actually B.V.3 which corresponds to the laboratory situation. B.V.2, which is independent of geometry, is a much simpler problem but as with I.V.2 only a study of the full problem (B.V.1 or B.V.2) can delimit its validity.*

* I.V.2 and B.V.2 will be referred to as dispersion problems.

With regard to usefulness and difficulty of the various situations we have

$$\text{usefulness} < \text{difficulty} ,$$

the perversity law.

GOVERNING EQUATIONS

On physical grounds, sound propagation is justified as a linear theory.* We shall therefore consider only linearized theory and make no apology for its use.

Two approaches can be taken. The first is by means of continuum equations. Denoting the equilibrium conditions by zero subscripts, the conservation equations are

$$(3.1) \quad \left\{ \begin{array}{l} \frac{1}{\rho_0} \frac{\partial \rho}{\partial t} + \frac{\partial u}{\partial x} = 0 \\ \frac{\partial u}{\partial t} + \frac{1}{\rho_0} \frac{\partial p}{\partial x} = \frac{\partial p_{11}}{\partial x} \\ \frac{\partial e}{\partial t} + \frac{p_0}{\rho_0} \frac{\partial u}{\partial x} = -\frac{1}{\rho} \frac{\partial Q}{\partial x} \end{array} \right.$$

where ρ , u , e , p are the perturbation density velocity, internal energy, and pressure; and p_{11} , Q the stress and heat conduction. These equations of course express the conservation of mass, momentum, and energy.

The second approach is through the Boltzmann equation of kinetic theory,

* In the linearizations no restriction need be placed on the size of derivatives. These in fact become large.

$$(3.2) \quad \frac{\partial g}{\partial t} + \xi \frac{\partial}{\partial x} g = \nu L(g) = \nu \int f_0(\xi_1) [g(\xi'_*) + g(\xi') - g(\xi_*) - g(\xi)] B(\theta, |\xi_* - \xi|) d\epsilon d\theta d\xi_*$$

Denoting the mass distribution function by f , g is defined by

$$(3.3) \quad f = f_0(1+g)$$

where

$$(3.4) \quad f_0 = \frac{\rho_0}{(2\pi RT_0)^{3/2}} e^{-\frac{\xi^2}{2RT_0}}$$

For later purposes the collision frequency ν has been extracted from the "cross-section" $B(\theta, |\xi_* - \xi|)$. The latter involves the details of the molecular interaction and the reader is referred to any standard book on kinetic theory for details.* The primed molecular velocities ξ'_* , ξ' are linearly related

$$(3.5) \quad \begin{cases} \xi'_* = \xi_* + (\xi - \xi_*) \cdot \frac{\mathbf{H}}{H} \frac{\mathbf{H}}{H} \\ \xi' = \xi + (\xi_* - \xi) \cdot \frac{\mathbf{H}}{H} \frac{\mathbf{H}}{H} \end{cases}$$

This follows from the conservation of momentum and energy in a two-body collision. The unit vector $\frac{\mathbf{H}}{H}$ orients a collision. Choosing $\xi_* - \xi$ as the polar axis we write

$$\frac{\mathbf{H}}{H} = (\cos\theta, \sin\theta \cos\epsilon, \sin\theta \sin\epsilon).$$

*See for example "The Mathematical Theory of Non-Uniform Gases"¹¹ by Chapman and Cowling.

With some reservations the second approach contains the first. For the hydrodynamical moments can be found from the distribution function, as follows

$$(3.6) \quad \left\{ \begin{array}{l} \rho = \int f^0 g d\xi, \quad \rho_0 u = \int f^0 g \xi_1 d\xi \\ p = \int f^0 g \frac{\xi^2}{3} d\xi \\ e = \frac{1}{\rho_0} \int f^0 g \frac{\xi^2}{2} d\xi - \frac{e_0}{\rho_0} \int f^0 g d\xi = \frac{3}{2} \frac{k}{m} T = C T \end{array} \right.$$

where k is Boltzmann's constant, m the molecular mass, and T the perturbed temperature. In addition we have,

$$(3.7) \quad \left\{ \begin{array}{l} p_{11} = - \int f^0 \xi_1^2 g d\xi \\ Q = \int \frac{1}{2} f^0 g \xi_1 (\xi^2 - 5RT) d\xi \end{array} \right.$$

From the conservation of mass, momentum, energy in a two-body collision one obtains

$$(3.8) \quad \int \begin{bmatrix} 1 \\ \xi_1 \\ \xi^2 \end{bmatrix} f^0 L(g) d\xi = 0$$

On taking the moments indicated by (3.8) one obtains the conservation laws (3.1).

The reservations are as follows

(1) While (3.1) is exact (3.2) is not.* (3.1) follows from

* Within this linear framework.

conservation of mass, momentum and energy. On the other hand, the derivation of (3.2) needs in addition to these laws, a number of additional assumptions. (2) The conservation laws (3.1) are more general. For (3.6) shows immediately that certain very specific state equations are implied in this formulation which is not the case for (3.1). (3) Also in this vein is the fact that the kinetic theory stress, (3.8), only takes into consideration the mechanical transport of momentum.* The exact stress should also incorporate the effect of intermolecular forces.

Of course the immediate shortcoming to (3.1) is that it forms an incomplete system. More unknowns, than than equations are appear. Various schemes are available for the closure of the conservations equations. One of these, the Chapman-Enskog procedure, in fact terminates (3.1) through (3.2). The procedure seeks a solution (sometimes called a normal solution) to (3.2) by iteration, assuming that $v \rightarrow \infty$. From this one finds explicit expressions which terminate (3.1). For example in the first two approximations (known as Navier-Stokes and Burnett respectively)

$$p_{11} = \frac{4}{3} \mu \left(\frac{\partial u}{\partial x} + \frac{\mu}{p_0 \rho_0} \frac{\partial^2 p}{\partial x^2} - \frac{3\mu}{5T_0 \rho_0} \frac{\partial^2 T}{\partial x^2} \right) + O\left(\frac{1}{v^3}\right)$$

*And corresponding statement for heat conduction.

$$Q = -\kappa \frac{\partial T}{\partial x} - \frac{\kappa}{5C} \left(\frac{3\kappa}{\rho} - \frac{4\mu}{\rho} \right) \frac{\partial^2 u}{\partial x^2} + O\left(\frac{1}{v^3}\right)$$

where the viscosity, μ , and heat conductivity κ are each $O\left(\frac{1}{v}\right)$. It is implicit in this procedure that $\frac{\partial}{\partial t}, \frac{\partial}{\partial x}$ are small compared with v and therefore one expects that such a theory is accurate in the upper right-hand corner of the earlier diagram. Except for some illustrative examples in the next section we will not consider this method of investigating of sound propagation. We shall see in fact that B.V.2 and I.V.2 by this method can more efficiently be obtained by other means.

ILLUSTRATIVE EXAMPLES

In order to illustrate the various problems of section 2 we now consider the continuum formulation. In fact it will suffice for our purposes to consider only a model of the continuum approach. This will give at least a qualitative understanding of the various situations.

First we replace the energy equation by the condition that $T = 0$, and then we terminate the system by taking

$$(4.1) \quad p_{11} = \frac{4}{3} \mu \frac{\partial \mu}{\partial x}.$$

For convenience we introduce

$$(4.2) \quad L = \frac{4\mu}{3\rho\sqrt{RT}}$$

which is roughly the mean-free-path and the normalization

$$(4.3) \quad \frac{\rho}{\rho_0} = \rho', \quad \frac{u}{\sqrt{RT}} = u', \quad \frac{x}{L} = x', \quad \frac{t\sqrt{RT}}{L} = t'.$$

This results in

$$(4.4) \quad \begin{cases} \frac{\partial \rho}{\partial t} + \frac{\partial u}{\partial x} = 0 \\ \frac{\partial u}{\partial t} + \frac{\partial \rho}{\partial x} = \frac{\partial^2 u}{\partial x^2} \end{cases}$$

where the primes have dropped.

I.V.1 Writing the initial data as

$$(4.5) \quad \begin{cases} \rho(t=0) = e^{ikx} \rho^0(k) \\ u(t=0) = e^{ikx} u^0(k) \end{cases}$$

from linearity we seek a solution by taking

$$\frac{\partial}{\partial x} = ik$$

which yields the solution

$$(4.6) \quad \begin{bmatrix} \rho \\ u \end{bmatrix} = e^{-\begin{bmatrix} 0 & ik \\ ik & k^2 \end{bmatrix} t} \begin{bmatrix} \rho^0(k) \\ u^0(k) \end{bmatrix}$$

The matrix is easily diagonalized and has the eigenvalues

$$(4.7) \quad \sigma_{\pm} = \frac{k^2 \pm \sqrt{k^4 - 2k^2}}{2}$$

For $k^2 > 2$ propagation ceases. For $k \sim 0$

$$\sigma = \pm ik + k^2$$

which signifies propagation to the right and left with speed $\sqrt{RT_0}$, i.e., the isothermal speed. To solve a general initial value problem one takes the Fourier integral of (4.6)*.

I.V.2 This is immediately solved by 4.7.

To consider the B.V. problems we consider B.V.3 from which the others follow.

B.V.3

$$\begin{aligned} \text{Boundary conditions: } u &= u^0 e^{i\omega t} & x &= 0 \\ u &= 0 & x &= D \end{aligned}$$

* This problem is solved in "On the Structure of Wakes and Waves" Tech. Rep. 56 NONR 562(07) 13 Brown University.

From linearity we can seek a steady state solution, i.e., we take $\frac{\partial}{\partial t} = i\omega$ and so eliminate time dependence from the problem. (This ignores the transient in a real situation.)

Then eliminating density from the system (4.4)

$$(4.8) \quad i\omega u - \frac{1}{i\omega} \frac{\partial^2 u}{\partial x^2} - \frac{\partial^2}{\partial x^2} u = 0$$

This of course has exponential solutions of the form e^{sx} , where s satisfies.

$$(4.9) \quad i\omega + s^2 \left(\frac{i}{\omega} - 1 \right) = 0$$

and

$$(4.10) \quad s = \pm \frac{i\omega}{\sqrt{i\omega + 1}}$$

This has one root with positive real part s_+ , the other, s_- , has a negative real part. The solution to B.V.3 is then

$$(4.11) \quad A e^{s_- x} + (u^0 - A) e^{s_+ x} = u$$

with A such that

$$A e^{s_- D} + (u^0 - A) e^{s_+ D} = 0$$

so that

$$(4.12) \quad A = \frac{u^0 e^{s_+ D}}{e^{s_+ D} - e^{s_- D}}$$

This solves B.V.3 and we shall discuss it in a moment. To solve B.V.1 let $D \rightarrow \infty$ which implies $u^0 = A$ and so

$$(4.13) \quad u = u_0 e^{s_- x}.$$

The solution to B.V.2 is obviously given by (4.9) and B.V.1, (4.13), tells us to only consider s_- , the root with negative real part. It is in fact (4.13) which implies that only B.V.2 need be considered for a determination of wave speed and attenuation rate.

For comparison with later results we plot the speed and attenuation as given by (4.10). Writing

$$s = \alpha + i\beta$$

one finds

$$(4.14) \quad \frac{\alpha}{\omega} = \sqrt{\frac{-1 + \sqrt{1 + \omega^2}}{2(1 + \omega^2)}}$$

$$(4.15) \quad \frac{\beta}{\omega} = \frac{\omega}{\sqrt{2(1 + \omega^2)}(-1 + \sqrt{1 + \omega^2})}$$

and this is sketched in the diagram

One easily sees that

$$\frac{\alpha}{\omega} = \frac{\sqrt{RT}}{v_s}$$

and

$$\frac{\beta}{\omega} = \frac{\beta' \sqrt{RT}}{\omega'}$$

where v_s is the wave speed and primes denote dimensional quantities. The abscissa can also be written as

$$\frac{1}{\omega} = \frac{3}{4} \frac{p_0}{\omega' \mu}$$

Note that the reciprocal speed starts from its equilibrium value and falls to zero algebraically as $\omega \rightarrow \infty$. The normalized attenuation rate starts at zero achieves a maximum and vanishes algebraically as $\omega \rightarrow \infty$. Without change the same is true for any approximation of the Chapman-Enskog theory.

Returning to B.V.3 we see that $A \sim u^0$ if $\omega \rightarrow \infty$.

In fact this will be true for $D\alpha \gg 1$. Many of the sound measurements of interest take place in a regime for which $D\alpha = O(1)$. Both terms of (4.11) must then be retained for a description of the pressure field. Actually in an experiment the wall at $x=D$ is the detector so that only the pressure field at D is of interest. For the isothermal case under study $p \sim \rho$ and a simple calculation yields

$$\rho(x=D) = \frac{iu^0}{\omega} \left[\frac{2s_-}{e^{s_+D} - e^{s_-D}} \right]$$

In a more exact description more modes appear and in this regime many more terms appear in the analogue of this expression.

From these remarks we must conclude that B.V.2 is of questionable value when $D\alpha = 0(1)$. In spite of this we now take up the question of solving B.V.2 and I.V.2 for the Boltzmann equation (3.2).

METHOD OF WANG CHANG AND UHLENBECK

Wang Chang and Uhlenbeck set out, in a path breaking report, to examine plane waves (B.V.2 and I.V.2) for all values of the Knudsen number based on wave length K_λ . To do this they of course had to start with the Boltzmann equation, (3.2). We now briefly review their method and results. To start with we introduce an unspecified frequency, λ , and the following notation and normalization

$$(5.1) \quad \left\{ \begin{array}{l} t\lambda = t', \quad \frac{x\lambda}{\sqrt{RT_0}} = x', \quad \frac{\xi}{\sqrt{RT_0}} = \xi' \\ \omega = \frac{1}{(2\pi)^{3/2}} e^{-\frac{\xi'^2}{2}}, \quad \frac{Bv_0}{\lambda} = B' \\ (f, g) = \int \omega g f d\xi' \\ \frac{vL}{\lambda} = L' \end{array} \right.$$

These are inserted into (3.1), and after dropping the primes we obtain

$$(5.2) \quad \left(\frac{\partial}{\partial t} + \xi_1 \frac{\partial}{\partial x} \right) g = L(g) = \int w_* [g(\xi'_*) + g(\xi') - g(\xi_*) - g(\xi)] B d\xi d\theta d\xi_*$$

where all quantities are dimensionless. Also for instance

$$(1, g) = \rho$$

$$(\xi_1, g) = u$$

are the dimensionless, perturbed density and velocity

Following Wang Chang and Uhlenbeck* we restrict attention to interaction laws for which

$$(5.3) \quad B = B(\theta)^{**}$$

They discovered that in this case the eigenfunctions of L are given by[†]

* "On the Propagation of Sound in Monatomic Gases" Engr. Res. Inst., University of Michigan.

** A case in point are Maxwell molecules for which the interaction force is inversely proportional to the fifth power of the distance between molecules. This case was considered by Wang Chang and Uhlenbeck.

† They actually showed that the angular dependence is $\sim P_l^m(\cos\theta)e^{im\theta}$. However for our one-dimensional flow (5.4) suffices.

$$(5.4) \quad \psi_{r\ell} = \frac{S_{\ell+\frac{1}{2}}^r (\frac{1}{2}\xi^2) \xi^\ell P_\ell(\cos \theta)}{\left[\frac{2^{\ell+1} \Gamma(r+\ell+\frac{3}{2})}{\pi^{\frac{1}{2}} r! (2\ell+1)} \right]^{\frac{1}{2}}}$$

where $S_{\ell+\frac{1}{2}}^r$ and P_ℓ are Laguerre and Legendre polynomials respectively. In the form written we have

$$(5.5) \quad (\psi_{r\ell}, \psi_{r'\ell'}) = \delta_{rr'} \delta_{\ell\ell'}.$$

To demonstrate that

$$(5.6) \quad L(\psi_{r\ell}) = \lambda_{r\ell} \psi_{r\ell}.$$

we remark first that the angular dependence of $\psi_{r\ell}$ is immediate since L is an isotropic operator. Next we observe that $L(\psi_{r\ell})$ produces a polynomial in ξ of the same degree as $\psi_{r\ell}$, i.e. of degree $2r+\ell$. Therefore since

$$(5.6) \quad (\psi_{r'\ell'}, L \psi_{r\ell}) = (L \psi_{r'\ell'}, \psi_{r\ell})$$

we have

$$2r' + \ell = 2r + \ell$$

but from the previous remark $\ell = \ell'$ and therefore $r = r'$.

Several examples of the $\psi_{r\ell}$ are

$$\psi_{00} = 1$$

$$\psi_{01} = \xi_1$$

$$\psi_{10} = \left(\frac{3}{2}\right)^{\frac{1}{2}} \left(1 - \frac{1}{3} \xi^2\right)$$

From the conservation laws the corresponding eigenvalues are all zero.

The functions $\psi_{r\ell}$ form a complete set in velocity space and we can expand g in these. For later purposes we define the following operator

$$(5.7) \quad P_N = \sum_{r\ell}^N \psi_{r\ell} (\psi_{r\ell},)$$

and we can therefore write

$$(5.8) \quad g = P_\infty g, \quad L = \sum_{r\ell}^\infty \lambda_{r\ell} \psi_{r\ell} (\psi_{r\ell},)$$

Making the planewave assumption, i.e. writing

$$(5.9) \quad g = g(\xi) e^{\sigma t + s x}$$

the Boltzmann equation becomes

$$(5.10) \quad (\sigma + s \xi_1) g = L g$$

Substituting (5.8) in this and forming

$$(5.11) \quad (\psi_{r,\ell}, \{\sigma + s \xi_1 - L\} g) = 0$$

yields an infinite system of linear equations, which since, as is easily shown,

$$(5.12) \quad \xi_1 \psi_{r\ell} = (\ell+1) \left\{ \psi_{r,\ell+1} \left[\frac{(r+\ell + \frac{3}{2})^2}{(2\ell+1)(2\ell+3)} \right]^{\frac{1}{2}} \right.$$

$$\begin{aligned}
& -\psi_{r-l+1} \left[\frac{2r}{(2l+3)(2l+1)} \right]^{\frac{1}{2}} \Bigg\} + l \left\{ \psi_{r,l-1} \left[\frac{2(r+l+\frac{1}{2})}{(2l+1)(2l-1)} \right]^{\frac{1}{2}} \right. \\
& \left. - \psi_{r+l,l-1} \left[\frac{2r+l}{(2l-1)(2l+1)} \right]^{\frac{1}{2}} \right\}
\end{aligned}$$

has a relatively simple coupling. In fact any finite cutoff of the equations has only two more coefficients (ψ_{rl}, g) than equations.

Wang Chang and Uhlenbeck consider the truncated determinants or dispersion relations. Formally, they consider the linear homogeneous system of equation generated from

$$(5.13) \quad P_N(\sigma + s\xi_1 - L)P_N g = 0.$$

The resulting algebraic equation has a root $(\sigma, s) = (0, 0)^*$ and continuing this in the neighborhood of the origin power series for either I.V.2 or B.V.2 are found from the determinant of

(5.13) For example for I.V.2**

$$\begin{aligned}
(5.14) \quad \sigma = i \left(\frac{5}{3} \right)^{\frac{1}{2}} & \left[k + k^3 \left(\frac{-2}{5\lambda_{02}\lambda_{11}} + \frac{1}{10\lambda_{11}^2} + \frac{8}{15\lambda_{02}^2} \right) \right] \\
& + k^2 \left(\frac{1}{3\lambda_{11}} + \frac{2}{3\lambda_{02}} \right) + O(k^4)
\end{aligned}$$

* This is of multiplicity more than one.

** See Phys. Flu. 6, 10, 1963.

A remarkable feature of this calculation is that the coefficients in the series are exactly determined at successive truncations (This is due to the recursion relation (5.17)). In the form given by (5.13) the calculation may be carried out for arbitrary intermolecular force laws*. The previous feature however is lost, i.e. coefficients are no longer determined exactly but after a sufficient number of truncations they only change slightly. The series obtained in this way is exactly that obtained through the Chapman-Enskog theory.

It is very likely the case that these series diverge. This is shown to be the case in the appendix, for a kinetic model which is introduced in the following section.

If we choose λ of (5.1) to be the largest eigenvalue (or the largest constant in any other case) then it is clear that all coefficients in the series expansion are $O(1)$. Hence the series can be expected to be inaccurate when k (or ω in B.V.2) is $O(0)$. If we regard the determinant of (5.13) in its entirety, we obtain an algebraic expression for the roots, as for example is given by (4.14,15). In spite of the above comments on the nature of the series, we might attempt using the algebraic express for even large values of wavenumber or frequency. This approach was taken by Pekeris and his coworkers.

* The Maxwell eigenfunctions are still retained.

They in fact used the Wang-Chang-Uhlenbeck scheme to obtain determinants up to order 483 for Maxwell molecules and up to 105 for rigid spheres. Their results in the Maxwell molecule case are sketched below for the attenuation rate.*

METHOD OF KINETIC MODELS

We now consider an entirely different method of examining plane waves via the Boltzmann equation. We rewrite the Boltzmann equation as

$$\left(\frac{\partial}{\partial t} + \xi_1 \frac{\partial}{\partial x} + \Lambda \right) g = (L + \Lambda) g$$

where Λ is a constant to be specified. A kinetic model is taken to be

$$(6.1) \quad \left(\frac{\partial}{\partial t} + \xi_1 \frac{\partial}{\partial x} + \Lambda \right) g = (L + \Lambda) P_N g$$

* This is taken from "Symposium on Num. Treatment of O.Q.E. and I.D.E. of P.I.C.C. (Birkhauser-Verlog, Basel, 1960) pp. 388-398.

with $-\Lambda$ equal to the $N+1^{\text{st}}$ eigenvalue.* In passing, we mention that (6.1); (1) preserves the conservation laws, (2) has the linearized form of the H-theorem (3) gives correctly at least $N+2$ eigenvalues, (4) leads to the free flow operator for large Knudsen number (5) in a relaxation theory yields relaxing high moments which is at least qualitatively correct.

Items (1) and (2) are the "sacred laws" of kinetic theory and it is deemed important that these properties be preserved.**

Since

$$(6.2) \quad P_N L = L P_N$$

for Maxwell molecules we can also write

$$(6.3) \quad \left(\frac{\partial}{\partial t} + \xi \frac{\partial}{\partial x} + \Lambda \right) g = P_N (L + \Lambda) P_N g .$$

This furnishes suitable kinetic model for non-Maxwellian molecules[†]. As will be seen momentarily a most important feature of these models is the appearance of only a finite number of moments on the right-hand side.

* L is negative semi-definite.

** For $N=3$, (6.1) gives the BGK kinetic model, Phys. Rev. 94, 511, 1954. For other values of N this is equivalent to the Gross-Jackson procedure, Phys. Flu. 2, 432, 1959.

† See Phys. Flu. 5, 908, 1962.

Choosing λ in (5.1) such that $\Lambda = 1$, the plane wave problem leads to

$$(6.4) \quad (\sigma + \xi s + 1)g = P_N(L+1)P_N g$$

Before proceeding to what must obviously be done, we perform a short calculation which is instructive. Although the result will be true in general, we consider I.V.2 for Maxwell molecules,

$$(6.5) \quad (\sigma + ik\xi + 1)g = (L+1)P_N g$$

Since complex numbers have been introduced we allow the previous inner product to be the complex inner product.

