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THE UNIVERSITY OF ALBERTA

ON THE PENETRATION OF FAST CHARGED PARTICLES

BY

DAVID J. PERRY

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To my father, John Joseph Perry

Without him, this work would never have started

To my mother, Mary Elizabeth Perry

Without her, this work would never have finished

Abstract

The work presented here is intended to provide theoretical support for medical physicists who are interested in improving radiotherapy treatment plans involving charged particle beams. These plans still rely heavily on emperical behavior rather than theory as a basis for making predictions. In the most frequent therapy applications, electron beams, typically with initial energies between 5-20 MeV, penetrate materials of low atomic number. Energy loss is predominately by ionization and the effects of multiple scattering by repeated Coulomb deflections from nuclei are of primary interest.

Our development is strongly influenced by these applications and so we begin our work with a review of Fermi-Eyges theory. This theory and ideas which were equivalent to it have dramatically improved electron beam treatment plans over the last several years, as is now generally recognized. This theory also has significant limitations due to the approximations or assumptions that it makes. Since we can improve and extend these results by relaxing some of the key assumptions, we continue by considering some generalizations of this basic theory and we discuss those which were given by Snyder-Scott, Lewis and Yang in some detail.

Yang's theory had significant potential for applications but this theory will not work properly unless its time development is handled differently. This leads us to present a wave solution to the penetration problem in our final chapter. Sample calculations of the most important distributions are given there as well.

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I. Introduction

Medical physicists' association with accelerator-produced charged particle beams is about three and one half decades old. In that time a number of important problems in radiation dosimetry have been successfully solved and are presently managed rather well. Others have been more persistent and no such success can be claimed.

To a medical physicist concerned with therapy, the most important quantity is the absorbed dose, the energy absorbed by an infinitesimal bit of matter during the course of an irradiation. If the target is a homogeneous medium of tissue-like material, e.g., a tank full of water or sheets of solid plastic, the measurement of absorbed dose is a satisfactorily solved problem. The calculation of absorbed dose, even under these limited conditions, is not. A more difficult question which arises frequently in actual irradiations is the calculation of dose within inhomogeneous tissue, when a beam will penetrate mixtures of material of different composition. The recent advances in computerized axial tomography, which makes detailed anatomical information available, has stimulated renewed interest in the inhomogeneity topic although the importance of the problem was recognized long ago.

This work aims to extend the earlier effort of Perry and Holt[1]. Along with a number of other papers that began to appear mostly after 1975, but especially also those of Goitein[2] and Hogstrom and Almond[3], a number of problems were being solved for medical physicists which had been in their literature for decades. The explicit topic discussed by

these papers was the inhomogeneity problem and the various means which had been taken to address it used methods which were equivalent to Fermi's[4] theory or the Eyges[5] extension of it. Most medical physicists concerned with this topic have now recognized that this approach has been successful in that it has led to progress and is quite promising[6]. Its success rests squarely on the fact that it is analytic. Its greatest value and level of difficulty was not in the production of results which were directly and immediately useful, treatment planning computer programs, but in the identification and development of an applicable theory which was required as a prerequisite to this. It is this aspect of the approach that we aim to extend here.

In the charged particle applications most frequently met by treatment planners, electron beams, typically with initial energies between 10-15 MeV, penetrate materials of low atomic number. Here energy loss is predominantly by ionization, the stripping of orbital electrons, and the effects of multiple scattering by repeated Coulomb deflection, "collisions" with nuclei that cause an angular spread, are of primary interest. Within this context we will generally consider the following problem: A group of fast charged particles is injected into a homogeneous medium within a burst of extremely short duration. Sometime later, where are they?

The penetrability of a beam into a material is an extremely important piece of information. A medical physicist, who usually summarizes this information into what is called a depth dose curve, will often use it to characterize and completely represent a beam's interaction with a

material. It is an essential component of every treatment plan. For this reason special emphasis will be given to the longitudinal or penetration aspects of the problem.

Our treatment of multiple scatter will be organized in the following way: In Chapter II we give a background discussion of Fermi's model. Since this section is also intended to serve as an introduction to the multiple scattering problem we take advantage of the opportunity to introduce a few ideas which will later be met in more elaborate ways. In Chapter III we discuss two small angle generalizations of Fermi's model, Snyder and Scott's[7] and that of Yang[8]. Lewis' theory[9], which may be regarded as a generalization of Snyder and Scott's work, will also be introduced there but then considered in more detail in Chapter IV. Each of these theories contained pivotal information but also had difficulties which were significant enough to prevent the emergence of a working theory of charged particle penetration. In Chapter V we define a theory free of these difficulties, a theory which may well prove to be valuable in medical physics applications. We also give some sample calculations and discuss some of its more important predictions.

II. Small Angle Lateral Transport

We first consider the question of the lateral transport of charged particles in its simplest form. A charged particle moving through a material will be deflected by the Coulomb potential of any nucleus that it passes close to. If the charged particle is fast, meaning difficult to deflect, its change in direction from any one collision is typically through a very small angle. We are interested here in the case of a large number of collisions, statistically large, but still small enough so that even a resultant deflection remains a small angle and we may write $\sin\theta = \theta$, $\cos\theta \approx 1$. Changes in direction of movement will be accompanied by changes in particle positions. Our first question is to decide how to describe the situation.

A. Statistical Approach

The simplest problem considers particle motion in a plane, say $x - z$. The initial direction of particle movement can define the z axis and, as a result of scattering, a particle will acquire a small velocity component perpendicular to it, which we denote by θ_x. To determine a particle's direction of movement after n scatterings, we sum over all its individual directional changes. If we call our particle α, then

$$\theta_x^{\alpha}(n) = \sum_{i=1}^{n} \delta\theta_x^{\alpha}(i) \qquad (1)$$

where $\delta\theta_x^{\alpha}(i)$ is the particle's change in direction due to the i^{th} collision. The lateral distance that a particle will travel after n collisions is computed similarly

$$x^{\alpha}(n) = \sum_{i=1}^{n} \delta x^{\alpha}(i) = \sum_{i=1}^{n} \theta_x^{\alpha}(i)\, \delta\ell \qquad (2)$$

where $\delta\ell$ is the distance that a particle drifts between collisions. This distance is usually called the mean free path and will be denoted by μ. If ℓ is the particle's pathlength, then $n = \ell\mu^{-1}$. We are not particularly interested in describing one particle but a very large number of them, N. Of particular interest are group averages which we denote by bars, e.g.,

$$\overline{\theta_x(n)} = \frac{1}{N}\sum_{\alpha=1}^{N} \theta_x^{\alpha}(n) \qquad (3)$$

$$\overline{x(n)} = \frac{1}{N}\sum_{\alpha=1}^{N} x^{\alpha}(n) \qquad (4)$$

To actually compute such group averages requires the use of the deflecting cross section. Thus

$$\overline{\theta_x(n)} = \sum_{i=1}^{n} \left\{ \frac{1}{N}\sum_{\alpha=1}^{N} \delta\theta_x^{\alpha}(i) \right\}$$

$$= \sum_{i=1}^{n} \left\{ \frac{\int d\theta_x \int d\theta_y\, \theta_x \frac{d\sigma}{d\Omega}(i)}{\int d\theta_x \int d\theta_y \frac{d\sigma}{d\Omega}(i)} \right\}$$

$$\equiv \sum_{i=1}^{n} \langle \delta\theta_x(i) \rangle \qquad (5)$$

Since a particle will deflect right as often as left, $\langle \delta\theta_x(i)\rangle = 0$ and we have $\overline{\theta_x(n)} = 0$. Similarly $\overline{x(n)} = 0$. The first non-vanishing quantities involve squares

$$\overline{\theta_x^2(n)} = \frac{1}{N}\sum_{\alpha=1}^{N} \sum_{i=1}^{n} \delta\theta_x^{\alpha}(i) \sum_{j=1}^{n} \delta\theta_x^{\alpha}(j)$$

$$= \sum_{i=1}^{n}\sum_{j=1}^{n} \langle \delta\theta_x(i)\, \delta\theta_x(j) \rangle \qquad (6)$$

If $i \neq j$, $\langle \delta\theta_x(i)\,\delta\theta_x(j)\rangle = \langle \delta\theta_x(i)\rangle \langle \delta\theta_x(j)\rangle$ because different collisions are independent and this product is zero as above. So $i=j$ and

$$\overline{\theta_x^2(n)} = \sum_{i=1}^{n} \langle (\delta\theta_x(i))^2 \rangle$$

$$= \sum_{i=1}^{n} \frac{1}{\sigma(i)} \int\int d\theta_x\, d\theta_y\, \theta_x^2\, \frac{d^2\sigma(i)}{d\theta_x\, d\theta_y} \qquad (7)$$

If we ignore energy losses, the collision cross section never changes so that $\langle \delta\theta_x^2(i)\rangle = \langle \delta\theta_x^2\rangle$ and

$$\overline{\theta_x^2(n)} = n \langle \delta\theta_x^2 \rangle \qquad (8)$$

Similar steps would give

$$\overline{x^2(n)} = \overline{\theta_x^2(n)}\; l^2/3 \qquad (9)$$

Using the central limit theorem of statistics we could prove that the angular distribution becomes Gaussian as $n \to \infty$ so that

$$f(l, \theta_x) = \frac{1}{(2\pi\overline{\theta_x^2})^{1/2}}\, e^{-\theta_x^2/2\overline{\theta_x^2}} \qquad (10)$$

can represent the probability that a particle will be travelling in the directional interval $(\theta_x, \theta_x + d\theta_x)$ after making n collisions. We would use (8) to obtain $\overline{\theta_x^2}$. We would also write

$$f(l, x) = \frac{1}{(2\pi\overline{x^2})^{1/2}}\, e^{-x^2/2\overline{x^2}} \qquad (11)$$

to represent the spatial probability distribution, and use (9) for

$\overline{x^2(\ell)}$. Equations (10 and (11) do not tell us everything about what is happening. If a particle has the direction θ_x we do not yet have an equation telling us where it is; similarly, if a particle is located at x we do not know its direction of movement. Equations (10) and (11) say nothing about how the variables θ_x and x are correlated. To completely describe the situation we need a joint probability distribution $f(\ell, \theta_x, x)$ which has the properties

$$\int dx\, f(\ell, \theta_x, x) = f(\ell, \theta_x) \tag{12}$$

$$\int d\theta_x\, f(\ell, \theta_x, x) = f(\ell, x) \tag{13}$$

$$\int\int d\theta_x\, dx\, f(\ell, \theta_x, x) = 1 \tag{14}$$

A more elaborate version of the above argument using the same type of steps leads to

$$f(\ell, \theta_x, x) = \frac{1}{(2\pi\,\overline{\theta_x^2}/4)^{1/2}} e^{-(\theta_x - \frac{3}{2}x/\ell)^2/(2\,\overline{\theta_x^2}/4)} \frac{1}{(2\pi\,\overline{x^2})^{1/2}} e^{-x^2/2\overline{x^2}} \tag{15}$$

which is equation (A8) in the appendix of Perry and Holt. The remaining details of the derivation are given there as well.

B. Fermi's Transport Equation

Fermi[4] pursued the observation that $\overline{\theta_x^2(\ell)} \sim \ell$ while $\overline{x^2(\ell)} \sim \ell^3$, as in (8) and (9), and are different order infinitesimals if we let

$\ell \to d\ell \to 0$. The first order effect is to produce an angular distribution, but since the spatial width is zero to this order, the spatial distribution is a point. Spatial distributions will only develop thereafter, in subsequent infinitesimals as particles begin to fly apart due to an angular distribution developed earlier. Thus, a particle moving through a distance $d\ell$ will simply drift from one point to another along its initial line of motion, but be represented as a spray of different directions when it gets there (Fig. 1). Fermi had identified the nature of the problem as a shower or multiplication problem. Collecting his observations he wrote

$$f(\ell+d\ell,\theta_x,x) = \int_{-\infty}^{\infty} d\theta_x' \; f(\ell,\theta_x', x-\theta_x' d\ell) \; f(d\ell,\theta_x'-\theta_x) \qquad (16)$$

which says that a particle which arrives at the point x has come from the point $x' = x - \theta_x' \, d\ell$,if θ_x' was its direction of movement when it started. In the process of moving it can change direction and be scattered from the initial value θ_x' into the final direction θ_x . This feature is described by the probability distribution $f(d\ell, \theta_x' \to \theta_x)$. The integral adds up all the contributions. Fermi used

$$f(d\ell, \theta_x' \to \theta_x) = f(d\ell, \theta_x'-\theta_x) = \frac{1}{(\pi K d\ell)^{1/2}} e^{-(\theta_x'-\theta_x)^2/K d\ell} \qquad (17)$$

to describe the angular changes by moving through an infinitesimal distance $d\ell$, the step that incorporates the Gaussian approximation into his work. Expanding (16) and keeping terms up to first order in $d\ell$

gives

$$f(\ell,\theta_x,x) + \frac{\partial f}{\partial \ell}(\ell,\theta_x,x)\,d\ell + \dots \tag{18}$$

$$= \int_{-\infty}^{\infty} d\theta_x' \left[f(\ell,\theta_x, x-\theta_x d\ell) + \frac{\partial}{\partial \theta_x} f(\ell,\theta_x, x-\theta_x d\ell)(\theta_x'-\theta_x) \right.$$

$$\left. + \frac{1}{2!}\frac{\partial^2 f}{\partial \theta_x^2}(\ell,\theta_x, x-\theta_x d\ell)(\theta_x'-\theta_x)^2 + \dots \right] f(d\ell, \theta_x'-\theta_x)$$

where the Taylor expansion on the right is motivated by the fact that $f(d\ell,\ \theta_x' \to \theta_x)$ becomes an even more sharply peaked function about θ_x as $d\ell \to 0$. Continuing we have

$$f(\ell,\theta_x,x) + \frac{\partial f}{\partial \ell}(\ell,\theta_x,x)\,d\ell + \dots \tag{19}$$

$$= \left[f(\ell,\theta_x,x) - \theta_x \frac{\partial f}{\partial x}(\ell,\theta_x,x)\,d\ell \right] \left[\int_{-\infty}^{\infty} d\theta_x' f(d\ell, \theta_x' \to \theta_x) = 1 \right]$$

$$+ \left[\frac{\partial f}{\partial \theta_x}(\ell,\theta_x, x-\theta_x d\ell) \right] \left[\int_{-\infty}^{\infty} d\theta_x' (\theta_x'-\theta_x) f(d\ell, \theta_x'-\theta_x) = 0 \right]$$

$$+ \frac{1}{2!}\frac{\partial^2 f}{\partial \theta_x^2}(\ell,\theta_x,x) \left[\int_{-\infty}^{\infty} d\theta_x' (\theta_x'-\theta_x)^2 f(d\ell, \theta_x'-\theta_x) = \frac{K\,d\ell}{2} \right]$$

So that

$$\frac{\partial f}{\partial \ell}(\ell,\theta_x,x) = -\theta_x \frac{\partial f}{\partial x} + \frac{K}{4}\frac{\partial^2 f}{\partial \theta_x^2} \tag{20}$$

is obtained as an exact equation of motion. Fermi also gave the solution to (20) as

$$f(\ell,\theta_x,x) = \frac{\sqrt{3}}{2\pi\ell^2}\left(\frac{4}{K}\right) e^{-\frac{4}{K}\left(\frac{\theta_x^2}{\ell} - \frac{3\theta_x x}{\ell^2} + \frac{3x^2}{\ell^3}\right)} \tag{21}$$

which is equation (1.62) of Rossi and Griesen[4] and is valid for constant K . They also showed that (21) had the initial conditions

$$f(\ell=0,\theta_x) = \delta(\theta_x) \quad ; \quad f(\ell=0,x) = \delta(x) \tag{22}$$

If we use

$$\overline{\theta_x^2(\ell)} = \frac{1}{2}\left(\overline{\theta_x^2(\ell)} + \overline{\theta_y^2(\ell)}\right) = \frac{K\ell}{2} \tag{23}$$

we easily establish that (15) and (21) are identical expressions although the derivations were quite different. The argument leading to (15) was a moments approach in which the form of the solution, obtained from the central limit theorem, was combined with a few average beam features which, in this case, could be computed without great difficulty. Moments and moment related arguments are important and will be a frequently recurrent theme. However, Fermi's method, which was also based on a moments argument, was superior because he used much better calculational machinery. This would show up in several different ways. For example, from it we can obtain the exact solution without ever making use of the central limit theorem. Writing the differential equation is the essential first step in the theory and Fermi's contribution was to give such a clear exposition on how to do this. It is also a step upon which it is easy to generalize.

C. The Eyges Extension

Equation (21) is the solution to (20) in the sense that it works in the differential equation. It is not the best form for use, (15) is

better, and we have said nothing about how to solve (20) in a systematic way. Some insight on the latter question was given by Eyges who solved

$$\frac{\partial f(\ell,\theta_x,x)}{\partial \ell} = -\theta_x \frac{\partial f}{\partial x} + \frac{K(\ell)}{4}\frac{\partial^2}{\partial \theta_x^2} f \qquad (24)$$

with the initial condition

$$f(\ell=0,\theta_x,x) = \delta(\theta_x)\,\delta(x) \qquad (25)$$

The difference between (24) and (20) is that we have allowed K to become path length dependent, $K \rightarrow K(\ell)$. A particle moving through a material will generally be losing energy and the ability of the material to deflect it may, and generally will, be dependent on this. This is the problem that Eyges addressed. Letting

$$f(\ell,\theta_x,x) = \frac{1}{(2\pi)^2}\int_{-\infty}^{\infty} d\tau_x \int_{-\infty}^{\infty} dp_x\; e^{i(\tau_x\theta_x + p_x x)}\, f(\ell,\tau_x,p_x) \qquad (26)$$

and then using it in (24) gives the differential equation for the Fourier transform of the solution

$$\frac{\partial f}{\partial \ell}(\ell,\tau_x,p_x) = p_x \frac{\partial}{\partial \tau_x} f - \frac{K(\ell)}{4}\tau_x^2 f \qquad (27)$$

With a change of variable Eyges solved (27) and then gave a form which is equivalent to

$$f(\ell,\tau_x,p_x) = e^{-(A_1(\ell)\tau_x^2 + A_2(\ell)\tau_x p_x + A_3(\ell)p_x^2)} \qquad (28)$$

where

$$A_1(\ell) = \int_0^{\ell} d\ell'\, K(\ell')/4 \qquad (29a)$$

$$A_2(\ell) = 2\int_0^{\ell} d\ell'\,(\ell-\ell')\,K(\ell')/4 \qquad (29b)$$

$$A_3(\ell) = \int_0^{\ell} d\ell'\,(\ell-\ell')^2\,K(\ell')/4 \qquad (29c)$$

which are Eyges' equations (13 a,b,c) in our notation. The initial conditions on $A_\kappa(\ell)$ are $A_\kappa(0) = 0$, which are the same as (25). Eyges then inverted the transforms using (26) and (28) to obtain $f(\ell, \theta_\kappa, \chi)$, a straightforward step since it only involves standard integrals, and then gave the solution in the form (21) except that the terms ℓ, ℓ^2, ℓ^3 are replaced by more complicated expressions involving $A_\kappa(\ell)$. For future reference we rewrite equations (29) in the form

$$\frac{d A_1(\ell)}{d\ell} = \frac{K(\ell)}{\gamma} \qquad (30a)$$

$$\frac{d A_2(\ell)}{d\ell} = 2 A_1(\ell) \qquad (30b)$$

$$\frac{d A_3(\ell)}{d\ell} = A_2(\ell) \qquad (30c)$$

Since we have been using the approximation $\cos\theta = 1$, we also have $\ell = z$, and (24) with ℓ replaced by z everywhere will now describe a beam traversing a medium that has varying scattering properties. This is the inhomogeneity problem, or at least a simple form of it, and the fact that this theory can describe it is a key reason why medical physicists have shown an interest in the Fermi-Eyges equations. Since the replacement $\ell \to z$ turns an energy dependent homogeneous scattering problem into an inhomogeneity problem, it is evident that both have the same character. Of the two, homogeneous versus inhomogeneous, it is the homogeneous problem which is the more difficult and the more valuable. Our work in later sections will be generally restricted to homogenous solutions and it will be left to medical physicists to pursue the topic further, adapting them to handle inhomogeneous confi-

gurations.

