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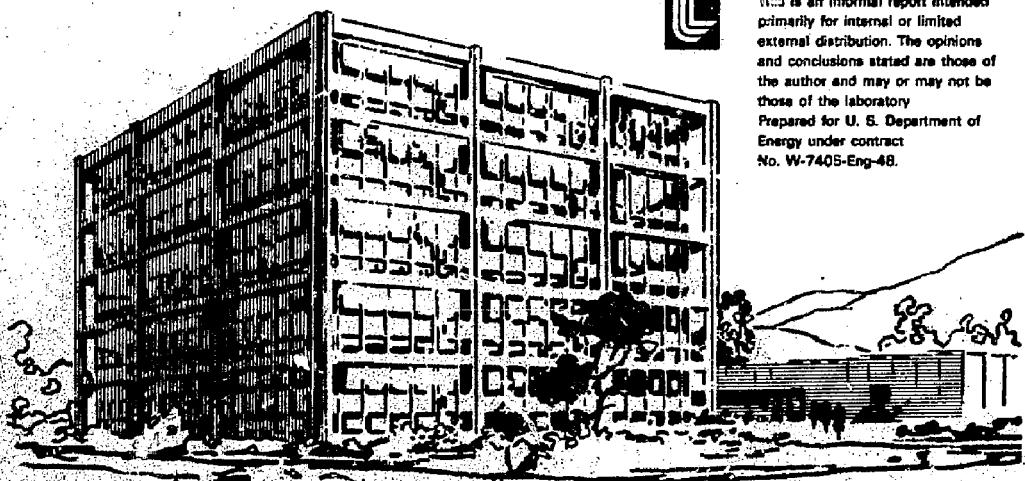
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Abstract

   Using the technique developed by Chapman and Enskog for deriving the
Navier-Stokes equations from the Boltzmann equation, a framework is set up
for deriving diffusion theories from the transport equation. The procedure
is first applied to give a derivation of isotropic diffusion theory and
then of a completely new theory which is naturally flux-limited. This new
flux-limited diffusion theory is then compared with asymptotic diffusion theory.

Introduction

In many problems involving transport theory one is often forced by computational or cost considerations to adopt some approximate method to handle the transport phenomena. By far the most common such methods in use today involve approximating the angular information by various forms of diffusion approximation, typically based on equilibrium diffusion theory (EDT),[1a] isotropic diffusion theory (IDT),[2] or asymptotic diffusion theory (ADT).[1b,3,4] All these theories impose restrictions on significant spatial variations over distances of a mean free path and all yield expressions for the flux which can violate causality (the magnitude of the flux can be no greater than the density times the maximum transport speed) when these restrictions are exceeded. While these constraints are reasonable for many physical problems, they are often violated in problems that arise in plasma physics and astrophysics. In the past this has led to the ad hoc introduction of a flux-limiter,[4] usually with some degree of arbitrariness, in order to preserve causality in the presence of large spatial gradients. It is one purpose of this paper to present a diffusion theory which is naturally flux-limited, and thus circumvents some of the restrictions usually imposed. It will be called flux-limited diffusion theory (FDT).

The setting of what follows will be radiation transport theory, although the result makes no special use of this fact and may be applied to any one speed transport problem. For simplicity, only the case of isotropic elastic scattering will be treated here but the procedure can be generalized to handle anisotropic and weakly inelastic scattering. The transport equation for the specific intensity $I(\overline{\Omega}, \overline{r}, t)$ of photons has the form

$$\frac{1}{c} \partial_t I + \overline{\Omega} \cdot \overline{\nabla} I + \sigma_T I = \frac{c}{4\pi} (\sigma_A B + \sigma_S U) \qquad (1)$$

where $\overline{\Omega}$, $\overline{r}$, and t are the angular, spatial, and temporal variables, c is the speed of light, $\sigma_A(\overline{r},t)$ is the absorption coefficient, $\sigma_S(\overline{r},t)$ is the scattering coefficient, $\sigma_T = \sigma_A + \sigma_S$ is the total interaction coefficient, $B(\overline{r},t)$ is the black body energy density, and $U(\overline{r},t)$ is the energy density as defined by

$$U(\overline{r},t) = \frac{1}{c} \int_{4\pi} I(\overline{\Omega}, \overline{r}, t) \, d\Omega \qquad (2)$$

These equations may be considered to be either frequency-dependent with the frequency parameter suppressed or gray equations.