Then

$$(6.6) \quad \sigma(g, g) + ik(g, \xi g) = (g, (L+1)P_N g) - (g, g)$$

and therefore

$$(6.7) \quad \operatorname{Re} \sigma = \frac{(g, (L+1)P_N g)}{(g, g)} - 1$$

and hence

$$(6.8) \quad -1 \leq \operatorname{Re} \sigma \leq 0.$$

Other arguments then show that k is bounded for σ in this region. This same effective cutoff of planewaves occurs in the B.V.2 case also. If the normalization is removed so that the lower limit goes to ∞ in (6.8) (since L is unbounded for Maxwell molecules) and therefore the condition (6.8) is "unphysical". We will return to this point momentarily.

Returning to (6.4) we form

$$(6.8) \quad P_N g = P_N \frac{1}{\sigma+1+\xi s} P_N^{(L+1)} P_N g$$

which is exact for (6.4). This only involves the (N+1) coefficients*

$$(6.9) \quad (\psi_{r(i)\ell(i)}, g), \quad i = 0, \dots, N,$$

and so we are lead to only a finite determinant. Comparing

(6.8) with (5.13) we see that the present method can also be regarded as a sequence of approximations to the exact situation and not just a model of it.

A typical term in the determinant of (6.8) is

$$(6.10) \quad s \int_{-\infty}^{\infty} \frac{\omega \psi_{r\ell} \psi_{r'\ell'}}{\frac{\sigma+1}{s} + \xi_1} d\xi$$

The integral in (6.10) is readily integrated in terms of the error and Gaussian functions of the variable $z = \frac{\sigma+1}{s}$. It is analytic everywhere save $z = 0, \infty$ where essential singularities occurs.

On regarding (6.10) we see that two analytic functions are defined by the integral - one each for $\text{Im } z > 0$ and $\text{Im } z < 0$. Realizing this we can remove the mystery associated with the planewave cutoff given by (6.8). To do this we consider I.V.1, i.e. $s = ik$. In fact for simplicity we consider k fixed so that the initial disturbance is sinesoidal. Then denoting the initial data by g^0 , the transformed equation is

* It is convenient for discussion and calculation to reduce the two dimensional array (r, ℓ) to a one-dimensional array.

$$(6.11) \quad (\sigma + ik\xi + 1)g = P_N(L+1)P_N g + g^0$$

and

$$(6.12) \quad g = \frac{1}{\sigma + ik\xi + 1} P_N(L+1)P_N g + \frac{g^0}{\sigma + ik\xi + 1}$$

We see that only

$$(6.13) \quad (\psi_{r(i), \ell(i)}, g) = a_i, \quad i=0, \dots, N$$

appear on the righthand side. Writing

$$(6.14) \quad a_i^0 = \left(\psi_{r(i), \ell(i)}, \frac{g^0}{\sigma + ik\xi + 1} \right)$$

and

$$A_{ij} a_j = \left(\psi_{r(i), \ell(i)}, P_N(L+1)P_N g \right)$$

we can represent solution to (6.12) by

$$a - Aa = a^0$$

and

$$a = (1-A)^{-1} a^0,$$

Inverting the Laplace transform we obtain

$$a(t) = \int_{\uparrow} e^{\sigma t} (1-A)^{-1} a^0 d\sigma$$

where the $\uparrow$ denotes a Bromwich path. On moving the path of integration to the left in the complex σ plane we pick up the poles of $\det(1-A)$. We may move as far to the left as we please*, but this is permitted by the Cauchy theorem only if the analytic function of the integrand is continued. This means that only one of the two analytic functions defined by

* If a^0 has a barrier at $\operatorname{Re} \sigma = -1$, this is not true.

(6.10) is used (which depends on the sign of k). From analytic function theory we know that the locus of zeroes of $\det (1-A)$ cannot end in the finite plane (at least for finite k) and so the condition (6.8) would seem to be removed. Actually what has happened is that the dispersion relation has been given an analytic continuation. Although poles are picked up to the left of $\text{Re } \sigma < -1$ these do not lead to plane waves. The plane wave associated with such a pole cannot be dissociated from an infinity of other plane waves which have poles in the continued portion of the plane. In contrast to this are the poles for which $-1 < \text{Re } \sigma \leq 0$, and which are pure plane waves. For such waves initial data can be found which lead to the appearance of this wave and only this wave.

As already mentioned the position of the cutoff line moves to the left as N increases, and hence this cutoff can be regarded as unphysical. From actual calculation we find that the analytic continuation of the sound root of the dispersion relation falls, with a high degree of accuracy, upon the pure wave roots of a larger N calculation. This of course suggests that the analytically continued result should be used without apology. The plots given below are self-explanatory and demonstrate the close agreement which the method just described has with experiment.*

* Taken from Jour. Acous. Soc., 37, 329, 1965.

Appendix
Low Frequency Expansions

In this section we take up the nature of formal power series expansion of $\sigma(s)$ (or equivalently $s = s(\sigma)$). This is of basic importance in as much as the Chapman-Enskog theory is closely related to this expansion. We shall show that this expansion is in fact divergent. Earlier, on page 20, we mentioned that the truncated Boltzmann equations lead to the exact determination of coefficients in the formal expansion (for $B = B(\theta)$). This then brings up the question of the value of truncated Boltzmann equations in the present connection. Ford* has shown (for a kinetic model) that the roots of the dispersion relation arising from successively truncated Boltzmann equations do in fact converge to the series of the exact dispersion relation. Bearing in mind the extensive numerical work of Pekeris et al, we must conclude that this convergence is extremely slow.

Our demonstration of the non-convergence of the formal expansion for $\sigma(s)$ will be for the following simplified kinetic model (referred to as the isotheric model)

$$(1) \quad (\sigma + s\xi + 1)g = a_1 \psi_0 .$$

Taking the inner product of (1) with $\psi_0 = 1$ we obtain

* See these lecture notes.

$$(2) \quad a_1 = a_1 \int \frac{\Omega d\xi}{\sigma + s\xi_1 + 1}$$

Carrying out the integration of ξ_2 and ξ_3 we left with the dispersion relation

$$(3) \quad \sigma = \lambda \int \frac{e^{-\frac{\xi_1^2}{2}} d\xi}{\lambda - i\xi_1} - 1 = M(\lambda) - 1$$

where

$$(4) \quad \lambda = \frac{1 + \sigma}{is}$$

As can be easily verified the function M satisfies

$$(5) \quad \frac{dM}{d\lambda} = \left(\lambda + \frac{1}{\lambda}\right) M - \lambda$$

Setting

$$(6) \quad -x = s^2$$

and using (3) and (4) we find after some manipulation

$$(7) \quad 2 \frac{d\sigma}{dx} = \frac{\sigma}{x} + \frac{1}{x} + \frac{1}{\sigma}$$

Further setting

$$(8) \quad \varphi = \frac{\sigma}{x}$$

we find

$$(9) \quad 2x^2 \varphi \frac{d\varphi}{dx} + x\varphi^2 = \varphi + 1$$

Formally writing

$$(10) \quad \varphi = \sum_{r=0}^{\infty} a_r x^r$$

and substituting we find

$$(11) \quad a_{r+1} = (r+1) \sum_{j=0}^r a_{r-j} a_j$$

For the isosteric model only one discrete root exists, and is in fact $\sigma = 0 = x$, which satisfies (3). From (9) we see that $\varphi = -1$ for $x = 0$, so that $a_0 = -1$. An induction argument immediately yields that $a_{2r} > 0$ and $a_{2r+1} < 0$. Induction also shows that $|a_r| > r!$, for $r > 1$. This concludes the demonstration.

The above method of showing the divergence of the formal power series can in principle be applied to more refined models. This however has proven too tedious to carry out. In the absence of such work we cannot, with rigor, conclude the divergence of similar series for other models and of course not for Boltzmann equations. On the other hand the present work is work which highly suggests this conclusion.

- I. THE METHOD OF AVERAGING
- II. THE KINETIC EQUATION FOR MODERATELY DENSE GASES

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I. THE METHOD OF AVERAGING

I must first of all tell you that most of what I know about the method of averaging I have learned from my colleague, K. M. Case. He has been working with the method for the past year and most of the general formalism and applications I will tell you about today are due to him.¹⁾

As do most of the methods of non-linear mechanics, the method of averaging goes back at least to Poincare. A brief introduction is given in the last chapter of the book of Bogoliubov and Mitropolsky.²⁾

Let me tell you now what the method is. Consider the first order differential equation:

$$\frac{dx}{dt} = \epsilon F(x, t) \quad (1)$$

where ϵ is a small parameter. In general, we may consider x to be a vector with, say, n components, but for the moment we think of a single dependent variable. We desire the solution of (1) which is valid for times long compared with ϵ^{-1} . To see what the trouble is, consider the trivial example

$$\dot{x} = -\epsilon(1 + \cos t)x \quad (2)$$

Following the usual methods of time dependent perturbation theory, known to every physicist, we convert this equation into an integral equation:

$$x(t) = x(0) - \epsilon \int_0^t (1 + \cos t') x(t') dt' \quad (3)$$

and solve by iteration:

$$\begin{aligned} x(t) &= x(0) - \epsilon \int_0^t dt' (1 + \cos t') x(0) + \dots \\ &= \{1 - \epsilon(t + \sin t) + \frac{1}{2}\epsilon^2(t + \sin t)^2 + \dots\}x(0) \end{aligned} \quad (4)$$

We even know that the series indicated here converges for all t , yet it is of no use if t is of order ϵ^{-1} . This is because of the secular terms ϵt , $(\epsilon t)^2$, etc., which become very large when t is of order ϵ^{-1} . Now the exact solution of (2) is, of course,

$$\begin{aligned} x(t) &= e^{-(t + \sin t)} x(0) \\ &= e^{-\epsilon t} \{1 - \epsilon \sin t + \frac{1}{2}\epsilon^2 \sin^2 t + \dots\}x(0) \end{aligned} \quad (5)$$

Here we see that the secular terms all add up to a slowly varying exponential factor, and that the remaining terms are rapidly varying but bounded for all t . Hence, for sufficiently small ϵ , the first few terms are a good approximation for all t . The method of averaging is designed to make this separation of slowly varying and rapidly varying terms in the general case where $F(x, t)$ may be non-linear.

What one does is to seek a solution of (1) which is of the form

$$x = \xi + \epsilon A^{(1)}(\xi, t) + \epsilon^2 A^{(2)}(\xi, t) + \dots \quad (6)$$

where ξ is a new dependent variable which obeys an equation of the form:

$$\frac{d\xi}{dt} = \epsilon B^{(1)}(\xi) + \epsilon^2 B^{(2)}(\xi) + \dots \quad (7)$$

Here we require that $A^{(n)}(\xi, t)$ have no secular terms in t , and that ξ be a slowly varying function of t , which is implied by the fact that the $B^{(n)}(\xi)$ are independent of t . Inserting (6) in (1), using (7), and then equating powers of ϵ , we get the following sequence of equations for the determination of $A^{(n)}$ and $B^{(n)}$.

$$\frac{\partial A^{(1)}}{\partial t}(\xi, t) + B^{(1)}(\xi) = F(\xi, t) \quad (8a)$$

$$\frac{\partial A^{(2)}}{\partial t}(\xi, t) + B^{(2)}(\xi) = \frac{\partial F(\xi, t)}{\partial \xi} A^{(1)}(\xi, t) - \frac{\partial A^{(1)}}{\partial \xi}(\xi, t) B^{(1)}(\xi) \quad (8b)$$

etc.

The first of these equations is typical of them all, since the right-hand side of each is known if the previous equations have been solved. To determine $A^{(1)}(\xi, t)$ we note that ξ appears only parametrically in (8) and that for fixed ξ , $A^{(1)}(\xi, t)$ is to have no secular terms in t . This means that $B^{(1)}(\xi)$ must be chosen

to cancel the terms in $F(\xi, t)$ which would lead to such secular terms. This will be so if we choose $B^{(1)}(\xi)$ to be the time average of $F(\xi, t)$ for fixed ξ :

$$B^{(1)}(\xi) = \overline{F(\xi, t)} = \lim_{t \rightarrow \infty} \frac{1}{t} \int_0^t dt F(\xi, t) \quad (9)$$

Clearly, we must assume this limit exists.³⁾ The equation may now be integrated directly to give

$$A^{(1)}(\xi, t) = \int dt [F(\xi, t) - \overline{F(\xi, t)}]. \quad (10)$$

This is the indefinite integral, with the constant of integration an arbitrary function of ξ alone. Depending upon the problem, we generally find it convenient to choose this constant of integration either so that

$$\overline{A^{(n)}(\xi, t)} = 0 \quad (11)$$

in which case ξ is the "mean value" of x , or to choose

$$A^{(n)}(\xi, 0) = 0. \quad (12)$$

in which case the initial value of ξ is equal to the initial value of x .

Let us now see how this works for a number of examples.

Consider first the simple equation

$$\frac{dy}{dt} = -\alpha y + \epsilon y^2, \quad (13)$$

where $\alpha > 0$, and ϵ is a small parameter. We must first prepare the equation in the canonical form (1). This we do by writing

$$y = e^{-\alpha t} x \quad (14)$$

Then x is a solution of

$$\dot{x} = \epsilon e^{-\alpha t} x^2, \quad (15)$$

which is in standard form. We now make the expansion (6) and (7). The equation (8a) becomes

$$\frac{\partial A^{(1)}}{\partial t} + B^{(1)} = e^{-\alpha t} \xi^2 \quad (16)$$

The time average of the right-hand side vanishes so

$$B^{(1)} = 0, \quad (17)$$

and we have

$$A^{(1)}(\xi, t) = -\frac{1}{\alpha} \xi^2 (e^{-\alpha t} - 1), \quad (18)$$

where we have chosen the constant of integration so that

$A^{(1)}(\xi, 0) = 0$. Similarly from (8b) we find

$$B^{(2)} = 0 \quad (19)$$

and

$$A^{(2)}(\xi, t) = \frac{\xi^3}{\alpha^2} (e^{-\alpha t} - 1)^2 \quad (20)$$

Hence we have $\xi = x(0)$ is a constant through second order in

ϵ and

$$x(t) = x(0) - \frac{\epsilon}{\alpha} x^2(0) (e^{-\alpha t} - 1) + \frac{\epsilon^2}{2\alpha} x^3(0) (e^{-\alpha t} - 1)^2 + \dots \quad (21)$$

Note that $x(t)$ is bounded in every order, so if the series (21) converges, it follows that $y(t)$ vanishes for large t . This is a special case of the Poincaré-Lyapunov theorem which states that if all solutions of the linear equation $dy/dt = -Ay$ go to zero as $t \rightarrow \infty$, and if ϵ is sufficiently small, then the solution of (13) goes to zero for large t . We can verify these properties for our special case by inspection of the exact solution, which is

$$y(t) = \frac{x(0)e^{-\alpha t}}{1 - \epsilon x(0) \frac{1 - e^{-\alpha t}}{\alpha}} \quad (22)$$

Hence, if $\epsilon < \alpha/x(0)$, the series (21) converges and the Poincaré-Lyapunov theorem holds.

Consider now a less trivial problem drawn from physics. The classical nuclear magnetic resonance experiment is one in which a sample containing paramagnetic nuclei (i.e. nuclei which have a spin, and hence an associated magnetic moment) is introduced into a uniform field H_0 .

The result is that the nuclear spins precess about the magnetic field direction, which we take to be the z-axis. The angular velocity of this precession is

$$\omega_0 = \gamma H_0 \quad (23)$$

Fig. 1.

where γ is the so-called gyromagnetic ration of the nucleus. The experiment consists in applying an oscillating magnetic field along, say, the x-axis, of the form

$$2H_1 \cos \omega t \quad (24)$$

(the 2 is conventional). When ω is near ω_0 , it is observed that a kind of resonance occurs in which the nuclear spins precess about the x-axis. This change in the character of the spin rotation in the sample is easily detected and, hence, one has a method of measuring ω_0 . Since H_0 can be separately measured, the method leads to measurement of γ , which is the quantity of interest. The resonance in fact does not occur exactly at

$\omega = \omega_0$, there is a slight shift, called the Bloch-Siegert shift, which depends on the magnitude of the oscillating field. Our aim now will be to calculate that shift.

I consider for simplicity only the special case of spin $\frac{1}{2}$ ⁵⁾. The Schrödinger equation for the spin motion in a magnetic field is

$$i \frac{d\psi}{dt} = -\frac{1}{2} \gamma \vec{\sigma} \cdot \vec{H} \psi, \quad (25)$$

where ψ is a two component spinor (a two vector):

$$\psi = \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} \quad (26)$$

and $\sigma_x, \sigma_y, \sigma_z$ are the 2×2 Pauli spin matrices given by

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (27)$$

In our case, where $H_x = 2H_1 \cos \omega t$, $H_y = 0$, $H_z = H_0$, (25) becomes

$$i \frac{d\psi}{dt} = -\left(\frac{\omega_0}{2} \sigma_z + \omega_1 \cos \omega t \sigma_x \right) \psi, \quad (28)$$

where $\omega_1 = \gamma H_1$. In the experimental situations ω_1 is generally small compared with ω_0 . To put (28) into a form like (1), we make a change of variables by putting

$$\psi = e^{\frac{i\omega t}{2}\sigma_z} \varphi. \quad (29)$$

This corresponds to a rotation about the z-axis through angle ωt . It is then true that φ satisfies the equation

$$i \frac{d\varphi}{dt} = \left(\frac{\omega - \omega_0}{2} \sigma_z - \omega_1 e^{-i \frac{\omega t}{2} \sigma_z} \sigma_x e^{i \frac{\omega t}{2} \sigma_z} \cos \omega t \right) \varphi \quad (30)$$

$$\text{But } e^{-i \frac{\omega t}{2} \sigma_z} \sigma_x e^{-i \frac{\omega t}{2} \sigma_z} = \cos \omega t \sigma_x + \sin \omega t \sigma_y. \quad (31)$$

Hence, (30) becomes:

$$i \frac{d\varphi}{dt} = \frac{\epsilon}{2} \left[(\omega - \omega_0) \sigma_z - \omega_1 (1 + \cos 2\omega t) \sigma_x - \omega_1 \sin 2\omega t \sigma_y \right] \varphi \quad (32)$$

Here I have inserted a factor of ϵ , which I shall later set equal to unity. The effective magnitude of ϵ is the ratio ω_1/ω , which is assumed small. You could see this more clearly if we were to introduce a dimensionless time $\tau = \omega t$ and note that $\omega - \omega_0$ is of order ω_1 for the frequencies of interest.

We now apply the method of averaging to equation (32).

Write

$$\varphi = \theta + \epsilon F^{(1)}(t) \theta + \epsilon^2 F^{(2)}(t) \theta + \dots \quad (33)$$

where

$$i \frac{d\theta}{dt} = \epsilon B^{(1)} \theta + \epsilon^2 B^{(2)} \theta + \dots \quad (34)$$

Inserting the expansion (33) in (32) and then using (34)

we find upon equating coefficients of powers of ϵ .

$$i \frac{dF^{(1)}}{dt} + B^{(1)} = \frac{1}{2}[(\omega - \omega_0)\sigma_z - \omega_1(1 + \cos 2\omega t)\sigma_x - \omega_1 \sin 2\omega t \sigma_y] \quad (35)$$

and

$$i \frac{dF^{(2)}}{dt} + B^{(2)} = -F^{(1)} R^{(1)} + \frac{1}{2}[(\omega - \omega_0)\sigma_z - \omega_1(1 + \cos 2\omega t)\sigma_x - \omega_1 \sin 2\omega t \sigma_y] F^{(1)} \quad (36)$$

etc.

According to our general prescription, we must choose $B^{(1)}$ to be equal to the time average of the right-hand side of (35).

That is

$$B^{(1)} = \frac{1}{2}[(\omega - \omega_0)\sigma_z - \omega_1 \sigma_x] \quad (37)$$

With this choice of $B^{(1)}$ we find upon integrating (35) that

$$F^{(1)}(t) = +i \frac{\omega_1}{4\omega} (\sin 2\omega t \sigma_x - \cos 2\omega t \sigma_y). \quad (38)$$

Here I have chosen the constant of integration so that the time average of $F^{(1)}(t)$ vanishes. The wave function θ will describe, therefore, the slowly moving mean spin motion, which is just what one measures.

Knowing $F^{(1)}$, we determine $B^{(2)}$ from (36) where we must choose $B^{(2)}$ to be the time average of the right-hand side. That is

$$B^{(2)} = i \frac{\omega_1^2}{16\omega} (\sigma_x \sigma_y - \sigma_y \sigma_x) = -\frac{\omega_1^2}{8\omega} \sigma_z. \quad (39)$$

Here I have used the fact that $\sigma_x \sigma_y - \sigma_y \sigma_x = 2i\sigma_z$. We could go on to determine $F^{(2)}$, then $B^{(3)}$ etc., but I'll stop here.

The equation for the mean spin motion through second order, is then

$$i \frac{d\theta}{dt} = \frac{1}{2} \left[(\omega - \omega_0 - \frac{\omega_1^2}{4\omega}) \sigma_z - \omega_1 \sigma_x \right] \theta, \quad (40)$$

where I have set $\epsilon = 1$. We can write this equation as

$$i \frac{d\theta}{dt} = -\frac{1}{2} \vec{\sigma} \cdot \vec{\Omega} \theta, \quad (41)$$

where $\vec{\Omega}$ is the angular velocity of the mean spin motion, whose components are

$$\Omega_x = -\omega_1, \quad \Omega_y = 0, \quad \Omega_z = \omega - \omega_0 - \frac{\omega_1^2}{4\omega}. \quad (42)$$

The observed resonance occurs when the mean spin rotates about the x direction, i.e. when

$$\omega_0 = \omega - \frac{\omega_1^2}{4\omega}. \quad (43)$$

The term $\omega_1^2/4\omega$ is the Bloch-Siegert shift.

I hope that with these examples I have been able to give you some idea of how the method of averaging works and of how it might be useful in the solution of problems in physics. I will turn next to a more ambitious, and at the same time more speculative, application of the method to the derivation of a kinetic equation for moderately dense gases.

FOOTNOTES

- 1^o See Richard Y. Y. Lee, "On a new perturbation method"
Thesis, University of Michigan, 1964.
- 2^o N. N. Bogoluibov and Y. A. Mitropolsky, "Asymptotic
methods in the theory of non-linear oscillations"
(Hindustani Publ. Co., India, 1961).
- 3^o The generalization of the method to the case where this
limit does not exist is not difficult. See ref. 1 and
K. M. Case, to be published.
- 4^o F. Bloch and A. J. F. Siegert, Phys. Rev. 57, 522 (1940).
- 5^o The discussion for arbitrary spins is given in the thesis
of Lee, ref. 1.

II. THE KINETIC EQUATION FOR MODERATELY DENSE GASES

INTRODUCTION

The problem of determining the corrections to the Boltzmann kinetic equation due to the non-ideality of the gas has occupied a host of researchers, and there are many papers on the subject. One thing is clear in all these papers: there has been in the past no unanimity about how one should even approach the problem. There is, however, a thread, starting with the classic work of Bogoliubov¹⁾, then on to the work of Uhlenbeck and his student Choh²⁾, and most recently appearing in the works of Cohen and of M. S. Green^{3,4)} which is generally agreed to be a correct, if not necessarily unique, approach to the problem. Other approaches I should mention are those of Prigogine and Resibois⁵⁾, and of Frieman and Sandri⁶⁾, and of Lewis⁷⁾ who by different techniques arrive at similar conclusions. My purpose here is to show how the method of averaging can be of use in the discussion of the problem. Those who are familiar with the works mentioned above, will know that what I do is not entirely original, and that I have learned from each of them.