D. The Need For a Better Theory

Returning to Fermi's transport equation (20) and integrating it over all space gives

$$\frac{\partial f(\ell,\theta_s)}{\partial \ell} = \frac{K}{4}\frac{\partial^2}{\partial \theta_s^2} f \qquad (31)$$

as the equation for the directional distribution, recognizable as the familiar diffusion equation with path length playing the role of time. The diffusion of direction brought about by multiple scattering and described by (31) then leads to diffusion in space. It is easily verified using (9) that the spatial density satisfies

$$\frac{\partial f(\ell,x)}{\partial \ell} = \frac{K\ell^2}{4}\frac{\partial^2 f}{\partial x^2} \qquad (32)$$

which has the same form as (31) except that our diffusion constant has become time dependent. To obtain (32) or equivalently (9) from (20) requires that we first find the complete solution $f(\ell,\theta_s,x)$, then integrate out the angular variables, leaving the spatial density, $f(\ell,x)$. This is a much more elaborate procedure than was required to obtain the equation for the directional distribution (31).

We will generally show more interest in spatial distributions than in directional distributions. They contain more information,which is why they are more difficult to solve for. They also contain the kind

of information that medical physicists should be interested in because they are very closely related to energy release and absorption calculations. Our pursuit of angular distributions will be in part because they can tell us something about spatial distributions, give us some insights, and in part because we need to develop angular information concurrently, i.e., we need to go through the motion in order to construct a configuration.

Fermi's theory combines both transport and diffusion. We can eliminate the diffusive aspects of the theory by allowing $K \to 0$ in (20). The remaining equation of motion

$$\frac{\partial f(\ell, \theta_x, x)}{\partial \ell} = -\theta_x \frac{\partial f}{\partial x} \qquad (33)$$

merely describes radiation moving from one place to another in a rectilinear straight line fashion. For example, if we choose the initial conditions to be $f(\ell=0, \theta_x, x) = \delta(\theta_x - \theta_{x_0})\,\delta(x - x_0)$ then the solution of (33) is $f(\ell, \theta_x, x) = \delta(\theta_x - \theta_{x_0})\,\delta(x - x_0 - \theta_{x_0}\ell)$. It is easily shown that the Gaussians which solve (31), (32), (20) and (24) collapse back into infinitely narrow beams, i.e., rays, as $K \to 0$. The medium becomes scatterless in this limit.

Before medical physicists became interested in the development of Fermi's theory, a ray picture in one form or another (Fig. 1a) was almost universally and exclusively adopted by treatment planners. We should call it the zero order theory because the probability fields have no degrees of freedom. Because the radiation fields do not do

anything, except go straight, medical physicists had to rely extensively on experiments in order to infuse this model with some "predictive" power. In practice this meant drawing straight lines, then extrapolating and interpolating measured values to make predictions. Trying to amend and correct the deficiencies of a theory by inserting empirical behavior whenever the theory fails is an approach we should wish to avoid; it does not improve our understanding of the situation; it has many practical difficulties associated with it; it may also give incorrect predictions even when conducted with apparent care. The alternative is to get a better theory, one capable of making genuine predictions on its own.

Fermi had a first order theory with $\sin\theta = \theta$ and $\cos\theta = 1$. It contains the ray picture exactly but is superior to it because it gives the probability fields a lateral degree of freedom. Particles penetrating a medium now spread out over an infinitely thin flat surface perpendicular to the initial line of movement (Fig 1b). An example of the inadequacy of the ray model predictions in an inhomogeneity problem is shown in our Fig. 2 which was taken from Perry and Holt. As that diagram also shows, the agreement between predictions and experimental results dramatically improves once the lateral movement of charged particles is taken into account.

Models which incorporate only the lateral movement can't be expected to do everything for us. If our questions concerned the longitudinal movement, which is correlated with the lateral motion, there was either no prediction at all, or a prediction was made which was

incorrect. Depth dose information, the most pivotal information of a treatment plan, had to be inserted empirically into the models of Goitein, Perry and Holt, Hogstrom and Almond, etc., because the Fermi-Eyges equations tell us nothing about it. Our Fig. 3, also taken from Perry and Holt, gives an example of an incorrect prediction. The lateral spreading is predicted to increase monotonically with increasing depth in the Fermi-Eyges picture, but experimentally it reaches a maximum then falls to zero again at deeper penetrations, a systematic error.

Removing these difficulties requires another degree of freedom, allowing particle distributions to develop in the direction parallel to the initial line of motion. Fermi's theory works well near the surface of the material and cannot simply be discarded, so we build on it. Noting that particles which are scattered wide won't be as deep, the flat surfaces of Fermi's model may be redrawn as curved, bent slightly back towards their origin (Fig. 1c). If we keep the small angle formalism, we would now use $\sin\theta = \theta$, $\cos\theta = 1 - \theta^2/2$, giving a second order theory. Since $\cos\theta \neq 1$, $\ell \neq z$, and particle distributions now have a longitudinal degree of freedom not present in Fermi's theory. This leads us to Yang's theory, discussed in the next chapter, and a central topic of this work.

E. Diffusion Calculations

Most medical physicists interested in treatment planning applications would view a small angle energy independent theory with considerable suspicion. Many would dismiss it out of hand as being unrealistically simple. This could easily lead to a significant misevaluation and we might well be discarding an invaluable result by underestimating it.

The two volume text of Morse and Feshbach[10] is an excellent source of background remarks concerning the nature of diffusion and the way a diffusion calculation is supposed to work. Although their remarks are scattered throughout both volumes and it requires a bit of an effort to dig them out, there is probably no finer reference on this matter. Their key observations are as follows: Diffusion is always a blurring, dulling, smearing and eroding process. An ongoing diffusion process will invariably lead us from sharper and more distinctive distributions into smoother and more rounded forms. Since sharp distributions are always more difficult to describe than round ones, the mathematical structure of a diffusion calculation cannot (or should not) develop into something which becomes more complicated with time. The pivotal part of a diffusion calculation is therefore in the earliest stages of its development where small angle energy independent approximations are expected to be valid. Relaxing these approximations is not expected then to complicate an analysis by requiring that we find extra or additional structure, but by leading us to more difficult additions instead, e.g., more difficult integrals. The Eyges' extension of Fermi's theory, for example, certainly had this character.

The remarks of Morse and Feshbach clearly identify the small angle energy independent analysis as being crucial. We therefore examine two such generalizations of Fermi's theory in the next chapter (III), Snyder and Scott's and Yang's.

Calculations allowing for energy dependence or large angles should be classified, according to the above remarks, as applied calculations. To be sure, it is often necessary to know how to do them. Meaningful comparisons between theory and experiments sometimes can't be done without them. They would be necessary for credible inhomogeneity calculations. The point made above, however, was that a correct theoretical solution, even one obtained by small angle energy independence approximations, should contain and develop enough structural information to handle these applied topics as well.

We can use these remarks in more than one way. For example, if the underlying analysis has a fundamental difficulty accomodating either of these effects, then this might well be a signal that there is something fundamentally wrong with that analysis. The Snyder and Scott calculation had a most interesting difficulty with a large angle effect; Yang's analysis cannot handle any energy dependence. Both calculations had problems with moments. Both had problems with their time development. The difficulties in these key analyses were not resolved in later works, but were incorporated and assimilated into them. Applications floundered very badly because of it. The end result for medical physicists is that they were left without a working theory of electron penetration.

We discuss the theories in more detail in chapters III and IV, which should be helpful in identifying more precisely just what the problems were. We redo the fundamental analyses in chapters IV and V, which leads to a theory free from these problems. We also give some examples of applied calculations, which are sufficient to demonstrate that the theory is working properly.

III. Generalizations of the Transport Equation

Very many generalizations of Fermi's equation (20) are possible. Each feature that we add to the description leads to an altered equation of motion and could technically be called a different theory. Some changes are more important than others and the most dramatic are those which give the probability fields more degrees of freedom because they lead to different kinds of predictions. This work will be primarily interested in Yang's theory because it included the longitudinal degree of freedom, allowing us to calculate true penetration phenomena. Yang's solution to the transport equation was not only exact and completely analytic but also completely contains Fermi's theory exactly within it, much as Fermi's theory contains the ray model exactly within it. To the present day treatment planner, whose charged particle applications are overwhelmingly concerned with electron beams having initial energies between 5-20 MeV and penetrating low Z materials, there is no theory which is more important.

A. Multiple Scattering Equations

Our discussion begins with a generalization of Fermi's argument (16) and aims to derive all the transport equations that will be considered in this work. Harder's[11] discussion is also noteworthy here.

The equations that we shall be concerned with neglect all secondary particles and follow only the primaries. In the electron problems to which we will eventually wish to apply this theory, there

are both knock-on or secondary electrons as well as bremsstrahlung photons. We would try to argue that neither is a cause of great concern to us, e.g., that the secondary electrons are of such low energy and short range that they are immediately absorbed at the site of production, that the photons are of such long range that they escape the region of interest altogether and deposit their energy somewhere off at infinity. Neither statement is altogether true in practice and the applicability of the theory discussed here will be limited to the extent that they are not. References 6,12,18,22 provide ample background on this topic.

Our picture will assume that a particle moving through matter traces out a continuous trajectory and the distance along its path back to its origin will be denoted by ℓ. We specify the status of a single particle at a given time by stating its direction of movement $\hat{\Omega}$, its spatial coordinates $\vec{x}$, and its energy E. The instantaneous status of a large number of particles is then completely defined by the probability distribution $f(\ell, E, \hat{\Omega}, \vec{x})$; the number of particles within the energy interval (E, dE), and the directional interval $(\hat{\Omega}, d\hat{\Omega})$ and the spatial volume $(\vec{x}, d\vec{x})$ is $f(\ell, E, \hat{\Omega}, \vec{x})\, dE\, d^2\Omega\, d^3x$ if they have all traveled a distance ℓ. We obtain the differential equation as before, by constructing $f(\ell+d\ell, E, \hat{\Omega}, \vec{x})$ from $f(\ell, E, \hat{\Omega}, \vec{x})$ and then looking at the difference. We write

$$f(\ell+d\ell, E, \hat{\Omega}, \vec{x}) = \iiint dE'\, d^2\Omega'\, d^3x'\; f(\ell, E', \hat{\Omega}', \vec{x}')\, f(d\ell, E'\to E, \hat{\Omega}'\to\hat{\Omega}, \vec{x}'\to\vec{x}) \tag{34}$$

where $f(d\ell, E'\to E, \hat{\Omega}'\to\hat{\Omega}, \vec{x}'\to\vec{x})\, dE\, d^2\Omega\, d^3x$ gives the fraction of particles that would scatter from $E', \hat{\Omega}', \vec{x}'$ into the interval

$dE\,d\hat{\Omega}\,d^3x$ in the course of moving through a distance dl. This equation is written with the understanding that we intend to take the limit as $dl \to 0$, which will mean in practice that we only need to keep first order differentials. Particles simply drift from $\vec{x}' \to \vec{x}$ along their initial line of movement, as discussed earlier, so that

$$f(dl, E' \to E, \hat{\Omega}' \to \hat{\Omega}, \vec{x}' \to \vec{x}) = f(dl, E' \to E, \hat{\Omega}' \to \hat{\Omega})\, \delta(\vec{x}' + dl\,\hat{\Omega}' - \vec{x}) \qquad (35)$$

In the theory that we will be concerned with, energy loss is by one mechanism while deflection is by another. The two processes are assumed to have nothing to do with each other. When electrons of several MeV penetrate a low material, for example, the major part of energy loss is to orbital electrons with only negligible scattering while deflection is produced by Coulomb scattering off the nucleus with only negligible energy loss. Since the two are independent we can write

$$f(dl, E' \to E, \hat{\Omega}' \to \hat{\Omega}) = f(dl, E' \to E)\, f(dl, \hat{\Omega}' \to \hat{\Omega}) \qquad (36)$$

and then continue the right side of (36) into (37)

$$= \left[\frac{dl}{\mu_1}\,\frac{d\sigma_1(E' \to E)}{\sigma_1\, dE} + \left(1 - \frac{dl}{\mu_1}\right)\delta(E' - E)\right]\left[\frac{dl}{\mu_2}\,\frac{d\sigma_2(E, \hat{\Omega}' \to \hat{\Omega})}{\sigma_2\, d\omega} + \left(1 - \frac{dl}{\mu_2}\right)\delta(\hat{\Omega}' - \hat{\Omega})\right]$$

where μ_1, μ_2 and σ_1, σ_2 are the mean free paths and cross sections associated with each of these processes. Continuing with (37) gives

$$\begin{aligned} f(l + dl, E' \to E, \hat{\Omega}' \to \hat{\Omega}) &= \delta(E' - E)\,\delta(\hat{\Omega}' - \hat{\Omega}) + \delta(\hat{\Omega}' - \hat{\Omega})\left(\frac{dl}{\mu_1}\right)\left[\frac{1}{\sigma_1}\frac{d\sigma_1(E' \to E)}{dE} - \delta(E' - E)\right] \\ &\quad + \delta(E' - E)\left(\frac{dl}{\mu_2}\right)\left[\frac{1}{\sigma_2}\frac{d\sigma_2(E, \hat{\Omega}' \to \hat{\Omega})}{d\omega} - \delta(\hat{\Omega}' - \hat{\Omega})\right] \end{aligned} \qquad (38)$$

if we keep only terms up to first order in $d\ell$. Using the delta functions to do the integrals, (34) then becomes

$$\frac{\partial f(\ell,E,\hat{\Omega},\vec{x})}{\partial \ell} = -\hat{\Omega}\cdot\vec{\nabla}f + \frac{1}{\mu_1}\int dE'\left[\frac{1}{\sigma_1}\frac{d\sigma_1(E'\to E)}{dE} - \delta(E'-E)\right] f(\ell,E',\hat{\Omega},\vec{x})$$
$$+ \frac{1}{\mu_2}\int d^2\Omega'\left[\frac{1}{\sigma_2}\frac{d\sigma_2}{d\omega}(E,\hat{\Omega}'\to\hat{\Omega}) - \delta(\hat{\Omega}'-\hat{\Omega})\right] f(\ell,E,\hat{\Omega}',\vec{x}) \qquad (39)$$

the third term on the right of (39) may be written

$$\frac{1}{\mu_2}\int d^2\Omega' \frac{1}{\sigma_2}\frac{d\sigma_2}{d\omega}(E,\hat{\Omega}'\cdot\hat{\Omega})\left[f(\ell,E,\hat{\Omega}',\vec{x}) - f(\ell,E,\hat{\Omega},\vec{x})\right]$$

while the second, if we assume that the significant energy variation depends only on the energy difference $\epsilon = E'-E$, becomes

$$\frac{1}{\mu_1}\int d\epsilon \frac{1}{\sigma_1}\frac{d\sigma_1}{d\epsilon}(E,\epsilon)\left[f(\ell,E+\epsilon,\hat{\Omega},\vec{x}) - f(\ell,E,\hat{\Omega},\vec{x})\right]$$

We further assume that the mechanism of energy loss involves only very small energy charges in a given interaction so that only the first non-vanishing term from the difference $f(\ell,E+\epsilon,\hat{\Omega},\vec{x}) - f(\ell,E,\Omega,\vec{x})$ needs to be kept. This term becomes

$$\left[\frac{1}{\mu_1}\int d\epsilon\ \epsilon\ \frac{d\sigma_1(E,\epsilon)}{d\epsilon} \Big/ \int d\epsilon\ \frac{d\sigma_1(E,\epsilon)}{d\epsilon} = \frac{\langle\epsilon\rangle}{\mu_1}\right]\frac{\partial f(\ell,E,\hat{\Omega},\vec{x})}{\partial E}$$

This last step incorporates into the theory what is frequently referred to as the continuous energy loss or continuous slowing down approximation. If we now write $f(\ell,E,\hat{\Omega},\vec{x}) = f(\ell,E)f(\ell,\hat{\Omega},\vec{x})$ the transport

equation (39) decomposes into two equations

$$\frac{\partial f(\ell,\epsilon)}{\partial \ell} = \frac{\langle \epsilon \rangle}{\mu_\epsilon} \frac{\partial f(\ell,\epsilon)}{\partial \epsilon} \tag{40a}$$

$$\frac{\partial f(\ell,\hat{\Omega},\vec{x})}{\partial \ell} = -\hat{\Omega}\cdot\vec{\nabla} f + \frac{1}{\mu_s}\int d^2\Omega' \frac{d\sigma(\epsilon,\hat{\Omega}'\cdot\hat{\Omega})}{\sigma d\omega}\left[f(\ell,\hat{\Omega}',\vec{x}) - f(\ell,\hat{\Omega},\vec{x})\right] \tag{40b}$$

If the energy distribution is initially a delta function, then the solution to the first is always a delta function connecting the energy of the particle to its distance of travel. The effect is to make pathlength, time and energy equivalent variables. We will choose pathlength as the variable of interest, but will frequently refer to it as if it were time. $\langle \epsilon \rangle / \mu_\epsilon$ is the average energy lost per interaction over the average distance between (energy loss) interactions. This information is most usually presented as a stopping power $S(\epsilon)$

$$S(E) \equiv \frac{1}{\rho}\left\langle \frac{dE_{loss}}{d\ell} \right\rangle_\epsilon \tag{41}$$

where ρ is the density of the material. The delta function relation

$$\ell(\epsilon) = \frac{1}{\rho}\int_\epsilon^{E_o} dE' \frac{1}{S(E')} \tag{42}$$

is the result of solving (40a). If we set ϵ equal to the rest energy of the particle, then (42) defines the range R of the particle in a given material if it initially had energy E_o. Stopping power information is fairly accessible to medical physicists and we will assume that there is no problem in obtaining or using range-energy relationships[12]. The ultra-sharp correspondence between R and E_o is an

idealization that will be used or assumed throughout this work. Had we not wished to retain it, we would be required to keep at least the next term $\frac{\partial^2}{\partial E^2} f(\ell, E, \hat{\Omega}, \vec{x})$ in the expansion of the energy difference. This would allow a distribution of energies to develop for a given pathlength.

Lewis' theory[9] is essentially equations (40a) and (40b), although he developed the theory further. If we made an expansion of the difference $f(\ell, \hat{\Omega}', \vec{x}) - f(\ell, \hat{\Omega}, \vec{x})$, a worthwhile idea if the deflecting cross section is expected to redirect a particle's direction of motion by only a slight amount in any one collision, the first term would integrate to zero and the first non vanishing term involves the second derivative in angular variables. The transport equation (40b) would then simplify and become

$$\frac{\partial f(\ell, \hat{\Omega}, \vec{x})}{\partial \ell} = -\hat{\Omega} \cdot \vec{\nabla} f + \frac{1}{4} \frac{\langle \theta^2 \rangle}{\mu_s} \nabla_{\Omega}^2 f \qquad (43)$$

where $\langle \theta^2 \rangle$ may be written

$$\langle \theta^2 \rangle = \frac{1}{\sigma_s} \int_{-\infty}^{\infty} \int d\theta_x \, d\theta_y \, (\theta_x^2 + \theta_y^2) \frac{d^2\sigma}{d\theta_x \, d\theta_y} (\theta_x, \theta_y) \qquad (44)$$

since small angle notation is clearly appropriate here. When derived in this manner the transport equation (43) is called the Fokker-Planck approximation and it is obviously an approximation. An equation of the same form can be derived more directly by first writing

$$f(\ell + d\ell, \hat{\Omega}, \vec{x}) = \int\int d^2\Omega' \, d^3x' \, f(\ell, \hat{\Omega}', \vec{x}') \, \delta(\vec{x}' + \hat{\Omega}' d\ell - \vec{x}) \, f(d\ell, \hat{\Omega}' \to \hat{\Omega}) \qquad (45)$$

and then inserting

$$f(d\ell, \hat{\Omega}' \to \hat{\Omega}) = \frac{e^{-\theta^2/K d\ell}}{\pi K d\ell} \qquad (46)$$

where $\cos\theta = \hat{\Omega}\cdot\hat{\Omega}'$ and taking the limit of $\Delta\ell \to 0$. With $K = \langle\sigma\rangle\mu_s^{-1}$ we would again obtain (43), but now as an exact equation of motion although it would be called the Gaussian approximation. If we use a spherical description for $\hat{\Omega}$ and Cartesian spatial coordinates it is explicitly

$$\frac{\partial f(\ell,\hat{\Omega},\vec{x})}{\partial \ell} = -\left[\sin\theta\cos\phi\,\frac{\partial}{\partial x} + \sin\theta\sin\phi\,\frac{\partial}{\partial y} + \cos\theta\,\frac{\partial}{\partial z}\right] f + \frac{K(\ell)}{4}\left[\frac{1}{\sin\theta}\,\frac{\partial}{\partial\theta}\left(\sin\theta\,\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\,\frac{\partial^2}{\partial\phi^2}\right] f \qquad (47)$$

We have allowed for energy dependence simply through the notation $K(\ell)$. We would choose the initial conditions on (47) and (40b) as

$$f(\ell=0,\hat{\Omega},\vec{x}) = \delta(\hat{\Omega}-\hat{z})\,\delta(\vec{x}) \qquad (48)$$

which places the coordinate origin at the point where the particle originates and defines the z axis as the initial direction of movement.