Integrating (1) over $\overline{\Omega}$ shows that $U(\overline{r},t)$ satisfies

$$\partial_t U + \overline{\nabla}\cdot\overline{F} + c\sigma_A(U-B) = 0 \quad , \qquad (3)$$

where $\overline{F}(\overline{r},t)$, the energy flux, is defined by

$$\overline{F}(\overline{r},t) = \int_{4\pi} \overline{\Omega} I(\overline{\Omega}, \overline{r}, t) \, d\Omega \qquad (4)$$

If one can obtain an expression for $\overline{F}$ in terms of U then equation (3) would determine $U(\overline{r},t)$ completely. By (4) it clearly suffices to derive an expression for I in terms of U, and the second purpose of this paper is to demonstrate the power of the Chapman-Enskog technique to derive such expressions.

The Chapman-Enskog Technique

The idea of Chapman-Enskog[5] is to derive an expression for I in terms of U such that whenever U satisfies equation (3) then I(U) will at least approximately solve equation (1). This requirement is turned into a nonlinear functional differential equation for I in terms of U which is then solved

approximately. The procedure is as follows.

Let $I(U)$ be some functional for I in terms of U with the $\overline{\Omega}$ dependence suppressed. The corresponding functional for $\overline{F}$ is obtained using equation (4) and a consistency condition is obtained from equation (2). The functional derivative of I with respect to U is denoted $\frac{\delta I}{\delta U}$ and defined by the formula

$$\frac{\delta I}{\delta U} H = \frac{d}{dt} I (U+tH)\Big|_{t=0}$$

$\frac{\delta I}{\delta U}$ is a linear operator acting on H, an infinitesmal displacement of U. Using this notation, one may rewrite equations (1) and (3) as

$$\frac{1}{c} \frac{\delta I}{\delta U} \partial_t U + \frac{\delta I}{\delta U} (\overline{\Omega} \cdot \overline{\nabla} U) + \sigma_T I = \frac{c}{4\pi} (\sigma_A B + \sigma_S U) \tag{5a}$$

$$\partial_t U + \frac{\delta \overline{F}}{\delta U} \cdot \overline{\nabla} U + c\sigma_A (U-B) = 0 \tag{5b}$$

Since it is assumed U satisfies (5b), it may be used to eliminate $\partial_t U$ from (5a). The resulting equation is the previously mentioned nonlinear functional differential equation

$$\frac{\delta I}{\delta U} (\overline{\Omega} \cdot \overline{\nabla} U - \frac{1}{c} \frac{\delta \overline{F}}{\delta U} \cdot \overline{\nabla} U - \sigma_A (U-B)) + \sigma_T I = \frac{c}{4\pi} (\sigma_A B + \sigma_S U) \tag{6}$$

Clearly now, if $I(U)$ solves (6) and $U(\overline{r},t)$ solves (5b), then $I(\overline{\Omega},\overline{r},t) = I(U)$ solves (5a).

Finding the general solution of (6) is fully as difficult as solving the general initial value problem for (1); however, that is not the goal here. All that is needed to complete our theory is one solution of (6), and the difficulty lies solely in picking which one. The choice is narrowed considerably

by looking only for solutions that primarily depend on the local values of U. That is, to first approximation $I(U)$ is an explicit function of U and its spatial derivatives. Such solutions can be found approximately by employing standard asymptotic techniques which suppress the functional derivatives in (6).

There is just one fine point to watch when carrying out such a procedure. Observe that, as a direct consequency of its derivation, one finds upon integrating (6) over all angles ($\int d\Omega$) an identity is obtained. Therefore consistency requires that any asymptotic procedure satisfy this identity to all orders.

A Derivation of IDT

As an illustrative example of the procedure for obtaining approximate solutions of the nonlinear functional differential equation (6), a derivation of isotropic diffusion theory (IDT) is presented. A formal parameter, ε, is introduced into (6) as

$$\varepsilon \frac{\delta I}{\delta U} (\overline{\Omega} \cdot \overline{\nabla} U - \frac{1}{c} \frac{\delta \overline{F}}{\delta U} \cdot \overline{\nabla} U) + \varepsilon \frac{\delta I}{\delta U} (\sigma_A(B-U)) - \varepsilon \frac{c}{4\pi} \sigma_A(B-U)$$

$$+ \sigma_T (I - \frac{c}{4\pi} U) = 0 \qquad (7)$$

Here the first two epsilons suppress the functional derivatives and the third insures consistency of the asymptotic scheme. This is clearly the simplest implementation of the considerations at the end of the preceding section.