Before proceeding let me briefly summarize the problem. The one particle distribution function $f(\vec{r}, \vec{p}, t)$ is defined so that $f(\vec{r}, \vec{p}, t) d\vec{r} d\vec{p}$ is the number of gas particles at time t whose momentum is in the range $d\vec{p}$ about $\vec{p}$ and whose position is in the range $d\vec{r}$ about $\vec{r}$. Thus

$$\iint d\vec{r} d\vec{p} f(\vec{r}, \vec{p}, t) = N \quad (1.1)$$

is the number of gas particles. For the monoatomic gas, whose atoms may be considered as spherically symmetric centers of force, the Boltzmann equation takes the form⁸⁾:

$$\frac{\partial f}{\partial t} + \frac{1}{m} \vec{p} \cdot \frac{\partial f}{\partial \vec{r}} = \int d\vec{p}_1 \int d\Omega g I(g, \theta) [f' f'_1 - f f_1] \quad (1.2)$$

Here m is the mass of a gas particle, $I(g, \theta)$ is the differential scattering cross section for a collision between two atoms in which the relative velocity, whose magnitude is g , is rotated through an angle θ into solid angle $d\Omega$. The prime and the index on the f 's refer to the four momenta of the binary collision $(\vec{p}, \vec{p}_1) \rightarrow (\vec{p}', \vec{p}'_1)$, e.g. $f_1 = f(\vec{r}, \vec{p}_1, t)$. The classical derivation of the Boltzmann equation is very persuasive, but it has the defect that it involves a probabilistic assumption, the famous Stosszahlansatz. It is clear also that the equation can be valid only for very low densities, since only then can the effects of triple and higher collisions

be neglected. Thus there are two closely related problems: first to give a satisfactory derivation of the Boltzmann equation, and second to determine the corrections to it due to multiple collisions.

It is generally believed that the solution of these problems will take the form of a systematic derivation of a kinetic equation for f which may be written:

$$\frac{\partial f}{\partial t} = B^{(1)}(f) + B^{(2)}(f) + \dots, \quad (1.3)$$

where

$$B^{(1)}(f) = -\frac{1}{m} \vec{p} \cdot \frac{\partial f}{\partial \vec{r}} \quad (1.4)$$

is the Boltzmann streaming term.

$$B^{(2)}(f) = \int d p_1 \int d \Omega g I(g, \theta) [f' f'_1 - f f_1] \quad (1.5)$$

is the Boltzmann binary collision term, and in general $B^{(n)}(f)$ will be an n -tuple collision term. Since the probability of an n -tuple collision is proportional to the n 'th power of the density of the gas, the expansion indicated on the righthand side of (1.3) will be an expansion in powers of the density. An important property which this kinetic equation is expected to have is that $B^{(n)}(f)$ will not depend explicitly upon the time. What this means is that the kinetic equation affords a closed deterministic description of the motion of the gas in the sense that the distribution function

$f(\vec{r}, \vec{p}, t)$ is determined by its initial value alone. We call this a contracted description since the number of variables is much less than that required to determine the mechanical state of the gas⁹⁾. That such a description should exist is paradoxical, since it is hard to believe that it could be an exact consequence of the microscopic mechanical laws which underlie the motion of the gas. So our task is not only to discover the form of the kinetic equation, but also to show in what sense it approximates the true motion.

SOME FORMAL PROPERTIES OF THE MECHANICAL MOTION¹⁰⁾

We consider the mechanical motion of a system of N particles, which is governed by the Hamiltonian:

$$H = \sum_{j=1}^N \left[\frac{1}{2m} \vec{p}_j^2 + \omega(\vec{r}_j) \right] + \sum_{j < k} \varphi(|\vec{r}_j - \vec{r}_k|), \quad (2.1)$$

where the interparticle force potential $\varphi(r)$ is spherically symmetric and is assumed to have a hard core and a finite range. In this expression $\omega(\vec{r})$ is the potential energy of the outside forces, including the wall force which keeps the particles in their container. We shall use for the Hamiltonian (2.1) the compact notation

$$H(1, 2, \dots, N), \quad (2.2)$$

indicating only the labels of the N particles whose canonical variables appear in H . Thus

$$\begin{aligned} H(1) &= \frac{1}{2m} \vec{p}_1^2 + \omega(\vec{r}_1) \\ H(1, 2) &= \frac{1}{2m} \vec{p}_1^2 + \omega(\vec{r}_1) + \frac{1}{2m} \vec{p}_2^2 + \omega(\vec{r}_2) + \varphi(r_{12}) \end{aligned} \quad (2.3)$$

etc.

The system of N particles may be described by the probability distribution in the $6-N$ dimensional phase space of the system:

$$D(1, 2, \dots, N; t) \equiv D(x_1, x_2, \dots, x_N; t), \quad (2.4)$$

where

$$x_k = (\vec{r}_k, \vec{p}_k) \quad (2.5)$$

denotes the coordinates and momenta of the k^{th} particle.

This distribution is normalized so the total probability is unity;

$$\int \dots \int dx_1 dx_2 \dots dx_N D(1,2,\dots,N;t) = 1 \quad (2.6)$$

The identity of the particles requires that D be a symmetric

function of $x_1, x_2, \dots, x_N$. The change of D with time is given

by the Liouville equation:

$$\frac{\partial D}{\partial t} = [H, D], \quad (2.7)$$

where the Poisson bracket, for any pair of functions F and

G , is defined to be

$$[F, G] \equiv \sum_{k=1}^N \left(\frac{\partial F}{\partial \vec{r}_k} \cdot \frac{\partial G}{\partial \vec{p}_k} - \frac{\partial F}{\partial \vec{p}_k} \cdot \frac{\partial G}{\partial \vec{r}_k} \right). \quad (2.8)$$

The formal solution of the Liouville equation may be written:

$$D(1,2,\dots,N;t) = S(1,2,\dots,N;t)D(1,2,\dots,N;0), \quad (2.9)$$

where the streaming operator is defined so that

$$\begin{aligned} S(1,2,\dots,N;t)F(1,2,\dots,N) &\equiv e^{t[H, \cdot]} F(1,2,\dots,N) \\ &\equiv F + t[H, F] + \frac{t^2}{2!} [H, [H, F]] + \dots, \end{aligned} \quad (2.10)$$

for any function F .

Note that $S(1,2,\dots,N;-t)$ is the inverse of $S(1,2,\dots,N;t)$.

An important property of the motion is that

$$\int \dots \int dx_1 dx_2 \dots dx_N [H, F] = 0 \quad (2.11)$$

for any function F which vanishes fast enough at infinity.

To prove this, note that

$$[H, F] = \sum_{k=1}^N \frac{\partial}{\partial p_k} \cdot \frac{\partial H}{\partial r_k} F - \frac{\partial}{\partial r_k} \cdot \frac{\partial H}{\partial p_k} F \quad (2.12)$$

Hence the integral in (2.11) can be transformed into a surface integral, which vanishes if F vanishes for sufficiently large values of the coordinates and momenta. From (2.10) it follows that for any such F ,

$$\begin{aligned} \int \dots \int dx_1 \dots dx_N S(1,2,\dots,N;t) F(1,2,\dots,N) \\ = \int \dots \int dx_1 \dots dx_N F(1,2,\dots,N). \end{aligned} \quad (2.13)$$

This is the famous integral invariant of Poincare; it follows from the application of (2.11) term by term to the definition (2.10) of the streaming operator.

Finally, it should be clear that the solution of the Liouville equation (2.7) is equivalent to a complete solution of the equation of motion for the N particles. It should be clear that if we are given the initial values of all the coordinates and momenta, which I denote by a prime,

then by solving the equations of motion we can find the coordinates and momenta at time t . I indicate this schematically by

$$(x'_1, x'_2, \dots, x'_N) \xrightarrow[t]{H} (x_1, x_2, \dots, x_N). \quad (2.14)$$

We say that the initial state $(x'_1, \dots, x'_N)$ goes into the final state $(x_1, x_2, \dots, x_N)$ under the action of the Hamiltonian H during the time t . It is not difficult to verify that the solution (2.9) of the Liouville equation is

$$D(1, 2, \dots, N; t) = D(1', 2', \dots, N'; 0) \quad (2.15)$$

or that

$$x'_j = S(1, 2, \dots, N; t)x_j. \quad (2.16)$$

Here (2.15) is the solution of the Liouville equation given the complete solution of the equation of motion, and (2.16) is the solution of the equation of motion given the streaming operator, i.e. given a complete solution of the Liouville equation. From (2.16) we are led to the fruitful interpretation of $S(1, 2, \dots, N; t)$ as a substitution operator. The result of acting with $S(1, 2, \dots, N; t)$ upon any function of $(x_1, x_2, \dots, x_N)$ is to replace x_1 by x'_1 , x_2 by x'_2 , ..., x_N by x'_N , where $(x'_1, x'_2, \dots, x'_N)$ is the initial state indicated in (2.16). The operator $S(1, 2, \dots, N; t)$, interpreted as a substitution operator, carries the motion backward a time t .

THE EXPRESSION OF THE DISTRIBUTION FUNCTIONS IN TERMS OF THEIR INITIAL VALUES

The s-particle (generic) distribution function is defined by the expression:

$$f(1,2,\dots,s;t) \equiv \frac{N!}{(N-s)!} \int \dots \int dx_{s+1} \dots dx_N D(1,2,\dots,N;t). \quad (3.1)$$

Since D is normalized to unity,

$$\int \dots \int dx_1 \dots dx_s f(1,2,\dots,s;t) = \frac{N!}{(N-s)!} \quad (3.2)$$

is the number of ordered s-tuples of gas particles. Thus, $f(1,2,\dots,s;t)$ is the distribution function for the number of ordered s-tuples in the gas. In particular $f(1;t) \equiv f(\vec{r}_1, \vec{p}_1;t)$ is the one particle distribution introduced in Section 1.

These partial distribution functions can be expressed formally in terms of their initial values. We shall do so only for the one particle distribution function, but the generalization to higher distribution functions is not difficult. Consider

$$\begin{aligned} f(1;t) &= \frac{N!}{(N-1)!} \int \dots \int dx_2 \dots dx_N D(1,2,\dots,N;t) \\ &= \frac{N!}{(N-1)!} \int \dots \int dx_2 \dots dx_N S(1,2,\dots,N;t) D(1,2,\dots,N;0), \end{aligned} \quad (3.3)$$

where we have used (2.9). We introduce now a generalized Ursell expansion of the streaming operators¹¹⁾:

$$S(1) = R(1),$$

$$S(1,2) = R(1,2) + R(1)S(2), \quad (3.4)$$

$$S(1,2,3) = R(1,2,3) + R(1,2)S(3) + R(1,3)S(2) + R(1)S(2,3),$$

etc.

The N'th expression in this sequence is obtained as follows: Consider a partition of the labels $2, 3, \dots, N$ into two (ordered) blocks. Associate with this partition a product of an R operator whose variables have the labels of the first block together with the label 1 and an S operator whose variables have the labels of the second block. Then $S(1, 2, \dots, N)$ is equal to the sum over all such partitions of the associated product.

The sequence (3.4) defines, recursively, the R operators in terms of the S operators. Thus

$$R(1) = S(1)$$

$$R(1,2) = S(1,2) - S(1)S(2)$$

$$R(1,2,3) = S(1,2,3) - S(1,2)S(3) - S(1,3)S(2) - S(2,3)S(1) + 2 S(1)S(2)S(3), \quad (3.5)$$

etc.

In general, $R(1, 2, \dots, N)$ is equal to the sum over all partitions of the labels $1, 2, \dots, N$ into any number of blocks; the terms in the sum are products of S-operators

whose labels are the labels in the blocks of the partitions and each term is multiplied by a factor $(1)^{k-1}(k-1)!$, where k is the number of blocks in the partition. The R operators are just the cluster functions associated with the S operators¹¹⁾.

When the expansion (3.4) for $S(1,2,\dots,N;t)$ is put in (3.3) we find

$$f(1;t) = \frac{N!}{(N-1)!} \sum_{m=1}^N \binom{N-1}{m-1} \int \dots \int dx_2 \dots dx_N R(1,2,\dots,m;t) \times S(m+1,m+2,\dots,N;t) D(1,2,\dots,N;0), \quad (3.6)$$

where we have used the symmetry of D and the fact that there are $\binom{N-1}{m-1} = (N-1)! [(N-m)!(m-1)^{-1}]$ partitions of the $N-1$ labels into a block of $m-1$ labels and a block of $N-m$ labels. The S operators in (3.6) may be replaced by unity, because of the general property (2.13), and then, using the definition (3.1) of the partial distribution functions, we get the result:

$$f(1;t) = \sum_{m=1}^N \frac{1}{(m-1)!} \int \dots \int dx_2 \dots dx_m R(1,2,\dots,m;t) f(1,2,\dots,m;0). \quad (3.7)$$

This is the desired expression for $f(1;t)$ in terms of the initial values of the partial distribution functions.

It will be convenient for us to introduce an auxiliary distribution function defined by

$$g(1;t) \equiv S(1;-t)f(1;t). \quad (3.8)$$

In the spatially homogeneous case g is identical with f ; the general point in introducing g is that the time dependence of g comes only from collisions. Using the property (2.13) of the S operators, we obtain from (3.7) the following expression for g .

$$g(1;t) = \sum_{m=1}^N \frac{1}{(m-1)!} \int \cdots \int dx_2 \cdots dx_m \mathcal{R}(1,2,\dots,m;t) f(1,2,\dots,m;0). \quad (3.9)$$

Here we have introduced the reduced streaming operator:

$$\mathcal{R}(1,2,\dots,m;t) = \prod_{j=1}^m S(j;-t) R(1,2,\dots,m;t). \quad (3.10)$$

Note that, since $R(1;t) = S(1;t)$, $\mathcal{R}(1,t) = 1$.

If we form the time derivative of both sides of (3.9) we get the equation

$$\frac{\partial g(1)}{\partial t} = \sum_{m=2}^N \frac{1}{(m-1)!} \int \cdots \int dx_2 \cdots dx_m \dot{\mathcal{R}}(1,2,\dots,m;t) f(1,2,\dots,m;0), \quad (3.11)$$

where the dot indicates the derivative of the operator with respect to time. In the next section, we take up the task of eliminating the initial data between equations (3.9) and (3.11) to obtain a single equation for g alone.

THE ELIMINATION OF THE INITIAL VALUES

Our aim is to eliminate the initial values between equations (3.9) and (3.11) to obtain a single equation for the distribution function g alone. This requires that we make some assumption about the initial values $f(1,2,\dots,s;0)$ of the s -particle distribution functions. Certainly, an obvious choice is to assume that there are no correlations in the initial state of the gas, i.e. we assume:

$$f(1,2,\dots,s;0) = \prod_{j=1}^s f(j;0) \quad (4.1)$$

Although this is a very special assumption, it is the key in all the derivations of the kinetic equation, (sometimes appearing in a disguised form). In my opinion, one should view this assumption as follows. Our aim is to discover the kinetic equation which, if it exists, will be of the form (1.3) independent of the initial state of the system. Hence, if we find a kinetic equation under this assumption, it should be the correct one. Once we have found the kinetic equation, we can then consider the problem of proving that all, or at least a large class, of initial correlations leads to the same equation. Here I should mention the attempts by Green and Piccerelli and by Cohen in this direction¹²⁾.

Let us consider the consequences of this assumption. Inserting (4.1) in the expansion (3.9) it takes the form:

$$g(1) = \sum_{m=1}^{\infty} \frac{1}{(m-1)!} \int \dots \int dx_2 \dots dx_m \dot{R}(1, 2, \dots, m; t) \prod_{j=1}^m f(j; 0) \quad (4.2)$$

$$= f(1; 0) + \int dx_2 \dot{R}(1, 2; t) f(1; 0) f(2; 0) + \dots$$

Similarly, equation (3.11) becomes

$$\frac{\partial g(1)}{\partial t} = \sum_{m=2}^{\infty} \frac{1}{(m-1)!} \int \dots \int dx_2 \dots dx_m \dot{R}(1, 2, \dots, m; t) \prod_{j=1}^m f(j; 0) \quad (4.3)$$

$$= \int dx_2 \dot{R}(1, 2; t) f(1; 0) f(2; 0)$$

$$+ \frac{1}{2} \int dx_2 \int dx_3 \dot{R}(1, 2, 3; t) f(1; 0) f(2; 0) f(3; 0) + \dots$$

We can clearly invert the series (4.2) term by term to obtain an expansion of $f(1; 0)$ in terms of g . Putting this expansion in the righthand side of (4.3) we get an equation for g which may be written:

$$\frac{\partial g(1)}{\partial t} = \sum_{k=2}^{\infty} \frac{1}{(k-1)!} \int \dots \int dx_2 \dots dx_k A(1; 2, 3, \dots, k; t) \prod_{j=1}^k g(j) \quad (4.4)$$

where

$$A(1; 2) = \dot{R}(1, 2)$$

$$A(1; 2, 3) = \dot{R}(1; 2, 3) - \dot{R}(1, 2) \dot{R}(1, 3) - \dot{R}(1, 2) \dot{R}(2, 3) - \dot{R}(1, 3) \dot{R}(1, 2) - \dot{R}(1, 3) \dot{R}(1, 2)$$

$$\dots \text{etc.} \quad (4.5)$$

The general prescription for obtaining the A operators is not difficult to obtain, but I won't bother to give it here since we will need only the first few.

Equation (4.4), which I call the dynamical equation for the distribution function, is similar in form to the desired kinetic equation. Indeed, in the spatially homogeneous case, the kinetic equation obtained by Green, Cohen, and others is just equation (4.4) in which the A-operators are replaced by their limits as $t \rightarrow \infty$ ¹³⁾. In the next section I shall show how we can systematically obtain the kinetic equation from this dynamical equation.

Let me conclude with a number of remarks about the dynamical equation and its derivation. First, our expansions are purely formal. We do not know, for example, that the series on the righthand side of (4.4) converges, even for the case where g is the equilibrium Maxwell distribution. The situation here may be very bad indeed, as is indicated by the fact that if we insert for the initial values in the expansion (3.7) the exact equilibrium distribution functions, the terms do not vanish individually. Rather there is an intricate cancellation, between the terms while each term beyond the first in fact diverges as $t \rightarrow \infty$. There are indications of similar difficulties in the expansion of the dynamical equation¹⁴⁾.

Leaving aside these difficulties, the dynamical equation is a formally exact consequence of the equations of motion, assuming only that the initial correlations vanish. Thus, the dynamical equation is invariant under time reversal, i.e. if $g(1;t)$ is a solution of (4.4), so is $g(1;-t)$. This is in contrast with the kinetic equation, which does not have this invariance property.

For the case of hard spheres, the total potential energy of the gas diverges for the correlationless initial state. This can easily be remedied by modifying the assumption (4.1) to take the form:

$$f(1,2,\dots,s;0) = W(1,2,\dots,s) \prod_{j=1}^s f(j;0), \quad (4.6)$$

where $W(1,2,\dots,s)$ is a function of the relative positions which vanishes for configurations with infinite potential energy. A simple choice would be

$$W(1,2,\dots,s) = \exp \left\{ -\alpha \sum_{j < k} \varphi(r_{jk}) \right\} \quad (4.7)$$

where α is a positive constant. The only change in the dynamical equation is that in the expression (4.5) for the A operators, one must insert a W factor after each $\mathcal{R}$ operator, i.e.

$$\mathcal{R}(1,2,\dots,s) \rightarrow \mathcal{R}(1,2,\dots,s) W(1,2,\dots,s) \quad (4.8)$$

THE KINETIC EQUATION

The dynamical equation (4.4) may be written:

$$\frac{\partial g(l)}{\partial t} = \sum_{k=2}^{\infty} \frac{\epsilon^{k-1}}{(k-1)!} \int \cdots \int dx_2 \cdots dx_k A(1;2,\dots,l;t) \prod_{j=1}^k g(j), \quad (5.1)$$

where ϵ is a parameter inserted to help keep track of the order of magnitude of the terms; we will later set ϵ equal to unity. The effective magnitude of ϵ is not hard to determine. Since g , like f , is normalized so that

$$\int dx_1 g(l) = N \quad (5.2)$$

is the number of particles, it follows that g itself is proportional to the number density, n , of gas particles.

But at any instant in time, the operator $A(1;2,\dots,k;t)$ vanishes unless all k particles are within some multiple of the range, r_0 , of the interparticle forces. Hence, the effective magnitude of ϵ is

$$\epsilon \sim n r_0^3. \quad (5.3)$$

We are concerned with the case of nearly ideal gases for which the effective magnitude of $\epsilon \ll 1$.

It is also instructive to consider ϵ as the ratio of the two natural times which appear in the equation. These are the collision time $T \sim r_0/v_{av}$, where v_{av} is an average velocity, and the mean free time $t_0 \sim (n r_0^2 v_{av})^{-1}$. Clearly $\epsilon \sim T/t_0$, and $T \ll t_0$. It is important to recognize that these two times appear in different ways in equation (5.1). The short collision time appears as the natural time scale for the explicit time dependence of the A operators, since this time dependence arises from the dynamics of collisions involving only a finite number of particles. On the other hand, the relatively long mean free time appears in the order of magnitude of the terms on the righthand side of the equation.

The temporal development of the solution $g(l;t)$ of the dynamical equation will also exhibit these two time scales. For times of order t_0 , in what is called the kinetic stage, the fast motion will in general appear as fluctuations about the slower mean motion. It is this mean motion which is governed by the kinetic equation and it is our task to separate the two motions in a systematic manner.

To accomplish this I use the method of averaging.

I write first:

$$g(l) = h(l) + \sum_{k=2}^{\infty} \frac{\epsilon^{k-1}}{(k-1)!} \int \cdots \int dx_2 \cdots dx_k C(l; 2, 3, \dots, k; t) \prod_{j=1}^k h(j). \quad (5.4)$$

The idea here is that h is to be the mean distribution function, which varies slowly in time, with the fluctuations about h given in successive orders by the C-operators. This mean distribution function satisfies the kinetic equation, which takes the form:

$$\frac{\partial h(1)}{\partial t} = \sum_{k=2}^{\infty} \frac{\epsilon^{k-1}}{(k-1)!} \int \dots \int dx_2 \dots dx_k B(1;2,\dots,k) \prod_{j=1}^k h(j) \quad (5.5)$$

Note particularly that the B operators have no explicit time dependence, since such time dependences are on the fast scale and we require that h exhibit only the slow scale motion.