B. Snyder-Scott Theory

If we integrate (40b) over the z coordinate, eliminating it from the equation, and also restrict the discussion to small angles, the transport equation may be written

$$\frac{\partial f(\ell,\theta_x,\theta_y,x,y)}{\partial \ell} = -\left(\theta_x\frac{\partial}{\partial x} + \theta_y\frac{\partial}{\partial y}\right) f + \frac{1}{\mu_s\sigma}\iint d\theta_x'\,d\theta_y'\,\frac{d\sigma}{d\Omega}(\theta)\left[f(\ell,\theta_x',\theta_y',x,y) - f(\ell,\theta_x,\theta_y,x,y)\right] \qquad (49)$$

where the deflection angle for a single collision is $\{(\theta_x'-\theta_x)^2+(\theta_y'-\theta_y)^2\}^{1/2}$ The Snyder and Scott[7] development thus began with a generalization of Fermi's lateral transport equation (20) in which the generalization was to use a very realistically chosen cross section to redirect particles rather than assume the Gaussian approximation. We could, of course, recover two equations of the form (20) simply by expanding the difference $f(\ell,\theta_x',\theta_y',x,y)-f(\ell,\theta_x,\theta_y,x,y)$ and retaining only the first non-vanishing terms.

Snyder and Scott worked in the projection plane, obtained by integrating one dimension away

$$f(\ell,\theta_x,x)=\int_{-\infty}^{\infty}d\theta_y\int_{-\infty}^{\infty}dy\ f(\ell,\theta_x,\theta_y,x,y) \tag{50}$$

If we also integrate over the remaining spatial coordinate, the transport equation (49) then becomes

$$\frac{\partial f(\ell,\theta_x)}{\partial \ell}=\frac{1}{\mu_s\sigma}\int d\theta_x'\ \sigma_{proj}(\theta_x-\theta_x')\left[f(\ell,\theta_x')-f(\ell,\theta_x)\right] \tag{51}$$

where

$$\sigma_{proj}(\theta_x)=\int_{-\infty}^{\infty}d\theta_y\ \frac{d\sigma}{d\Omega}\left((\theta_x^2+\theta_y^2)^{1/2}\right) \tag{52}$$

which is the equation satisfied by the (projected) angular distribution, the topic their work was concerned with. One may obtain a formal solution to (51) by using Fourier transforms defined by

$$f(\ell,\theta_x)=\frac{1}{2\pi}\int_{-\infty}^{\infty}d\mathcal{T}_x\ e^{i\mathcal{T}_x\theta_x}f(\ell,\mathcal{T}_x) \tag{53a}$$

$$\sigma_{proj}(\theta_x)=\frac{1}{2\pi}\int_{-\infty}^{\infty}d\mathcal{T}_x\ e^{i\mathcal{T}_x\theta_x}\sigma_{proj}(\mathcal{T}_x) \tag{53b}$$

When (53a) and (53b) are inserted into (51) and a few straightforward integrals are done, (51) then becomes

$$\frac{\partial f(\ell,T_v)}{\partial \ell} = -\frac{1}{\mu_s}\left[1-\frac{\sigma_{proj}(T_v)}{\sigma}\right] f(\ell,T_v) \qquad (54)$$

The solution of (54) that we want is

$$f(\ell,T_v) = e^{-\frac{\ell}{\mu}\left[1-\frac{\sigma_{proj}(T_v)}{\sigma}\right]} \qquad (55)$$

since it has the initial condition $f(\ell=0,T_v) = 1$, or equivalently by (53a), $f(\ell=0,\theta_v) = \delta(\theta_v)$. To obtain (54) we would also need to use $\sigma_{proj}(T_v=0) = \sigma$, a relation easily obtained from (53b) and (52). To obtain results with this approach we insert (55) into (53a) and then invert the Fourier transform, a major part of the problem.

Snyder and Scott then chose the differential cross section derived in the Born approximation for scattering from a screened Coulomb potential, $V(r) = (ze^2/r)\, e^{-r/a}$, a rather realistic model, as the starting point to begin deriving their results. They used the small angle version of

$$\frac{d\sigma(\theta)}{d\Omega} = \left(\frac{zz'e^2E}{2p^2c^2}\right)^2 \frac{1}{\left[sine^2(\theta/2)+(\theta_s/2)^2\right]^2}$$

$$\simeq \left(\frac{2zz'e^2E}{p^2c^2}\right)^2 \frac{1}{(\theta^2+\theta_s^2)^2} \qquad (56)$$

where $\theta_s = (p_{inc}\,a)^{-1}$ is the screening angle, p_{inc} the wave number of the approaching particle and a , the screening radius was given its

conventional value $a = a_0/Z^{1/3}$ where a_0 is the Bohr radius of hydrogen. With the form (56), the integral (52) is done directly giving

$$\sigma_{proj}(\theta_x) = \left(\frac{2zz'e^2E}{p^2c^2}\right)^2 \left[\frac{\pi}{2}\frac{1}{(\theta_x^2+\theta_s^2)^{3/2}}\right] \qquad (57)$$

Using the modified Bessel function integral representation

$$K_\nu(xz) = \frac{\Gamma(\nu+1/2)}{\pi^{1/2}}\frac{(2z)^\nu}{x^\nu}\int_0^\infty dt\,\frac{\cos xt}{(t^2+z^2)^{\nu+1/2}} \qquad (58)$$

for $\nu=1$, the Fourier transform of (57) gives

$$\sigma_{proj}(J_x) = \pi\left(\frac{2zz'e^2E}{p^2c^2\theta_s}\right)^2 (J_x\theta_s)\,K_1(J_x\theta_s) \qquad (59)$$

we also get

$$\sigma_{proj}(J_x=0) = \sigma = \pi\left(\frac{2zz'e^2E}{p^2c^2\theta_s}\right)^2 \qquad (60)$$

So that

$$1 - \frac{\sigma_{proj}(J_x)}{\sigma} = 1 - J_x\theta_s\,K_1(J_x\theta_s) \qquad (61)$$

and, with (55)

$$f(l,J_x) = e^{-\frac{l}{\mu_s}\left(1 - J_x\theta_s K_1(J_x\theta_s)\right)} \qquad (62)$$

The only remaining step is to use (62) in (53a), which may be written

$$f(l,\theta_x) = \frac{1}{\pi}\int_0^\infty dJ_x\,\cos(J_x\theta_x)\,f(l,J_x) \qquad (63)$$

To generate numerical values for the modified Bessel function K_1, Snyder and Scott used an ascending series representation

$$K_1(z) = \frac{1}{z} + \frac{z}{2}\left\{\ln\left(\frac{z}{2}\right) + \frac{1}{2}(2\gamma - 1)\right\} + \\ + \frac{z^3}{16}\left\{\ln\left(\frac{z}{2}\right) + \frac{1}{2}\left(2\gamma - \frac{5}{2}\right)\right\} + \ldots \quad (64)$$

where γ is Euler's constant = .5772, and then numerically evaluated the integrals (63) very carefully. The presentation of their results was somewhat facilitated by the fact that their integrals depended only on ratios ℓ/μ, the number of collisions, and θ_*/θ_c.

Snyder and Scott quoted many results but the two that are most noteworthy are reproduced on our Fig. 4. Together they indicate that the exact numerical prediction is more sharply peaked at very small angles than is suggested by the Gaussian approximation. The results fall below the Gaussian at slightly larger angles only to rise above it again, being several orders of magnitude above the Gaussian at large angles where it approaches the single scattering prediction asymptotically.

As an interesting or noteworthy calculation, the Snyder and Scott analysis was unobjectionable. However, as a theory, it was seriously defective. The chief difficulty was that these authors had generated all their results using a specific cross section. The solution of the transport equation is actually a function of the deflecting cross section, so one can't solve it by choosing a particular case. The example

that they chose to examine, charged particle multiple scattering, is certainly the one that we are most interested in. It is also a pathological case. It becomes a poor theoretical example to choose, especially if we only have one, because the pathological peculiarities of the problem will be contained in its results.

Difficulties in their analysis began with line (56). The pathological features of this particular cross section become evident when we try to computee its moments, i.e.,

$$\langle \theta^2 \rangle = \frac{\iint d\theta_x\, d\theta_y\, (\theta_x^2+\theta_y^2)\, \frac{d\sigma}{d\Omega}(\theta)}{\iint d\theta_x\, d\theta_y\, \frac{d\sigma}{d\Omega}(\theta)} \sim \int_0^\infty d\theta^2 \frac{\theta^2}{(\theta^2+\theta_s^2)^2} \to \ln\infty \tag{65}$$

which undefined. Higher moments $\langle \theta^4 \rangle, \langle \theta^6 \rangle, \ldots$ will diverge even faster and won't exist either. Because the moments of the single scattering cross section don't exist, the moments of the complete multiple scattering angular distribution don't exist, e.g.,

$$\overline{\theta_x^2(l)} = \left(\int_{-\infty}^{\infty} d\theta_x\, \theta_x^2\, f(l,\theta_x) \Big/ \int_{-\infty}^{\infty} d\theta_x\, f(l,\theta_x) \right) \to \infty \tag{66}$$

as is easily demonstrated if we use the general relation (53a) and the particular form (62). Since

$$\overline{\theta_x^2(l)} = -\frac{\partial^2}{\partial J_x^2} f(l,J_x)\Big|_{J_x=0} \tag{67}$$

as can be shown easily from (53a), these derivatives will not exist, a feature traceable to the presence of log terms in the expansion (64). Since moments of the angular distribution did not exist, moments of the spatial distribution would not exist either, Taylor expansions would

not exist, and the analytic structure of the whole problem has been ruined. These difficulties are all traceable back to the choice (56). The root difficulty is that charged particle multiple scattering is not strictly a small angle problem. The Rutherford (single scattering) tail, a characteristic feature of any realistically chosen charged particle differential cross section, imparts large angle features to the problem which the small angle formalism can't accomodate properly. The end result was a highly accurate numerical description built out of specific functions which were analytically impossible.

Snyder and Scott made no mention of the moments problem. Scott, in his article "Small Angle Multiple Scattering of Charged Particles" written for the Reviews of Modern Physics more than a dozen years later, a work often considered to be a definitive treatment of the topic, finally acknowledges and addresses the problem after a brief discussion of Snyder and Scott theory. Moments, of course they exist, he writes. His next choice of topics indicates how to solve this problem to his satisfaction, with cutoffs and shaveoffs. Thus, numerical fix up is the answer. The real reason for the infinities is that we are attempting to solve an essentially three dimensional problem in two dimensions, and cutoffs or shaveoffs won't address it. Apart from the difficulty with moments and the significant limitations due to numerical analysis, the problem of constructing spatial distributions, a problem significantly more complicated than angular distributions, had not been addressed either.

C. Lewis' Theory

Lewis[9] began by writing (40b). The main purpose of his work was to describe a method of obtaining exact results without the small angle approximation. His equation is, for the most part, a large angle generalization of (49) although he also included the longitudinal coordinate and did derive some exact relations concerning it. His investigation of this integro-differential equation included both its angular and spatial parts. We will discuss both briefly, beginning with angular distribution, which is simpler.

Integrating (40b) over all spatial coordinates out to infinity leaves the equation for the angular distribution, irrespective of position. If we also ignore energy losses, which would not be important to the discussion here, it becomes

$$\frac{\partial f(\ell,\hat{\Omega})}{\partial \ell} = \frac{1}{\mu_s}\int d^2\Omega' \frac{1}{\sigma_s}\frac{d\sigma(\hat{\Omega}\cdot\hat{\Omega}')}{d\omega}\left[f(\ell,\hat{\Omega}') - f(\ell,\hat{\Omega})\right] \qquad (68)$$

The initial condition would then be the space integral of (48), $f(\ell=0,\hat{\Omega}) = \delta(\hat{\Omega}-\hat{z})$. Equivalently, if we use spherical coordinates $f(\ell=0,\hat{\Omega}) = (2\pi)^{-1}\delta(1-\cos\theta)$. The most general form of the solution would then be

$$f(\ell,\cos\theta,\phi) = \sum_{j=0}^{\infty}\left(\frac{2j+1}{4\pi}\right) f_j(\ell)\, P_j(\cos\theta) \qquad (69a)$$

because of the cylindrical symmetry of the problem. The initial conditions require that $f_j(\ell=0)=1$. If we also decompose the differential cross section into its Legendre components

$$\frac{1}{\sigma}\frac{d\sigma}{d\Omega}(\cos\theta) = \sum_{j=0}^{\infty}\left(\frac{2j+1}{4\pi}\right)\left(\frac{1}{\sigma}\frac{d\sigma}{d\Omega}\right)_j P_j(\cos\theta) \qquad (69b)$$

and then insert (69a) and (69b) into (68), we obtain

$$\frac{df_j(\ell)}{d\ell} = -\frac{1}{\mu_s}\left[1-\left(\frac{1}{\sigma}\frac{d\sigma}{d\Omega}\right)_j\right] f_j(\ell) \qquad (70)$$

if we use the addition theorem for spherical harmonics and use the orthogonality of the Legendre polynominals to do the remaining integrals. The solution to (70) with the correct initial conditions is

$$f_j(\ell) = e^{-\frac{\ell}{\mu_s}\left[1-\left(\frac{1}{\sigma}\frac{d\sigma}{d\Omega}\right)_j\right]} \qquad (71)$$

Since the coefficients $\left(\frac{1}{\sigma}\frac{d\sigma}{d\Omega}\right)_j$ are given by

$$\left(\frac{1}{\sigma}\frac{d\sigma}{d\Omega}\right)_j = 2\pi\int_{-1}^{1} d\cos\theta\; P_j(\cos\theta)\;\frac{1}{\sigma}\frac{d\sigma}{d\Omega}(\cos\theta) \qquad (72)$$

as one obtains by inverting (69b), we may alternatively write

$$f_j(\ell) = e^{-K_j\ell} \qquad (71)'$$

where

$$K_j = \frac{2\pi}{\mu_s}\int_{-1}^{1} d\cos\theta\;\left(1-P_j(\cos\theta)\right)\;\frac{1}{\sigma}\frac{d\sigma}{d\Omega}(\cos\theta) \qquad (73)$$

which is equivalent to the form which was given by Lewis. The steps should look familiar. (69a) and (69b) are analogues of (53a) and (53b), while (70) and (71) are analogues of (54) and (55) respectively. Lewis' theory, as far as the angular distribution is concerned, is essentially Snyder-Scott theory redone with large angle machinery. The corresponding expressions would have looked even more similar if Snyder and Scott had used a cylindrical rather than a Cartesian (projected angle) description. Energy dependence, had we included it, would only have led to the replacements $K_j \rightarrow K_j(\ell)$, $K_j\ell \rightarrow \int_0^\ell d\ell'\, K_j(\ell')$.

This example was intended to serve as an illustration of the comments made in section II.E concerning diffusion calculations, namely, that the pivotal theoretical analysis is the small angle energy independent analysis, the analysis which pertains at the earliest possible times because it is expected to develop a mathematical structure sufficient to handle the problem at all subsequent times, and sufficient to handle it rather easily. We should also point out that this will only be the case if this early time analysis is impeccable. Should it contain a flaw, or even less, such as a misleading feature, then the problem of constructing distributions correctly at later times can become extremely difficult. This is particularly true of large angle problems which can turn very ugly, into almost intractable analyses. The small angle analysis needs to be perfect and suggest exactly the correct route to take.

Lewis initiated work on the construction of spatial distributions, the topic of principle importance to us. Consider the longitudinal part of the multiple scattering problem which we define by integrating away lateral variables

$$f(\ell, \cos\theta, z) = \int_0^{2\pi} d\phi \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy \quad f(\ell, \cos\theta, \phi, x, y, z) \qquad (74)$$

The equation of motion for this distribution function, obtained by applying these integrals to (40b), becomes

$$\frac{\partial f(\ell, \cos\theta, z)}{\partial \ell} + \cos\theta \frac{\partial}{\partial z} f \qquad (75)$$
$$= \frac{1}{\mu_s} \int d\phi \int d\cos\theta' \; \frac{1}{\sigma} \frac{d\sigma}{d\omega}(\epsilon, \cos\Theta) \left[f(\ell, \cos\theta', z) - f(\ell, \cos\theta, z) \right]$$

where

$$\cos\Theta = \cos\theta\cos\theta' + \sin\theta\sin\theta'\cos(\phi-\phi') \qquad (76)$$

Our problem would be simpler, considerably simpler, if we could integrate over $\cos\theta$ as well, turning (75) into a direct differential equation for the density. Unfortunately this can't be done and it becomes necessary to solve for angular information simultaneously. If we write

$$f(\ell,\cos\theta,z) = \sum_{j=0}^{\infty} \frac{2j+1}{2} f_j(\ell,z)\, P_j(\cos\theta) \qquad (77)$$

as a first step toward solving (75), then by inserting (77) and (69b) into (75), and then using the orthogonality of the Legendre polynominals we obtain

$$\frac{\partial f_j(\ell,z)}{\partial \ell} = -\frac{\partial}{\partial z}\left[\frac{j}{2j+1} f_{j-1}(\ell,z) + \frac{(j+1)}{2j+1} f_{j+1}(\ell,z)\right] - K_j(\ell) f_j(\ell,z) \qquad (78)$$

which is exactly equivalent to (75). The moments approach to the problem, which Lewis pursued, applies additional integrals to (78). Defining the n^{th} moment of the j^{th} distribution by

$$f_{j,n}(\ell) = \int_{-\infty}^{\infty} dz\, z^n f_j(\ell,z) \qquad (79)$$

then (78) becomes

$$\frac{d f_{j,n}(\ell)}{d\ell} = n\left[\frac{j}{2j+1} f_{j-1,n-1}(\ell) + \frac{(j+1)}{(2j+1)} f_{j+1,n-1}(\ell)\right] - K_j(\ell) f_{j,n}(\ell) \qquad (80)$$

Setting n=0 in (80) gives the equation for the angular distribution discussed earlier, so the complete set of Legendre coefficients $f_{j0}(\ell)$ gives the directional distribution, irrespective of position. The

coefficients $f_{on}^{(\ell)}$ give the moments of the spatial distribution irrespective of direction. The fact that we can solve for them from (80) and the possibility that we can construct a spatial distribution from a knowledge of its moments is the reason for writing (80).

To solve for them we would begin by solving for $f_{j=0,n=0}$, a trivial equation. To solve for the next spatial moment, $f_{0,n=1}$, we would first have to solve for $f_{j=1,n=0}$. A procedure which aims to compute f_{oN} will involve computing all coefficients f_{jn} for which $j+n \leq N$. The procedure, which begins with almost trivial equations, develops enormous and burgeoning complexity as we try to compute more moments, largely because the number of integrations to be performed rapidly increases. Any reasonable individual trying to solve these equations with his hands would begin to question the sense of his effort beyond $n = 3$. Really determined individuals, diehards, would begin dropping out after 5. The complexity of these equations is a practical limitation, not a theoretical one, since numerical integration by computer can yield results for higher n. Lewis stated that the set $f_{o,n}^{(\ell)}$ for all n constituted a solution in principle, although he did mention that the moments approach might not be that useful.

Sooner or later we would have to specify the K_j. For the case of charged particles, Lewis suggested the forms

$$K_j = A\frac{j(j+1)}{2}\left[\ln(1/\beta) + 1 - 2\sum_{m=1}^{j}(1/m)\right] \qquad (81)$$

$$\simeq A\frac{j(j+1)}{2}\left[\ln(1/\beta) + 1 - 2(\gamma + \ln(j+1/2))\right]$$

where $A = 2\pi N Z^2 e''/\rho^2 v^2$, $\mathcal{B} = (\eta_0/2)^2$, γ is Euler's constant. He arrived at these expressions by beginning with the definition (73), the large angle differential cross section (56) which had been quoted (but not used) by Snyder and Scott, and some difficult arguments with Legendre polynominals. These expressions would agree with the first few terms of the ascending series representation which had been used by Snyder and Scott. Thus Lewis' work clearly contained the Snyder-Scott analysis within it, but was more general. It also contained the problems of the Snyder-Scott analysis, but was now beginning to add a few of its own.

There are two new questions that have come up. The first is whether or not a knowledge of all the moments of a distribution actually constitutes a solution in principle. The second is whether the moments of a distribution are numbers or not, i.e., do we need analytical expressions for the moments or is it sufficient to compute them numerically? Both questions can be answered at once.