Now look for a formal solution of the form

$$I = I_0 + \varepsilon I_1 + \varepsilon^2 I_2 + \ldots$$

and define

$$\overline{F}_k = \int_{U_\pi} \overline{\Omega} I_k(\overline{\Omega}) d\Omega$$

Solving (7) to zero order yields

$$I_0 = \frac{c}{4\pi} U \qquad\qquad (8)$$

which implies

$$\overline{F}_0 = 0$$

$$\frac{\delta I_0}{\delta U} = \frac{c}{4\pi}$$

$$\frac{\delta \overline{F}_0}{\delta U} = 0$$

Making use of these results, one can solve (7) to first order and arrive at

$$I_1 = -\frac{c}{4\pi} \frac{1}{\sigma_T} \overline{\Omega} \cdot \overline{\nabla} U \qquad\qquad (9)$$

which gives Fick's law

$$\overline{F}_1 = -\frac{c}{3\sigma_T} \overline{\nabla} U \quad .$$

Then using

$$\frac{\delta I_1}{\delta U} = -\frac{c}{4\pi} \frac{1}{\sigma_T} \overline{\Omega} \cdot \overline{\nabla}$$

$$\frac{\delta \overline{F}_1}{\delta U} = -\frac{c}{3\sigma_T} \overline{v}$$

one can solve (7) to second order. In general, for $n \geq 1$, one can write down the following recursion formula for I_{n+1} as a function of lower order terms:

$$I_{n+1} = -\frac{1}{\sigma_T} \left[\frac{\delta I_n}{\delta U} (\overline{\Omega} \cdot \overline{v} U) - \frac{1}{c} \sum_{k=1}^{n} \frac{\delta I_{n-k}}{\delta U} (\frac{\delta \overline{F}_k}{\delta U} \cdot \overline{v} U) + \frac{\delta I_n}{\delta U} (\sigma_A (B-U)) \right]$$

It is a straightforward matter to check that for $n \geq 1$

$$\int_{4\pi} I_n(\overline{\Omega}, U) \, d\Omega = 0$$

as was insured by the consistency requirement.

Taking   as the approximate solution of (6) the first two terms of the above expansion as given by (8) and (9) yields

$$I \sim \frac{c}{4\pi} (U - \frac{1}{\sigma_T} \overline{\Omega} \cdot \overline{v} U) \tag{10a}$$

$$\overline{F} = -\frac{c}{3\sigma_T} \overline{v} U \tag{10b}$$

and using (10b) in equation (3) produces the well-known IDT result:

$$\partial_t U - \overline{v} \cdot (\frac{c}{3\sigma_T} \overline{v} U) + c\sigma_A (U-B) = 0 \tag{11}$$

The Derivation of FDT

Clearly if more information is going to be extracted from equation (6), a little more information will have to be put into it. This is provided by

the preceding derivation of IDT which showed that, to leading order, $I \sim \dfrac{c}{4\pi} U$. This motivates the introduction of the new dimensionless quantit. as ϕ and $\overline{f}$ which are defined by the formulas

$$I = cU\phi \tag{12a}$$

$$\overline{F} = cU\overline{f} \tag{12b}$$

Equations (2) and (4) then reduce to

$$I = \int_{4\pi} \phi(\overline{\Omega})\ d\Omega \tag{13a}$$

$$\overline{F} = \int_{4\pi} \overline{\Omega}\phi(\overline{\Omega})\ d\Omega \tag{13b}$$

To leading order IDT gave the result $\phi \sim \dfrac{1}{4\pi}$. The goal now is to transform equation (6) into an equation for ϕ and solve the transformed equation by asymptotic methods.