The B and C operators are determined by inserting the expansions (5.4) in the dynamical equation (5.1) and using (5.5); equating powers of ϵ gives the following sequence of equations.

$$\int dx_2 [\dot{C}(1;2;t) + B(1;2)] h(1)h(2) = \int dx_2 A(1;2;t) h(1)h(2) \quad (5.6a)$$

$$\begin{aligned} \iint dx_2 dx_3 [\dot{C}(1;2,3;t) + B(1;2,3)] h(1)h(2)h(3) = \\ \iint dx_2 dx_3 [A(1;2,3;t) + A(1;2;t)C(1;3;t) \\ + A(1;2;t)C(2;3;t) + A(1;3;t)C(3;3;t) \\ + A(1;3;t)C(1;2;t) - C(1;2;t)B(1;3) \\ - C(1;2;t)B(2;3) - C(1;3;t)B(3;2) \\ - C(1;3;t)B(1;2)] h(1)h(2)h(3) \end{aligned} \quad (5.6b)$$

$$\begin{aligned}
& \iiint dx_2 dx_3 dx_4 [C(1;2,3,4;t) + B(1;2,3,4)] h(1)h(2)h(3)h(4) = \\
& \iiint dx_2 dx_3 dx_4 [A(1;2,3,4;t) + A(1;2,3;t)C(1;4;t) \\
& \quad + A(1;2,4;t)C(1;3;t) + A(1;3,4;t)C(1;2;t) \\
& \quad + A(1;2,3;t)C(2;4;t) + A(1;2,4;t)C(2;3;t) \\
& \quad + A(1;2,3;t)C(3;4;t) + A(1;2,4;t)C(4;3;t) \\
& \quad + A(1;3,4;t)C(4;2;t) + A(1;3,4;t)C(3;2;t) \\
& \quad + A(1;2;t)C(2;3,4;t) + A(1;3;t)C(3;2,4;t) \\
& \quad + A(1;4;t)C(4;3,2;t) + A(1;2;t)C(2;3,4;t) \quad (5.6c) \\
& \quad + A(1;2;t)C(1;3;t)C(2;4;t) + A(1;2;t)C(1;4;t)C(2;3;t) \\
& \quad + A(1;3;t)C(1;2;t)C(3;4;t) + A(1;3;t)C(3;2;t)C(1;4;t) \\
& \quad + A(1;4;t)C(1;2;t)C(4;3;t) + A(1;4;t)C(1;3;t)C(4;2;t) \\
& \quad - C(1;2;3;t)B(1;4) - C(1;2,4;t)B(1;3) - C(1;3,4;t)B(1;2) \\
& \quad - C(1;2,3;t)B(2;4) - C(1;2,4;t)B(2;3) - C(1;2,3;t)B(3;4) \\
& \quad - C(1;2,4;t)B(4;3) - C(1;3,4;t)B(4;2) - C(1;3,4;t)B(3;2) \\
& \quad - C(1;2;t)B(2;3,4) - B(1;3;t)B(3;2,4) - C(1;4;t)B(4;3,2) \\
& \quad - C(1;2;t)B(2;3,4) - C(1;3;t)B(1;3,4) - C(1;3;t)B(1;2,3) \\
& \quad - C(1;2;t)B(1;3)B(2;4) - C(1;2;t)B(1;4)B(2;3) \\
& \quad - C(1;3;t)B(1;2)B(3;4) - C(1;3;t)B(3;2)B(1;4) \\
& \quad - C(1;4;t)B(1;2)B(4;3) - C(1;4;t)B(1;3)B(4;2)] h(1)h(2)h(3)h(4) \\
& \text{etc.}
\end{aligned}$$

In these expressions the integrands have been made explicitly symmetric under permutation of the labels of the integration variables. A graphical method for determining the general term in this sequence of equations can be given, but since we shall need only the first few, I won't bother with it here. As you can see, the equations in this sequence are all of the same general form, which, for convenience, I write as

$$\begin{aligned} \int \cdots \int dx_2 \cdots dx_k [C(1;2,\dots,k;t) + B(1;2,\dots,1;t)] h(1)h(2)\dots h(k) \\ = \int \cdots \int dx_2 \cdots dx_k D(1;2,\dots,k;t) h(1)h(2)\dots h(k) \end{aligned} \quad (5.7)$$

Here $D(1;2,\dots,k;t)$ stands for the operator appearing in the integrand on the righthand side of the equation. It is a long sum of products of A, B, and C operators, as you can see from (5.6), but it is in principle known from the solution of the previous equations in the sequence. The two operators, C and B are to be determined from (5.7). This we can do uniquely if we impose the requirement that the time average of the C-operators be zero. More specifically, we require

$$\lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T dt \int \cdots \int dx_2 \cdots dx_k C(1;2,\dots,k;t) h(1)h(2)\dots h(k) = 0. \quad (5.8)$$

Note that the time average is only with respect to the explicit time dependence of the C operator; the functions $h(1), h(2), \dots, h(k)$ are held fixed during the averaging process. This condition can be imposed on the solution C of (5.7) only if the integral involving B is chosen to be equal to the time average of the righthand side.

$$\int \dots \int dx_2 \dots dx_k B(1; 2, \dots, k) h(1) h(2) \dots h(k) = \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T dt \int \dots \int dx_2 \dots dx_k D(1; 2, \dots, k; t) h(1) h(2) \dots h(k) \quad (5.9)$$

The operator C is then given by

$$\int \dots \int dx_2 \dots dx_k C(1; 2, \dots, k; t) h(1) h(2) \dots h(k) = \int dt \int \dots \int dx_2 \dots dx_k [D(1; 2, \dots, k; t) - B(1; 2, \dots, k)] h(1) h(2) \dots h(k), \quad (5.10)$$

where in this indefinite integral over time, the constant of integration is chosen so that the condition (5.8) is satisfied.

Let me emphasize that the choice (5.9) for B is necessary, since only then can the lefthand side of (5.10) be free of secular terms (terms growing proportional to t), and, hence, allow the imposition of the requirement (5.8).

Thus, we have a complete prescription for successively determining the B and C operators from the sequence of equations (5.6). I hope you are able to see that this is just an application of the method of averaging outlined in the first lecture.

THE BOLTZMANN EQUATION

In order to show you more explicitly how the method works, I will show you how the Boltzmann equation comes out.

The first equation in the sequence (5.6) may be written:

$$\int dx_2 [\dot{C}(1;2;t) + B(1;2)] h(1)h(2) = \int dx_2 \dot{\mathcal{R}}(1;2;t) h(1)h(2) \quad (6.1)$$

where we have used the expression given in (4.5) for $A(1;2;t)$.

According to the prescription given in the previous section, the term on the lefthand side containing the operator $B(1;2)$ must be equal to the time average of the righthand side.

That is

$$\int dx_2 B(1;2) h(1)h(2) = \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T dt \int dx_2 \dot{\mathcal{R}}(1;2;t) h(1)h(2) \quad (6.2)$$

But, from (3.5) and (3.10) we have

$$\mathcal{R}(1;2;t) = \mathcal{P}(1;2;t) - 1 \quad (6.3)$$

where

$$\mathcal{P}(1;2;t) = S(1;-t)S(2;-t)S(1;2;t) \quad (6.4)$$

is the reduced streaming operator¹⁵⁾. Hence, since the dot indicates the derivative with respect to time, (6.2)

becomes

$$\int dx_2 B(1;2) h(1)h(2) = \lim_{T \rightarrow \infty} \int dx_2 \frac{\mathcal{P}(1,2;T)-1}{T} h(1)h(2). \quad (6.5)$$

I assert now that this, in the spatially homogeneous case, is the Boltzmann collision term (1.2). To see this, note first that in the spatially homogeneous case

$$h(1) = h(\vec{p}, t) \quad (6.6)$$

is independent of $\vec{r}$. Next consider the effect of the streaming operator (6.4). It follows from the interpretation of the streaming operator as a substitution operator that

$$S(1,2;T)h(\vec{p}_1)h(\vec{p}_2) = h(\vec{p}'_1)h(\vec{p}'_2) \quad (6.7)$$

where $\vec{p}'_1$ and $\vec{p}'_2$ are the momenta of particles a time T in the past which go into $\vec{p}_1$ and $\vec{p}_2$ under the influence of the Hamiltonian $H(1,2)$. The operators $S(1;-t)S(2;-t)$ in (6.4) can be neglected in the spatially homogeneous case since they only produce a translation of the positions of the particles. Hence we have the result

$$\int dx_2 B(1;2)h(1)h(2) = \int d\vec{p}_2 \int d\vec{r}_2 \frac{h(\vec{p}'_1)h(\vec{p}'_2) - h(\vec{p}_1)h(\vec{p}_2)}{T} \quad (6.8)$$

FIGURE 2

Relative Motion in a Binary Collision.

Clearly, the integrand vanishes except for those positions $\vec{r}_2$ for which the particles will have undergone a collision a time T in the past, since only then so $\vec{p}_1', \vec{p}_2'$ differ from $\vec{p}_1, \vec{p}_2$.

Looking at the relative motion, (see Figure 1), we see that, for collisions in which the impact parameter is between b and $b+db$, this implies that $\vec{r}_2$ must lie within the collision cylinder, which is a cylinder of length gT , oriented along the relative velocity $\vec{g} = (\vec{p}_2 - \vec{p}_1)/m$, with base $bdbd\phi$, where ϕ is the azimuthal angle. The volume of this cylinder is $gTbdbd\phi$, so we have

$$\int dx_2 B(1;2)h(1)h(2) = \int d\vec{p}_2 \int bdbd\phi [h(\vec{p}_1')h(\vec{p}_2') - h(\vec{p}_1)h(\vec{p}_2)] \quad (6.9)$$

This becomes identical with the Boltzmann collision operator occurring in (1.2) when we identify

$$bdbd\phi = I(g, \theta) d\Omega. \quad (6.10)$$

I have only briefly sketched this derivation of the Boltzmann collision term, since it is by now quite a standard discussion¹⁶⁾.

REMARKS AND ACKNOWLEDGEMENTS

The derivation in sections 2, 3 and 4 of the dynamical equation, although it is completely equivalent to that of Cohen, Green and Piccirelli, Lewis, and others, is not identical with these derivations. It seems to me to be particularly natural and simple, and I am surprised that it has not yet appeared in the literature. In conversations with J. Groeneveld I have learned that he has a very similar derivation.

The application of the method of averaging in section 5 I consider to be somewhat speculative. One might think that it could lead to the solution of the divergence problem since there is a possibility of a cancellation of the divergences in the A operators by the products of B and C operators which appear on the righthand sides of equations (5.6b), (5.6c), etc.¹⁷⁾. This does not appear to be the case, but the discussion is very complicated and it is difficult to be certain of what happens.

I want especially to acknowledge many conversations with E. G. D. Cohen, from whom I have learned much about the derivation of kinetic equations.

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- 9 See ref. 8, Ch. I, esp. pp. 14-16.
- 10 See e.g. H. Goldstein, "Classical Mechanics" (Addison Wesley Publishing Co., Cambridge, Mass., 1951).
- 11 Such generalized Ursell expansion were first introduced by J. de Boer, Rept. Prog. Phys. XII, 305 (1949).
See also G.W. Ford and G.E. Uhlenbeck, "The Theory of Linear Graphs" appearing in "Studies in Statistical Mechanics" Vol. 1, Ed. J. de Boer and G.E. Uhlenbeck (North Holland Publishing Co., Amsterdam, 1962).
- 12 See e.g. ref. 4.
- 13 See e.g. M.S. Green, Phys. Rev. 136, A905(1964).
- 14 J.R. Dorfman and E.G.D. Cohen, Physics Lett. 16, 124(1965).
- 15 Note that this definition of the S-operators differs from that of most other authors (see e.g. Cohen, ref. 3).
In the spatially homogeneous case there is no difference.
- 16 See ref. 8, pp. 77-79 and pp. 130-131.
- 17 The discovery of the divergences is quite recent. See ref. 14.

BROWNIAN MOTION MODELS

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INTRODUCTION¹✓

I am going to talk about a subject which has been under investigation for about 135 years - ever since the English botanist, Robert Brown, observed the animated motion of pollen grains suspended in a liquid. The first "theory" concerning the nature of this Brownian motion attributed the agitation to a "life force" associated with the pollen grains. This theory was shown to have certain shortcomings when particles from a ground up portion of the Sphinx exhibited the same behavior as the pollen grains. A real understanding of the phenomenon of Brownian motion came in the period 1905-17 through the work of Einstein, Smoluchowski, Langevin, Fokker, and Planck. Subsequent work by Ornstein and Uhlenbeck was concerned with the development of equations of motion for the probability distribution function describing the state of the Brownian particle.

In order to supply some direction or motivation to the investigation of the class of models with which we will be concerned, I am going to compress and distort history to some extent. A common feature of all mechanical systems exhibiting Brownian motion is the large mass of the Brownian particle relative to the mass of the molecules in the surrounding medium. This observation applies equally to Brown's pollen

grains or to a small torsion mirror suspended on a quartz fiber in a gas at low density. The first starting point for the study of Brownian motion is the Langevin equation, which is simply Newton's equation of motion. In the case of a "free" Brownian particle moving in one space dimension, the Langevin equation is assumed to have the form

$$(1) \quad M \dot{v}(t) = -M \beta v(t) + M A(t) ,$$

where $v(t)$ is the velocity of the particle. The force on the Brownian particle of mass M is assumed to be the sum of two terms (a) a viscous resistance or dynamic friction which is proportional to the instantaneous velocity of the particle where β is a friction constant (per unit mass) and (b) an uncorrelated random force which is the resultant of the random impacts of the surrounding molecules on the particle. This random force per unit mass $A(t)$ is uncorrelated in the sense that

$$(2) \quad \langle A(t) A(t+\tau) \rangle = D \delta(\tau) ,$$

where the brackets denote either a time or ensemble average, $\delta(\tau)$ is a delta-function, and the constant D , which characterizes the intensity of the fluctuating force, is proportional to the absolute temperature of the medium. In addition, $A(t)$ is independent of position. In treating a Brownian particle in an external force field, e.g., a Brownian oscillator, an additional term must be added to the righthand side of

equation (1). The Langevin equation provides a description of the behavior of the particle in terms of the two phenomenological constants β and D . For example, equation (1) can be solved formally for $\dot{x}(t)$ in terms of $\dot{x}(0)$ and the fluctuating force $A(t)$. With the aid of equation (2) (and suitable generalizations), ensemble or time averages of $v(t)$, $v^2(t)$, $v(t)v(t+\tau)$, $v^3(t)$... with respect to the possible values of $A(t)$ can be computed. A particularly interesting moment is the normalized velocity autocorrelation function

$$(3) \quad \langle v(t)v(t+\tau) \rangle / \langle v^2(t) \rangle = e^{-\beta\tau}.$$

The particular form of equation (3) follows from equations (1) and (2). In general, for any stationary random variable $y(t)$ with zero mean, Wiener and Khintchine have shown that the normalized autocorrelation function admits the representation

$$(4) \quad \langle y(t)y(t+\tau) \rangle / \langle y^2(t) \rangle = \frac{1}{2\pi} \int_0^\infty dw G(w) \cos w\tau$$

where $G(w)$, the "spectral density", is non-negative. [Wiener and Khintchine actually proved considerably more.] We will see later for the models treated how the autocorrelation functions can be cast in the form shown in equation (4).

The entire set of moments taken together define a distribution function for the velocity. Fokker and Planck derived an equation of motion for this distribution function. This line of development brings us to the second starting point,

an equation of motion for the full conditional probability distribution function (p.d.f.) of position and velocity $P(v, u, t | v_0, u_0, 0)$ for a Brownian particle in a field of force. This equation is a generalized one-particle Liouville equation which includes the effects of friction and thermal agitation, and has been derived by Kramers and Chandrasekhar

$$(5) \quad \frac{\partial P}{\partial t} + v \frac{\partial P}{\partial u} - K(u) \frac{\partial P}{\partial v} = \frac{\partial}{\partial v} (\beta v P) + q \frac{\partial^2 P}{\partial v^2}$$

where u is the position coordinate, $K(u)$ is the external force per unit mass, and q is a constant related to D in equation (2). If one solves equation (5) for the initial condition

$$(6) \quad P(v, u, 0 | v_0, u_0, 0) = \delta(u - u_0) \delta(v - v_0),$$

then one is led to the conditional p.d.f. $P(v, u, t | v_0, u_0, 0)$. An additional assumption is required in the derivation of equation (5): the evolution of the trajectory of the Brownian particle depends only on the instantaneous values of u and v and is entirely independent of its previous history. A precise definition of this Markoffian property is

$$(7) \quad P(v_2, u_2, t_2 | v_1, u_1, t_1; v_0, u_0, t_0) = P(v_2, u_2, t_2 | v_1, u_1, t_1)$$

where $t_2 \geq t_1 \geq t_0$. For future reference we note that: (a) the solutions of equations (5) for the initial condition (6) in the case of the free particle and the harmonic oscillator

($K(u) = 0$ and $K(u) = -ku$, respectively) can be obtained;
 (b) these solutions are gaussian and the moments agree with those obtained from the Langevin equation; and (c) for any other external force, the solution of equation (5) (although not known) is not gaussian. However, the pair of random variables $\{u, v\}$ are necessarily Markoffian.

COUPLED OSCILLATOR MODELS²

We now consider a classical system of coupled oscillators for which it is possible to determine formally exact expressions for joint p.d.f.'s such as $W(v_0, u_0, t_0; v_1, u_1, t_1; v_2, u_2, t_2)$ and conditional p.d.f.'s such as $P(v_2, u_2, t_2 | v_1, u_1, t_1; v_0, u_0, t_0)$ and $P(v_2, u_2, t_2 | v_1, u_1, t_1)$, where $\{v_i, u_i\}$ are the velocity and position, respectively, of a particular particle at time t_i . Consider a system of N coupled oscillators with Hamiltonian expressed in matrix notation as

$$(8) \quad H = \frac{1}{2} \underline{P}^T \underline{M}^{-1} \underline{P} + \frac{1}{2} \underline{x}^T \underline{V} \underline{x}$$

where $\underline{P}$ and $\underline{x}$ are N -vectors whose k^{th} components are, respectively, the momentum and the displacement from equilibrium of the k^{th} particle. $\underline{M}$ is a diagonal $N \times N$ matrix whose k^{th} diagonal element is m_k the mass of the k^{th} particle. $\underline{V}$ is the potential energy matrix, which for the time being is assumed to be positive definite (i.e., $\underline{V}^{-1}$ exists). The superscript T denotes the transpose. The equations of motion in matrix

notation are

$$(9) \quad \underline{M} \ddot{\underline{x}} = -\underline{V} \underline{x}$$

where

$$(10) \quad \underline{M} \dot{\underline{x}} = \underline{p}.$$

The problem of determining the p.d.f.'s for particle 0 consists of two parts. We first solve the equations of motion and express the position and velocity of particle 0 as a linear combination of initial conditions; and next treat the statistical problem of determining the p.d.f.'s for these sets of linear combinations of initial conditions.

It is convenient to replace the variables $\underline{x}$ by $\underline{M}^{-1/2}$ in equation (9)

$$(11) \quad \ddot{\underline{y}} = -\underline{M}^{-1/2} \underline{V} \underline{M}^{-1/2} \underline{y} \\ = -\underline{W} \underline{y}.$$

Next introduce the orthogonal matrix $\underline{S}$ whose j^{th} column is the j^{th} eigenvector of $\underline{W}$ and so diagonalize $\underline{W}$. With $\underline{Q} = \underline{S}^T \underline{y}$ equation (11) takes the simple form

$$(12) \quad \ddot{\underline{Q}} = -\underline{\Omega}^2 \underline{Q}$$

where $\underline{S}^T \underline{W} \underline{S} = \underline{\Omega}^2$, is a diagonal matrix whose j^{th} diagonal element is the square of the frequency of the j^{th} normal mode. The positions and velocities of the particles in the system can be expressed in terms of the initial values of the normal

coordinates and velocities $\underline{Q}(0)$ and $\dot{\underline{Q}}(0)$

$$(13) \quad \underline{x}(t) = \underline{M}^{-\frac{1}{2}} \underline{S} [\underline{\Omega}^{-1} \sin \underline{\Omega} t \dot{\underline{Q}}(0) + \cos \underline{\Omega} t \underline{Q}(0)]$$

and

$$(14) \quad \dot{\underline{x}}(t) = \underline{M}^{-\frac{1}{2}} \underline{S} [\cos \underline{\Omega} t \dot{\underline{Q}}(0) - \underline{\Omega} \sin \underline{\Omega} t \underline{Q}(0)] .$$

In order to express the position and velocity of particle 0 concisely we introduce the vector $\underline{\Delta}$, all of whose components are zero except the zeroth component which is one. Thus we have

$$(15) \quad \underline{x}(0,t) = \underline{\Delta}^T \underline{M}^{-\frac{1}{2}} \underline{S} \underline{\Omega}^{-1} \sin \underline{\Omega} t \dot{\underline{Q}}(0) + \underline{\Delta}^T \underline{M}^{-\frac{1}{2}} \underline{S} \underline{\Omega} \sin \underline{\Omega} t \underline{Q}(0) .$$

and

$$(16) \quad \dot{\underline{x}}(0,t) = \underline{\Delta}^T \underline{M}^{-\frac{1}{2}} \underline{S} \cos \underline{\Omega} t \dot{\underline{Q}}(0) - \underline{\Delta}^T \underline{M}^{-\frac{1}{2}} \underline{S} \underline{\Omega} \sin \underline{\Omega} t \underline{Q}(0) .$$

We now turn to the statistical problem. We assume that the initial distribution of coordinates and momenta is one of thermal equilibrium. In terms of normal coordinates and velocities, the canonical distribution is

$$(17) \quad (kT/2\pi)^N \left(\prod_{i=1}^N \Omega_i \right)^{-N} \exp \left\{ \frac{-1}{2kT} \dot{\underline{Q}}(0)^T \dot{\underline{Q}}(0) - \frac{1}{2kT} \underline{Q}(0)^T \underline{\Omega}^2 \underline{Q}(0) \right\} .$$

The canonical distribution function, equation (17), which characterizes thermal equilibrium, is an example of a multivariate normal p.d.f. We will summarize three theorems

concerning these distributions which will be useful in our analysis.³

Theorem 1. If the p.d.f. of the components of an m-dimensional vector $\underline{Y}$ is

$$(18) \quad (2\pi)^{-m/2} (|\Sigma^{-1}|)^{1/2} \exp\{-\frac{1}{2}(\underline{Y}-\underline{u})^T \Sigma^{-1}(\underline{Y}-\underline{u})\},$$

where Σ^{-1} is an mxm positive definite matrix and $|\Sigma^{-1}|$ denotes the determinant of Σ^{-1} , then the mean value of $\underline{Y}$ is $\underline{u}$ and the covariance matrix is Σ (the inverse of Σ^{-1}). The i, j^{th} element of Σ is the covariance or expected value of the product of the i^{th} and j^{th} components of $\underline{Y}-\underline{u}$,

$$(19) \quad \Sigma_{ij} = \left\langle (Y_i - u_i) (Y_j - u_j) \right\rangle.$$

A multivariate normal distribution such as (18) is completely specified by $\underline{u}$ and Σ ; thus the p.d.f. (18) can be denoted as $n\{\underline{Y}|\underline{u}, \Sigma\}$.

Theorem 2. If $\underline{Y}$ is distributed according to the p.d.f. $n\{\underline{Y}|\underline{u}, \Sigma\}$, then a set of p linearly independent combinations of the m components of $\underline{Y}$, $\underline{Z} = \underline{D}\underline{Y}$, is distributed according to the p.d.f. $n\{\underline{Z}|\underline{D}\underline{u}, \underline{D} \Sigma \underline{D}^T\}$, where $\underline{D}$ is a pxm matrix.