If we had an infinite set of expressions, $f_{\nu=0,n}$, we would look to organize all of them into a single equation as the very first step. Otherwise, we would simply have a large number of disjointed expressions that might just as well not have anything to do with each other. If we define the Fourier transform of the distribution by

$$f(\ell, z) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dQ \; e^{iQz} f(\ell, Q) \qquad (82)$$

then by inverting the transform and expanding the exponential we have

$$f(\ell, Q) = f^{(\ell)}_{n=0} - \frac{iQ}{1!} f^{(\ell)}_{n=1} + \frac{(-iQ)^2}{2!} f^{(\ell)}_{n=2} + \ldots \qquad (83)$$

which is simply a Taylor expansion of $f(\ell,Q)$ about the point Q=0, where the n derivatives with respect to Q are the moments of the distribution (e.g., defined by (79)). This accomplishes the first objective, putting all the moments into one equation. The next step in constructing the distribution would be to invert the Fourier transform (82). In general we would not be able to do this because it is typical of such series expressions that they will not converge from $Q=0\rightarrow\infty$. Thus $f(\ell,Q)$, if defined by (83), simply won't have definition across the range required by the integral.

Singularities in the complex plane will cause this series to diverge. Within some circle of convergence, say from $Q=0\rightarrow Q_1$, the series (83) will be meaningful and converge. Outside it, the series is meaningless and needs to be given extended meaning by redefining it in a manner so that it will always converge suitably. Thus the principle by which the moments approach works is analytic continuation. Without such a redefinition, and the information required to accomplish it, the series (83) is not a solution in principle. What we have instead is a representation of a solution, i.e., we have something to work with even though we don't know what the solution actually is.

Whether we can evaluate moments numerically or not will depend on the problem. Sometimes we can, sometimes we can't, but we should not simply assume that we can and blindly go ahead and start evaluating them numerically as a first step. If we were to do this, we might well be destroying the structural information that would have allowed us to make a meaningful analytic continuation. If it turns out to be mean-

ingful to evaluate moments of a distribution numerically, then we should be able to prove this before we actually go ahead and do it.

Lewis' work on spatial distributions was taken rather seriously because it had the appearance of being very thorough and quite studious, because of the high degree of plausibility of his remarks, because he had been able to derive some exact relations concerning them. There were nonetheless significant practical and theoretical difficulties intrinisic to the whole approach. These problems were to be even further compounded by Yang's analysis, an analysis which should have shed considerable light on the problem instead.

D. Yang's Theory

Yang[8] began by writing a transport equation which is equivalent to the small angle version of (43),

$$\frac{\partial f(\ell,\theta_x,\theta_y,x,y,z)}{\partial \ell} = -\left[\theta_x \frac{\partial}{\partial x} + \theta_y \frac{\partial}{\partial y} + \left(1-\left(\frac{\theta_x^2+\theta_y^2}{2}\right)\right)\frac{\partial}{\partial z}\right] f + \frac{K}{4}\left(\frac{\partial^2}{\partial \theta_x^2} + \frac{\partial^2}{\partial \theta_y^2}\right) f \qquad (84)$$

The essential generalization of Fermi's transport equation (20) is the introduction of the z or longitudinal coordinate. The assumptions of energy independence, small angles and the Gaussian approximation are retained in (84), exactly as they were in Fermi's theory. Introducing the spatial variable $\Delta = \ell - z$ and Fourier transforms (85)

$$f(\ell,\theta_x,\theta_y,x,y,\Delta) = \frac{1}{(2\pi)^3}\iiint d p_x\, d p_y\, d q\; e^{i(p_x x + p_y y + q\Delta)} f(\ell,\theta_x,\theta_y,p_x,p_y,q)$$

then by inserting (85) into (84) we obtain

$$\frac{\partial f(\ell,\theta_x,\theta_y,p_x,p_y,g)}{\partial \ell} = -i\left[\theta_x p_x + \theta_y p_y + g\left(\frac{\theta_x^2+\theta_y^2}{2}\right)\right] f + \frac{K}{4}\left(\frac{\partial^2}{\partial\theta_x^2}+\frac{\partial^2}{\partial\theta_y^2}\right) f \qquad (86)$$

The equation is separable into x-y parts. If we let

$$f(\ell,\theta_x,\theta_y,p_x,p_y,g) = f(\ell,\theta_x,p_x,g)\, f(\ell,\theta_y,p_y,g) \qquad (87)$$

then (86) becomes two equations

$$\frac{\partial f(\ell,\theta_x,p_x,g)}{\partial \ell} = \left(\frac{K}{4}\frac{\partial^2}{\partial\theta_x^2} - ig\frac{\theta_x^2}{2} - ip_x\theta_x\right) f(\ell,\theta_x,p_x,g) \qquad (88)$$

with the same equation for y. Yang recognized them as being reducible to a form identical to Schrodinger's equation for a harmonic oscillator with the only difference being that the frequency here would be complex. With $\theta_x' = \theta_x + \frac{p_x}{g}$ and $f(\ell,\theta_x,p_x,g) = \psi(\ell,\theta_x',g)\, e^{\frac{ip_x^2\ell}{2g}}$, (88) becomes

$$\frac{\partial \psi}{\partial \ell}(\ell,\theta_x',g) = \left(\frac{K}{4}\frac{\partial^2}{\partial\theta_x'^2} - ig\frac{\theta_x'^2}{2}\right)\psi \qquad (89)$$

which he solved by the eigenvalue approach. Letting $\psi = \phi e^{-\omega\ell}$ the time variable is eliminated and we are led to solve

$$\omega_n \phi_n(\theta_x',g) = \left(-\frac{K}{4}\frac{d^2}{d\theta_x'^2} + ig\frac{\theta_x'^2}{2}\right)\phi_n(\theta_x',g) \qquad (90)$$

for all the eigenfunctions and eigenvalues. Letting $F = \alpha\theta_x'$, where $K\alpha^2/4 = ig/2\alpha^2 \equiv \omega_0(g)$, (90) is put into the dimensionless form

$$\lambda_n \phi_n(F) = \left(-\frac{d^2}{dF^2} + F^2\right)\phi_n(F) \qquad (91)$$

where $\lambda_n = \frac{\omega_n}{\omega_0}$. The eigenvalues of (91) are well known from the quantum theory of the harmonic oscillator, $\lambda_n = 2n+1$ where $n = 0,1,2,..$, as are its eigenfunctions (see Schiff[14], Chapter 4)

$$\phi_n(\xi) = C_n H_n(\xi) e^{-\frac{1}{2}\xi^2} \tag{92}$$

where the H_n are Hermite polynominals , $C_n = (2^n n! \pi^{1/2})^{-1/2}$ are normalization constants determined by

$$\int_{-\infty}^{\infty} d\xi \; \phi_n(\xi) \phi_{n'}(\xi) = \delta_{nn'} \tag{93}$$

Since the eigenfunctions form a complete set, the general form of the solution to (88) may be written

$$f(\ell, \theta_x, p_x, \beta) = \sum_{n=0}^{\infty} A_n \phi_n(\xi) \; e^{\left(\frac{p_x^2}{2\beta} - (2n+1)\omega_0(\beta)\right)\ell} \tag{94}$$

where the A are constants determined by the initial conditions. If we take the initial condition on (84) as $f(\ell=0, \theta_x, \theta_y, x, y, z) = \delta(\vec{\theta})\delta(\vec{x})$, then the initial condition on (88) would become $f(\ell=0, \theta_x, p_x, \beta) = \delta(\theta_x)$ so that

$$A_n = \int_{-\infty}^{\infty} d\xi \; \delta(\theta_x) \phi_n(\xi) = \alpha \phi_n\left(\frac{\alpha p_x}{\beta}\right) \tag{95}$$

Yang actually had two variables, Δ_x, Δ_y, rather than just Δ that we used in (85). Our presentation altered this feature in order to conform to our own usage. In Yang's[8] original work, particle distributions were confined to infinitely thin, geometrically flat planes, exactly as in Fermi's theory. Z had the meaning of a scattering foil thickness and a distribution in $\Delta = \ell - Z$ gave the variation of pathlengths, ℓ , for particles which emerged through the foil. In our

usage, ℓ is the common distance that all particles travel within a material. A distribution in Δ develops because particles will be located at different depths, z . Particles will then be found within curved surfaces (Fig 1c). For the case of small angles, the two pictures are complimentary and equivalent.

In order to compute spatial distributions using this theory, we also need to invert the Fourier transforms (85). We consider the most important spatial distribution of the theory defined by

$$f(\ell,\Delta) = \iiiint d\theta_x\, d\theta_y\, dx\, dy\, f(\ell,\theta_x,\theta_y,x,y,\Delta) \qquad (96)$$

which gives the longitudinal or penetration density irrespective of lateral position or direction of movement. The integrals over dx dy in (85) give $(2\pi)^2\,\delta(p_x)\,\delta(p_y)$, so that the p_x, p_y integrals are trivial. Then

$$f(\ell,\Delta) = \frac{1}{2\pi}\int_{-\infty}^{\infty} d\beta\, e^{i\beta\Delta}\int_{-\infty}^{\infty} d\theta_x \int_{-\infty}^{\infty} d\theta_y\, f(\ell,\theta_x,\theta_y,0,0,\beta) \qquad (97)$$

where

$$f(\ell,\theta_x,\theta_y,0,0,\beta) = \sum_{n,m=0}^{\infty} \alpha^2\, \phi_n(\alpha\theta_x)\,\phi_m(\alpha\theta_y)\,\phi_n(0)\,\phi_m(0)\, e^{-2(n+m+1)\omega_0\ell} \qquad (98)$$

Some of the quantities needed to evaluate (97) can be obtained from the generating function for Hermite polynominals defined by

$$S(F,s) = e^{-s^2+2sF} = \sum_{n=0}^{\infty} H_n(F)\frac{s^n}{n!} \qquad (99)$$

If we set $\xi = 0$ in (99), we get

$$e^{-s^2} = 1 - s^2 + \frac{(s^2)^2}{2!} - + \cdots = \sum_{n=0}^{\infty} H_n(0)\,\frac{s^n}{n!} \qquad (100)$$

from which we obtain

$$\begin{aligned} H_n(0) &= (-1)^{n/2}\,\frac{n!}{(n/2)!} && n = \text{even} \\ H_n(0) &= 0 && n = \text{odd} \end{aligned} \qquad (101)$$

so that $\phi_n(0) = N_n H_n(0)$, where Nm are defined by (92), $H_n(0)$ by (101). Integrals of the form $\int_{-\infty}^{\infty} d\theta_n\, \phi_n(\alpha\theta_n) = \int d\xi\, \phi_n(\xi)$ can also be evaluated this way. With

$$\int_{-\infty}^{\infty} d\xi\; S(\xi, s)\, e^{-\frac{1}{2}\xi^2} = \sum_{n=0}^{\infty} \frac{s^n}{n!} \int_{-\infty}^{\infty} d\xi\; H_n(\xi)\, e^{-\frac{1}{2}\xi^2} \qquad (102)$$

the integral on the left is easily done directly and then expanded, i.e.,

$$\int_{-\infty}^{\infty} d\xi\; e^{-s^2 + 2s\xi}\, e^{-\frac{1}{2}\xi^2} = (2\pi)^{1/2} e^{s^2} = (2\pi)^{1/2}\left\{1 + s^2 + \frac{s^4}{2!} + \cdots\right\} \qquad (103)$$

so that a comparison of (103) and (102) gives

$$\begin{aligned} \int_{-\infty}^{\infty} d\xi\; H_n(\xi)\, e^{-\frac{1}{2}\xi^2} &= (2\pi)^{1/2}\,\frac{n!}{(n/2)!} && n = \text{even} \\ &= 0 && n = \text{odd} \end{aligned} \qquad (104)$$

Thus, in (97),

$$\iint d\theta_x\, d\theta_y\, f(\ell, \theta_x, \theta_y, 0, 0, \xi) = \sum_{\substack{n,m=0 \\ \text{even}}}^{\infty} \frac{(-1)^{\frac{n+m}{2}}}{2^{n+m-1}}\,\frac{n!\,m!}{\left[\frac{n}{2}!\,\frac{m}{2}!\right]^2}\, e^{-2(n+m+1)\omega_0(\xi)\ell} \qquad (105)$$

and the remaining part of (97) is to do the q integral. Since $\omega_0 = (iqK/\delta)^{1/2}$ by its initial definition, all the integrals have the form

$$\frac{1}{2\pi}\int_{-\infty}^{\infty} dq\, e^{iq\Delta}\, e^{-M\omega_0(q)\ell}$$

where M is an integer, and to do them along the real q axis requires some definition of the choice of phase. Yang chose them so that the real part of ω_0 is always positive, i.e., $(iq)^{1/2} \to 2^{-1/2}(1\pm i)|q|^{1/2}$ if q is $\pm$ real .

The above integral becomes

$$\frac{Re}{\pi}\int_0^{\infty} dq\, e^{iq\Delta}\, e^{-(1+i)\left(q\frac{M^2K\ell^2}{16}\right)^{1/2}} = \left(\frac{M^2K\ell^2}{32\pi\Delta^3}\right)^{1/2} e^{-\frac{M^2K\ell^2}{32\Delta}} \tag{106}$$

With (106) and (105), (97) becomes

$$f(\ell,\Delta) = \sum_{\substack{n,m=0\\ \text{even}}} \frac{(-1)^{\frac{n+m}{2}}}{2^{n+m-1}} \frac{n!\,m!}{\left[\frac{n}{2}!\,\frac{m}{2}!\right]^2} \frac{(n+m+1)K\ell^2}{(32\pi)^{1/2}\Delta^{3/2}}\, e^{-\frac{(n+m+1)K\ell^2}{8\Delta}} \tag{107}$$

Yang expressed this result (his Case I) more simply by using the variable $v = 8\Delta/K\ell^2$ and defining the function $f(\ell,v)$ by $f(\ell,v)\,dv = f(\ell,\Delta)\,d\Delta$. Then (107) becomes

$$f(\ell,v) = \frac{2}{\pi^{1/2}}\frac{1}{v^{3/2}}\left\{e^{-1/v} - 3e^{-9/v} + 5e^{-25/v} - +\ldots\right\} \tag{108}$$

once we work out the coefficients. Yang also gave the asymptotic approximations to this result, valid to within 1% in the regions indicated, as

$$f(\ell,v) = \frac{2}{\pi^{1/2}}\frac{1}{v^{3/2}}\left(e^{-1/v} - 3e^{-9/v}\right) \qquad v \le 2$$

$$f(\ell,v) = \frac{\pi}{4}\, e^{-\pi^2 v/16} \qquad v \ge 2 \tag{109}$$

For the case of small angles and energy independence that we are using here, it is easily shown that $\bar{\Delta} = K z/4$ where $\bar{\Delta}$ is the average value of the longitudinal distribution. The two regions of (109) are then

$$\Delta \leq \bar{\Delta} \ , \ \Delta \geq \bar{\Delta} \ .$$

Many of the eigenstates ϕ_{nm} which were required for a solution of (84) did not appear in the final calculation of the longitudinal density (108). The integrals over the lateral coordinates gave conditions that n,m be even integers, which removed them from the summations. Instead, we could have formulated a more restrictive but simpler one dimensional problem by integrating over these coordinates right from the very beginning. The equation of motion (84) would then become

$$\frac{\partial f(\ell, \theta_x, \theta_y, z)}{\partial \ell} = -\left[1 - \tfrac{1}{2}\left(\theta_x^2 + \theta_y^2\right)\right] \frac{\partial f}{\partial z} + \frac{K}{4}\left(\frac{\partial^2}{\partial \theta_x^2} + \frac{\partial^2}{\partial \theta_y^2}\right) f \tag{110}$$

Since the problem is cylindrically symmetric it makes better sense to use cylindrical variables θ, ϕ rather than Cartesian θ_x, θ_y. By integrating over the ϕ variable (110) becomes

$$\frac{\partial f(\ell, \theta, z)}{\partial \ell} = -\left(1 - \frac{\theta^2}{2}\right) \frac{\partial f}{\partial z} + \frac{K}{4}\left(\frac{\partial^2}{\partial \theta^2} + \frac{1}{\theta}\frac{\partial}{\partial \theta}\right) f \tag{111}$$

With

$$f(\ell, \theta, z) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dq \, e^{iq(\ell - z)} f(\ell, \theta, q) \tag{112}$$

as the analogue of (85), we obtain

$$\frac{\partial f(\ell, \theta, q)}{\partial \ell} = \left[\frac{K}{4}\left(\frac{\partial^2}{\partial \theta^2} + \frac{1}{\theta}\frac{\partial}{\partial \theta}\right) - \frac{iq}{2}\theta^2\right] f(\ell, \theta, q) \tag{113}$$

as the analogue of (89). The eigenvalue approach $f(\ell,\theta,\beta) = \psi(\theta,\beta)\, e^{-\omega\ell}$ now leads us to solve

$$\omega_N \psi_N = \left[-\frac{K}{4}\left(\frac{d^2}{d\theta^2} + \frac{1}{\theta}\frac{d}{d\theta}\right) + i\frac{\beta\theta^2}{2}\right]\psi_N \qquad (114)$$

as the analogue of (90). Letting $\mathcal{F} = \alpha\,\theta$ where $\alpha = \left(\frac{2i\beta}{K}\right)^{1/4}$ (114) becomes

$$\lambda_N \psi_N = \left[-\left(\frac{d^2}{d\mathcal{F}^2} + \frac{1}{\mathcal{F}}\frac{d}{d\mathcal{F}}\right) + \mathcal{F}^2\right]\psi_N \qquad (115)$$

where $\lambda_N = \frac{\omega_N}{\omega_0}$ and $\omega_0 = \frac{K\alpha^2}{4}$ as were defined earlier. The eigenvalues of (115) are $\lambda_N = 2(2N+1)$ where $N = 0,1,2,\ldots$, so that $\omega_N = 2(2N+1)\omega_0$. The eigen functions of (115) are where L_N are the Laguerre polynominals.

$$\psi_N(\Xi) = C_N\, L_N(\xi^2)\, e^{-\frac{1}{2}\Xi^2} \qquad (116)$$

where the L_N are Laguerre polynominals. The normalization constants can be determined by the requirement

$$\int_0^\infty \Xi\, d\Xi\ \psi_N(\Xi)\,\psi_{N'}(\Xi) = \delta_{NN'} \qquad (117)$$

The generating function for Laguerre polynominals

$$U(\rho,s) = \frac{1}{1-s}\, e^{-\rho s/(1-s)} = \sum_{N=0}^{\infty} \frac{s^N}{N!}\, L_N(\rho) \qquad (118)$$

can be used to do these integrals and we would find $C_N = 2^{1/2}/N!$. The most general form of the solution to (113) would then be

$$f(\ell,\theta,\beta) = \sum_N A_N\, \psi_N(\Xi)\, e^{-\omega_N(\beta)\ell} \qquad (119)$$

where the constants A_N are determined by the initial condition $f(0,\theta,\xi) = \delta(\theta^2/2)$ giving

$$A_N = \int_0^\infty \xi\, d\xi\ \delta(\theta^2/2)\ \psi_N(\xi) = \alpha^2 \psi_N(0) \qquad (120)$$

Setting $\rho = 0$ in (118) gives $L_N(0) = N!$, so that the solution of (113) becomes

$$f(\ell,\theta,\xi) = \sum_{N=0}^{\infty} \frac{2\alpha^2}{N!} L_N(\xi^2)\, e^{-\xi^2/2} e^{-\omega_N(\xi)\ell} \qquad (121)$$

If we integrate over all angles, (121) becomes

$$f(\ell,\xi) = \sum_{N=0}^{\infty} \frac{2}{N!} \left\{ \int_0^\infty \xi\, d\xi\, L_N(\xi)\, e^{-\xi^2/2} \right\} e^{-\omega_N(\xi)\ell}$$

$$= \sum_{N=0}^{\infty} 2(-1)^N e^{-\omega_N(\xi)\ell} \qquad (122)$$

in agreement with (105). Inverting the Fourier transform leading to (108) would be done as before.

The above example was suggested by a section of Spencer and Coyne[15], who generally pursued the one dimensional longitudinal problem. The eigenfuctions (116) are exact machinery and are potentially valuable for doing calculations in which we modify some aspect of the penetration problem. Spencer and Coyne generally used them with variational type calculations. We will refer to them again as a starting point for perturbation calculations. The fact that Laguerre polynomials will solve the two dimensional cylindrically symmetric oscillator problem isn't very surprising, however, since the three dimensional spherically symmetric oscillator is known to be solved by associated Laguerre polynomials, a well studied example in nuclear physics. One

of the strengths of Yang's quantum oscillator recognition was the fact that it gives us access to a great deal of free information. Also noteworthy is a known symmetry of the oscillator problem, that the eigenfunctions in configuration or momentum space are of identical type. In the same angle multiple scattering problem we could rewrite an equation like (89) as

$$\frac{\partial \psi(\ell, x, \beta)}{\partial \ell} = \left(i\beta \frac{\partial^2}{\partial x^2} - \frac{K}{4} x^2 \right) \psi \qquad (89)'$$

if we use Fourier transforms of the kind defined by (53a, 53b). The eigenfunctions and eigenvalues that solve (89) will obviously solve (89)'.