Using the identities

$$\frac{1}{c}\ \frac{\delta I}{\delta U} = \phi + U\ \frac{\delta \phi}{\delta U}$$

$$\frac{1}{c}\ \frac{\delta \overline{F}}{\delta U} = \overline{f} + U\ \frac{\delta \overline{f}}{\delta U}$$

equation (6) may be rewritten as

$$U\ \frac{\delta \phi}{\delta U}\ ((\overline{\Omega}-\overline{f})\cdot\overline{\nabla}U - U\ \frac{\delta \overline{f}}{\delta U}\cdot\overline{\nabla}U - \sigma_A(U-B)) + (\sigma_A B + \sigma_S U + (\overline{\Omega}-\overline{f})\cdot\overline{\nabla}U - U\ \frac{\delta \overline{f}}{\delta U}\cdot\overline{\nabla}U)$$

$$= \frac{1}{4\pi}\ (\sigma_A B + \sigma_S U) \tag{14}$$

A formal parameter, ε, is then introduced that suppresses all the functional derivatives.

$$\varepsilon U \frac{\delta \phi}{\delta U} \left((\overline{\Omega} - \overline{f}) \cdot \overline{\nabla} U - U \frac{\delta \overline{f}}{\delta U} \cdot \overline{\nabla} U - \sigma_A (U-B) \right) - \varepsilon U \phi \frac{\delta \overline{f}}{\delta U} \cdot \overline{\nabla} U$$

$$+ (\sigma_A B + \sigma_S U + (\overline{\Omega} - \overline{f}) \cdot \overline{\nabla} U) \phi = \frac{1}{4\pi} (\sigma_A B + \sigma_S U) \qquad (15)$$

This scheme is asymptoticly consistent without having to suppress any additional terms as in IDT.

Now look for a formal solution of the form

$$\phi = \phi_0 + \varepsilon \phi_1 + \varepsilon^2 \phi_2 + \ldots$$

and define

$$\overline{f}_k = \int_{4\pi} \overline{\Omega} \phi_k(\overline{\Omega}) \, d\Omega \qquad (16)$$

Solving (15) to zero order gives

$$\phi_0 = \frac{\omega}{4\pi} \frac{1}{\omega + \overline{f}_0 \cdot \overline{X} - \overline{\Omega} \cdot \overline{X}} \qquad (17)$$

where $\omega = \dfrac{\sigma_A B + \sigma_S U}{\sigma_T U}$ is the effective albedo and $\overline{X} = -\dfrac{\overline{\nabla} U}{\sigma_T U}$ is the dimensionless gradient. Normalizing ϕ_0 to either (12a) or (12b) relates $\overline{f}_0$ to $\overline{X}$ as

$$\overline{f}_0 = \lambda\left(\frac{X}{\omega}\right) \frac{1}{\omega} \overline{X} \qquad (18)$$

where $X = |\overline{X}|$ and*

$$\lambda(R) = \frac{1}{R} \left(\coth R - \frac{1}{R} \right) \qquad (19)$$

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*see appendix

The fact that both normalizations are equivalent follows from the consistency of the scheme. Using (19) one can now write ϕ_0 directly in terms of $\overline{X}$ and

$$\phi_0 = \frac{\omega}{4\pi} \; \frac{1}{X \; \coth \; (\frac{X}{\omega}) - \overline{\Omega} \cdot \overline{X}} \tag{20}$$

In general, a recursive formula for ϕ_{n+1} as a function of lower order terms can be written down. This involves solving the linear equation

$$(\omega + \overline{f}_0 \cdot \overline{X} - \overline{\Omega} \cdot \overline{X}) \phi_{n+1} + \phi_0 \overline{X} \cdot \overline{f}_{n+1} = J_n \tag{21}$$

where J_n contains terms of order n and less. Multiplying this equation by $\dfrac{\overline{X} \cdot \overline{\Omega}}{(\omega + \overline{f}_0 \cdot \overline{X} - \overline{\Omega} \cdot \overline{X})}$ and integrating and using (16) gives

$$\frac{\sinh 2X}{2X} \; \overline{X} \cdot \overline{f}_{n+1} = \int_{4\pi} \frac{\overline{X} \cdot \overline{\Omega}}{\omega + \overline{f}_0 \cdot \overline{X} - \overline{\Omega} \cdot \overline{X}} \; J_n \; d\Omega$$

which when substituted back up into (20), produces

$$\phi_{n+1} = \frac{1}{\omega + \overline{f}_0 \cdot \overline{X} - \overline{\Omega} \cdot \overline{X}} \left[J_n - \frac{2X}{\sinh X} \; \phi_0 \int_{4\pi} \frac{\overline{X} \cdot \overline{\Omega}}{\omega + \overline{f}_0 \cdot \overline{X} - \overline{\Omega} \cdot \overline{X}} \; J_n \; d\Omega \right]$$

It can then be checked directly from (21) that

$$\int_{4\pi} \phi_{n+1} (\overline{\Omega}) d\Omega = 0$$

as was insured by the consistency requirement.