Theorem 3. Let the components of $\underline{Y}$ be divided into two groups composing the subvectors $\underline{Y}^{(1)}$ and $\underline{Y}^{(2)}$. Suppose the mean $\underline{u}$ is similarly divided into $\underline{u}^{(1)}$ and $\underline{u}^{(2)}$ and suppose the covariance matrix Σ of $\underline{Y}$ is divided into Σ_{11} , Σ_{12} , Σ_{22} , the

covariance matrices of $\underline{Y}^{(1)}$, of $\underline{Y}^{(1)}$ and $\underline{Y}^{(2)}$, and of $\underline{Y}^{(2)}$, respectively. Then if the p.d.f. of $\underline{Y}$ is $n\{\underline{Y}|\underline{u}, \underline{\Sigma}\}$, the conditional p.d.f. of $\underline{Y}^{(1)}$ given $\underline{Y}^{(2)}$ is

$$n\{\underline{Y}^{(1)} | \underline{u}^{(1)} + \underline{\Sigma}_{12} \underline{\Sigma}_{22}^{-1} (\underline{Y}^{(2)} - \underline{u}^{(2)}), \underline{\Sigma}_{11} - \underline{\Sigma}_{12} \underline{\Sigma}_{22}^{-1} \underline{\Sigma}_{21}\}.$$

Let us now consider the problem of obtaining the joint probability that the velocity $\dot{x}(0,t)$ and position $x(0,t)$ of particle zero are v_0 and u_0 at t_0 , v_1 and u_1 at $t_1, \dots$, and v_{r-1}, u_{r-1} at t_{r-1} . The set of linear relations between $v_0, \dots, v_{r-1}, u_0, \dots, u_{r-1}$ and the initial conditions can be represented by the partitioned matrix expression

$$(20) \begin{pmatrix} v_0 \\ \vdots \\ v_{r-1} \\ u_0 \\ \vdots \\ u_{r-1} \end{pmatrix} = \begin{pmatrix} \underline{\Delta}^T \underline{M}^{-\frac{1}{2}} \underline{S} \cos \underline{\Omega} t_0 & -\underline{\Delta}^T \underline{M}^{-\frac{1}{2}} \underline{S} \underline{\Omega} \sin \underline{\Omega} t_0 & \vdots \\ \vdots & \vdots & \vdots \\ \underline{\Delta}^T \underline{M}^{-\frac{1}{2}} \underline{S} \cos \underline{\Omega} t_{r-1} & -\underline{\Delta}^T \underline{M}^{-\frac{1}{2}} \underline{S} \underline{\Omega} \sin \underline{\Omega} t_{r-1} & \vdots \\ \underline{\Delta}^T \underline{M}^{-\frac{1}{2}} \underline{S} \underline{\Omega}^{-1} \sin \underline{\Omega} t_0 & \underline{\Delta}^T \underline{M}^{-\frac{1}{2}} \underline{S} \cos \underline{\Omega} t_0 & \vdots \\ \vdots & \vdots & \vdots \\ \underline{\Delta}^T \underline{M}^{-\frac{1}{2}} \underline{S} \underline{\Omega}^{-1} \sin \underline{\Omega} t_{r-1} & \underline{\Delta}^T \underline{M}^{-\frac{1}{2}} \underline{S} \cos \underline{\Omega} t_{r-1} & \vdots \end{pmatrix} \begin{pmatrix} \dot{\underline{Q}}(0) \\ \underline{Q}(0) \end{pmatrix}$$

or

$$\begin{pmatrix} \underline{v} \\ \underline{u} \end{pmatrix} = \underline{D} \begin{pmatrix} \dot{\underline{Q}}(0) \\ \underline{Q}(0) \end{pmatrix}$$

where the components of the partitioned vector $\begin{pmatrix} \underline{v} \\ \underline{u} \end{pmatrix}$ are $v_0, \dots, v_{r-1}, u_0, \dots, u_{r-1}$, and $\underline{D}$ is the partitioned matrix on the right-hand side of equation (20). The p.d.f. of the initial conditions equation (17) is

$$(21) \quad n \left\{ \begin{pmatrix} \dot{\underline{Q}}(0) \\ \underline{Q}(0) \end{pmatrix} \middle| \begin{pmatrix} \underline{0} \\ \underline{0} \end{pmatrix}, \begin{pmatrix} kT\underline{1} & \underline{0} \\ 0 & kT\underline{\Omega}^{-2} \end{pmatrix} \right\}.$$

From theorem 2, the p.d.f. of $\begin{pmatrix} \underline{v} \\ \underline{u} \end{pmatrix}$ is

$$(22) \quad W(\underline{v}_0, \underline{u}_0, t_0; \dots; \underline{v}_{r-1}, \underline{u}_{r-1}, t_{r-1}) = n \left\{ \begin{pmatrix} \underline{v} \\ \underline{u} \end{pmatrix} \middle| \begin{pmatrix} \underline{0} \\ \underline{0} \end{pmatrix}, \underline{D} \begin{pmatrix} kT\underline{1} & \underline{0} \\ \underline{0} & kT\underline{\Omega}^{-2} \end{pmatrix} \underline{D}^T \right\}.$$

The covariance matrix

$$\begin{pmatrix} kT\underline{1} & \underline{0} \\ \underline{D} & \underline{0} & kT\underline{\Omega}^{-2} \end{pmatrix} \underline{D}^T$$

reduces to a symmetric partitioned matrix

$$(23) \quad \begin{pmatrix} \underline{\Sigma}^{\underline{v}, \underline{v}} & \underline{\Sigma}^{\underline{v}, \underline{u}} \\ \underline{\Sigma}^{\underline{u}, \underline{v}} & \underline{\Sigma}^{\underline{u}, \underline{u}} \end{pmatrix}$$

where the elements of the rxr submatrices $\underline{\Sigma}^{\underline{v}, \underline{v}}$, $\underline{\Sigma}^{\underline{v}, \underline{u}}$, $\underline{\Sigma}^{\underline{u}, \underline{v}}$, and $\underline{\Sigma}^{\underline{u}, \underline{u}}$ are

$$(24) \quad \underline{\Sigma}_{i,j}^{\underline{v}, \underline{v}} = (kT)^{-1} \underline{\Delta}^T \underline{M}^{-\frac{1}{2}} \underline{S} \cos \underline{\Omega}(t_i - t_j) \underline{S}^T \underline{M}^{-\frac{1}{2}} \underline{\Delta}$$

$$(25) \quad \underline{\Sigma}_{i,j}^{\underline{v}, \underline{u}} = -(kT)^{-1} \underline{\Delta}^T \underline{M}^{-\frac{1}{2}} \underline{S} \underline{\Omega}^{-1} \sin \underline{\Omega}(t_i - t_j) \underline{S}^T \underline{M}^{-\frac{1}{2}} \underline{\Delta}$$

$$(26) \quad \underline{\Sigma}_{i,j}^{\underline{u}, \underline{v}} = (kT)^{-1} \underline{\Delta}^T \underline{M}^{-\frac{1}{2}} \underline{S} \underline{\Omega}^{-1} \sin \underline{\Omega}(t_i - t_j) \underline{S}^T \underline{M}^{-\frac{1}{2}} \underline{\Delta}$$

and

$$(27) \quad \underline{\Sigma}_{i,j}^{\underline{u}, \underline{u}} = (kT)^{-1} \underline{\Delta}^T \underline{M}^{-\frac{1}{2}} \underline{S} \underline{\Omega}^{-2} \cos \underline{\Omega}(t_i - t_j) \underline{S}^T \underline{M}^{-\frac{1}{2}} \underline{\Delta}.$$

The functions of the time $t = t_i - t_j$ which appear in equations (24)-(27) have a dynamical interpretation in terms of a special initial condition. In particular, if we take as initial conditions

$$(28) \quad \begin{aligned} \dot{\underline{x}}(0) &= \underline{\Delta} & \text{and} & \quad \underline{x}(0) = \underline{0} \\ \dot{\underline{q}}(0) &= \underline{S}^T \underline{M}^{+\frac{1}{2}} \underline{\Delta} & \text{and} & \quad \underline{q}(0) = \underline{0} \end{aligned}$$

then the position and velocity at time t are given by

$$(29) \quad \underline{X}(t) = \underline{M}^{-\frac{1}{2}} \underline{S} \underline{\Omega}^{-1} \sin \Omega t \underline{S}^T \underline{M}^{+\frac{1}{2}} \underline{\Delta}$$

and

$$(30) \quad \dot{\underline{X}}(t) = \underline{M}^{-\frac{1}{2}} \underline{S} \cos \Omega t \underline{S}^T \underline{M}^{+\frac{1}{2}} \underline{\Delta}$$

where $\underline{X}(t)$ denotes the solution of the equation of motion (9) for the special condition equation (28). The position and velocity of particle zero are

$$(31) \quad \underline{X}[0,t] = \underline{\Delta}^T \underline{M}^{-\frac{1}{2}} \underline{S} \underline{\Omega}^{-1} \sin \Omega t \underline{S}^T \underline{M}^{+\frac{1}{2}} \underline{\Delta}$$

and

$$(32) \quad \dot{\underline{X}}[0,t] = \underline{\Delta}^T \underline{M}^{-\frac{1}{2}} \underline{S} \cos \Omega t \underline{S}^T \underline{M}^{+\frac{1}{2}} \underline{\Delta}.$$

Thus we have established a connection between the covariances in equations (24), (25) and (26) and the solution of a special initial value problem, namely

$$(33) \quad \Sigma_{i,j}^{v,v} = (m_0 kT)^{-1} \dot{\underline{X}}[0, t_i - t_j]$$

and

$$(34) \quad \Sigma_{i,j}^{v,u} = -(m_0 kT)^{-1} \underline{X}[0, t_i - t_j] = -\Sigma_{i,j}^{u,v}$$

where we have used the relation $\underline{M}^{-\frac{1}{2}} \underline{\Delta} = m_0^{-1} \underline{M}^{+\frac{1}{2}} \underline{\Delta}$. The function $\Sigma_{i,j}^{u,u}$ also has a simple independent significance which can be exhibited by noting that $\underline{X}(t)$ is a solution of equation (9)

$$(35) \quad \underline{M} \ddot{\underline{X}} = - \underline{V} \underline{X}.$$

If we integrate the set of equations (35) from 0 to t, we obtain

$$(36) \quad \underline{M} \dot{\underline{X}} - \underline{M} \dot{\underline{X}}(0) = - \underline{V} \int_0^t \underline{X}(s) ds.$$

Equation (36) can be written as

$$\underline{M} \frac{d^2}{dt^2} \int_0^t \underline{X}(s) ds = m_0 \underline{\Delta} - \underline{V} \int_0^t \underline{X}(s) ds.$$

Thus the integral

$$(37) \quad \int_0^t \underline{X}(s) ds = \underline{M}^{-\frac{1}{2}} \underline{S} \underline{\Omega}^{-2} (1 - \cos \underline{\Omega} t) \underline{S}^T \underline{M}^{\frac{1}{2}} \underline{\Delta}$$

is a solution of the equation of motion

$$(38) \quad \underline{M} \ddot{\underline{X}} = m_0 \underline{\Delta} - \underline{V} \underline{X}$$

for the set of oscillators when a constant force of magnitude m_0 is suddenly applied to a particle 0 at time $t=0$ and when the initial velocities and displacements are all 0,

$$(39) \quad \underline{X}(0) = \underline{0}, \quad \dot{\underline{X}}(0) = \underline{0}.$$

From equation (37) we find that

$$(40) \quad \underline{M}^{-\frac{1}{2}} \underline{S} \underline{\Omega}^{-2} \cos \underline{\Omega} t \underline{S}^T \underline{M}^{\frac{1}{2}} \underline{\Delta} = \underline{M}^{-\frac{1}{2}} \underline{S} \underline{\Omega}^{-2} \underline{S}^T \underline{M}^{\frac{1}{2}} \underline{\Delta} - \int_0^t \underline{X}(s) ds \\ = m_0 \underline{V}^{-1} \underline{\Delta} - \int_0^t \underline{X}(s) ds,$$

and further that

$$(41) \quad \underline{\Delta}^T \underline{M}^{-\frac{1}{2}} \underline{S} \underline{\Omega}^{-2} \cos \underline{\Omega} t \underline{S}^T \underline{M}^{\frac{1}{2}} \underline{\Delta} = (\underline{V}^{-1})_{0,0} - m_0^{-1} \int_0^t \underline{X} \left[\begin{smallmatrix} 0, s \end{smallmatrix} \right] ds.$$

As a result we have the following expression for the covariance

$$\Sigma_{i,j}^{u,u} \quad (42) \quad \Sigma_{i,j}^{u,u} = (kT)^{-1} \left\{ (V^{-1})_{0,0}^{-1} \int_0^t X[0,s] ds \right\},$$

where $\int_0^t X[0,s] ds$ is obtained from the solution of equation (38) for the initial conditions (39).

We now obtain an expression for the conditional p.d.f $P(v_1, u_1, t | v_0, u_0, 0)$ from the joint p.d.f. $W(v_0, u_0, 0; v_1, u_1, t)$. The joint p.d.f. $W(v_0, u_0, 0; v_1, u_1, t)$ is

$$(43) \quad n \left\{ \begin{pmatrix} v_0 \\ v_1 \\ u_0 \\ u_1 \end{pmatrix} \middle| \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} \right\} \left\{ \begin{pmatrix} kTm_0^{-1} & kTm_0^{-1} X[0,t] & 0 & +kTm_0^{-1} X[0,t] \\ kTm_0^{-1} X[0,t] & kTm_0^{-1} & -kTm_0^{-1} X[0,t] & 0 \\ 0 & -kTm_0^{-1} X[0,t] & kT(V^{-1})_{0,0} & kT(V^{-1})_{0,0}^{-1} \int_0^t X[0,\sigma] d\sigma \\ +kTm_0^{-1} X[0,t] & 0 & kT(V^{-1})_{0,0}^{-1} \int_0^t X[0,\sigma] d\sigma & kT(V^{-1})_{0,0} \end{pmatrix} \right\}.$$

Using theorem 3, with

$$\underline{Y}^{(2)} = \begin{pmatrix} v_0 \\ u_0 \end{pmatrix}, \quad \underline{Y}^{(1)} = \begin{pmatrix} v_1 \\ u_1 \end{pmatrix}, \quad \Sigma_{11} = \begin{pmatrix} kTm_0^{-1} & \\ 0 & kTV^{-1}_{00} \end{pmatrix}, \quad \Sigma_{22} = \Sigma_{11}$$

and

$$\Sigma_{12} = \begin{pmatrix} kTm_0^{-1} X[0,t] \\ kTm_0^{-1} X[0,t] \end{pmatrix} \quad kT \begin{pmatrix} -kTm_0^{-1} X[0,t] \\ (V^{-1})_{0,0}^{-1} \int_0^t X[0,\sigma] d\sigma \end{pmatrix},$$

we obtain the joint conditional p.d.f.

$$(44) \quad P(v_1, u_1, t | v_0, u_0, 0) = n \left\{ \begin{pmatrix} v_1 \\ u_1 \end{pmatrix} \left| \begin{pmatrix} v_0 \dot{x}[0, t] - u_0 v x[0, t] \\ v_0 x[0, t] + u_0 \left[1 - v \int_0^t x[0, \sigma] d\sigma \right] \end{pmatrix} \right. \right\}, \underline{\Sigma} \right\},$$

where

$$(45) \quad \left\{ \begin{aligned} & k T m_0^{-1} \left\{ 1 - \dot{x}^2[0, t] - v x^2[0, t] \right\} \quad k T m_0^{-1} x[0, t] \left\{ 1 - \dot{x}[0, t] - v \int_0^t x[0, \sigma] d\sigma \right\} \\ & T m_0^{-1} x[0, t] \left\{ 1 - \dot{x}[0, t] - v \int_0^t x[0, \sigma] d\sigma \right\} \quad k T m_0^{-1} \left\{ 2 \int_0^t x[0, \sigma] d\sigma - x^2[0, t] - v \left(\int_0^t x[0, \sigma] d\sigma \right)^2 \right\} \end{aligned} \right\}$$

and where

$$(46) \quad v = \left[m_0 (V^{-1})_{0,0} \right]^{-1}.$$

It can be seen in Equations (43), (44) and (45) that some of the moments in Equation (43) are infinite if $\underline{V}$ is only positive semi-definite because the zero eigenvalue(s) of $\underline{V}$ are associated with free translation of the oscillator system. Nevertheless all the conditional moments in Equations (44) and (45) are bounded.

We conclude this section with a few general observations:

- 1) All p.d.f.'s are gaussian, and all moments are expressed in terms of the three functions $\dot{x}[0, t]$, $x[0, t]$ and $\int_0^t x[0, s] ds$.

2) These three functions describe the state of particle zero for special initial value problems - either (9), (28) or (38), (39).

3) The defining relation for $\dot{X}[0,t]$ given in Equation (32) can be written as

$$(47) \quad \dot{X}[0,t] = \sum_j S_{0j}^2 \cos \Omega_j t,$$

where S_{0j} is the amplitude of particle 0 in the j^{th} normal mode. The function $\dot{X}[0,t]$ is the normalized velocity autocorrelation function and bears a formal resemblance to the Wiener-Khinchine formula (4).

SPECIAL COUPLED OSCILLATOR SYSTEMS

Having solved the problem of obtaining an expression for the conditional p.d.f. $P(v_1, u_1, t | v_0, u_0, 0)$ for one of the particles in a general harmonically coupled system of particles, we now consider two special systems in which the time-dependent behavior of the moments of $P(v_1, u_1, t | v_0, u_0, 0)$ can be determined explicitly.

1) Heavy Lattice Particle.³ The first system is a modified n -dimensional lattice with nearest-neighbor central and noncentral harmonic forces and with periodic boundary conditions. There are assumed to be $2N+1$ lattice points in each of the lattice directions, labelled from $-N$ to $+N$. A particle in the lattice

is designated by the n -component vector $\underline{R}$ whose components r_j are integers such that $-N \leq r_j \leq N$, $j = 1, \dots, n$. The principal modification of the conventional lattice model which is introduced is that the mass of particle $\underline{R} = \underline{0} = \{0, \dots, 0\}$ is M whereas the mass of each of the other lattice particles is m (where $m < M$). A second modification which is introduced merely as a formal convenience to make the potential energy matrix positive-definite, is that each particle is held to its equilibrium position by an additional harmonic force (strength = k'). Ultimately we shall be interested in the limit $k' \rightarrow 0$. The moments of the conditional p.d.f. $P(v_1, u_1, t | v_0, u_0, 0)$ for the heavy particle are expressible in terms of the functions $\dot{X}[0, t]$, $X[0, t]$, and $\int_0^t X[0, s] ds$ which are solutions of the equations of motion for a special initial condition. The equations of motion of the system for particle displacements in any lattice direction are independent of the displacements in other lattice directions. The equations of motion for the x component are

$$(48) \quad [m + (M - m) \delta_{\underline{0}, \underline{R}}] \ddot{x}[\underline{R}, t] = -k' x[\underline{R}, t] + \sum_{j=1}^n k_j \{x[\underline{R} + \underline{1}_j, t] - 2x[\underline{R}, t] + x[\underline{R} - \underline{1}_j, t]\}$$

where $x[\underline{R}, t]$ is the displacement of particle $\underline{R}$ from equilibrium in the x -direction and where a dot above x denotes differentiation with respect to the time t . The vector $\underline{1}_j$ is a unit vector in

lattice direction j . The various nearest-neighbor force constants are denoted by k_j and the Kronecker delta is

$$\delta_{\underline{0}, \underline{R}} = \begin{cases} 1 & \text{if } \underline{R} = \underline{0} \\ 0 & \text{if } \underline{R} \neq \underline{0} \end{cases}.$$

We must solve Equations (48) for the special initial condition

$$x[\underline{R}, 0] = 0, \quad \text{all } \underline{R}$$

and

$$\dot{x}[\underline{R}, 0] = 0, \quad \underline{R} \neq \underline{0}$$

$$\dot{x}[\underline{0}, 0] = 1.$$

(49)

The velocity and position of particle $\underline{0}$ will then be identical with the functions $\dot{X}[\underline{0}, t]$ and $X[\underline{0}, t]$ in Equations (43)-(45); and the function $\int_0^t X[\underline{0}, s] ds$ can be obtained as well.

Equations (48) are solved by introducing a generating function. If we multiply the equation for $\ddot{x}[\underline{R}, t]$ by $(2N+1)^{-n/2} \exp \left[\frac{2\pi i}{2N+1} \underline{s} \cdot \underline{R} \right]$ and sum the resulting set of equations we obtain

$$\ddot{G}[\underline{s}, t] + (2N+1)^{-n/2} Q \ddot{x}[\underline{0}, t] = -\gamma' G[\underline{s}, t] - 2 \sum_{j=1}^n \gamma_j \left\{ 1 - \cos \frac{2\pi s_j}{2N+1} \right\} G[\underline{s}, t], \quad (50)$$

where the vector $\underline{s}$ has integer components $s_1, \dots, s_n$ and $-N \leq s_j \leq N$. The generating function $G[\underline{s}, t]$ is, by definition,

$$G[\underline{s}, t] = (2N+1)^{-n/2} \sum_{\{\underline{R}\}} x[\underline{R}, t] \exp \left[\frac{2\pi i}{2N+1} \underline{s} \cdot \underline{R} \right] \quad (51)$$

where the sum is over all particles $\underline{R}$. The parameters Q , γ' , and γ_j are, respectively $(M-m)/m$, k'/m , and k_j/m . The initial values of $G[\underline{s}, 0]$ and $\dot{G}[\underline{s}, 0]$ corresponding to the initial conditions (49) are

$$G[\underline{s}, 0] = 0 \text{ and } \dot{G}[\underline{s}, 0] = (2N+1)^{-n/2}. \quad (52)$$

Equation (50) for the generating function can be solved by the method of Laplace transforms. The Laplace transform of Equation (50) is

$$\begin{aligned} -(2N+1)^{-n/2} + P^2 \Gamma[\underline{s}, P] + (2N+1)^{-n/2} \{-Q + QP^2 \xi[\underline{Q}, P]\} \\ = -\gamma' \Gamma[\underline{s}, P] - 2 \sum_{j=1}^n \gamma_j \left\{ 1 - \cos \frac{2\pi s_j}{2N+1} \right\} \Gamma[\underline{s}, P] \end{aligned} \quad (53)$$

where

$$\begin{aligned} \Gamma[\underline{s}, P] &= \int_0^\infty e^{-Pt} G[\underline{s}, t] dt \\ &= (2N+1)^{-n/2} \sum_{\{\underline{R}\}} \xi[\underline{R}, P] \exp \left[\frac{2\pi i}{2N+1} \underline{s} \cdot \underline{R} \right] \end{aligned} \quad (54)$$

and

$$\xi[\underline{R}, P] = \int_0^\infty e^{-Pt} x[\underline{R}, t] dt.$$

If we solve Equation (53) for $\Gamma[\underline{s}, P]$, we obtain

$$\Gamma[\underline{s}, P] = (2N+1)^{-n/2} \frac{Q+1+QP^2 \xi[\underline{Q}, P]}{P^2 + \gamma' + 2 \sum_{j=1}^n \left\{ 1 - \cos \frac{2\pi s_j}{2N+1} \right\}}. \quad (55)$$

Equation (55) is an implicit equation for $\xi[\underline{0}, P]$ since it appears on both the left- and right-hand sides. An equation for determining $\xi[\underline{0}, P]$ can be obtained by multiplying Equation (55) by $(2N+1)^{-n/2}$ and summing over all values of $\{\underline{s}\}$

$$\xi[\underline{0}, P] = \{Q+1+QP^2\xi[\underline{0}, P]\}\zeta[\underline{0}, P] \quad (56)$$

$$\text{where } \zeta[\underline{0}, P] = (2N+1)^{-n} \sum_{\{\underline{s}\}} \left[P^{2+\gamma'+2\sum_{j=1}^n \gamma_j} \left\{ 1 - \cos \frac{2\pi s_j}{2N+1} \right\} \right] \quad (57)$$

Thus from Equation (56) one obtains an explicit expression for $P\xi[\underline{0}, P]$, the Laplace transform of $X[\underline{0}, t]$,

$$P\xi[\underline{0}, P] = \frac{Q+1}{QP + \frac{1}{P\zeta[\underline{0}, P]}}, \quad (58)$$

or

$$\dot{X}[\underline{0}, t] = \frac{Q+1}{2\pi i} \int_L \frac{e^{Pt} dp}{QP + \{P\zeta[\underline{0}, P]\}^{-1}}, \quad (59)$$

where L , the path of integration, is parallel to the imaginary P -axis, and lies to the right of all singularities of the integrand. Equation (59) is equivalent to the expression

obtained earlier for $\dot{X}[0,t]$ in Equation (47)

$$\dot{X}[0,t] = \sum_j s_{0j}^2 \cos \Omega_j t. \quad (47)$$

Thus the only singularities of the integrand in Equation (59)

are poles located on the imaginary P-axis.