Let us briefly consider practical applications of this theory, applications of the type that treatment planners might be interested in. Their applications would include energy dependent and large angle effects. The introduction of any energy dependence into the problem, done by allowing $K \rightarrow K(\ell)$, causes eigenfunctions and eigenvalues to disappear. They don't exist anymore. If we were to try to adapt this machinery to handle an energy dependent problem we might consider breaking up the problem into several regions where the scattering parameters are constant within each region but differ from region to region. Yang's theory would give us a solution within each region and we would only have to connect the various sectional solutions to solve this problem. In principle we could do it, in practice we could not. To connect results from one region to the next we would have to overlap a set of eigenfunctions of one frequency with another set of a different frequency. Harmonic oscillator wave functions have many nice

mathematical properties, but the overlapping of two sets with different fundamental frequencies is not one of them. The overlap coefficients are quite complicated and an eigenfunction from one region will connect to every other eigenfunction of the next region in a difficult way. We would quickly give up this calculation as altogether intractable. Extension to large angles also appears to be very dubious. Rather than writing differential equations in the small angle case, we would be led to write difference equations in the large angle case. To represent a solution we would need all the eigenfunctions and eigenvalues, so we can expect to be working with NxN matrices to obtain them. Analytic work with 3x3 matrices is already becoming difficult, NxN seems out of the question. If we recall the statements that were made in section IIE, we have a signal that there is something the matter with this theory.

There are several other aspects of the theory that suggest that something is wrong. While there is no doubt that Yang solved the equations in a convincing and elegant manner, physical interpretations are quite difficult with this type of machinery. What do these calculations actually explain? What is a quantum oscillator doing in the middle of a classical diffusion problem? This is no clear correspondence between the mathematics and the physics and the theory doesn't make any apparent physical sense. Time development, for example, is exceptionally special in Yang's problem and all distributions and simply grow larger with time. The longitudinal density given by (108) or (109) is only one example of this. It is a function of a dimensionless ratio $\Delta/\bar{\Delta}$, so its shape never changes. We should have expected

to see something different in a diffusion problem, distributions deforming continuously with time. This special time development severely limits our ability to interpret what is happening; we need to see change, not perfect replication. We could have the suggestion now that Yang chose a problem with too much symmetry in it. To make it intelligible as a diffusion theory we should mess up the problem a bit, remove and ruin some of the exquisite oscillator symmetry. To accomplish this technically we will have to change something in the way the problem was formulated and this will lead us, in Chapters 4 and 5, to relax the approximations which were being made. The three approximations, the Gaussian approximation, small angles, energy independence apply constraints to the problem and each prevents the solution from developing or changing in some way. Relaxing these approximations will give us greater freedom for promoting change while also allowing for more realistic description.

The $\beta \to 0$ limit of Yang's theory is also worth pursuit. The limit of Yang's differential equation (88) is Fermi's differential equation (20). Therefore Yang's solution should collapse down to Fermi's solution if we take the $\beta \to 0$ limit of his results. This will clearly involve more than simply setting $\beta = 0$ in all of his expressions because we would have trouble making sense out of his terms like $\phi_n\left(\alpha \frac{\rho_i}{\beta}\right)$ in (95), where $\alpha = (a i \beta / \kappa)^{1/4}$. The connection back to Fermi's solution is not immediately apparent. Further, there has been nothing in Yang's theory which indicates that the modification of Fermi's theory has geometrical meaning, i.e., that the main alteration is to

curve or bend the distributions as was drawn in (Fig. 1c).

The $g \to 0$ limit of Yang's theory is worthy of pursuit for another reason, moments. As already noted in connection with equations (78), (80), (81), if the density and its Fourier transform are related by

$$f(\ell,\Delta) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dg\, e^{ig\Delta} f(\ell,g) \tag{123a}$$

$$f(\ell,g) = \int_{-\infty}^{\infty} d\Delta\, e^{-ig\Delta} f(\ell,\Delta) \tag{123b}$$

then an expansion of the exponential in (123b) gives the moment series

$$f(\ell,g) = \sum_{m=0}^{\infty} \frac{\overline{\Delta^m(\ell)}}{i^m}\,\frac{g^m}{m!} \tag{124}$$

where the moments of the distribution would be defined by

$$\overline{\Delta^m(\ell)} = \int_{-\infty}^{\infty} d\Delta\, \Delta^m f(\ell,\Delta) \tag{125}$$

Since (124) is also a Taylor expansion, $\overline{\Delta^m} = i^m \frac{\partial^m}{\partial g^m} f(g)\Big|_{g=0}$

If we use Yang's result (122) and proceed (rather blindly) to take its first derivative we might write

$$\overline{\Delta(\ell)} = i\frac{\partial}{\partial g}\sum_{N=0}^{\infty} 2(-1)^N e^{-2(2N+1)\omega_0(g)\ell}\Big|_{g=0} \tag{126}$$

$$= i\sum_{N} 2(-1)^N \frac{\partial}{\partial g} e^{-2(2N+1)\omega_0(g)\ell}\Big|_{g=0} \tag{127}$$

$$\longrightarrow \infty \quad \text{because} \quad \omega_0(g) \sim g^{1/2}$$

None of its higher derivatives would exist either. Equivalently, none of the terms in (108) have sensible moments. Individually the terms in (108) do not have moments, collectively they do. The error in going from (126) to (127) was that we interchanged a derivative and an infinite summation. This is only permissible sometimes. The way around this problem is to first sum the series and then take its derivative.

We can sum the series because of the linear spacing between oscillator levels. Thus (122) should be written

$$f(\ell,\varphi) = 2\, e^{-2\omega_0 \ell} \sum_{N=0}^{\infty} (-1)^N \left[e^{-4\omega_0}\right]^N \tag{128}$$

$$= \frac{2\, e^{-2\omega_0 \ell}}{1+e^{-4\omega_0 \ell}} = \left(\cosh(2\omega_0 \ell)\right)^{-1} \tag{129}$$

All the derivatives of (129) can be evaluated at $\varphi=0$ and the difficulty with moments illustrated in (127) has disappeared, e.g.,

$$\overline{\Delta(\ell)} = i \frac{\partial}{\partial \varphi} \left(\cosh 2\omega_0(\varphi)\ell\right)^{-1} \Big|_{\varphi=0} \tag{130}$$

$$= \frac{2\ell}{i} \left[\frac{\sinh(2\omega_0 \ell)}{\cosh^2(2\omega_0 \ell)} \frac{d\omega_0(\varphi)}{d\varphi}\right]_{\varphi=0} = \frac{K\ell^2}{4}$$

Other series expressions resulting from Yang's oscillator theory can also be summed, e.g., (121) becomes

$$f(\ell,\theta,\varphi) = 2\alpha^2 e^{-2\omega_0 \ell} e^{-F^2/2} \sum_{N=0}^{\infty} \frac{\left[e^{-4\omega_0 \ell}\right]^N}{N!} L_N(\xi^2) \tag{131}$$

and with the use of the generating function (118) this becomes

$$f(\ell,\theta,\varphi) = 2\alpha^2 e^{-2\omega_0 \ell} e^{-F^2/2} \frac{e^{-F^2\left(\frac{e^{-4\omega_0 \ell}}{1-e^{-4\omega_0 \ell}}\right)}}{\left(1-e^{-4\omega_0 \ell}\right)} \tag{132}$$

$$= \frac{\alpha^2}{\sinh 2\omega_0 \ell} e^{-F^2/2\left(\frac{\cosh 2\omega_0 \ell}{\sinh 2\omega_0 \ell}\right)} \tag{133}$$

The $\varphi \to 0$ limit of (133) is $f(\ell,\theta,\varphi\to 0) = \frac{e^{-\theta^2/K\ell}}{K\ell}$ (134)

a Gaussian angular distribution of width $K\ell$, the correct result, but one which would not be obtained by setting $\beta=0$ first in (121).

The expressions (129), (133) are far more compact than their counter parts (122), (121) and have superior analytic properties. The summations which were used to obtain them have had an interesting by-product, they have completely removed everything of the quantum oscillator from the results. We will suggest here and later demonstrate that Yang's quantum oscillator was elegant but irrelevant computational machinery. It introduced an elaborate and very misleading structure into the theory.

A result contained within Yang's theory that we can pursue is the singularity structure contained within (129). When $\cosh 2\omega_0(\beta)\ell = 0$ the Fourier transform of the longitudinal density diverges. This occurs for special values of β which we obtain from

$$\frac{2\omega_0(\beta_n)\ell}{i} = \pm(2n+1)\frac{\pi}{2} \qquad (135)$$

where n=0,1,2,. With the definition for ω_0, (135) becomes

$$\beta_n = +\frac{i(2n+1)^2\pi^2}{2K\ell^2} \qquad (136)$$

This allows us to invert the Fourier transform by complex contour integration. Closing a contour in the upper half complex β plane gives

$$f(\ell,\Delta) = \frac{1}{2\pi}\oint_{u\,HP} d\beta\,\frac{e^{i\beta\Delta}}{\cosh 2\omega_0(\beta)\ell} = \sum_{n=0}^{\infty} i\beta_n\, e^{i\beta_n\Delta} \qquad (137)$$

where the β_n are the residues at the poles ξ_n. If we work out the β_n and express this result using the variable $v = 2\Delta/\pi$ we have with $\bar{\Delta} = K\ell^2/4$

$$f(\ell, v) = \frac{\pi}{4} \sum_{n=0}^{\infty} (-1)^n (2n+1)\, e^{-\frac{(2n+1)^2 \pi^2 v}{16}} \qquad (138)$$

as an alternative to (108).

The quantum oscillator machinery that we used to obtain this series isn't providing us with sufficient guidance to say very much about it. We can nonetheless pursue the suggestion that (138) is more fundamental than (108), e.g., in an energy dependent problem eigenvalues must disappear but poles might remain, providing us with a different way of representing the solution and analyzing the problem. The small angle energy dependent analysis given in Chapter (V) will answer questions like this and also provide us with the machinery necessary to handle the large angle problem.

E. The Moments Development

We will refer to the works of Spencer[16], Adawi[17] and Kessaris[18] as the moments development. The general objective was the construction of spatial distributions by the moments method, especially longitudinal or penetration distributions. This development, which used Lewis' equation as the equation of motion, essentially began where Lewis had stopped.

Spencer, being the first to actually construct distributions using

the moment relations, faced a number of problems. His methods of handling them were discussed in his 1955 work and he later presented the results of a large number of electron calculations done in many different materials with various initial energies. Adawi followed and extended the approach into a higher and more therapeutically useful energy region. Both Spencer and Adawi had focused their attention on energy dissipation curves. Since they are closely related to energy absorption distributions, both are potentially important in medical physics applications. Kessaris, working in the same energy region as Adawi, recomputed these curves more carefully by computing more moments (than Adawi) and also considerably broadened the scope of the calculations by constructing a number of other relevant distributions as well. Kessaris, who had produced calculations that treatment planners should have been very interested in, had followed, like Adawi, Spencer's ideas very closely.

Spencer, who laid the groundwork for this applied development, found it necessary to introduce and incorporate the function fitting approach into his calculations. The approach had two essential steps. First we compute the numerical values of the moments of the distribution, then we find a function or functions that will reproduce those numbers. Both steps require elaboration but we will concern ourselves here only with the first.

Spencer noted that attempts to construct distributions from a knowledge of the first few numerical values of moments were generally

unsatisfactory because the information contained seemed insufficient for such a construction. While he felt that a knowledge of all the numerical values of moments should theoretically yield the distribution, he also noted that in practice only a finite number of them could actually be computed, and even these only with imperfect accuracy. In Spencer's opinion, constructing a spatial distribution was equivalent to extrapolating the finite set of imperfectly known numerical values of moments, which we could compute, to infinite order. The essential information which was missing, according to Spencer, was something which would allow us to make this extrapolation with confidence. Spencer identified this something as the asymptotic behavior of the distribution, its $\Delta \to 0$ behavior, which he labeled "the deep penetration trend".

This behavior had already been calculated by Wick[19] and so Spencer sometimes called it a Wick-type asymptotic behavior. Wick, who had earlier been solving a neutron penetration problem, made the small angle approximation at the end of his paper, recognized the Schrodinger equation, then made the Gaussian approximation and calculated the $\Delta \to 0$ part of the distribution from the most deeply bound state of a quantum harmonic oscillator. Yang's calculation with the quantum oscillator was complete, exact and fully analytic. It superceded Wick's work. The behavior being referred to is the $\nu \to 0$ term in (108), $f(\ell, \nu \to 0) = 2 e^{-\nu/\nu} / \pi^{1/2} \nu^{3/2}$ which had as its Fourier transform $2 e^{-2\omega_0 \ell}$.

Thus, in Spencer's development, the behavior of the spatial distribution should be $f(\ell, \Delta \to 0) \sim \Delta^{-3/2} e^{-b/\Delta}$ where b is some number, or

something equivalent to it such as $f(x \to l) \sim (-\ln(x/l))^{-3/2} e^{b/\ln(x/l)}$, as he stated in his Section 5.

The numerical values of the spatial moment integrals would then have the form $(\pi/b)^{1/2} e^{-[4b(n+1)]^{1/2}}$ for high n, as he writes in his equation #30. This suggested to Spencer that the computed numerical values of moments would plot up into a straight line, for high n, if one plotted the logarithims of the numerical values of moments against $(n+1)^{1/2}$.

Spencer also worked out recursion relations that allowed him to compute the numerical values of many moments of the spatial distributions. When he plotted up the first twenty in the manner just discussed, they did indeed plot into straight lines. Spencer gave an example of this in his Fig. 2, which we have reproduced as our Figure 5. Spencer thus stated that he could very clearly recognize the trend predicted by a Wick-type asymptotic calculation. It was the "break" that made the construction of spatial distributions possible, as he writes in the second page of his introductory remarks. Spencer still had many problems related to finding functions that would reproduce these numbers, but we will not be concerned with that part of his development here.

Spencer's demonstrations had not proved anything. He seems never to have considered the possibility that the numerical values of moments might not be meaningful numbers. It would not then be meaningful to compute them, to plot them, to extrapolate them, to work out recursion

relations for them or to find functions that would reproduce them. We can illustrate the incorrectness of argument by choosing an example from Kessaris' work.

Kessaris[18] considered the problem of high energy electron beams (10-20 MeV) penetrating water, the example of greatest interest to treatment planners. His calculation of the time dependent (primary) particle density was his most important calculation. His result (Kessaris' equation (26)) expressed in our notation was

$$f(\ell, z) = \pi^{-1/2} d\, e^{2d(1+A)^{1/2}} \frac{z^A}{\ell^{A+1}} \frac{e^{d^2/\ln(z/\ell)}}{[-\ln z/\ell]^{3/2}} \qquad (139)$$

where d and A are numbers which are to be read off a graph (Kessaris' Fig. 6). He obtained this result by numerically integrating Lewis' spatial moment equations, (80). At each time of interest he computed the numerical values of the first ten moments of the spatial distribution. He plotted these values on semilog paper against $(n+1+A)^{1/2}$ and obtained a straight line (to within an accuracy of 1/2% or less) when A was suitably chosen. Thus, his result not only reproduced the numerical values of moments, but also contains the deep-penetration or $z \to \ell$ behavior of Spencer's analysis, the behavior that Spencer felt would allow him to extrapolate the finite set of numbers actually computed to infinite order with confidence.

Kessaris' calculation was elaborate and required a high degree of computer force to conduct it. He appears to have made every effort to

produce results which were both accurate and reliable and he generally conducted his calculation with great diligence, as had Spencer. Kessaris did this calculation for three different initial energies, 10, 15 and 20 MeV electrons. All three calculations worked the same way and exhibited the same type of behavior. It will suffice to take an example from only one.

Let us choose the case of 20 MeV electrons after they have travelled a distance of 1 cm in water. This distance corresponds to approximately 10^4 collisions, so the Gaussian approximation would be reasonably good. The approximations of small angles and energy independent scattering would also be unobjectionable under these conditions, so a comparison of Kessaris' result against that of Yang is then valid and the two should agree. The comparison is shown in our Fig (6). Kessaris' result is in error by about an order of magnitude and all three of his calculations contain similar errors. If we had made many comparisons with Kessaris' results, we would find that the size of his error depends on the time at which we choose to look at it. Generally speaking, the longer the time the better his result, the earlier the time the larger the error. If we recall the remarks of Chapter II Section D, the proper way to evaluate a diffusion theory is to look early into it, in the earliest stages of its development. Thus, when the moments development is examined properly, at early times as in Fig. (6), it is seen to be in significant error.

The greatest error of the function-fitting approach was not the size of the numerical errors that it was capable of, nor even the fact

that its arguments were fundamentally unreliable and incorrect. It was the manner in which the information was being carried. Functions like (139), and all the functions of Spencer's function-fitting approach, come from tables of integrals and have nothing to do with the problem. This makes them theoretically worthless. Kerraris' results, even if they had been highly accurate numerically, would have been practically worthless in treatment planning applications as well. The high degree of computer muscle required to obtain them would have been sufficient to disqualify the whole approach there.

Each theory discussed in this section had theoretical difficulties associated with it. As the theory developed, problems from previous analyses were being carried along and compounded. Spencer, for example, had misidentified the missing information, the complex plane structure, and pursued a misleading and irrelevant structure, the quantum oscillator. The end result, the moments development, was so thoroughly riddled with error it is unsalvagable. To solve the multiple scattering problem in a theoretically meaningful way we begin by going back and redoing the most pivotal analyses. Developing the theory further then leads to a theory which has practical potential in the applications of interest.

IV. Re-examination of Lewis' Theory

Much of the content within Lewis' theory was simply being lost because it had been pursued by numerical analysis. The first and most pivotal problems had been introduced by Snyder and Scott on line (56), as we have already noted, where they chose a specific functional form for the deflecting cross-section. We therefore begin by re-examining the angular distribution without any specific choice of cross-section but we retain the small angle approximation. We then make a continuous passage to large angles which requires the more general Lewis formalism. We finally consider spatial distributions, the topic that we are most interested in. We ignore any energy dependence throughout this chapter since it would unnecessarily complicate the arguments.

A. The Angular Distribution

We consider the angular distribution associated with (49)

$$\frac{\partial f(l,\theta_x,\theta_y)}{\partial l} = \frac{1}{\mu_s \sigma} \iint d\theta_x' \, d\theta_y' \, \frac{d\sigma(\theta)}{d\Omega} \left[f(l,\theta_x',\theta_y') - f(l,\theta_x,\theta_y) \right] \tag{140}$$

here $\theta = \{ (\theta_x' - \theta_x)^2 + (\theta_y' - \theta_y)^2 \}^{1/2}$ as before. We first rewrite (140) the basic Snyder-Scott (small angle) equation in a way that exhibits the cylindrical symmetry of the problem. This is a bit repetitious but necessary since the transition from small angles requires that we have our equations in this form. We define the two dimensional Fourier transforms

$$f(l,\theta_x,\theta_y) = \frac{1}{(2\pi)^2} \iint d\tau_x \, d\tau_y \, e^{i \vec{\tau} \cdot \vec{\theta}} f(l,\tau_x,\tau_y) \tag{141a}$$

$$d\sigma(\theta_x,\theta_y) = \frac{1}{(2\pi)^2} \iint d\tau_x \, d\tau_y \, e^{i \vec{\tau} \cdot \vec{\theta}} \, d\sigma(\tau_x,\tau_y) \tag{141b}$$

which are the analogues of (53a) and (53b). The cylindrical symmetry derives from the fact that $d\sigma$ depends only on the magnitude of its argument, θ , rather than its Cartesian projections θ_x, θ_y separately. Its Fourier transform then depends only on $(\tau_x^2 + \tau_y^2)^{1/2}$ and not τ_x, τ_y separately, while the same is true for $f(\ell, \tau_x, \tau_y)$ which can be replaced by $f(\ell, \tau)$. With (141a), (141b), the equation of motion (140) becomes

$$\frac{\partial f(\ell,\tau)}{\partial \ell} = - K(\tau) f(\ell,\tau) \tag{142}$$

where

$$K(\tau) = \frac{1}{\mu_s}\left[1 - \frac{1}{\sigma}\frac{d\sigma(\tau)}{d\Omega}\right] = \frac{1}{\mu_s \sigma}\left[\frac{d\sigma(\tau=0)}{d\Omega} - \frac{d\sigma}{d\Omega}(\tau)\right] \tag{143}$$

The quantity $d\sigma(\tau)$ is defined by the inversion of (141b)

$$\frac{d\sigma}{d\Omega}(\tau_x,\tau_y) = \iint d\theta_x\, d\theta_y\, e^{-i\vec{\tau}\cdot\vec{\theta}} \frac{d\sigma(\theta)}{d\Omega} = \int_0^\infty \theta\, d\theta \frac{d\sigma(\theta)}{d\Omega} \int_0^{2\pi} d\alpha\, e^{-i\tau\theta\cos\alpha} \tag{144}$$

With the integral representation for the zero order Bessel function

$$J_0(\tau\theta) = \frac{1}{2\pi}\int_0^{2\pi} d\alpha\, e^{i\tau\theta\cos\alpha} \tag{145}$$

(144) becomes

$$\frac{d\sigma(\tau)}{d\Omega} = 2\pi \int_0^\infty \theta\, d\theta\, J_0(\tau\theta) \frac{d\sigma(\theta)}{d\Omega} \tag{146}$$

so that (143) may be written

$$K(\tau) = \frac{2\pi}{\mu_s}\int_0^\infty \theta\, d\theta \left[1 - J_0(\tau\theta)\right] \frac{1}{\sigma}\frac{d\sigma(\theta)}{d\Omega} \tag{147}$$

The solution of (142) with the initial condition $f(\ell=0,\tau)=1$ is

$$f(\ell,\tau) = e^{-K(\tau)\ell} \tag{148}$$

and the angular distribution (141a) then becomes

$$f(\ell,\theta,\phi) = \frac{1}{2\pi}\int_0^\infty \tau\, d\tau\, J_0(\tau\theta)\, f(\ell,\tau) \qquad (149)$$

in cylindrical variables. There is no explicit azimuthal dependence in (149) because of the cylindrical symmetry of the problem. To construct an angular distribution we need only (147), (148) and (149). They are the small angle analogues of Lewis' equations (73), (71)' and (69a) respectively.