So taking (20) as the approximate solution of (6) and defining

$$D_f(\omega, X) = \frac{1}{\omega} \; \lambda (\frac{X}{\omega}) \tag{22}$$

allows the FDT expression for the flux to be written as

$$\overline{F} = -D_f(\omega,X) \frac{c}{\sigma_T} \overline{\nabla}U \qquad (23)$$

and upon using this result in equation (3) gives

$$\partial_t U - \overline{\nabla} \cdot (D_f(\omega,X) \frac{c}{\sigma_T} \overline{\nabla}U) + c\sigma_A(U-B) = 0 \qquad (24)$$

It should be pointed out that in the limit of X and $\omega-1$ being small, FDT reduces to IDT as it should.

Comparisons with ADT

Asymptotic Diffusion Theory (ADT) gives an expression for the flux[1b,3,4]

$$\overline{F} = -D_a(\omega) \frac{c}{\sigma_T} \overline{\nabla}U$$

which while not being flux-limited, is albedo-dependent. The diffusion coefficient is defined by

$$D_a(\omega) = \frac{1-\omega}{\alpha^2}$$

where α solves

$$\alpha = \tanh \frac{\alpha}{\omega}$$

When $\omega \leq 1$, α is real, when $\omega \geq 1$, α is imaginary, and when $\omega = 1$, $D_a(\omega) = \frac{1}{3}$.

ADT and FDT can be related as follows:

For $\omega < 1$ $D_a(\omega) < D_f(\omega,X)$ when $X < \alpha$

                     $D_a(\omega) = D_f(\omega,\alpha)$

                     $D_a(\omega) > D_f(\omega,X)$ when $X > \alpha$

For $\omega > 1$ $D_a(\omega) > D_f(\omega,X)$

For $\omega \to 0$ $D_a(\omega) \sim 1-\omega$

                     $D_f(\omega,X) \sim \frac{1}{X}\left(1 - \frac{\omega}{X}\right)$

For $\omega \to \infty$ $D_a(\omega) \sim \frac{4}{\pi^2\omega}$

                     $D_f(\omega,X) \sim \frac{1}{3\omega}$

In Figure 1 a graphic comparison is shown between $D_f(\omega,0)$, $D_a(\omega)$, and $D_f(\omega,1)$. For $0 < X < 1$ one has

$$D_f(\omega,1) < D_f(\omega,X) < D_f(\omega,0)$$

with $D_f(\omega,X)$ intersecting $D_a(\omega)$ at $\omega = \dfrac{X}{\tanh^{-1} X}$, while for $X > 1$

$$D_f(\omega,X) < D_f(\omega,1)$$

Summary

The power of the Chapman-Enskog procedure has been demonstrated by showing that it may be employed in a very natural way to derive an intrinsically flux-limited diffusion theory (FDT). This theory gives a diffusion coefficient which depends on both the albedo, ω, and the magnitude of a dimensionless gradient, X. In the limit of small gradients and albedos near unity, it reduces to IDT as it should. When the gradient is related to the albedo, as it is in the slab penetration problem in ADT, then FDT agrees with ADT.

Furthermore, it agrees qualitatively with ADT over a large range of ω and X in which one would expect ADT to be valid. However, most importantly, as X gets large, FDT will not violate causality.

Thus FDT provides a very promising approach toward replacing the very disparate collection of ad hoc flux-limiters currently in use with a theoretically consistent and hopefully more accurate method. Detailed evaluation of this approach is currently underway in a number of Laboratory transport codes.

Appendix: $\lambda(R)$

In equation (19) the function $\lambda(R)$ was defined by

$$\lambda(R) = \frac{1}{R} \left(\coth R - \frac{1}{R} \right)$$

This monotonically decreasing function in $R \geq 0$ has the following limiting forms

$$\lambda(R) \sim \frac{1}{3} - \frac{R^2}{45} + 0(R^4) \qquad \text{for } R \ll 1$$

$$\lambda(R) \sim \frac{1}{R} - \frac{1}{R^2} + 0(e^{-2R}) \qquad \text{for } R \gg 1$$

A simple rational approximation is

$$\lambda_R(R) = \frac{2+R}{6+3R+R^2}$$

which was fit by the requirements

$$\lambda_R(0) = \frac{1}{3}$$

$$\lambda_R'(0) = 0$$

$$\lambda_R(R) \sim \frac{1}{R} - \frac{1}{R^2} + 0(\frac{1}{R^3}) \qquad \text{for } R \gg 1$$

In Table 1 this approximation is compared with the exact expression. It is seen that the maximum relative error occurs around $R = 2.5$ and is about 7.2%.