At this stage, we consider the limiting behavior of the heavy particle as the number of particles in the lattice approaches infinity and as the added force constant k' approaches zero. The explicit dependence of the function $\dot{X}[0,t]$ on the number of lattice particles is contained in $\zeta[0,P]$. Since we are primarily concerned with velocity relaxation and possible Brownian-like properties of the model, the fact that the period of Poincare cycles in the system approaches infinity in this limit is of no consequence. In fact, the analysis of Equation (59) is simplified in the limit $N = \infty$. The sums in Equation (57) are replaced by integrals (the discrete variables $2\pi s_j/(2N+1)$ are replaced by the continuous variables θ_j) so that Equation (57) becomes

$$\zeta[0,P] = \left(\frac{1}{2\pi}\right)^n \int_{-\pi}^{\pi} d\theta_1 \dots \int_{-\pi}^{\pi} d\theta_n \left[P^2 + 2\gamma \sum_{j=1}^n (1 - \cos \theta_j) \right]^{-1} \quad (60)$$

where we have also set $k' = 0$. We now study the properties of

$\dot{X}[0,t]$ for the 1-dimensional lattice in the limit $N = \infty$,
 $k' = 0$ when $M/m \gg 1$ (i.e. $Q \gg 1$). The value of $\zeta[0,P]$ is

$$\begin{aligned}\zeta[0,P] &= \frac{1}{2\pi} \int_{-\pi}^{\pi} d\theta [P^2 + 2\gamma(1 - \cos \theta)]^{-1} \\ &= P^{-1} [P^2 + 4\gamma]^{-\frac{1}{2}}\end{aligned}\quad (61)$$

Substituting Equation (61) in the integral representation (59) for $\dot{X}[0,t]$, we obtain

$$\dot{X}[0,t] = \frac{Q+1}{2\pi i} \int_L \frac{e^{Pt}}{QP + [P^2 + 4\gamma]^{\frac{1}{2}}} dP. \quad (62)$$

If the branch points at $\pm 2i\gamma^{\frac{1}{2}}$ in (62) are connected by a cut along the imaginary axis, and if the path of integration is wrapped around the cut, an equivalent expression for the integral in Equation (62) is

$$\dot{X}[0,t] = \frac{2}{\pi} (Q+1) \int_0^{2\gamma^{\frac{1}{2}}} \frac{(4\gamma - \omega^2)^{\frac{1}{2}} \cos \omega t}{(Q^2 - 1)\omega^2 + 4\gamma} d\omega. \quad (63)$$

This last expression has the same form as Equation (4) or (47). The spectral density is

$$G(\omega) = \begin{cases} 2\pi^{-1} (Q+1) [4\gamma - \omega^2]^{\frac{1}{2}} / [(Q^2 - 1)\omega^2 + 4\gamma], & 0 \leq \omega \leq 2\gamma^{\frac{1}{2}} \\ 0, & 2\gamma^{\frac{1}{2}} < \omega \end{cases}$$

In the case in which the mass of particle 0 is the same as that of the other lattice particles, $Q = 0$ and the spectral density

$$G(\omega) = \begin{cases} 2/\pi[4\gamma - \omega^2]^{\frac{1}{2}}, & 0 \leq \omega \leq 2\gamma^{\frac{1}{2}} \\ 0, & 2\gamma^{\frac{1}{2}} < \omega \end{cases}$$

is identical with the density of the vibrational frequency spectrum of the perfect lattice. In the limit $N = \infty$, the density of vibrational frequencies is not changed as the mass of particle 0 is increased. Consequently, on the basis of the similarity between Equations (47) and (63), we can regard the quantity

$$S_0^2(\omega) = \frac{(Q+1)(4\gamma - \omega^2)}{(Q^2 - 1)\omega^2 + 4\gamma} \quad (64)$$

as the limiting form of S_{0j}^2 , the square of the amplitude of the heavy particle in the j^{th} normal mode. The function $S_0^2(\omega)$ is strongly peaked near $\omega = 0$ when $Q \gg 1$.

The initial value of $X[0, t]$ is $X[0, 0] = 1$. In order to estimate the integral in Equation (62) at later values of the time, it is convenient to connect the branch points at $\pm 2i\gamma^{\frac{1}{2}}$ by a semicircular cut in the left half of the complex P -plane. As a result, a pole of the integrand is uncovered at

$P = -2\gamma^{\frac{1}{2}}/(Q^2-1)^{\frac{1}{2}}$. When the original path of integration L is wrapped around the semi-circular cut and the contribution of the residue at $P = -2\gamma^{\frac{1}{2}}/(Q^2-1)^{\frac{1}{2}}$ is accounted for, one obtains

$$\begin{aligned} \dot{X}[0, t] - \frac{Q}{Q-1} e^{-\frac{2\gamma^{\frac{1}{2}}t}{(Q^2-1)^{\frac{1}{2}}}} \\ = \frac{Q+1}{2\pi} \int_{\frac{3\pi}{2}}^{\frac{\pi}{2}} d\theta \exp\{i\theta + 2\gamma^{\frac{1}{2}}te^{i\theta}\} \left[\frac{1}{Qe^{i\theta} + (1+e^{2i\theta})^{\frac{1}{2}}} - \frac{1}{Qe^{i\theta} - (1+e^{2i\theta})^{\frac{1}{2}}} \right] \end{aligned}$$

(65)

where the integral on the right-hand side represents the contribution from the semi-circular cut. It is a simple matter to show that the magnitude of this integral is bounded by $2^{\frac{1}{2}}(Q+1)/(Q^2-2)$. Therefore, when $Q \gg 1$, the magnitude of the difference between $\dot{X}[0, t]$ and the exponential $\frac{Q}{Q-1} \exp\left[\frac{-2\gamma^{\frac{1}{2}}t}{(Q^2-1)^{\frac{1}{2}}}\right]$ is small compared to the initial value $\dot{X}[0, 0] = 1$ for all $t \geq 0$, i.e.,

$$\left| \dot{X}[0, t] - \frac{Q}{Q-1} \exp\left[\frac{-2\gamma^{\frac{1}{2}}t}{(Q^2-1)^{\frac{1}{2}}}\right] \right| < 2^{\frac{1}{2}}(Q+1)/(Q^2-2) \ll 1. \quad (66)$$

For $Q \gg 1$, the inequality (66) can be replaced by the slightly more simple one

$$\left| \dot{X}[0, t] - e^{-2\gamma^{\frac{1}{2}}t/Q} \right| < cQ^{-1} \quad (67)$$

where c is of order unity.

Equation (65) can be used to obtain similar precise estimates for $X[0, t]$ and $\int_0^t X[0, s]ds$ by integrating both the left- and right-hand sides with respect to the time from 0 to t . The results analogous to (67) are

$$2\gamma^{\frac{1}{2}} \left| X[0, t] - \frac{Q}{2\gamma^{\frac{1}{2}}} \left(1 - e^{-2\gamma^{\frac{1}{2}}t/Q} \right) \right| < c_1/Q \quad (68)$$

and

$$4\gamma \left| \int_0^t X[0, s]ds - \frac{Q}{4\gamma} \left[2\gamma^{\frac{1}{2}}t - Q \left(1 - e^{-2\gamma^{\frac{1}{2}}t/Q} \right) \right] \right| < [x_2 + c_3(2\gamma^{\frac{1}{2}}t)]Q^{-1} \quad (69)$$

where c_1 , c_2 , and c_3 are of order unity.

The only quantity appearing in the expression for the conditional p.d.f. for the heavy particle in a one-dimensional crystal lattice which we have not estimated is $(V^{-1})_{0,0}$ in Equation (46). Montroll and Potts obtained an expression for $(V^{-1})_{0,0}$ in the limit of an infinite lattice which in our notation is

$$(V^{-1})_{0,0} = \left(\frac{1}{2\pi} \right)^n \int_{-\pi}^{\pi} d\theta_1 \dots \int_{-\pi}^{\pi} d\theta_n \left[k' + 2 \sum_{j=1}^n k_j (1 - \cos \theta_j) \right]^{-1}.$$

In the case of the one- and two-dimensional lattices, in the limit $N = 0$ and $k' \rightarrow 0$, $(V^{-1})_{\underline{0},\underline{0}}$ diverges as $(k')^{-\frac{1}{2}}$ and $-\ln k'$, respectively, whereas for $n \geq 3$, $(V^{-1})_{\underline{0},\underline{0}}$ is finite. In particular, when $n = 3$, and $k_1 = k_2 = k_3 = k$,

$$\lim_{k' \rightarrow 0} (V^{-1})_{\underline{0},\underline{0}} = \zeta_0 / 4k$$

where ζ_0 is a constant which is approximately 1.019. In the one-dimensional example, $v = 0$ in the limit $k' = 0$ since

$$v = \left[M(V^{-1})_{0,0} \right]^{-1}.$$

On substituting the one-dimensional values of v ,

$\int_0^t X[0,s]ds$, $X[0,t]$, and $\dot{X}[0,t]$; Equations (67)-(69), in the general expression for $P(v_1, u_1, t | v_0, u_0, 0)$, Equation (44),

we obtain

$$P^{(1)}(v_1, u_1, t | v_0, u_0, 0) = n \left\{ \begin{pmatrix} v_1 \\ u_1 \end{pmatrix} \middle| \begin{pmatrix} \langle v_1 \rangle \\ \langle u_1 \rangle \end{pmatrix}, \Sigma \right\}, \quad (70)$$

with

$$\begin{pmatrix} \langle v_1 \rangle \\ \langle u_1 \rangle \end{pmatrix} = \begin{pmatrix} v_0 e^{-bt} \\ v_0 b^{-1} [1 - e^{-bt}] + u_0 \end{pmatrix}, \quad (71)$$

and

$$\Sigma = \begin{pmatrix} kTM^{-1}[1-e^{-2bt}] & kTM^{-1}b^{-1}[1-e^{-bt}]^2 \\ kTM^{-1}b^{-1}[1-e^{-bt}]^2 & kTM^{-1}b^{-2}[2bt-3+4e^{-bt}-e^{-2bt}] \end{pmatrix}, \quad (72)$$

where $b = 2\gamma^{\frac{1}{2}}Q^{-1}$. It is noteworthy that the conditional mean value $\langle v_1 \rangle$ is independent of u_0 , and is simply an exponential function of the time. Such behavior is characteristic of a free particle undergoing Brownian motion. In fact, the result in Equations (70)-(72) is identical with the conditional pdf obtained from the Kramers' equation for a free Brownian particle, i.e., the fundamental solution of the equation

$$\partial P / \partial t = -v(\partial P / \partial u) + (\partial / \partial v)(bvP) + q(\partial^2 P / \partial v^2), \quad (73)$$

corresponding to the initial condition $P(v, u, 0) = \delta(v - v_0)$

$\times \delta(u - u_0)$. Thus, to within the accuracy of the equalities in Equations (71) and (72), the random thermal motion of a heavy particle in a 1D lattice of a temperature T is described by Kramers' equation for a free Brownian particle, Equation (73), in which the phenomenological constants b and q are, respectively, $2\gamma^{\frac{1}{2}}Q^{-1}$ and $kTM^{-1}b$. It is also possible to determine a diffusion coefficient for the heavy particle from the variance

$$\langle (u_1 - \langle u_1 \rangle)^2 \rangle = 2kTM^{-1}Q(4\gamma)^{-1} \{ 2\gamma^{\frac{1}{2}}t - Q[1 - e^{-bt}] \}. \quad (74)$$

For times which are large compared to the velocity relaxation time b^{-1} , the phenomenological analog of Equation (74) is

$$\langle (u_1 - \langle u_1 \rangle)^2 \rangle = 2Dt;$$

and so the diffusion coefficient in Equation (74),

$$D = kTM^{-1}Q(4\gamma)^{-1}2\gamma^{\frac{1}{2}} = kTM^{-1}(2\gamma^{\frac{1}{2}})^{-1},$$

is independent of the mass of the heavy particle and depends only on the properties of the medium with which the heavy particle interacts, as should be expected.

The analysis of the functions $X[0,t]$, $X[0,t]$, and $\int_0^t X[0,s]ds$ is more involved in the case of the heavy particle in the two- and three-dimensional lattices. Even though we will not go into the details, the results are striking enough to warrant mentioning. Estimates of $X[0,t]$, $X[0,t]$ and $\int_0^t X[0,s]ds$ in the three-dimensional lattice have been obtained by Rubin. They are precise in the same sense as in the one-dimensional case in Equations (67)-(69). When these estimates are substituted in the expression for $P(v_1, u_1, t | v_0, u_0, 0)$, Equation (44), one obtains

$$P^{(3)}(v_1, u_1, t | v_0, u_0, 0) = n \left\{ \begin{pmatrix} v_1 \\ u_1 \end{pmatrix} \middle| \begin{pmatrix} \langle v_1 \rangle \\ \langle u_1 \rangle \end{pmatrix}, \Sigma \right\}, \quad (75)$$

with

$$\begin{pmatrix} \langle v_1 \rangle \\ \langle u_1 \rangle \end{pmatrix} = \begin{pmatrix} v_0 e^{-\frac{1}{2}\beta t} [\cos \omega t - \beta(2\omega)^{-1} \sin \omega t] - u_0 \omega e^{-\frac{1}{2}\beta t} \sin \omega t \\ v_0 \omega^{-1} e^{-\frac{1}{2}\beta t} \sin \omega t + u_0 e^{-\frac{1}{2}\beta t} [\cos \omega t + \beta(2\omega)^{-1} \sin \omega t] \end{pmatrix} \quad (76)$$

and

$$\begin{pmatrix} k_{TM}^{-1} \{1 - e^{-\beta t} [1 - \beta \omega^{-1} \sin \omega t \cos \omega t]\} & k_{TM}^{-1} \beta \omega^{-2} e^{-\beta t} \sin^2 \omega t \\ k_{TM}^{-1} \beta \omega^{-2} e^{-\beta t} \sin^2 \omega t & k_{TM}^{-1} Q \zeta_0 (4\gamma)^{-1} \{1 - e^{-\beta t} [1 + \beta \omega^{-1} \sin \omega t \cos \omega t]\} \end{pmatrix}. \quad (77)$$

The remarkable feature of Equations (75)-(77) is that

$P^{(3)}(v_1, u_1, t | v_0, u_0, 0)$ is identical in form with the fundamental solution of Kramers' equation for an underdamped harmonic oscillator,

$$(\partial P / \partial t) = -v(\partial P / \partial u) + (\partial / \partial v) [(\beta v + \omega^2 u)P] + q(\partial^2 P / \partial v^2). \quad (78)$$

Thus in the same sense as in the one-dimensional case the random thermal motion of a heavy particle in a 3D lattice at a temperature T is described by Kramers' equation for a harmonically bound particle, Equation (78), in which the frequency ω and the phenomenological constants β and q are, respectively,
 $\omega = 2\gamma^{\frac{1}{2}}(Q\zeta_0)^{-\frac{1}{2}}$, $\beta = 4\gamma^{\frac{1}{2}}\zeta_0^{-2}\pi^{-1}Q^{-1}$, and $q = k_{TM}^{-1}\beta$. The effective force constant associated with the frequency ω is $4k/\zeta_0$ or $[(V^{-1})_{0,0}]^{-1}$. As Q increases, the estimates of

$\dot{X}[0,t], \dots$ become more precise and the "Brownian oscillator" becomes more underdamped because $\beta \sim Q^{-1}$ and $\omega \sim Q^{-\frac{1}{2}}$.

In the case of the two-dimensional lattice analogous estimates of $\dot{X}[0,t], \dots$ in terms of elementary functions have not been obtained. Nevertheless Rubin has shown with the aid of Doob's theorem^{1c} that the position and velocity of the heavy particle constitute a non-Markoffian random process. Because $[(V^{-1})_{00}]^{-1}$ is zero in the one- and two-dimensional lattices, the condition which must be satisfied in Doob's theorem in order that the position and velocity of the heavy particle constitute a Markoffian random process reduces to

$$X[0, t_3 - t_1] = X[0, t_3 - t_2] X[0, t_2 - t_1]. \quad (79)$$

This condition is clearly satisfied in the one-dimensional case within the precision of the estimate in Equation (67).

It can be shown in the two-dimensional case that $X[0,t]$ is roughly of the form

$$\dot{X}[0,t] \approx ce^{-at} \cos(bt + \phi)$$

so that (79) cannot be satisfied in any reasonable sense.

2) Coupled Oscillator Model of Ford, Kac, and Mazur ⁴

From the general expression for the covariance Σ_{ij}^{vv} in Equation (33) and Equation (47), we have seen that

$$\Sigma_{ij}^{vv} = (m_0 kT)^{-1} \sum_k S_{0k}^2 \cos \Omega_k (t_i - t_j). \quad (80)$$

It was pointed out in discussing the one-dimensional crystal lattice model in the limit $N = \infty$ that the frequency spectrum of the lattice is fixed and, independent of the value of Q (for $Q \geq 0$), and that the $N = \infty$ limit of Σ_{ij}^{vv} can be written as

$$\Sigma_{ij}^{vv} = (m_0 kT)^{-1} \int_0^{2\gamma^{1/2}} \frac{(Q+1)(4\gamma - \omega^2)}{(Q^2 - 1)\omega^2 + 4\gamma^2} G(\omega) \cos \omega(t_i - t_j) d\omega$$

where

$$G(\omega) = 2\pi^{-1} [4\gamma - \omega^2]^{-1/2}$$

is the density of the vibrational frequency spectrum of the perfect lattice. In the limit as $Q \rightarrow \infty$, the form of the normal mode amplitude factor

$$S_0^2(\omega) = \frac{(Q+1)(4\gamma - \omega^2)}{(Q^2 - 1)\omega^2 + 4\gamma^2}$$

changes so that

$$\Sigma_{ij}^{vv} \rightarrow m_0 kT \exp[-2\gamma^{1/2} |t_i - t_j| / Q]$$

in a well-defined sense. Ford, Kac, and Mazur have treated a somewhat different one-dimensional system of N coupled oscillators with cyclic boundary conditions in which all particles have the same mass m and in which all particles are equivalent (V is cyclic). In this system Σ_{ij}^{vv} is the same for each particle. Formally we can use this fact to eliminate the normal mode amplitude factor from Equation (80), namely add up the expressions for Σ_{ij}^{vv} for each particle and divide by the total number N

$$\Sigma_{ij}^{vv} = (mkT)^{-1} \frac{1}{N} \sum_{k=1}^N \cos \Omega_k (t_i - t_j), \quad (81)$$

where we have used the fact that $\sum_R S_{Rk}^2 = 1$. Ford, Kac, and Mazur have considered the limit $N \rightarrow \infty$, and determined that smooth distribution of frequencies in Equation (81), for which

$$\Sigma_{ij}^{vv} = (mkT)^{-1} e^{-f|t_i - t_j|}.$$

The frequency versus wave number relation which they obtained is

$$\Omega = f \left| \tan \frac{\theta}{2} \right|, \quad -\pi < \theta < \pi.$$

Associated with this frequency or eigenvalue spectrum is a unique potential energy matrix in which the range of interaction between particles is infinite. In the first model studied, the frequency-wave number relation is

$$\Omega = 2\gamma^{\frac{1}{2}} \left| \sin \frac{\theta}{2} \right|, \quad -\pi < \theta < \pi$$

(in the one-dimensional case).

Both models exhibit the same limiting Brownian-like behavior. However, the propagation of disturbances (initial conditions) is radically different in the two models. In the first model, the group velocity is ⁵

$$(82) \quad v_g = \frac{d\Omega}{d\theta} = \gamma^{\frac{1}{2}} \cos \frac{\theta}{2}.$$

According to Equation (82), the group velocity decreases from $\gamma^{\frac{1}{2}}$ to zero as the frequency increases from zero to the maximum value $\Omega = 2\gamma^{\frac{1}{2}}$. There is a maximum velocity of propagation of disturbances, which is $\gamma^{\frac{1}{2}}$, the speed of sound. Consequently, there is a definite propagation time required (which is proportional to $\gamma^{-\frac{1}{2}}$) for a disturbance at one location to reach a second location. Subsequently, the disturbance persists at the second location as the higher frequency normal mode components arrive. In contrast to the behavior in the first model, the range of frequencies is infinite in the second model. The group velocity,

$$v_g = \frac{1}{2}f / \cos^2 \frac{\theta}{2},$$

increases from the minimum value $\frac{1}{2}f$ to an infinite value as the frequency increases from zero to infinity. As a consequence, there is an instantaneous response throughout the system to an initial localized disturbance; and there is a definite duration of the disturbance at any second location which is proportional to $2/f$, the reciprocal of the minimum group velocity.

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MATHEMATICAL PROBLEMS OF STATISTICAL MECHANICS

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GENERAL REMARKS

The purpose of statistical physics is to obtain from a knowledge of the underlying mechanics a "complete" description of the macroscopic behavior. One must be given both the constituents to be considered as fundamental, as well as the laws governing their descriptions. The macroscopic properties should then be determined.

To physicists this might seem like an involved, tedious process but not in principle difficult or profound and not yielding any new fundamental information. To mathematicians this might appear like a lengthy and boring process; but not likely to need interesting mathematics, let alone demand the creation of new mathematical ideas. I claim that neither of these contentions is true. To appreciate this, we shall look at the basic ideas of statistical mechanics.

Classical Mechanics

If the underlying mechanics is classical mechanics, the system is described by the Hamiltonian

$$H(p_1, \dots, p_n, q_1, \dots, q_n)$$

e.g. we might have

$$(1) \quad H = \sum_{i=1}^n \frac{p_i^2}{2m_i} + \sum_{i,j} V(q_i, q_j)$$

where the p 's and q 's are the momenta and positions of particles. Denote by $d\Gamma$ a volume element in the phase space

$$d\Gamma = dp_1, \dots, dp_n, dq_1, \dots, dq_n.$$

A complicated system is represented, described as an ensemble with ensemble density $\rho(p_1, \dots, p_n, q_1, \dots, q_n, t)$. Here $\rho d\Gamma$ denotes the number of particles to be found in the volume element $d\Gamma$ in the phase space. ρ satisfies the Liouville equation:

$$(2a) \quad \frac{\partial \rho}{\partial t} + \sum_{i=1}^n \frac{\partial \rho}{\partial p_i} \dot{p}_i + \frac{\partial \rho}{\partial q_i} \dot{q}_i = 0$$

Or making use of the Hamiltonian

$$(2b) \quad \frac{\partial \rho}{\partial t} = \{H, \rho\} \equiv \sum_{i=1}^n \frac{\partial \rho}{\partial p_i} \frac{\partial H}{\partial q_i} - \frac{\partial \rho}{\partial q_i} \frac{\partial H}{\partial p_i}$$

If we are given some function $Q(\vec{p}, \vec{q}, t)$ representing a measured quantity, then the basic observable is equal to the observed average of Q ,

$$\text{i.e.} \quad Q_{\text{obs}} = \frac{\int \rho Q d\Gamma}{\int \rho d\Gamma}$$

Remarks:

- 1) Strictly speaking, all one can give as prescribed data is $\rho(p, q, 0)$. (2b) then determines $\rho(p, q, t)$.