Two series developments of the angular distribution can be given which correspond to either very few or very many collisions. In the case of very few collisions we could expand (148) as

$$f(\ell,\tau) = 1 - K(\tau)\ell + \frac{(-K(\tau)\ell)^2}{2!} + \ldots \qquad (150)$$

and, after we invert the transform (149), we would have an expansion in which particles do not scatter, scatter only once, twice, etc. This was the series that Snyder and Scott pursued in their section (4). That series concerns very few particles if there are many collisions and we are far more interested in an alternative development which begins by utilizing the power series expansion of J_0 i.e.,

$$J_0(\tau\theta) = 1 - \frac{(\tau\theta)^2/4}{(1!)^2} + \frac{((\tau\theta)^2/4)^2}{(2!)^2} - \frac{((\tau\theta)^2/4)^3}{(3!)^2} + \ldots \qquad (151)$$

so that $K(\tau)$ from (147) becomes

$$K(\tau) = \frac{1}{\mu_s}\int_0^\infty 2\pi\theta\, d\theta \left\{ \frac{\tau^2\theta^2}{4} - \frac{1}{(2!)^2}\left(\frac{\tau^2\theta^2}{4}\right)^2 + \ldots \right\} \frac{1}{\sigma}\frac{d\sigma(\theta)}{d\Omega}$$

$$= \frac{1}{\mu_s}\left\{ \frac{\langle\theta^2\rangle}{(1!)^2}\left(\frac{\tau^2}{4}\right) - \frac{\langle\theta^4\rangle}{(2!)^2}\left(\frac{\tau^2}{4}\right)^2 + \ldots \right\} \qquad (152)$$

where $\langle\theta^2\rangle$ means that we average with the small angle cross-section, as before. We will temporarily exclude the pathological case of charged particles for which $\langle\theta^2\rangle, \langle\theta^4\rangle,$ ...would not exist. The expansion (152) is a moments expansion and is very general. It is important that it is not specific, i.e., we can represent the situation without stating exactly what the differential cross section actually looks like. Using (144), we could then expand the exponent around its leading term as

$$f(l,T) = e^{-l/\mu_s\left\{\langle\theta^2\rangle\frac{T^2}{4} - \frac{\langle\theta^4\rangle}{(2!)^2}\left(\frac{T^2}{4}\right)^2 + \frac{\langle\theta^6\rangle}{(3!)^2}\left(\frac{T^2}{4}\right)^3 - +\ldots\right\}}$$

$$= \left\{1 + \left(\frac{l}{\mu_s}\right)\left[\frac{\langle\theta^4\rangle}{(2!)^2}\left(\frac{T^2}{4}\right)^2 - \frac{\langle\theta^6\rangle}{(3!)^2}\left(\frac{T^2}{4}\right)^3 + -\ldots\right]\right.$$

$$\left. + \frac{1}{2!}\left(\frac{l}{\mu_s}\right)^2\left[\ \right]^2 + \frac{1}{3!}\left(\frac{l}{\mu_s}\right)^3\left[\ \right]^3 + ..\right\} e^{-\frac{l\langle\theta^2\rangle T^2}{\mu_s 4}}$$

with (153) in (149) we obtain (153)

$$f(l,\theta,\phi) = \left\{1 + n\left[\frac{\beta_2}{(2!)^2}\frac{L_2(\theta^2/\bar{\theta^2})}{n^2} - \frac{\beta_3}{(3!)^2}\frac{L_3(\theta^2/\bar{\theta^2})}{n^3} + \ldots\right]\right.$$

$$+ \frac{n^2}{2!}\left[\frac{\beta_2^2}{(2!)^4}\frac{L_4(\theta^2/\bar{\theta^2})}{n^4} - \frac{2\beta_2\beta_3}{(2!)^2(3!)^2}\frac{L_5(\theta^2/\bar{\theta^2})}{n^5} + ..\right]$$

$$\left. + \frac{n^3}{3!}\left[\ \right] + \ldots\right\}\frac{e^{-\theta^2/\bar{\theta^2}}}{\pi\,\bar{\theta^2}} \qquad (154)$$

where we have used the notation n for the number of collisions, l/μ, $\bar{\theta^2} = n\langle\theta^2\rangle$, Lm for Laguerre polynominals and $\langle\theta^{2m}\rangle/(\langle\theta^2\rangle)^m \equiv \beta_m$. In the limit of $n\to\infty$, but in a way that n remains finite, we have

$$\underset{n\to\infty}{f(l,\theta,\phi)} = \frac{e^{-\theta^2/\bar{\theta^2}}}{\pi\,\bar{\theta^2}} \qquad (155)$$

a result that we could have obtained separately and independently through the central limit theorem. This is, of course, the Gaussian approximation and means that the details of the deflecting cross section become less important with time and only its average features survive if we wait long enough. The additional terms in (154) show the approach towards the Gaussian limit and simply correct for the fact that n is not infinite. The closely related Fokker-Planck approximation keeps n finite but sets $\langle\theta^4\rangle, \langle\theta^6\rangle = 0$ achieving the same effect.

As a by-product of the above demonstration we have some additional machinery to work with, a different and general way of representing the expansion (152). We can use it to define spherical moments of the deflecting cross section which can replace the quantities $\langle\theta^2\rangle, \langle\theta^4\rangle \ldots$ that would not exist in a charged particle problem.

The large angle analogue of (147) is Lewis' expression (73). The replacement of $P_j(\cos\theta)$ by $J_0(J\theta)$ for small angles derives from the fact that Legendre's equation collapses into Bessel's equation for small angles. From that fact we would also derive the association $J^2 \leftrightarrow j(j+1)$. It would not be sufficient to use the usual Legendre polynominals etc. in expression (73). To insure continuous contact between the small and large angle expressions we would match K_j on $K(J)$ smoothly. This requires a series development of $P_j(\cos\theta)$ in powers of $j(j+1)$ analogous to the series development of $J_0(J\theta)$ in powers of J^2 which was used in (151). This is a Taylor series which takes derivatives with respect to order and has the form

$$P_j(\cos\theta) \to P(J^2, \cos\theta) = P(0, \cos\theta) + \left[\frac{\partial P}{\partial J^2}(0, \cos\theta)\right] J^2 + \left[\frac{\partial^2 P(0, \cos\theta)}{\partial (J^2)^2}\right] \frac{(J^2)^2}{2!} + \ldots \tag{156}$$

To obtain this series we integrate Legendre's equation beginning with $J^2 = 0$, and fix all integration constants by requiring that (156) agree with (151) for small angles. The first several terms may be written

$$P_j(\cos\theta) = 1 - j(j+1)\left\{ \sin^2\theta/2 + \tfrac{1}{2}(\sin^2\theta/2)^2 + \tfrac{1}{3}(\sin^2\theta/2)^3 + \ldots \right\}$$

$$+ (j(j+1))^2 \left\{ \tfrac{1}{4}(\sin^2\theta/2)^2 + \tfrac{2}{9}(\sin^2\theta/2)^3 + \tfrac{3}{16}(\sin^2\theta/2)^4 + \ldots \right\}$$

$$- + \ldots \qquad (157)$$

This recovers the usual Legendre polynominals for discrete values $j = 0, 1, \ldots$ but also allows transition to continuous J without difficulty. Thus (73) could be written

$$K_j = -\frac{1}{\mu_s}\left\{ \left\langle \frac{\partial P(0,\cos\theta)}{\partial J^2} \right\rangle j(j+1) + \left\langle \frac{\partial^2 P(0,\cos\theta)}{\partial (J^2)^2} \right\rangle \frac{(j(j+1))^2}{2!} + \ldots \right\} \qquad (158)$$

where $\langle\ \rangle$ now means average over 4π geometry using the large angle expression for $d\sigma/d\Omega$. A comparison of (152) and (158) then allows us to define spherical moments. For example, comparing the first term in each series, and using also (157) gives

$$\langle \theta^2 \rangle \longrightarrow 4 \left\langle \sin^2\theta/2 + \tfrac{1}{2}(\sin^2\theta/2)^2 + \tfrac{1}{3}(\sin^2\theta/2)^3 + \ldots \right\rangle \qquad (159)$$

This would eliminate the moments problem indicated in (65), if we use the first line of (56). By performing the average with the large angle cross section, the terms on the right exist even if the term on the left does not. However, this series of terms will converge so quickly that the first term dominates all the others and the approximation

$$\langle \theta^2 \rangle \simeq 4 \langle \sin^2\theta/2 \rangle \qquad (160)$$

would be more than adequate. Higher order terms $\langle\theta^4\rangle, \langle\theta^6\rangle \ldots$ could also be redefined by a comparison of (152) and (158).

The decomposition of K_j into the power series (158) was fundamental to Lewis' theory but was missing from it. The two functions $K(\tau)$ and K_j, which we can now use interchangably, control all the dynamics of the multiple scattering problem since it is only through them that the deflecting cross section enters our expressions. Any analytically acceptable representation of them requires that these expansions exist, but the numerically accurate representations of them which had been given in the literature were incompatible with it. Lewis' spatial moment equations, (80), for example, recognize and respect the spherical structure of K_j and won't work properly without it. Representing these functions correctly does not solve all of our difficulties; it is only a first step towards their solution.

B. Perturbing The Penetration Distribution

We consider the construction of a spatial distribution that corresponds to the angular distribution given by (154). We first solve

$$\frac{\partial f(\ell,\theta_x,\theta_y,\Delta)}{\partial \ell} = -\frac{\theta^2}{2}\frac{\partial f}{\partial \Delta} + \frac{1}{\mu_s \sigma}\iint d\theta_x' d\theta_y' \frac{d\sigma}{d\Omega}(\theta)\left[f(\ell,\theta_x',\theta_y') - f(\ell,\theta_x,\theta_y)\right] \tag{161}$$

in order to obtain $f(\ell,\Delta)$. With the Fourier transforms

$$f(\ell,\theta_x,\theta_y,\Delta) = \frac{1}{(2\pi)^3}\iiint d\tau_x d\tau_y d\xi\, e^{i(\vec{\tau}\cdot\vec{\theta}+\xi\Delta)} f(\ell,\tau,\xi) \tag{162}$$

(161) becomes

$$\frac{\partial f(\ell,J,\beta)}{\partial \ell} = \frac{i\beta}{2}\left(\frac{\partial^2}{\partial J^2} + \frac{1}{J}\frac{\partial}{\partial J}\right)f - K(J)\,f(\ell,J,\beta) \qquad (163)$$

and we would use the expansion (152) which we write as

$$K(J) = \frac{K}{4}J^2 + \delta K(J) \qquad (164)$$

where $K = \langle\theta^2\rangle/\mu_s$ and δK represents all the other terms in the expansion. We will treat the terms $\delta K(J)$ which appear in (163) as perturbations or corrections to

$$\frac{\partial f(\ell,J,\beta)}{\partial \ell} = \frac{i\beta}{2}\left(\frac{\partial^2}{\partial J^2} + \frac{1}{J}\frac{\partial}{\partial J}\right)f - \frac{K}{4}J^2 f \qquad (165)$$

which is a problem that can be solved exactly with Yang's eigenvalue approach. It is simply the Fourier transform of (113) and the two can be solved in the same manner. The solution to (165) also may be written in the form (119), where the eigenfunctions are given by (116). However, we would now use $\mathcal{J} = J/\alpha$, $\alpha = (2i\beta/K)^{1/4}$. The eigenvalues $\omega_N = (2N+1)2\omega_0$, with $\omega_0 = K\alpha^2/4$, are unchanged. With the initial conditions $f(\ell=0,J,\beta) = 1$, we have $A_N = 2^{1/2}(-1)^N$. Once we alter the problem by adding corrections terms δK, the eigenfunctions and eigenvalues all change, $\omega_N \to \omega_N + \delta\omega_N$, $\psi_N \to \psi_N + \delta\psi_N$. In the example below we consider only the first order changes for which non-degenerate (first order) perturbation theory gives[14]

$$\delta\omega_N = (\psi_N, \delta K\,\psi_N) \qquad (166a)$$

$$\delta\psi_N = \sum_{M\neq N} \frac{(\psi_M, \delta K\,\psi_N)}{(\omega_N - \omega_M)}\,\psi_M \qquad (166b)$$

Once we have worked out these expressions the solution to (163) will then have the form

$$f(\xi,\tau,\beta) = \sum_N A'_n \psi'_n e^{-\omega'_n \xi} \tag{167}$$

where the primes indicate that we use the new eigenfunctions and eigenvalues and new constants which are determined from the initial conditions. To obtain them we need the integrals

$$(\psi_m, \delta K \psi_N) = \int_0^\infty \xi\, d\xi \; C_m L_m(\xi^2) e^{-\xi^2/2} \cdot$$

$$\cdot \frac{1}{\mu_s}\left[-\frac{\langle\theta^4\rangle}{(2!)^2}\left(\frac{\alpha^2\xi^2}{4}\right)^2 + \frac{\langle\theta^6\rangle}{(3!)^2}\left(\frac{\alpha^2\xi^2}{4}\right)^3 - +\ldots\right] \cdot$$

$$\cdot C_N L_N(\xi^2) e^{-\xi^2/2} \tag{168}$$

where we have used $J = \alpha\xi$. The normalizing constants are $2^{N}/N!$ as before. These integrals are most easily evaluated by using the recursion relations for the Laguerre polynomials

$$\rho L_N(\rho) = (2N+1) L_N(\rho) - N^2 L_{N-1}(\rho) - L_{N+1}(\rho) \tag{169}$$

so that

$$\rho^2 L_N = (6N^2+6N+2) L_N - 4N^3 L_{N-1} - 4(N+1) L_{N+1} + N^2(N-1)^2 L_{N-2} + L_{N+2} \tag{170}$$

is obtained by applying (169) twice. It will be sufficient for our purposes to retain only the first term in the set of perturbations, the term containing ξ^4. Then

$$\int_0^\infty \xi\, d\xi \; C_m L_m(\xi^2) e^{-\xi^2/2} \; \xi^4 \; C_N L_N(\xi^2) e^{-\xi^2/2}$$

$$= (6N^2+6N+2)\delta_{mN} - 4N^2\delta_{m,N-1} - 4(N+1)^2\delta_{m,N+1}$$

$$+ N(N-1)\delta_{m,N-2} + (N+2)(N+1)\delta_{m,N+2} \tag{171}$$

So that

$$\delta\omega_N = \frac{1}{\mu_s}\left[-\frac{\langle\theta^4\rangle}{(2!)^2}\left(\frac{\alpha^2}{4}\right)^2\right](6N^2+6N+2) \tag{172a}$$

$$\delta\psi_N = -\frac{\langle\theta^4\rangle}{\mu_s(2!)^2}\left(\frac{\alpha^2}{4}\right)^2\left[\frac{-N^2}{\omega_0}\psi_{N-1} + \frac{(N+1)^2}{\omega_0}\psi_{N+1} + \frac{N(N-1)}{8\omega_0}\psi_{N-1} - \frac{(N+1)(N+2)}{8\omega_0}\psi_{N+2}\right] \tag{172b}$$

where we have used $\omega_N = (2N+1)2\omega_0$ in the denominator of (166b). Since the new eigenfunctions are still orthonormal, the initial condition $f(\ell=0,\tau,\beta)=1$ now gives

$$A'_N = \int_0^\infty \xi\, d\xi\, \psi'_N(\xi) = \int_0^\infty \xi\, d\xi\,\left(\psi_N(\xi) + \delta\psi_N(\xi)\right) \tag{173}$$

Since

$$\int_0^\infty \xi\, d\xi\, L_N(\xi^2)\, e^{-\xi^2/2} = (-1)^N (N!) \tag{174}$$

$$A'_N = 2^{1/2}(-1)^N\left[1 + \frac{1}{\mu_s}\frac{\langle\theta^4\rangle}{(2!)^2}\left(\frac{\alpha^2}{4}\right)^2\left\{\frac{5}{4}\,\frac{2N+1}{\omega_0}\right\}\right] \tag{175}$$

Since we are interested in the spatial density we integrate our solution over both angular variables. This is equivalent to setting $\tau = 0$ in (167), and we need the values of the new wavefunctions only at the origin. Since $\psi_n(0) = 2^{1/2}$, we have

$$\psi'_N(0) = 2^{1/2}\left[1 - \frac{\langle\theta^4\rangle}{\mu_s(2!)^2}\left(\frac{\alpha^2}{4}\right)^2\left\{\frac{3}{4}\,\frac{(2N+1)}{\omega_0}\right\}\right] \tag{176}$$

using also (172b). Then, using the notation $f(\ell,\tau=0,\beta) = f(\ell,\beta)$, (167) becomes

$$f(\ell,\beta) = \sum_N 2(-1)^N\left[1 + \frac{\langle\theta^4\rangle}{\mu_s(2!)^2}\left(\frac{\alpha^2}{4}\right)^2\frac{(2N+1)}{2\omega_0}\right] e^{-\omega'_N\ell} \tag{177}$$

by using (175) and (176). We can also make the replacement $e^{-(\omega+\delta\omega)_N \ell}$ $= (1-\delta\omega_N \ell)\, e^{-\omega_N \ell}$ since this is a first order calculation, and along with (172a), (177) becomes

$$f(\ell,\beta) = \sum 2(-1)^N \left[1+\frac{\langle\theta^4\rangle}{\mu_s(2!)^2}\left(\frac{\alpha^2}{4}\right)^2\left\{\frac{2N+1}{2\omega_0}+\ell\left(6N^2+6N+2\right)\right\}\right] e^{-\omega_N \ell} \tag{178}$$

to lowest order. The series expressions are now summed

$$2\sum_N (-1)^N e^{-\omega_N \ell} = \left(\cosh(2\omega_0 \ell)\right)^{-1} \tag{179a}$$

as in (129).

$$2\sum_N (-1)^N (2N+1)\, e^{-\omega_N \ell} = -\frac{1}{2\omega_0}\frac{\partial}{\partial \ell}\left(\cosh(2\omega_0 \ell)\right)^{-1} \tag{179b}$$

Since $(6N^2+6N+2) = 1/2 + 3/2\,(2N+1)^2$,

$$2\sum (-1)^N (6N^2+6N+2)\, e^{-\omega_N \ell} = \left[\frac{1}{2}+\frac{3}{2}\left(\frac{1}{2\omega_0}\right)^2\frac{\partial^2}{\partial \ell^2}\right]\left(\cosh(2\omega_0 \ell)\right)^{-1} \tag{179c}$$

With the definitions and (179), (178) becomes

$$f(\ell,\beta) = \left[1+\frac{\mu_s}{(2!)^2}\frac{\langle\theta^4\rangle}{(\langle\theta^2\rangle)^2}\left\{\frac{K\ell}{16}(i\beta)-\frac{1}{4}\frac{\partial}{\partial \ell}+\frac{3}{8}\ell\frac{\partial^2}{\partial \ell^2}\right\}\right]\left(\cosh(2\omega_0 \ell)\right)^{-1} \tag{180}$$

which allows us to invert the Fourier transform trivially by carrying the operators through the integral. Thus, the spatial density becomes

$$f(\ell,\Delta) = \left[1+\frac{\mu_s}{(2!)^2}\frac{\langle\theta^4\rangle}{(\langle\theta^2\rangle)^2}\left\{\frac{K\ell}{16}\frac{\partial}{\partial \Delta}-\frac{1}{4}\frac{\partial}{\partial \ell}+\frac{3}{8}\ell\frac{\partial^2}{\partial \ell^2}\right\}\right]\int_{-\infty}^{\infty}\frac{d\beta}{2\pi}\frac{e^{i\beta\Delta}}{\cosh 2\omega_0 \ell} \tag{181}$$

where the integral required in (181) was given in III D. If we use the infinite series that comes from this integral, take the indicated deri-

vatives, and then express it in terms of the variable v which was used in III D, we could rewrite (181) as

$$f^{(1)}(v) = f^{(0)}(v) + \frac{\gamma_2}{(2!)^2(2n_c)}\left[\frac{df^{(0)}}{dv} - \frac{v}{2}f^{(0)} + 3\frac{d^2}{dv^2}(v^2 f^{(0)})\right] \qquad (182)$$

where $f^{(0)}$ is the unperturbed result, given by (108) or (138), although the simplest form to use for evaluation would be (109). Here $\gamma_2 = \langle\theta^4\rangle/\langle\theta^2\rangle^2$, $n = \frac{\ell}{\mu_c}$ is the number of collisions, which is the notation used in association with (154). If we had a differential cross section of the form $d\sigma \sim e^{-\theta^2/\theta_0^2}$ then $\langle\theta^2\rangle = \theta_0^2$, $\langle\theta^4\rangle = 2\theta_0^4$, and the overall strength of the perturbation would be on the order of $\frac{\gamma_2}{2n_c} \sim \frac{1}{n_c}$. The rearrangement from the unperturbed result would be fairly small, even with as little as 10 collisions, for both the angular and spatial distributions. If we chose a more realistic charged particle cross section, e.g. (56), then γ_2 would be on the order of $\langle(\sin^2\theta/2)^2\rangle / \langle\sin^2\frac{\theta}{2}\rangle^2$, as the discussion leading to (160) indicates. Working out these integrals using (56) gives $\gamma_2 \cong [\theta_s \ln(2/\theta_s)]^{-2}$.