Table 1

R	$\lambda(R)$	$\lambda_R(R)$
0.0	.333	.333
0.25	.332	.330
0.5	.328	.323
1.0	.313	.300
1.5	.292	.275
2.0	.269	.250
2.5	.245	.228
3.0	.224	.208
3.5	.205	.191
4.0	.188	.177
4.5	.173	.164
5.0	.160	.152
6.0	.139	.133
7.0	.122	.118
8.0	.109	.106
9.0	.099	.094
10.0	.090	.088

FIGURE 1

FO : $D_\xi(\omega, 0) = \frac{1}{3\omega}$

A : $D_a(\omega)$

FI : $D_\xi(\omega, 1) = \coth\frac{1}{\omega} - \omega$
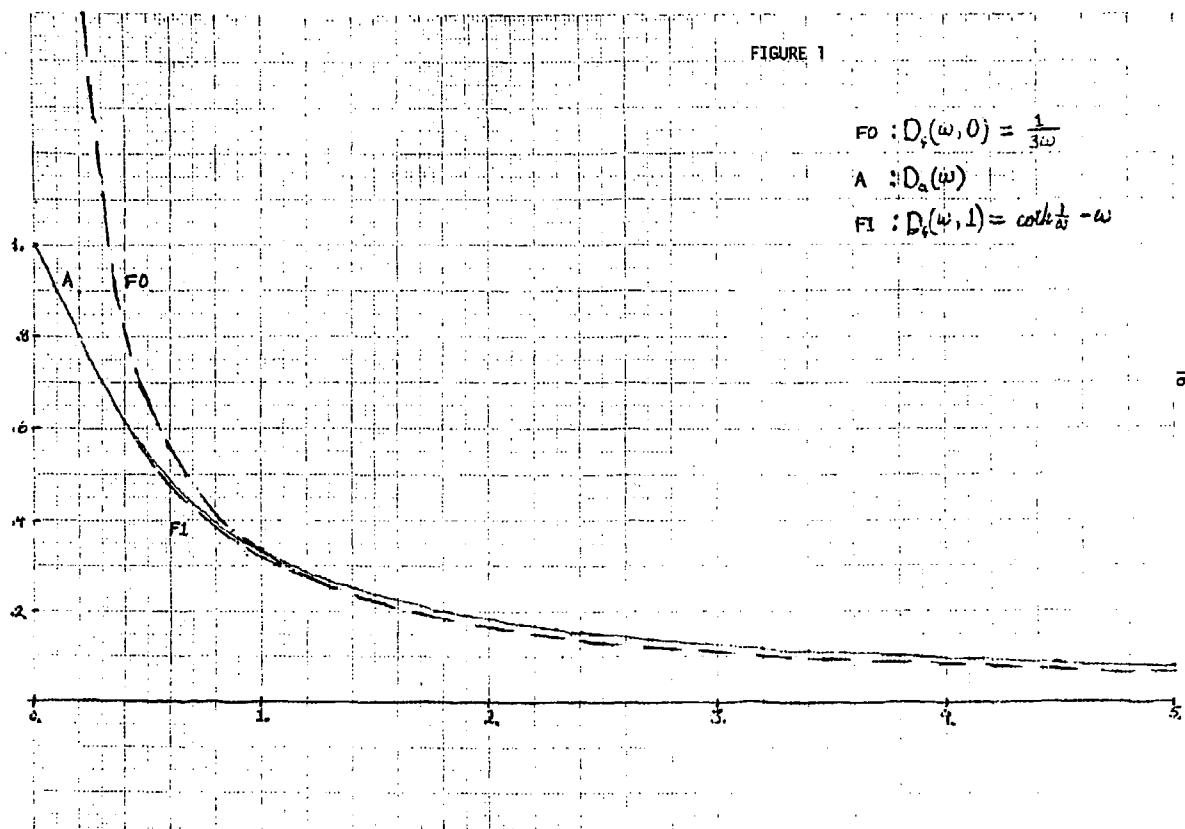
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