2) In equilibrium $\frac{d\rho}{dt} = 0$. This implies that $\rho = \rho(H)$.

Strictly, ρ is a function of all the integrals of the motion.

Quantum Mechanics

If the underlying mechanical principles are these of quantum mechanics, we again have a Hamiltonian H , an ensemble member is described by a Hilbert space vector $\psi^\alpha(q, t)$ (where the superscript labels the ensemble members), and h is an operator on the Hilbert space. Let $\{\varphi_n(q)\}$ be some orthonormal set and develop

$$(4) \quad |\psi^\alpha(q, t)\rangle = \sum_n a_n^\alpha(t) |\varphi_n(q)\rangle.$$

The analogue of the density function will now be a matrix ρ_{nm} , defined by

$$(5) \quad \rho_{mn} = \frac{1}{N_e} \sum_\alpha (a_m^\alpha) (a_n^\alpha)^*.$$

where N_e is the number of members in the ensemble.

Then

$$\rho_{mn}(0) = \frac{1}{N_e} \sum_\alpha a_m^\alpha(0) (a_n^\alpha(0))^* = \sum_m r_m^\alpha r_n^\alpha e^{i(\varphi_n^\alpha - \varphi_m^\alpha)}$$

where we have set

$$a_m^\alpha(0) = r_m^\alpha e^{i\varphi_m^\alpha}.$$

It is then easily seen that ρ now satisfies the equation

$$(6) \quad i \frac{d\rho}{dt} = \{H, \rho\}.$$

Again, in principle $\rho(o)$ determines $\rho(t)$. Also, if Q is some quantity to be measured, then Q has a representation as a matrix and

$$(7) \quad Q_{\text{obs}} = \text{trace } \rho Q.$$

Note that ρ_{nn} has a direct physical significance i.e., it is the probability that a system chosen at random from the ensemble will be in state n . The off-diagonal elements of ρ , i.e. ρ_{mn} , $m \neq n$, have no such direct meaning. In equilibrium, ρ is independent of time.

Does not this formal outline now substantiate the critical attitude towards statistical mechanics? After all, given that the system H is specified, one needs to (physically) give $\rho(o)$, solve (2a) or (6) and evaluate (3) or (7). That the matter is not so simple can be understood with the help of the following comments:

- (1) One can, as a matter of practice, not carry out these operations.

- (2) One can not deduce any of the macroscopic properties of a system; e.g., looking at (6) or (7) will not yield the color of CuSO_4 , or the strength of steel. Instead, one looks at limited pieces of the experimental material, and sees whether judicious approximations of the basic equations can reproduce these results.
- (3) In this sense most of equilibrium thermodynamics has been explained. Note that the thermodynamic explanation also leads to mathematical problems of unusual type. For example, one can show that in equilibrium, the thermodynamic properties of gas are determined by

$$\exp\left[-\frac{\Psi}{Kt}\right] = \frac{2\pi mkt}{h^2}^{\frac{3n}{2}} \frac{1}{N!} \int_{\Omega} \dots \int dx_1^3 \dots dx_N^3 e^{-\beta V(x_1, \dots, x_N)}$$

We would like to obtain from this the three physical states of a substance (i.e., gas, liquid, solid). Mathematically, this poses the question: can we show that

$$p = \frac{\partial \Psi}{\partial \Omega} \quad \text{as} \quad \begin{matrix} \Omega \rightarrow \infty \\ N \rightarrow \infty \end{matrix} \quad \frac{N}{\Omega} = \frac{1}{v}$$

consists of three separate analytical parts, for

$$V = \sum V(r_{ij})$$

where the general character of V is a short range repulsion and a long range attraction?

(4) To appreciate the scope of statistical physics, note that if

- a) quantum mechanics is the appropriate means to describe nuclei and
- b) the notion of an equivalent nuclear-nuclear force is again a statistical problem. Instead of predicting the number and kind of macroscopic parameters and macroscopic laws (as in usual statistical physics) one should now predict the characteristics of nuclei as a whole (nuclear bonding energies, nuclear surfaces, phase transitions, phase separations).

(5) If Chew is right in the sense that no strongly interacting particle is more fundamental than another (π meson, p , η , etc.) we still will need a statistical mechanics of strongly interacting objects, or one will have to explain why nuclei-composites of strongly interacting entities satisfy qualitatively different laws from their constituents.

This points to an important general moral. The laws and concepts used to describe the system as a whole will generally be quite different from those used to describe the constituents. It is only a rare instance that a purely mathematical analysis (contrasted to a descriptive

phenomenological one) yields even the appropriate variables and parameters to describe the system "macroscopically."

- (6) If quarks do exist, a new area of statistical mechanics opens up - the reconstruction of "fundamental particles" on the basis of quark mechanics.

The crucial concepts throughout are those of contraction and projection. The purely microscopic laws give too much information.

THE CONTRACTION AND PROJECTION TECHNIQUES

1. Contractions

The simplest way to roughen up the description is to integrate some variables - ; define

$$(9) \frac{1}{\Omega_s} f_s(x_1 \dots x_n, t) = \int \dots \int \rho(x_1 \dots x_n, t) dx_{s+1} \dots dx_n$$

$$x_1 \equiv (p_1, q_1) \quad \text{Let } n \rightarrow \infty \quad \frac{\Omega}{n} = v = \text{fixed}$$

$$(10) \frac{\partial f_1}{\partial t} + \frac{p_{1,\alpha}}{m} \frac{\partial f_1}{\partial p_{1,\alpha}} \frac{\partial V_o}{\partial q_{1,\alpha}} = \frac{1}{v} \iint dp_2 dq_2 \frac{\partial V(q_1 q_2)}{\partial q_{1,\alpha}} \frac{\partial f_2(p_1, q_1, p_2, q_2, t)}{\partial p_{1,\alpha}}$$

Now what does one do a) to give a "closed" contracted description

b) to yield irreversibility

c) to show the approach to equilibrium and compute it.

One uses:

- 1) An approximation procedure; f_2 is a functional of f_1
(Bogoliubov, Uhlenbeck); separate time scales
- 2) Truncation $f_2 = f_1 f_1$
- 3) Some additional averaging time averaging
course graining

- 4) Special initial conditions - factorization
 no long range correlations
- 5) Special systems - special interactions
- 6) Limit of large systems.

2. Projection Operator Techniques

These techniques are elegant and work both for classical and quantum systems.

Write the basic equation as

$$i \frac{\partial \rho}{\partial t} = [H, \rho] \equiv L\rho \quad (11)a$$

L is an operator, which constructs a new operator from an old one:

$$A = LB \equiv HB - BH \quad (11)b$$

(In the classical case $L = i \sum \frac{\partial H}{\partial q_i} \frac{\partial}{\partial p_i} - i \sum \frac{\partial H}{\partial p_i} \frac{\partial}{\partial q_i}$)

Note in matrix notation L has four indices.

$$A_{mn} = \sum L_{mnm'n'} B_{m'n'} \quad (12)a$$

$$L_{mnm'n'} = H_{mm'} \delta_{nn'} - \delta_{mm'} H_{n'n} \quad (12)b$$

Suppose one works in a definite representation; define D as the operator, which acting in a matrix projects into the off-diagonal part, or keeps the diagonal part:

$$(D M)_{ij} = \delta_{ij} M_{ij} = (\delta_{ij} M_{ii}) \text{ no summations} \quad (13)a$$

$$((1-D)M)_{ij} = (1-\delta_{ij}) M_{ij} \quad " \quad " \quad (13)b$$

$$\text{One has } D^2 = D \quad (14)a$$

$$(1-D)^2 = (1-D) \quad (14)b$$

D is also a matrix with four indices

$$(D M)_{ij} \equiv \sum_{kl} D_{ijkl} M_{kl} \quad \text{with}$$

$$D_{ijkl} = \delta_{ij} \delta_{kl} \delta_{ik} \quad \text{then}$$

$$\begin{aligned} (D M)_{ij} &= \sum_{kl} \delta_{ij} \delta_{kl} \delta_{ik} M_{kl} = \delta_{ij} \sum_k \delta_{ik} M_{kk} \\ &= \delta_{ij} M_{ii} \end{aligned}$$

Simple properties:

$$a) \quad D A = A \quad \text{if } A \text{ is diagonal} \quad (15)a$$

$$b) \quad D AB = A D B \quad " \quad " \quad " \quad (15)b$$

$$c) \quad e^{-is(1-D)L} (1-D)M = (1-D)e^{-isL(1-D)} M \quad (15)c$$

Proof:

$$\begin{aligned} e^{-is(1-D)L} (1-D)M &= \sum_n \frac{(is)^n}{n!} (1-D)L \dots (1-D)L (1-D)M \\ &\quad \text{n times} \\ &= (1-D) \sum_n \frac{(is)^n}{n!} L(1-D) \dots L(1-D)M = (1-D)e^{-isL(1-D)} M \\ &\quad \text{n times} \end{aligned}$$

Application:

Consider the equation for the density matrix; recall the different significance of diagonal and off-diagonal elements.

Define:

$$\rho' = D\rho \quad \rho'' = (1-D)\rho \quad \rho = \rho' + \rho'' \quad (16)$$

From $i \frac{\partial \rho}{\partial t} = L\rho$

$$a) \quad \left\{ \begin{array}{l} i \frac{\partial \rho'}{\partial t} = D L \rho' + D L \rho'' \end{array} \right. \quad (17)a$$

$$b) \quad \left\{ \begin{array}{l} i \frac{\partial \rho''}{\partial t} = (1-D)L \rho' + (1-D)L \rho'' \end{array} \right. \quad (17)b$$

Note (as expected) that ρ' and ρ'' are coupled.

Introduce the Green's function of (17)b.

$$K(t) = e^{-it(1-D)L}, \text{ then} \quad (18)a$$

$$\rho''(t) = K(t)\rho''(0) - i \int_0^t ds K(s) (1-D)L\rho'(t-s) \quad (18)b$$

[For consider (17)b, if the ρ' were not there

$$\rho''_0(t) = e^{-it(1-D)L}; \quad i \frac{\partial \rho''}{\partial t} = i(-i)(1-D)L e^{-it(1-D)L}$$

$$= (1-D)L \rho''_0, \text{ now write}$$

$$\rho'' = f e^{-it(1-D)L}; \text{ then}$$

$$i \frac{\partial \rho''}{\partial t} = i \frac{\partial f}{\partial t} e^{-it(1-D)L} + f(i)(-i)(1-D)L e^{-it(1-D)L}$$

But from (17)b we have:

$$i \frac{\partial \rho''}{\partial t} = (1-D)L \rho' + (1-D)L f e^{-it(1-D)L}$$

Comparing the two expressions, we get:

$$i \frac{\partial f}{\partial t} = e^{it(1-D)L} (1-D)L \rho'$$

$$f = -i \int_0^t e^{is(1-D)L} (1-D)L \rho'(s) ds + i \rho''(0)]$$

Substitute (18)b back into (17)a there results

$$i \frac{\partial \rho'}{\partial t} = D L \rho' - i \int_0^t ds D L K(s) (1-D)L \rho'(t-s) \quad (19)$$

$$+ D L K(t) \rho''(0)$$

- a) Note that this is an equation for ρ' alone;
the $\rho''(0)$ is an inhomogeneous term.
- b) If one picks the random phase approximation

$$\rho''(0) = 0; \quad (20)$$

one has a self contained equation, without
approximation for the probabilities only.

This is van Hove's master equation to general order.

- c) Note the triviality of the derivation, (apart from (20)).

$$J(t) = e^{-itD L} \quad (21)$$

Now

$$i \frac{\partial \rho''}{\partial t} = (1-D)L \rho'' - i(1-D)L \int_0^t ds J(t-s) D L \rho''(s) \quad (22)$$

$$+ (1-D)L J(t) \delta'(0)$$

One can now not impose the initial condition

$\rho'(0) = 0$, this conflicts with $\text{Tr}(\rho) = 1$. But dynamically ρ'' and $\rho'(0)$ are not coupled in (22). (22) is Janner's (van Hove's) master equation. H is as trivial as (19), (as exact, as reversible, as the Liouville equation.) The ideas of the projection operator can be applied generally to any equation of the form

$$\dots\dots i \frac{\partial x}{\partial t} = Lx \quad (\text{where } x(t) \text{ is a vector,} \quad (23)$$

$$L \text{ is a linear operator})$$

$$\text{Let } x = x' + x'' = Px + (1-P)x \quad (24)$$

P is a linear operator

then

$$i \frac{\partial x'}{\partial t} = PL x' - i \int_0^t ds PL K(s) (1-P) L x'(-s) \quad (25)$$

$$+ P L K(t) x''(0)$$

The obvious analogue of (19) $K(t) = e^{-it(1-P)L}$

In a sense, both (25) and (19) apply to objects which are elements in a Hilbert space. This is clear in (25); in (19) the elements of the Hilbert space are themselves (infinite)

matrices. The scalar product in that Hilbert space is the only aspect that needs definition. In a usual Hilbert space, the objects are vectors $u, v, \dots$ $(u, v) \equiv \sum_{\alpha} u_{\alpha}^* v_{\alpha}$, where the u_{α}, v_{α} are the components relative to a base. Suppose the matrices A, B have matrix elements A_{ij}, B_{kl} , relative to some base. Now (A_{ij}) can be written as (A_{α}) , (B_{kl}) as (B_{β}) , where α determines both i and j , β determines both k and l . In particular if $\alpha = \beta \rightarrow i = k, j = l$.

Now the scalar product of A and B is

$$(A, B) = \sum_{\alpha} A_{\alpha}^* B_{\alpha} = \sum_{i,j} A_{ij}^* B_{ij}$$

A CLASSICAL EXAMPLE

Consider a system of N particles $\vec{x}_1 \vec{p}_1 \dots \vec{x}_N \vec{p}_N$ and N scattering centers $\vec{r}_1 \dots \vec{r}_N$. $\vec{x}_i, \vec{p}_i$ can depend on t , the $\vec{r}_i$ cannot. The ensemble density describing the system is $\rho(\vec{x}_1 \vec{p}_1 \dots \vec{x}_N \vec{p}_N, \vec{r}_1 \dots \vec{r}_N, t)$, it satisfies the Liouville equation

$$i \frac{\partial \rho}{\partial t} = L_{2N} \rho \quad (26a)$$

$$L_{2N} = - \frac{i}{m} \sum_{j,s} p_{j,s} \frac{\partial}{\partial x_{j,s}} + i \sum_{j,\alpha,s} \frac{\partial V(x_j - r_\alpha)}{\partial x_{j,s}} \frac{\partial}{\partial p_{j,s}} \quad (26b)$$

Latin letters $i, j, \dots$ subscript the particles

Greek letters $\alpha, \beta, \dots$ subscript the scattering centers

Assumptions:

The particles do not interact with one another

do interact with the scattering centers

do possess kinetic energy

The scattering centers do not participate in dynamics

do not possess kinetic energy

do not exert forces on each other

do exert forces on the particles.

Introduce

$$(27) \quad f(\vec{x}, \vec{p}, \vec{r}_1 \dots \vec{r}_N) = \int \dots \int d^3x_2 d^3p_2 \dots d^3x_N d^3p_N \phi(\vec{x}, \vec{p}, \dots, \vec{x}_N \vec{p}_N, \vec{r}_1 \dots \vec{r}_N)$$

= prob. to find a particle at $\vec{x}$, with momentum $\vec{p}$
and the scattering centers at $\vec{r}_1 \dots \vec{r}_N$.

By straightforward integration from (26), f satisfies

$$(28)a \quad i \frac{\partial f}{\partial t} = L f$$

$$(28)b \quad L = - \frac{i}{m} p_s \frac{\partial}{\partial x_s} + i \sum_{\alpha} \frac{\partial V(\vec{x} - \vec{r}_{\alpha})}{\partial x_s} \frac{\partial}{\partial p_s}$$

$$(28)c \quad \int \dots \int d^3x d^3p d^4r_1 \dots d^4r_N f(x, p, r_1 \dots r_N, t) = 1$$

Note that the basic equation (28)a

$$(28)d \quad i \frac{\partial f}{\partial t} = - \frac{i}{m} p_s \frac{\partial f}{\partial x_s} + i \sum_{\alpha} \frac{\partial V(\vec{x} - \vec{r}_{\alpha})}{\partial x_s} \frac{\partial f}{\partial p_s}$$

is a partial differential equation, with variable coefficients
($V(x - r_{\alpha})$), depending on a set of parameters (r_{α}). This is not
a simple equation; due to the fact that the probability
function f describes both the particle and the centers; this
leads to correlations between the particle and the centers.
To see this attempt a further contraction, define

$$(29) \quad f_s(\vec{x}, \vec{p}, \vec{r}_1 \dots \vec{r}_s, t) = N^{s+1} \int \dots \int d^3r_{s+1} \dots d^3r_N f(\vec{x}, \vec{p}, \vec{r}_1 \dots \vec{r}_N, t)$$

$N-s$ integrations.

$$(29)a \quad f_0(\vec{x}, \vec{p}, t) = N \int \dots \int d^3 r_1 \dots d^3 r_N f(\vec{x}, \vec{p}, r_1 \dots r_N, t)$$

gives the pure particle distribution - without reference to the scattering centers. However it does not satisfy a differential equation. Integrate (28)d over all r's

$$\frac{1}{N} i \frac{\partial f_0}{\partial t} = \frac{1}{N} - \frac{i}{m} p_s \frac{\partial f_0}{\partial x_s} + i \int \dots \int d^3 r_1 \dots d^3 r_N \sum_{\alpha} \frac{\partial V(\vec{x} - \vec{r}_{\alpha})}{\partial x_s} \frac{\partial f(x, p, r_1 \dots r_N)}{\partial p_s}$$

$$\sum_{\alpha} \int d^3 r_{\alpha} \frac{\partial V(x - r_{\alpha})}{\partial x_s} \underbrace{\frac{\partial}{\partial p_s} \int \dots \int d^3 r_1 \dots d^3 r_N f(x, p, \dots r_{\alpha} \dots r_N)}_{\frac{1}{N^2} f_1}$$

$$(29)b \quad i \frac{\partial f_0}{\partial t} = - \frac{i}{m} p_s \frac{\partial f_0}{\partial x_s} + \sum_{\alpha} \frac{1}{N} \int d^3 r_{\alpha} \frac{\partial V(x - r_{\alpha})}{\partial x_s} \frac{\partial d_1(x, p, r_{\alpha})}{\partial p_s}$$

Notice that the typical coupled hierarchy feature shows up here.

Thus a discussion of f_0 , is not trivial.

Physically one wants to give f at $t = 0$; then one would like to obtain

- a) a proof that as $t \rightarrow \infty$, the distribution is spherically symmetric (if V is)
- b) How long does one have to wait for the spherical symmetry is established.

c) How long does it take for the initial value correlation to be washed out?

To give this discussion introduce a set of auxiliary functions $F_0, F_1, \dots, F_N$, defined recursively,

$$\begin{aligned} f_0(\vec{x}, \vec{p}, t) &= F_0(\vec{x}, \vec{p}, t) \\ f_1(x_1 p_1, r_1, t) &= \frac{N}{\Omega} F_0 + F_1(xp, r_1) \\ (30) \quad f_2(x_1 p_1 r_1 r_2 t) &= \frac{N^2}{\Omega^2} F_0 + \frac{N}{\Omega} F_1(xp, r_1) + \frac{N}{\Omega} F_1(xp r_2) \\ &\quad + F_2(xp, 1, 2) \\ f_N(xp, 1 \dots N) &= \left(\frac{N}{\Omega}\right)^N F(xp) + \left(\frac{N}{\Omega}\right)^{N-1} \sum_i F_1(xp, i, t) \\ &\quad + \left(\frac{N}{\Omega}\right)^{N-2} \sum_{i,j} F_2(xp, i, j, t) \\ &\quad + F_N(xp, 1 \dots N, t) \end{aligned}$$

Since by (24) $f_N = N^{N+1} f$, the last equation in (30) becomes

$$\begin{aligned} (30) \quad N \Omega^N f &= F_0(x_1 p) + \frac{\Omega}{N} \sum_i F_1(xp, i, t) \\ &\quad + \left(\frac{\Omega}{N}\right)^2 \sum_{i,j} F_2(xp, i, j, t) \\ &\quad + \left(\frac{\Omega}{N}\right)^N F_N(xp, 1 \dots N, t) \end{aligned}$$

Substitute (30) in the equation for f in (28)d.

(The usual definition of $f_s = N - \frac{N!}{(N-s)!} \int \dots f dr_{s+1} \dots dr_N$

has a different coefficient; from N^{s+1} , take the log

$$\log N + \log N! - \log(N-s)! \approx \log N + N \log N - N$$

$$= \log N + N \log N - N \left(1 - \frac{s}{N}\right) \log N \left(1 - \frac{s}{N}\right) - s$$

$$= \log N + N \log N - (N-s) \log N - (N-s) \log \left(\frac{s}{N} \dots\right) - s$$

large $N \approx \log N + s \log N = (1+s) \log N$; the same as the coefficient in (21).

Now note from (30)

$$\int f_1(xp, r_1, t) dr_1 = \frac{N}{\Omega} \int F_0 dr_1 + \int F_1(xp, r_1) dr_1$$

$$Nf_0(xp) = \frac{N}{\Omega} \int f_0(xp) dr_1 + \int F_1(xpr_1) dr_1$$

independent of r_1 gives

$$\frac{N}{\Omega} \int f_0, \text{ hence}$$

$$(33)a \quad \int dr_1 F_1(xpr_1) dr_1 = 0.$$

Next integrate the second term, over x_2

$$\begin{aligned} \int dr_2 f_2(xp, r_1, r_2, t) &= \frac{N^2}{\Omega} \int F_0(xp) dr_2 \\ &+ \frac{N}{\Omega} \int F_1(xp, r_1) dr_2 + \frac{N}{\Omega} \int F_1(xp, r_2) dr_2 \\ &+ \int F_2(xp, r_1, r_2) dr_2 \end{aligned}$$

$$\begin{aligned} N f_1(xp, r_1) &= \frac{N^2}{\Omega} + N F_1(xp) \\ &= \frac{N^2}{\Omega^2} F_0 + N F_1(r_1) + \int F_2(xp, r_1, r_2) dr_2 \end{aligned}$$

$$(33)b \quad \int dr_2 F_2(xp, r_1, r_2) = 0$$

One proves in general

$$(34) \quad \int dr_K F_s(xp, r_1 \dots r_K \dots r_s, t) = 0 \quad \begin{array}{l} s \geq 1 \\ 1 < K \leq s. \end{array}$$

The development of the reduced functions f_s , in terms of the function F_s , is like a cluster expansion; but not exactly the same.