The screening angle is given by $\theta_s = (k_{inc}\, a)^{-1}$, and if we use a wave number corresponding to 10 MeV electrons, and a typical atomic dimension $a \simeq 10^{-8}$ cm., then γ_2 is on the order of 10^5, and it takes a tremendous number of collisions before something as mild as a first order perturbation calculation, with only one correction term, can adequately represent the situation.

Keeping many correction terms in a perturbation calculation and pushing it to high order would not be theoretically interesting or practically useful. A fast procedure, useful at short times, e.g.,

$10^2 - 10^3$ collisions, would be to use the expressions for $K(J)$ and K_j given by Lewis and Snyder and Scott phenomenologically. One could define a convergence number, J_c, by the relation $K(J_c)\ell = 1$, and then replace the exact expression (148) by a phenomenological term $f^{phen.}(\ell, J) = e^{-J^2/J_c^2(\ell)}$. This would give Gaussian angular distributions and would only alter the way that we compute the parameters of the distributions. It would easily and accurately reproduce the numbers that Snyder and Scott generated, except for the part of the distribution associated with the Rutherford tail, but we will not pursue the topic further.

C. Spatial Moment Problems

The perturbation calculation given in the last section has certain exact features to it, features that would remain unaltered by keeping more terms or by going to higher orders. Here we examine these features and consider some of the implications.

If we return to (180) and take the indicated derivatives, the result may be written

$$f(\ell,q) = \left[1 + \frac{\langle\theta^4\rangle}{(2!)^2\langle\theta^2\rangle}\left(\frac{iq\ell}{8}\right)\left\{\frac{1}{2\omega_0\ell}\frac{\sinh 2\omega_0\ell}{\cosh 2\omega_0\ell} + 2 - \frac{3}{\cosh^2 2\omega_0\ell}\right\}\right]\left(\cosh 2\omega_0\ell\right)^{-1} \tag{183}$$

If we expand (183) in powers of q, keeping terms up to order q^2, it may be written as

$$f(\ell,q) = 1 - iq\left(\frac{K\ell^2}{4}\right) + \frac{(-iq)^2}{2!}\left(\frac{5}{3} + \frac{4}{3}\frac{B_2}{n_c}\right)\left(\frac{K\ell^2}{4}\right)^2 + \ldots \tag{184}$$

where $K = \langle \theta^2 \rangle \mu_i^{-1}$ by definition. By comparing with (124), we can simply read off the moments of the longitudinal distribution, where the moments were defined by (125). We obtain

$$\overline{\Delta^0(\ell)} = 1 \;,\; \overline{\Delta(\ell)} = K\ell^2/4 \;,\; \overline{\Delta^2(\ell)} = \left(\frac{5}{3} + \frac{4}{3}\frac{\beta_2}{n_c}\right)(\bar{a})^2 \qquad (185)$$

Within the context of the small angle approximation for which these expressions were derived, we can show that they are exact, that these three moments would be unaffected by higher orders or more terms in a perturbation calculation. To prove this we use a moments approach on (163) which derives exact expressions. The approach is a small angle analogue of Lewis' spatial moment procedure.

To begin, we chose a representation of the solution to (163) in the form

$$f(\ell, J, q) = \sum_{m=0}^{\infty} f^{(m)}(\ell, q)\,\frac{(J^2)^m}{m!} \qquad (186)$$

From this definition we have $f^{(m)}(\ell, q) = \dfrac{d^m}{d(J^2)^m} f(\ell, J, q)\Big|_{J^2=0}$. We also use an identical representation for $K(J)$, where the coefficients $K^{(m)}$ are defined by the expansion (152). Without the existence of this expansion, the procedure given below would not work. Inserting (186) and the expansion of $K(J)$ into (163) gives

$$\frac{d f^{(m)}(\ell, q)}{d\ell} = 2iq(m+1) f^{(m+1)}(\ell, q) - \sum_{n=0}^{m} \frac{m!}{n!(m-n)!} K^{(n)} f^{(m-n)}(\ell, q) \qquad (187)$$

by equating the coefficients of equal powers of J^2. The Fourier transform of the spatial density is what we are after, and is given by

$f^{(m=0)}(\ell,\xi) = f(\ell,\tau=0,\xi)$. Since we intend to compute the first three moments we need the first three equations which we write out explicitly

$$\frac{\partial f^{(m=0)}(\ell,\xi)}{\partial \ell} = 2i\xi\, f^{(m=1)}(\ell,\xi) \tag{188a}$$

$$\frac{\partial f^{(m=1)}(\ell,\xi)}{\partial \ell} = 2(2i\xi) f^{(m=2)}(\ell,\xi) - K^{(1)} f^{(m=0)}(\ell,\xi) \tag{188b}$$

$$\frac{\partial f^{(m=2)}(\ell,\xi)}{\partial \ell} = 3(2i\xi) f^{(m=3)}(\ell,\xi) - \left[2K^{(1)} f^{(m=1)}(\ell,\xi) + K^{(2)} f^{(m=0)}(\ell,\xi)\right] \tag{188c}$$

We don't use these equations as they stand, but expand them as

$$\frac{\partial}{\partial \ell}\left[f^{(0)}(\ell,\xi=0) + \frac{\partial f^{(0)}(\ell,\xi=0)}{\partial \xi}\xi + \frac{\partial^2 f^{(0)}(\ell,\xi=0)}{\partial \xi^2}\frac{\xi^2}{2!} + \dots\right] = 2i\xi\left[f^{(1)}(\ell,\xi=0) + \frac{\partial f^{(1)}(\ell,\xi=0)}{\partial \xi}\xi + \dots\right] \tag{189a}$$

$$\frac{\partial}{\partial \ell}\left[f^{(1)}(\ell,\xi=0) + \frac{\partial f^{(1)}(\ell,\xi=0)}{\partial \xi}\xi + \dots\right] = 2(2i\xi)\left[f^{(2)}(\ell,\xi=0) + \dots\right] - K^{(1)}\left[f^{(0)}(\ell,\xi=0) + \frac{\partial f^{(0)}(\ell,\xi=0)}{\partial \xi}\xi + \dots\right] \tag{189b}$$

$$\frac{\partial}{\partial \ell}\left[f^{(2)}(\ell,\xi=0) + \dots\right] = -\left[2K^{(1)} f^{(1)}(\ell,\xi=0) + K^{(2)} f^{(0)}(\ell,\xi=0) + \dots\right] \tag{189c}$$

Equating equal powers of ξ gives a system of six equations with six quantities to solve for, which we do using the initial condition $f^{(m)}(\ell=0,\xi) = 1$. The three that we are interested in have the solution

$$f^{(0)}(\ell,\xi=0) = 1\ ;\quad \frac{\partial f^{(0)}(\ell,\xi=0)}{\partial \xi} = \frac{K^{(1)}\ell^2}{i}\ ;\quad \frac{\partial^2 f^{(0)}(\ell,\xi=0)}{\partial \xi^2} = \frac{8}{3}K^{(2)}\ell^3 - \frac{5}{3}\left(K^{(1)}\ell^2\right)^2 \tag{190}$$

which are easily shown to be the same as (185), the result obtained

from the perturbation approach.

The first three moments of the distribution are by far the most important. If we were to attempt to construct a distribution from a knowledge of its moments only, we would not try to do it with less information. The zero-th moment tells us the number of particles in the distribution and was arbitrarily taken to be unity initially. We find that $\overline{\Delta^0}$ is always unity because particles are only redirected by multiple scattering, not created or destroyed. It is therefore independent of all scattering parameters $\langle\theta^2\rangle, \langle\theta^4\rangle, \ldots$. The first moment of the distribution, $\overline{\Delta}$, defines a point, the average location of all particles. It depends on $\langle\theta^2\rangle$ but is independent of all higher order terms $\langle\theta^4\rangle, \langle\theta^6\rangle, \ldots$. If we alter Yang's calculation by introducing correction terms $\mathcal{T}^4, \mathcal{T}^6, \ldots$, we would create distributions that look different from Yang's result, particles would be redistributed because of these additional terms, but all distributions created in this manner would have the same average value as appears in Yang's distribution. The next moment, $\overline{\Delta^2}$, would be expected to provide information about departures from average behavior and we would try to use it to define some physical extension for the distribution. For example, $\sigma^2 = \overline{\Delta^2} - (\overline{\Delta})^2$ is generally called the variance of the distribution and we would try to associate σ with the width of that distribution. It is in the second moment that problems with spatial moments appear.

The problem is that the first moment of the distribution is a meaningful number, but the second moment is not. If we use the expres-

sion for $\overline{\Delta^2}$ given by (185), which has contributions from two terms, part of this is a meaningful number, while part of it is not. The reason for the difference is due to the different types of mathematical objects that contribute. The $\frac{5}{3}(\bar{\Delta})^2$ part recieves contributions only from simple poles. The $\frac{4}{3}\frac{\beta_2}{n_c}\bar{\Delta}^2$ part receives contributions from first, second and third order singularities. To invert the transform correctly in the letter case we would have to seperate its terms and then apply different Cauchy rules. This can't be done if we have only a number representing it, the necessary structure is irretreviably missing.

If we had, somewhat blindly, been using a moments approach and had evaluated $\overline{\Delta^2}$ numerically in the process of obtaining it, we might not notice that we had done something wrong. This would be the case if we had been working with a true small angle differential cross section, e.g., $\frac{d\sigma(\theta)}{d\Omega} = \frac{d\sigma}{d\Omega}(\theta=0)\, e^{-\theta^2/\theta_0^2}$, where we have $\beta_2 \simeq 1$. The error becomes small after only a few collisions, since $5/3 \gg \frac{4}{3}\frac{\beta_2}{n_c}$ in a short time, and the meaningless numerical part is relatively minor by comparison. In the case of charged particle scattering, which is an exceptional and pathlogical small angle problem, β_2 is enormous, on the order of 10^5 for 10 MeV electrons, so even after 10^4 collisions we still have $\frac{4}{3}\frac{\beta_2}{n_c} \gg \frac{5}{3}$. The numerical value of $\overline{\Delta^2}$ is meaningless under these conditions and it would be equally meaningless to try to construct a distribution by using these numbers. This is exactly the type of error that was being illustrated in Fig. (6) in connection with Kessaris' result.

Kessaris had expressed his result (139) in a very complicated way and to discuss it more easily we considerd another function

$$f(\ell,\Delta) = N\, e^{-a/\Delta}\, \frac{1}{\Delta^{3/2}}\, e^{-\Delta/b} \qquad (139)'$$

which is closely related to the one that he used and has very similar properties. If the three parameters required to use (139)' are determined by the lowest three moments of the distribution, then (139)' will reproduce (139) very closely at all times and for all energies for which Kessaris did his calculation. For the distribution (139)', the moments are standard integrals and give

$$\int_0^\infty d\Delta\, f(\ell,\Delta) = 1 \quad \Rightarrow \quad N = \left(\frac{a}{\pi}\right)^{1/2} e^{2\left(\frac{a}{b}\right)^{1/2}} \qquad (191a)$$

$$\int_0^\infty d\Delta\, \Delta\, f(\ell,\Delta) = \bar{\Delta} = (ab)^{1/2} \qquad (191b)$$

$$\int_0^\infty d\Delta\, \Delta^2 f(\ell,\Delta) = \overline{\Delta^2} = a^{1/2} b^{3/2}\left[\frac{1}{2} + \left(\frac{a}{b}\right)^{1/2}\right] \qquad (191c)$$

We use these relations to eliminate N, a, b and replace them with expressions for moments. If we use Yang's scaled variable v, and the definition $\sigma^2 = \overline{\Delta^2} - (\bar{\Delta})^2$ along with (191), then (139)' may be written

$$f(\ell,v) = \left(\frac{e^{2/s}}{\pi s}\right)^{1/2} e^{-1/sv}\, \frac{1}{v^{3/2}}\, e^{-v/4s} \qquad (139)''$$

where $s = \sigma^2/(\bar{\Delta})^2$. This one number, S, completely controls the shape of the distribution and it is simply σ^2 expressed in dimensionless units. With a value of $s \simeq 1$, (139)'' would look reasonable, something like Yang's result if we were to plot it up. Kessaris, at the time referred to in Fig. (6), was using a value about 10 times this, so the shape of his distribution was altogether incorrect.

Kessaris had not used the Gaussian approximation but the more descriptive Lewis equation with the McKinley-Feshbach cross-section. This allowed for a few particles to be scattered directly to wide angles in a single collision thereby seperating them from the main group which was travelling with small angles. This part of the description was quite realistic since it even included a Rutherford tail, a small stream of trailing particles scattered all along the pathlength. Although this additional structure contains only a miniscule number of particles, a few tenths of one percent, its contribution to the numerical values of moments was disproportionate and overwhelming because of the relatively large distances it involves. Thus, Kessaris had constructed his distribution on the basis of the numbers derived from the most unrepresentative few. The incorrect step was the very first, the numerical evaluation of Lewis' moment expressions. They provided him with nothing more than a set of meaningless numbers.

Kessaris, however, actually did produce some reasonable looking numerical results and these results would be associated with times that were long enough so that the Rutherford tail dropped out of the problem. Eventually most particles scatter to large angles through a sequence of many deflections each of which is very small. The few which were earlier ejected from the main group by a single wide angle collision are then recovered and returned back into it. The Rutherford tail therefore begins to disappear, i.e., like $\frac{1}{n}, \frac{1}{n^2}$...in the angular distribution (154) and there is a corresponding loss of structure from the spatial distributions as well. Thus, Kessaris' results were best at the longest times considered in his calculation, which is when the

electrons had run out of energy and stopped or were nearly ready to stop. Evidently his calculations improved with more time not because his arguments or methods were improving but because of the way diffusion works. Diffusion is a process which eliminates details. The fact that Kessaris and Spencer had produced some good numerical results was the main reason why the moments development went unchallenged for decades and was generally passed along with satisfactory reviews. This was due much more to accident rather than to correct argument. Both authors, for example, drove their calculations to high orders, i.e., they aimed to achieve reliability and credibility by showing that they could reproduce the numerical values of many moments. To correctly compute more moments than were given by (185) we would be required to include more terms $\mathcal{T}^6, \mathcal{T}^8$ ... from the expansion (152), and also go to higher orders in a perturbation calculation. It is not difficult to see what effect this would have. $\mathcal{T}^2$ is a derivative operator, and in a small angle problem it can be replaced by

$$\mathcal{T}^2_{op} = \left(\frac{1}{i}\right)^2\left(\frac{\partial^2}{\partial\theta_x^2} + \frac{\partial^2}{\partial\theta_y^2}\right) \longrightarrow \left(\frac{1}{i}\right)^2\left(\frac{\partial^2}{\partial\theta^2} + \frac{1}{\theta}\frac{\partial}{\partial\theta}\right) \qquad (192)$$

where the last expression is true in a cylindrically symmetric problem. When $\mathcal{T}^2$ acts on a LaGuerre polynominal, as in (169), it produces power factors of N . If we have a perturbation $(\mathcal{T}^2)^3$, we apply the recursion relation three times, which produces higher factors of N, as in (170). Factors of N in the infinite series revert back to derivative operators, as in (179b) and (179c). The end result is that we would be led to take more and more derivatives of an expression which contains only simple poles in it, so the calculation contains higher and higher order

singularities in the complex χ plane as we drive it to higher orders. The numerical evaluation of moments is evidently less meaningful under these conditions than it was at low orders because the confusion of structure would be even greater.

Spencer, in trying to develop Lewis' theory, had used another argument which should not be trusted. When he first constructed distributions and compared them with experiment he found that he did not have satisfactory agreement. He felt, on inspecting his initial results, that the amount of scattering being predicted was too weak and that to achieve acceptable agreement with experiment it would have to be made stronger. Spencer's calculations concerned relativistic electrons scattering from atoms. His initial work included a factor of Z^2 in the calculation of the mean square deflection angle. This factor arises from electrons scattering off the nucleus. In looking for a way to increase the amount of scattering, Spencer suggested that the incident electrons would also scatter from the orbital electrons of the target. This provided Z more scattering objects and so Spencer redid his calculations using the replacement $Z^2 \rightarrow Z(Z+1)$. He was then able to achieve agreement with experiment. That argument is unreliable because there are two coordinate systems involved, the center of momentum frame in which we compute average deflection angles and the laboratory frame in which we do multiple scattering calculations. In the case of electrons of a few MeV scattering from a nucleus, the cm frame moves very slowly relative to the laboratory system because of the large target mass and the distinction between the two reference frames need not be drawn. In the case of equal mass par-

ticles, especially if one is relativistic, the distinction needs to be made as the effect of transforming from our system to another is to significantly reduce the amount of perceived scattering. A relativistic electron scattering elastically from another electron in the cm system will be viewed, in the lab frame, as one electron passing through relatively undeflected but losing a bit of recoil energy to the target electron.

Spencer, in his 1955 paper, demonstrated that he could, using Lewis' moment relations, construct distributions that were in agreement with experiment. When they were not in agreement, he discarded his results and fixed them up again until they were. Achieving agreement with experiment under conditions like this can hardly support or confirm the validity of the approach. Spencer consistently relied upon arguments which sounded plausible but were unsound, unreliable or incorrect. He appears not to have recognized the necessity of writing and solving the differential equations, as it is the only way that one can prove what one is talking about. Solution means analytic solution, left hand side equals right hand side, so that we have the force of a mathematical proof. Spencer had presesented what were essentially his opinions within a thick cloud of theoretical sounding statements which were generally supported by a numerical demonstration of one kind or another in an attempt to prove his remarks. Because of this, he had not developed the theory to the point of numerical application as he stated and probably believed. Instead, he had developed a numerical analysis. Spencer's theory of electron penetration was low energy electron beam phenomenology.

Significant and important information concerning Lewis' work had not been developed and that undeveloped information goes right to the heart of Lewis' whole approach. Lewis had proposed moments as a means of obtaining exact spatial results without the small angle approximation. Large angle effects, however, are a significant problem in the moments approach. In the longitudinal distribution they introduce large Δ effects. Because of the inverting properties of Fourier transforms, large Δ effects will show up at low ζ . More precisely, they can introduce high order singularities into a Fourier transform in the vicinity of $\zeta = 0$, the point about which the Taylor-moment expansion is done. A high order infinity a close distance away from the point at which an expansion is done will contain terms that can dominate that expansion. If we evaluate moments numerically, which does not deal with the nearby infinity properly, then even a relatively minor physical effect associated with large Δ can contribute to this number in a vastly exaggerated way making it quite unrepresentative of the distribution and worthless to even compute.