From (29) one sees again that

$$(35) \quad f_N(xp, r_1 \dots r_N, t) = N^{N+1} f(xp, r_1 \dots r_N, t)$$

The basic equation (28) refers to f , which via (35) and (30) is expanded as

$$\begin{aligned}
 (36) \quad \Omega^N N f &= \frac{\Omega^N}{N^N} f_N \\
 &= F(xp) + \left(\frac{\Omega}{N}\right) \sum_i F_1(xp, r_i, t) \\
 &\quad + \left(\frac{\Omega}{N}\right)^2 \sum_{i \neq j} F_2(xp, r_i, r_j, t) \\
 &\quad + \dots \left(\frac{\Omega}{N}\right)^N F_N(xp, r_1 \dots r_N, t)
 \end{aligned}$$

Application of Zwanzig's Result

If $i \frac{\partial x}{\partial t} = Lx$, and P is a projection operator

then

$$\begin{aligned}
 (37) \quad i \frac{\partial Px}{\partial t} &= P L Px(t) - i \int_0^t ds P L K(s) (1-P) L Px(t-s) ds \\
 &\quad + P L K(t) (1-P) x(0)
 \end{aligned}$$

For the application to this case let

$$(38)a \quad x = \Omega^N N f(xp, r_1 \dots r_N, t)$$

The projection operator

$$\begin{aligned}
 Px &= N \int \dots \int f(xp, r_1 \dots r_N, t) dr_1 \dots dr_N \\
 &= f_0(xp, t) \equiv F_0(xp, t)
 \end{aligned}$$

$$(38)b \quad P = \frac{1}{\Omega^N} \int \dots \int dr_1 \dots dr_N$$

$$(38)c \quad L_O = - \frac{i}{m} p_s \frac{\partial}{\partial x_s} = -i \vec{p} \cdot$$

$$(38)d \quad L_1 = i \sum_{\alpha} \frac{\partial V(\vec{x} - \vec{r}_{\alpha})}{\partial x_s} \frac{\partial}{\partial p_s}$$

$$(38)e \quad L = L_O + L_1$$

Show these properties:

$$(39)a \quad P^2 = P$$

$$(39)b \quad (1-P)^2 = (1-P)$$

$$(39)c \quad P L_O = L_O P$$

$$(39)d \quad P L_1 P = 0$$

$$(39)e \quad P L_O P = L_O P$$

Ad (39)a Act with P on a function $g(r_1 \dots r_N)$

$$Pg = \frac{1}{\Omega^N} \int \dots \int dr_1 \dots dr_N g(r_1 \dots r_N) = \text{member } X \text{ independent of } r$$

$$P^2 g = \frac{1}{\Omega^N} \int \dots \int dr_1 \dots dr_N \cdot \frac{1}{\Omega^N} \int \dots \int dr_1 \dots dr_N g$$

$$= \frac{1}{\Omega^N} \int \dots \int dr_1 \dots dr_N \cdot X = X = Pg$$

Ad (39)c L_0 and P refer to different variables

x_p and $r_1 \dots r_N$ respectively, hence commute.

Ad (39)d Let $g = g(x_p, r_1 \dots r_N)$

$$\begin{aligned}
 P L, P g &= \frac{1}{\Omega^N} \int \dots \int dr_1 \dots dr_N \cdot i \sum_{\alpha} \frac{\partial V(x-r_{\alpha})}{\partial x_s} \frac{\partial}{\partial p_s} \\
 &\quad \frac{1}{\Omega^N} \int \dots \int dr_1 \dots dr_N g(x_p, r_1 \dots r_N) X(p, s) \\
 &= \frac{1}{\Omega^N} \int \dots \int dr_1 \dots dr_N \sum_{\alpha} \frac{\partial V(x-r_{\alpha})}{\partial x_s} \frac{\partial}{\partial p_s} X(x_p) \\
 &= \frac{1}{\Omega^N} \int \dots \int dr_1 \dots dr_N \sum_{\alpha} \frac{\partial V(x-r_{\alpha})}{\partial r_{\alpha, s}} \frac{\partial X(x, p)}{\partial p_s}
 \end{aligned}$$

The r integrations can be carried out, if

go to zero, as $r \rightarrow \infty$, this term vanishes the potentials

hence (39)e.

One by (37) gets an equation for (P_x) , i.e. in

this case

$$\begin{aligned}
 &\frac{1}{\Omega^N} \int \dots \int dr_1 \dots dr_N \Omega^N N f(x_p, r_1 \dots r_N, t) \\
 &= N \int \dots \int dr_1 \dots dr_N f(x_p, r_1 \dots r_N, t) = f_0(x_p, t) \equiv F_0(x_p, t).
 \end{aligned}$$

The term $P L P(x(t))$ for example will be

$$P(L_0 + L_1)P(x(t)) = L_0 P x(t) = L_0 F_0$$

The term $P L K(s)(1-P)L P x(t-s)$

$$\begin{aligned} &= P(L_0 + L_1)K(s)(1-P)(L_0 + L_1)P x \\ &= P(L_0 + L_1)K(s)[(L_0 + L_1)P - L_0 P]x \\ &= P(L_0 + L_1)K(s) L_1 P x \end{aligned}$$

$$F_0$$

This means that the only unknown function involved is F_0 .

Actually the L_0 term (called a) can be left out altogether, for one has

$$e^{-is(1-P)L}(1-P)^M = (1-P)e^{-isL(1-P)}M$$

for any M . Now consider the term

$$\begin{aligned} &P L_0 K(s)(1-P)L P x \\ &= P L_0 e^{-is(1-P)L}(1-P) L P x \\ &= P L_0 (1-P)e^{-iLs(1-P)}(LPx) \\ &= L_0 P(1-P)e^{-iLs(1-P)}(LPx) = 0 \end{aligned}$$

Thus the integral term becomes just

$$-i \int_0^t P L_1 K(s) L_1 F_0(xp, t)$$

Finally study $P L K(t) (1-P) (x(o))$

clearly $x(o) = \Omega^N N f(xp, r_1 \dots r_N, o)$ can be expanded by (36), always in F 's at time o .

$$\text{Of course } P(x(o)) = F_0(o)$$

Thus one obtains the basic (and still rigorous) equation

$$(40) \quad i \frac{\partial F_0}{\partial t} = L_0 F_0 - i \int_0^t ds P L_1 K(s) L_1 F_0(xp, t-s) \\ + P L_1 K(t) \left[\frac{\Omega}{N} \sum_i F_1(xp, r_i, o) + \left(\frac{\Omega}{N} \right)^2 \sum_{i,j} F_2(xp, r_i, r_j, o) + \dots \right]$$

This is a self contained equation, which contains just the initial values of the higher correlation functions. At this point the van Hove assumption would be

$$F_s(xp, r_1 \dots r_s, o) = 0 \quad s = 1, 2, \dots$$

Prigogine assumption.

Let the F_s be so (initially) that there exists a length R , such that

$$(41) \quad F_s(xp, r_1 \dots r_s, o) = 0 \quad \text{if } |s - r_k| > R \\ \text{for } \underline{\text{any}} \ K \leq s \\ \text{and } \underline{\text{all}} \ s \geq 1$$

Thus the mathematical problem is to study (40) with the initial condition (41).

This is not easy a) the equation is non trivial, non

Markoffian integral equation.

b) the operator $K(t) = e^{-it(1-P)L}$ is complicated.

So one actually approximates K , and sees what happens to the equation. Then studies the solutions of that approximate equation.

Method

$$(42) \quad K(s) = \sum_{n=0}^{\infty} K^{(n)}(s)$$

$$K^{(n)}(t) = (-i)^n \int_0^t dt_1 e^{-i(1-P)L_0(t-t_1)} (1-P)L_1 \int_0^{t_1} dt_2 e^{-i(1-P)L_0(t-t_2)} (1-P)L_1 \\ \dots \int_0^{t_{n-1}} e^{-i(1-P)L_0(t-t_{n-1})} (1-P)L_1 \underbrace{e^{-i(1-P)L_0 t_n}}_{\text{}} dt_n$$

$$K^{(0)}(t) = e^{-i(1-P)L_0 t}$$

To see the character of these terms in the basic equation, one needs K_0 , in zero order

$$K^0 = e^{-i(1-P)L_0 t}$$

$$= 1 + (-i)(1-P)L_0 t + \frac{(-i)^2}{2!} (1-P)L_0 (1-P)L_0 \dots$$

Using that $P^\alpha = P$ and $L_0 P = P L_0$, one shows

$$(45) \quad K^0 = P + e^{-iL_0 t} (1-P); \text{ now there are no projection operators in the exponential.}$$

Now $e^{-iL_0 t} = e^{-\frac{ps}{m} t \frac{\partial}{\partial x_s}}$, is a shift operator,

so that

$$(46)a \quad e^{-iL_0 t} h(\vec{x}) = h(\vec{x} - \frac{\vec{p}}{m} t)$$

Check by differentiation that

$$(46)b \quad e^{-iL_0 t} L_1 = i \sum_{\alpha} \frac{\partial V(\vec{x} - \frac{\vec{p}t}{m} - \vec{r}_{\alpha})}{\partial x_s} \left(\frac{\partial}{\partial p_s} + \frac{t}{m} \frac{\partial}{\partial x_s} \right) e^{-iL_0 t}$$

The point to note is that the $e^{-iL_0 t}$ operator, hence K^0 , gives rise to potentials at shifted points, shifted just by the motion of the particles.

Thus a term such as

$P L_1 K^{(0)}(s) L_1 F_0(xp, t-s)$ will contain 2 potentials, (one from each L_1) but at different points, in fact one gets precisely for that term

$$\Sigma P \frac{\partial V(\vec{x}-\vec{r}_\alpha)}{\partial x_{s'}} \frac{\partial}{\partial p_{s'}} \frac{\partial V(\vec{x}-\vec{v}s-\vec{r}_\alpha)}{\partial x_{s''}} \left(\frac{\partial}{\partial p_{s''}} + \frac{s}{m} \frac{\partial}{\partial x_{s''}} \right) F_2(\vec{x}-\vec{v}s, t-s)$$

Now if $V(x-r_\alpha)$ vanishes whenever $x-r_\alpha > R$, one must have

$$|x-r_\alpha| < R$$

$$|x-\vec{v}s-r_\alpha| < R \quad \text{for a non vanishing}$$

result. On the memory term:

$$(47) \quad PL_1 K^0(s) L_1 F_0 = 0 \quad \text{if } s > \frac{2a}{v}$$

In general

$$(47)a \quad PL_1 K^{(n)}(s) L_1 F_0 = 0 \quad \text{if } s > \left(\frac{n}{2} + 1 \right) t_c$$

A similar argument for the correlation terms

yields

$$(48) \quad PL_1 K^0(t) [] = 0 \quad \text{unless } t < \frac{1}{2}t_c + t_R$$

$$(48)a \quad PL_1 K^{(n)}(t) F_\ell(0) = 0 \quad \text{for all } t \quad \text{if } \ell > n+1$$

$$(48)b \quad PL_1 K^{(n)}(t) F_\ell(0) = 0 \quad \text{for } t > \left(\frac{1}{2}(n-\ell) + \frac{3}{2} \right) t_c + t_R$$

$$PL_1 K^{(n)}(t) U_\ell(0) \quad \text{if } \ell \leq n+1$$

$$\text{not zero,} \quad \text{if } \ell \leq n+1$$

then only if t

Conclusions

a) The initial correlations of high order (high ℓ in F_ℓ) contribute only in high order perturbation theory. If the perturbation theory is good only $n = 0, 1, 2$ contribute the higher order correlations can be neglected.

b) All correlations vanish after some time, the length of time is longer as the order of perturbation theory increases

c) The time range contributing in the memory term, gets longer in higher order.

Using results a and b, one can in some sense say that for large t one can omit the correlation terms (this is of course not exact), then one obtains

$$(49) \quad i \frac{\partial F^0}{\partial t} = L_0 F_0 - i \int ds P L_1 K(s) L_1 F_2(xp, t-s)$$

One can reduce (49) further; replace $K(s)$ by K^0 , the time integration is non zero only for times $s > \frac{2a}{v}$. For large v this is small.

One finds the Boltzmann equation

$$(50) \quad \frac{\partial F_0}{\partial t} = - \frac{1}{mp_s} \frac{\partial}{\partial x_s} F_0(x_1 p, t) - m \left(\frac{N}{\Omega} \right) X \frac{\partial}{\partial p_s} \left(\frac{\delta_{ss'}}{p} - \frac{p_s p_{s'}}{p^3} \right) \frac{\partial F_0}{\partial p_s}$$

$$(50)a \quad X = \int_0^\infty \frac{d\alpha}{\alpha} \frac{\partial}{\partial \alpha} \int d^3 y V(y) V(y-\alpha)$$

Boltzmann Equation if V is repulsive

$$\underline{X < 0}$$

For the homogeneous case $\frac{\partial F_0}{\partial x_s} = 0$

$$F_0(\vec{p}, t) = \sum_{\ell m} C_{\ell m}(p, t) Y_\ell^m \quad C_{\ell m}(p, t) = A_{\ell m}(p) e^{\lambda(\ell, p)t}$$

$$\lambda = m \frac{N}{\Omega} X \frac{(\ell)(\ell+1)}{p^3}$$

$$\lambda = m \frac{N}{\Omega} X \frac{\ell(\ell+1)}{p^3}$$

Note that $\underline{X < 0}$, means that for long times all C 's $\rightarrow 0$, except C_0 , yielding spherical symmetry.

Unsolved a) Exact solution of (49)

b) non perturbation discussion of (40)

c) How long should one wait to obtain a given derivation from spherical symmetry?

d) One studies the solutions of the approximate equation $(K^{(n)})$. It is not obvious that the sequence of exact solutions to the approximate equation will converge to the exact solution of the exact equation. It is even less obvious that the approximate solutions of the approximate equation, will in any sense converge to the or an approximate solution of the exact equation.

A QUANTUM MECHANICAL EXAMPLE

1) The special feature of the Kac's models is that they allow both a precise description of the dynamics and the statistics. Thus the difference between a mechanistic treatment with certain pieces of information omitted, or averaged over can be directly compared to a discussion in which the time evolution itself is assumed to be governed by probability laws.

2) A special point is the fact that all these models are classical. It is always assumed that quantum mechanics makes no difference as far as statistical discussion are concerned. The quantum Kac model is so constructed to test this point.

The Classical Model

Kac ring, with n points

m markers

$$\frac{m}{n} = \mu$$

Dynamics, when a ball leaves a marker it will change color.

Problem At $t = 0$ all balls are white

$$N_W(\phi) = n$$

Asked color scheme as $t \rightarrow \infty$.

Set of markers S $\epsilon_p = -1$ yes marker at p

$\epsilon_p = +1$ no marker at p

dynamics $\eta_p(t) = +1$ ball at p white

$= -1$ ball at p black

$$(51) \quad \eta_{p+1}(t+1) = \epsilon_p \eta_p(t)$$

Statistical discussion

$$(52) \quad \left\{ \begin{array}{l} N_W + N_B = n \\ N_W(S', t) + N_B(S', t) = m \\ N_W(t+1) - N_W(t) = N_B(S, t) - N_W(S, t) \\ N_B(t+1) - N_B(t) = N_W(S, t) - N_B(S, t) \end{array} \right.$$

Assumption $N_W(S, t) = \frac{m}{n} N_W(t)$

$$(53) \quad \begin{aligned} \text{leads to} \quad \Gamma(t) &= \frac{1}{n} (N_W(t) - N_B(t)) \\ &= (1-2\mu)^t \Gamma(0) \end{aligned}$$

Wrong: Question is what sense is this correct?

Precise discussion

$$(54) \quad \eta_p(t) = \epsilon_{p-1} \epsilon_{p-2} \dots \epsilon_{p-t} \eta_{p-t}(0)$$

$$(54)a \quad \Gamma(t) = \frac{1}{n} \sum_p \epsilon_{p-1} \dots \epsilon_{p-t} \eta_{p-t}(0)$$

(53) is correct as a limit of an average (average over all markers positions). The probability to find a marker at p is μ . Hence $\text{Prob}(\epsilon_j = -1) = \mu$.

$$(55) \quad \text{Prob}(\epsilon_j = +1) = 1 - \mu$$

Thus

$$(56)a \quad g(s) = \frac{n!}{s!(n-s)!} \mu^s (1-\mu)^{n-s}$$

= prob. to find s markers

$$(56)b \quad \langle \epsilon_{p-1} \dots \epsilon_{p-t} \rangle = (1-2\mu)^t$$

average over the ensemble of Kac rings,

$$\begin{aligned} \text{Thus } \langle \Gamma(t) \rangle &= \frac{1}{n} \sum_p \langle \epsilon_{p-1} \dots \epsilon_{p-t} \rangle \eta_{p-t}(0) \\ &= (1-2\mu)^t \eta_{p-t}(0) \end{aligned}$$

in harmony with (53).

Other quantities can be similarly computed, e.g.

the number of white balls at time t

$$(57) \quad \lim_{n \rightarrow \infty} \frac{1}{n} \langle N_W(t) \rangle = \frac{1}{2} + \frac{1}{2}(1-2\mu)^t$$

Alternate derivation; let $f_p(t)$ be the probability that the ball at p at t is white ($1-f_p(t)$) black, then

$$(58) \quad f_{p+1}(t+1) = f_p(t)(1-\mu) + (1-f_p(t))\mu$$

white	black
no marker	yes marker

Given $f_{p+1}(t+1) = (1-2\mu)f_p(t) + \mu$

this yields by iteration

$$(59) \quad f_p(t) = \frac{1}{2} + \frac{1}{2}(1-2\mu)^t$$

The "self evident" equation (58) gives the result valid in the limit and the average.

Thus classically the master equation method in the averaged exact method (in the limit) give the same result for simple distributions

Ensembles Are Exact = Kinetic Area

$$EEA = KA$$

One now wants to introduce quantum ideas; in this same type model; leaving the dynamics as trivial as before; the only dynamics is again a color change. The essential quantum feature however, is to have states $|\eta_p(t)\rangle$ characterizing the state (color) of a ball. The state at point p at time t, is given by

$$(60) \quad |\eta_p(t)\rangle = c_1 |\eta_p^+\rangle + c_2 |\eta_p^-\rangle;$$

here $|\eta_p^+\rangle$ and $|\eta_p^-\rangle$ are eigenstates of the color operator.

A measurement of the color at p at time would yield a probability $|c_1|^2$ to a white, $|c_2|^2$ to be black.

The essential quantum feature is now that the time evolution (the dynamics) refer to $|\eta_p(t)\rangle$ the amplitudes, not the probabilities. To obtain a genuine quantum mechanical situation, one needs to construct a time evolution, which will provide a mixing of colors. Define E_p by

$$(61)a \quad E_p = \frac{1}{2}(1-\epsilon_p)S_p^- + \frac{1}{2}(1+\epsilon_p)S_p^+$$

clearly if $\epsilon_p = 1$, if there is no marker at p , then $E_p = S_p^+$.

Similarly if there is a marker at p , E_p is the same as S_p^- .

Call the white eigenstates $|\alpha_p\rangle$, the black eigenstate $|\beta_p\rangle$.

The operators S_p^+ and S_p^- are now defined by their action on the (time independent) eigenstates $|\alpha_p\rangle$ and $|\beta_p\rangle$

$$(62)a \quad S_p^+ |\alpha_p\rangle = |\alpha_{p+1}\rangle$$

$$(62)b \quad S_p^+ |\beta_p\rangle = |\beta_{p+1}\rangle$$

Thus the S^+ operator just perpetuates the color schemes

(Since $E_p = S_p^+$ in the case of no marker, this corresponds to the classical situation, in which the color is maintained from p to $p+1$, if no marker is present).

However S_p^- is defined by

$$(63)a \quad S_p^- |\alpha_p\rangle = \sqrt{1-\lambda} |\alpha_{p+1}\rangle + \sqrt{\lambda} |\beta_{p+1}\rangle$$

$$(63)b \quad S_p^- |\beta_p\rangle = -\sqrt{\lambda} |\alpha_{p+1}\rangle + \sqrt{1-\lambda} |\beta_{p+1}\rangle$$

This shows that if there is a marker at p , the mixing ratio of the amplitudes at $p+1$ is changed compared to that at p .

If $\lambda = 1$ a marker, would certainly (with probability 1) change a white ball into a black one. Thus λ plays the role of a coupling strength. One could of course solve the classical problem in which there is a probability of change of color. It is important to note that the classical problem with the probability built in, does not give the same results as the quantum mechanical situation.

The quantum equation of motion (Schrodinger equation) is now

$$(64) \quad |\eta_{p+1}(t+1)\rangle = E_p |\eta_p(t)\rangle$$

It is now straightforward, to iterate (64), one finds

$$(65) \quad |\eta_p(t)\rangle = E_{p-1} E_{p-2} \dots E_{p-t} |\eta_{p-t}(0)\rangle$$

If one assumes that the initial state was a pure state (say all white) $|\eta_{p-t}(0)\rangle = |\alpha_{p-t}\rangle$, one now has to use (61) and (63) to analyze the product. The state $|\eta_p(t)\rangle$ depends

of course on all the ϵ variables. The probability that at time t the ball at p is white is giving by the matrix element; $|\langle \eta_p(t) | \alpha_p \rangle|^2$. This quantity again will depend on the ϵ variables. One has to perform an (average 1 as before over the ϵ variables. The easiest way to carry this out and obtain $|\eta_p(t)\rangle$ is to adapt the method used in the classical case. Suppose that among the points $p-1, \dots, p-t$ there are r markers, then $|\eta_p(t)\rangle$ can be written as

$$(66) \quad |\eta_p(t)\rangle = (S^-)^n |\eta_{p-t}(0)\rangle \quad (\text{the locations without}$$

markers do not affect the states)

Now the matrix $S^- = \begin{pmatrix} \sqrt{1-\lambda} & -\sqrt{\lambda} \\ \sqrt{\lambda} & \sqrt{1-\lambda} \end{pmatrix}$ can be

diagonalized by $U = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ -i & i \end{pmatrix}$, therefore

$$(67) \quad |\eta_p(t)\rangle = U D^r U^{-1} |\eta_{p-t}(0)\rangle \quad \text{with}$$

$$(67)a \quad D = \begin{pmatrix} \sqrt{1-\lambda} + i\sqrt{\lambda} & 0 \\ 0 & \sqrt{1-\lambda} - i\sqrt{\lambda} \end{pmatrix}$$

Using this result, one finds; that if there are r markers at the points $p-1, \dots, p-t$, that the probability that at time t the ball at p is white is

$$(68) \quad P_p^{(r)}(t) = \frac{1}{4} |\lambda_+^r + \lambda_-^r| \equiv |\langle \alpha_p | \eta_p(t) \rangle|^2$$

$$(68)a \quad \lambda_+ = \sqrt{1-\lambda} + i\lambda \quad \lambda_- = \sqrt{1-\lambda} - i\sqrt{\lambda}$$

Using (56)a; one finds that the probability - to find a white ball at p, averaged over all marker positions is

$$(69) \quad W_p(t) = \frac{1}{2} \operatorname{Re} \left[1 + (1-2\lambda u + 2i\sqrt{\lambda-\lambda^2})^t \right]$$

It is important to stress that this result is essentially different from the classical result, one would obtain if merely the probability of a change in color were used to describe the dynamics. In that case the equation one would obtain is an obvious modification of (58) namely

(W_p' = probability that the ball at p at t is white)

$$(70)a \quad W_p'(t) = (1-\lambda)W_{p-1}'(t-1) + \lambda(1-W_{p-1}'(t-1)) \text{ for a marker at } p-1$$

$$(70)b \quad W_p'(t) = W_{p-1}'(t-1) \text{ for no marker at } p-1$$

Using the usual procedure, averaging over all marker positions one finds

$$(71) \quad \langle W_p'(t) \rangle = \frac{1}{2} [1 + (1-2\lambda u)^t]$$

Thus the Master equation method gives the classical result, in which just the probability of a marker is modified by the probability factor λ . The genuine quantum mechanical method, yields (69); the difference between a classical probability problem and an actual quantum mechanical treatment is quite explicit.