There are two such problems. The first is the Rutherford tail, as we have already discussed. Eliminating all difficulties associated with it is very easy, we use the Gaussian approximation which discards this structure and all of its problems completely. The second is due to boundaries. The exact solution to the transport equation must go to zero in the backward direction at $z \to -\ell$ in some manner analogous to the way that it goes to zero in the forward direction. Terms present in the exact transport equation that create the proper backward behavior can contribute to spatial moments and cause problems with them in

a manner that is entirely analogous to the problems which were associated with the Rutherford tail. Eliminating boundary effects is more difficult. We will begin by using a small angle analysis from which boundary effects are absent. For example, Yang's solution does not contain the correct backward boundary behavior even though his solution was ex[illegible] The reason is that Yang also used the small angle approximation. It has no backward direction and so the unwanted boundary effects don't appear when we use it. We then develop the small angle solution directly and continuously to large angles in a manner which will keep these boundary effects out of our description permanently. Yang's analysis did not provide the proper machinery for doing this and we find it necessary to repeat the small angle analysis in order to obtain it.

V. A Wave Solution to the Transport Problem

In this chapter we consider the calculation of spatial distributions that derive from

$$\frac{\partial f(\ell,\theta,\phi,x,y,\Delta)}{\partial \ell} = -\left[\sin\theta\cos\phi\frac{\partial}{\partial x} + \sin\theta\sin\phi\frac{\partial}{\partial y} + (1-\cos\theta)\frac{\partial}{\partial \Delta}\right] f + \frac{K(\ell)}{\mathcal{T}}\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right] f \tag{193}$$

which is (43) or (47) with $\Delta = \ell - z$ replacing z as the longitudinal coordinate. The first step in our approach will be to solve

$$\frac{\partial f(\ell,\theta_x,\theta_y,x,y,\Delta)}{\partial \ell} = -\left[\theta_x\frac{\partial}{\partial x} + \theta_y\frac{\partial}{\partial y} + \frac{1}{2}(\theta_x^2+\theta_y^2)\frac{\partial}{\partial \Delta}\right] f + \frac{K(\ell)}{\mathcal{T}}\left[\frac{\partial^2}{\partial\theta_x^2} + \frac{\partial^2}{\partial\theta_y^2}\right] f \tag{194}$$

which is (84) with Δ replacing z as the spatial coordinate.

A. Small Angles

With Fourier transforms

$$f(\ell,\theta_x,\theta_y,x,y,\Delta) = \frac{1}{(2\pi)^5}\int_{-\infty}^{\infty} d\mathcal{T}_x\, d\mathcal{T}_y\, dp_x\, dp_y\, d\mathcal{P}\; f(\ell,\mathcal{T}_x,\mathcal{T}_y,p_x,p_y,\mathcal{P})\, e^{i(\mathcal{T}_x\theta_x+\mathcal{T}_y\theta_y+p_x x+p_y y+\mathcal{P}\Delta)} \tag{195}$$

and separability

$$f(\ell,\mathcal{T}_x,\mathcal{T}_y,p_x,p_y,\mathcal{P}) = f(\ell,\mathcal{T}_x,p_x,\mathcal{P})\, f(\ell,\mathcal{T}_y,p_y,\mathcal{P}) \tag{196}$$

we obtain

$$\frac{\partial f(\ell,\mathcal{T}_x,p_x,\mathcal{P})}{\partial \ell} = \left(\frac{i\mathcal{P}}{2}\frac{\partial^2}{\partial\mathcal{T}_x^2} + p_x\frac{\partial}{\partial\mathcal{T}_x} - \frac{K(\ell)}{\mathcal{T}}\mathcal{T}_x^2\right) f \tag{197}$$

which is the Fourier transform of (88) where $K \to K(\ell)$ as well.

Yang's eigenvalue solution to this problem is possible only for constant K. It is that step that we wish to avoid and the replacement $K \to K(\ell)$ forces us to avoid it. The significance of the problem posed by (197) can be interpreted in more than one way. On the one hand, it allows for energy dependent scattering, a very practical question, routinely met in applications. On the other hand, it gives us a mechanism by which we can deform the solution, and quite generally if we allow $K(\ell)$ to be completely arbitrary. We want to see how the solution responds to these changes.

We solve (197) by constructing its time development operator and we use the fact that this equation is first order in time in order to do it. We consider first three separate problems that we can make up from (197), i.e.,

$$\frac{\partial f^{(1)}(\ell, J_x, \beta)}{\partial \ell} = \frac{i\beta}{2} \frac{\partial^2}{\partial J_x^2} f^{(1)} \tag{198a}$$

$$\frac{\partial f^{(2)}(\ell, J_x, p_x)}{\partial \ell} = p_x \frac{\partial}{\partial J_x} f^{(2)} \tag{198b}$$

$$\frac{\partial f^{(3)}(\ell, J_x)}{\partial \ell} = -\frac{K(\ell)}{4} J_x^2 f^{(3)} \tag{198c}$$

The solution of (198c) may be written

$$f^{(3)}(\ell, J_x) = f^{(3)}(\ell = 0, J_x)\, e^{-J_x^2 \int_0^\ell d\ell' \frac{K(\ell')}{4}} \tag{199}$$

but we would write it as

$$f^{(3)}(\ell + d\ell, J_x) = f^{(3)}(\ell, J_x)\, e^{-J_x^2 \frac{K(\ell)}{4} d\ell} \tag{200}$$

instead. The understanding will be that we keep only first order infi-

nitesimals. By writing it this way we have an operational rule which tells us how to take a solution at time ℓ and convert it into a solution of time $\ell+d\ell$. The analogous rule for (198b) is easily

$$f^{(2)}(\ell+d\ell, J_x, p_x) = f^{(2)}(\ell, J_x + p_x d\ell, p_x) \tag{201}$$

To obtain a rule for (198a) we can first take the Fourier transform of this equation. If $f^{(1)}(\ell, J_x, \gamma)$ is a solution of (198a) and we define $f^{(1)}(\ell, \theta_x, \gamma)$ by

$$f^{(1)}(\ell, \theta_x, \gamma) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dJ_x \, e^{i J_x \theta_x} f^{(1)}(\ell, J_x, \gamma) \tag{202}$$

then the inverse of (202) in (198a) gives simply

$$\frac{\partial f^{(1)}(\ell, \theta_x, \gamma)}{\partial \ell} = -\frac{i\gamma}{2} \theta_x^2 \, f^{(1)}(\ell, \theta_x, \gamma) \tag{203}$$

so that

$$f^{(1)}(\ell+d\ell, \theta_x, \gamma) = f^{(1)}(\ell, \theta_x, \gamma) \, e^{-i\gamma \frac{d\ell}{2} \theta_x^2} \tag{204}$$

which is the Fourier transform of the rule that we want. The inverse of (202) gives

$$f^{(1)}(\ell+d\ell, J_x, \gamma) = \int_{-\infty}^{\infty} d\theta_x \, e^{-i J_x \theta_x} f^{(1)}(\ell+d\ell, \theta_x, \gamma) \tag{205}$$

and if we insert (204) into the right side of (205) and then use the inverse of (202) again to eliminate $f^{(1)}(\ell, \theta_x, \gamma)$, we obtain

$$f^{(1)}(\ell+d\ell, J_x, \gamma) = \int_{-\infty}^{\infty} dJ_x' \, \frac{e^{-(J_x' - J_x)^2 / 2i\gamma d\ell}}{(2\pi i \gamma d\ell)^{1/2}} \tag{206}$$

after some manipulation. This is the form that we want since the rule, do an integral, refers to the same variables as our two previous rules.

Note that (206) is an identity for $d\ell=0$, so that

$$\lim_{d\ell\to 0} \frac{e^{-(J_x'-J_x)^2/2igd\ell}}{(2\pi i g d\ell)^{1/2}} = \delta(J_x'-J_x) \qquad (207)$$

For $d\ell\neq 0$ but still small, the integrand is sharply peaked about $J_x' \simeq J_x$ and the expansion

$$f^{(1)}(\ell,J_x',g) = f^{(1)}(\ell,J_x,g) + \frac{\partial f^{(1)}(\ell,J_x,g)}{\partial J_x}(J_x'-J_x)+\dots \qquad (208)$$

will give a quickly convergent result when used on the right of (206). One can use it to verify that (206) and (198a) are equivalent to lowest order in $d\ell$. Fermi had also used this argument in his derivation.

Combining the three rules (200), (201), and (206) independently gives

$$f(\ell+d\ell,J_x,p_x,g) = \int_{-\infty}^{\infty} dJ_x' \frac{e^{-\frac{(J_x'-J_x)^2}{2igd\ell}}}{(2\pi i g d\ell)^{1/2}} f(\ell,J_x'+p_x d\ell,p_x,g)\, e^{-J_x^2\frac{K(\ell)d\ell}{4}} \qquad (209)$$

as the equivalent of (197). The initial condition of (197) is $f(0,J_x,p_x,g)=1$. If we use it in (209) we obtain the result for the first infinitesimal, $f(d\ell,J_x,p_x,g) = e^{-\frac{K(0)d\ell}{4}J_x^2}$ which we insert back into (209). Inspection of the first few intervals establishes the form of solution as

$$f(\ell,J_x,p_x,g) = B(\ell,g)\, e^{-[A_1(\ell,g)J_x^2 + A_2(\ell,g)J_x p_x + A_3(\ell,g)p_x^2]} \qquad (210)$$

If we insert this into (197) we obtain

$$\frac{dA_1(\ell,g)}{d\ell} = -2igA_1^2 + \frac{K(\ell)}{4} \qquad \frac{dB(\ell,g)}{d\ell} = -igA_1 B \qquad (211a,d)$$

$$\frac{dA_2(\ell,g)}{d\ell} = -2igA_1A_2 + 2A_1 \qquad \frac{dA_3(\ell,g)}{d\ell} = -ig\frac{A_2^2}{2} + A_2 \qquad (211b,c)$$

by equating equal powers of transform coefficients. The initial conditions would now be $B(\ell=0,\xi)=1$, $A_\alpha(\ell=0,\xi)=0$. Note that the $\xi\to 0$ limit of the set (211) is the set (30), so that the Fermi-Eyges theory is contained as a limiting case.

The key equation of this set is (211a), the one which depends only on itself. With the transformation

$$A_1(\ell,\xi) = \frac{1}{2i\xi}\frac{1}{\psi(\ell,\xi)}\frac{d\psi(\ell,\xi)}{d\ell} = \frac{1}{2i\xi}\frac{d}{d\ell}\ln\psi(\ell,\xi) \qquad (212)$$

it becomes

$$\frac{d^2\psi}{d\ell^2} + \frac{\xi}{2i}K(\ell)\psi = 0 \qquad (213)$$

We may take the initial conditions as $\psi(0,\xi)=1$, $\psi'(0,\xi)=0$. With (212), the solution of (211c) is easily

$$B(\ell,\xi) = \psi^{-1/2}(\ell,\xi) \qquad (214)$$

Since the equation for A_2 is linear and first order with a well known general form of solution, we obtain

$$A_2(\ell,\xi) = \frac{1}{i\xi}\left(1-\frac{1}{\psi}\right) \qquad (215)$$

without difficulty. We can also integrate (211c) by recognizing $1/\psi^2$ as an exact differential. Defining $\chi(\ell,\xi)$ as the second solution of (213) with the initial conditions $\chi(0,\xi)=0$ and $\chi'(0,\xi)=1$, then

$$\frac{d}{d\ell}(\chi/\psi) = \frac{1}{\psi^2}\left(\psi\frac{d\chi}{d\ell} - \frac{d\psi}{d\ell}\chi\right) = \frac{1}{\psi^2} \qquad (216)$$

as is straightfoward to prove from (213). With (216), (211c) becomes

$$A_3(\ell,\xi) = \frac{1}{2i\xi}\left(\ell - \frac{\chi(\ell,\xi)}{\psi(\ell,\xi)}\right) \qquad (217)$$

Spatial distributions are our objective and we delete angular information by integration. Integrating (195) over all angles gives

$$f(\ell,x,y,\Delta)=\frac{1}{(2\pi)^3}\iiint d\rho_x\,d\rho_y\,d\rho\; e^{i(\rho_x x+\rho_y y+\rho\Delta)}\,f(\ell,T_x=T_y=0,\rho_x,\rho_y,\rho) \tag{218}$$

for the complete density, while the simpler longitudinal part, obtained by integrating over both lateral coordinates as well, is

$$f(\ell,\Delta)=\frac{1}{2\pi}\int d\rho\; e^{i\rho\Delta}\,f(\ell,T_x=T_y=0,\rho_x=\rho_y=0,\rho) \tag{219}$$

With (196), (210), (214) and (217), the transforms of interest are therefore

$$f(\ell,T=0,p,\rho)=f(\ell,p,\rho)=\frac{1}{\psi(\ell,\rho)}\,e^{-\frac{p^2\ell}{2i\rho}\left(1-\frac{\chi(\ell,\rho)/\ell}{\psi(\ell,\rho)}\right)} \tag{220}$$

and

$$f(\ell,T=0,p=0,\rho)=f(\ell,\rho)=1/\psi(\ell,\rho) \tag{221}$$

so that all the information that we would require is to be obtained by solving the wave equation (213). Before considering its solutions, we remove the small angle limitation. The objective is to give extended meaning and definition to the functions that were introduced here.

B. Large Angles

Consider first the longitudinal part of (193) which satisfies

$$\frac{\partial f(\ell,\cos\theta,\Delta)}{\partial\ell}=-(1-\cos\theta)\frac{\partial f}{\partial\Delta}+\frac{K(\ell)}{4}\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}f\right) \tag{222}$$

Its initial conditions would be $f(\ell=0,\cos\theta,\Delta)=\delta(1-\cos\theta)\,\delta(\Delta)$.

The most general form of solution may be written.

$$f(\ell,\cos\theta,\Delta)=\sum_{j=0}^{\infty}\left(\frac{2j+1}{2}\right)f_j(\ell,\Delta)\,P_j(\cos\theta) \tag{223}$$

where the P_j are the usual Legendre polynominals. We can always define a set of Fourier transforms by

$$f_j(\ell,\Delta) = \frac{1}{2\pi}\int_{-\infty}^{\infty} d\beta\; e^{i\beta\Delta} f_j(\ell,\beta) \tag{224}$$

and then (223) and (224) in (222) then give

$$\frac{d f_j(\ell,\beta)}{d\ell} = -i\beta\left[f_j - \frac{j}{2j+1} f_{j-1} - \frac{(j+1)}{(2j+1)} f_{j+1}\right] - \frac{K(\ell)}{4} j(j+1) f_j \tag{225}$$

which are equivalent to (222). The initial conditions are $f_j(\ell=0,\beta) = 1$. We are particularly interested in the first two of these relations, i.e.,

$$\frac{d f_0(\ell,\beta)}{d\ell} = -i\beta(f_0 - f_1) \tag{226}$$

$$\frac{d f_1(\ell,\beta)}{d\ell} = -i\beta\left(f_1 - \frac{1}{3} f_0 - \frac{2}{3} f_2\right) - \frac{K(\ell)}{2} f_1 \tag{227}$$

To solve them we need another relation and the form of the small angle solution provides it. The longitudinal part of the small angle solution is obtained from

$$f(\ell,\theta,\Delta) = \int_0^{2\pi} d\phi \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy\; f(\ell,\theta_x,\theta_y,x,y,\Delta) \tag{228}$$

where the Cartesian angles (θ_x,θ_y) would be replaced by their cylindrical equivalents θ,ϕ to match the spherical description (223) smoothly. Using (195), (196), (210) and (214), the integrals of (228) lead to

$$f(\ell,\theta,\Delta) = \frac{1}{2\pi}\int_{-\infty}^{\infty} d\beta\; e^{i\beta\Delta}\left(\int_0^{\infty} J\, dJ\, \mathcal{J}_0(J\theta)\, f(\ell,J,\beta)\right) \tag{229}$$

where J is the magnitude $J = (J_x^2 + J_y^2)^{1/2}$, $\mathcal{J}_0$ is a zero order Bessel function, and

$$f(\ell,J,\beta) = \frac{1}{\psi(\ell,\beta)}\, e^{-A_1(\ell,\beta) J^2} \tag{230}$$

Bessel's equation is the small angle limit of Legendre's equation and comparing them gives the associations $J_0(\tau\theta) \leftrightarrow P_j(\cos\theta)$, $\tau^2 \leftrightarrow j(j+1)$. Comparing (223), (224) against (229), (230) then gives

$$f_j(\ell,\beta) = \frac{1}{\psi(\ell,\beta)}\, e^{-A_1(\ell,\beta)\, j(j+1)} \tag{231}$$

as the form of solution. It does not define either or which is done by (226) and (227). With (226) and (231) we obtain a constraint between two functions

$$A_1(\ell,\beta) = -\frac{1}{2}\ln\left(1 + \frac{i}{\beta}\frac{1}{\psi}\frac{d\psi}{d\ell}\right) \tag{232}$$

With (232) we rewrite (231) as

$$f_j(\ell,\beta) = \frac{1}{\psi(\ell,\beta)}\left(1 + \frac{i}{\beta}\frac{1}{\psi}\frac{d\psi}{d\ell}\right)^{\frac{j(j+1)}{2}} \tag{233}$$

and then (233) in (227) gives

$$\frac{d^2\psi}{d\ell^2} + \left(1 + \frac{i}{\beta}\frac{1}{\psi}\frac{d\psi}{d\ell}\right)\frac{\beta}{2i}K(\ell)\psi = \frac{2}{3}\beta^2\psi\left(\frac{i}{\beta}\frac{1}{\psi}\frac{d\psi}{d\ell}\right)^3 \tag{234}$$

as the new definition of ψ. In (233) and (234) we have a complete solution to the longitudinal part of the transport problem. That solution is quite formal, however, since we still need to solve for ψ and then invert the Fourier transforms. These topics will be considered in section C of this chapter.

A more general argument begins with a spherical harmonic expansion

$$f(\ell,\theta,\phi,x,y,\Delta) = \sum_{jm}\left(\frac{2j+1}{4\pi}\right)^{1/2} f_{jm}(\ell,x,y,\Delta)\, Y_{jm}(\theta,\phi) \tag{235}$$

and allows us to include the lateral movement as well. The expansion (235) replaces (223) and aims to solve (193) rather than (222). We would again define spatial Fourier transforms

$$f_{jm}(\ell,x,y,\Delta) = \frac{1}{(2\pi)^3}\iiint d\rho_x d\rho_y d\beta\; e^{i(\rho_x x + \rho_y y + \beta\Delta)} f_{jm}(\ell,\rho_x,\rho_y,\beta) \tag{236}$$

which replace (224). Then (235) and (236) in (193) give

$$2(2j+1)\left[\frac{df_{jm}(\ell,p_x,p_y,q)}{d\ell} + \frac{K(\ell)}{4} j(j+1) f_{jm}\right] =$$

$$= -i(p_x+ip_y)\left\{-[(j+1+m)(j+2+m)]^{1/2} f_{j+1,m+1} + [(j-m)(j-m-1)]^{1/2} f_{j-1,m+1}\right\}$$

$$-i(p_x-ip_y)\left\{+[(j+1-m)(j+2-m)]^{1/2} f_{j+1,m-1} - [(j+m)(j+m-1)]^{1/2} f_{j-1,m-1}\right\}$$

$$-2iq\left\{(2j+1) f_{jm} - [(j+m)(j-m)]^{1/2} f_{j-1,m} - [(j+1+m)(j+1-m)]^{1/2} f_{j+1,m}\right\} \tag{237}$$

as the generalization of (225). Many of these relations are not independent. Because of cylindrical symmetry we have

$$f_{jm}(\ell,p_x,p_y,q) = e^{-im\beta} f_{jm}(\ell,p,0,q) \tag{238a}$$

$$f_{j,-m}(\ell,p,0,q) = (-1)^m f_{jm}(\ell,p,0,q) \tag{238b}$$

where $p = (p_x^2 + p_y^2)^{1/2}$, $\beta = \arctan(p_y/p_x)$.

In addition to these large angle expressions, we will also want to express the small angle result, the product of (196) and (210), which uses continuous variables J_x, J_y , in discrete notation j,m .

The p_x, p_y, q integrations of (195) are spatial transforms while the angular parts of this equations are concerned only with

$$\frac{1}{(2\pi)^2}\int_{-\infty}^{\infty} dJ_x \int_{-\infty}^{\infty} dJ_y \; e^{i(J_x\theta_x + J_y\theta_y)} f(\ell, J_x, J_y, p_x, p_y, q)$$

$$= \frac{1}{(2\pi)^2}\int_0^{\infty} J\,dJ \int_0^{2\pi} d\alpha \; e^{iJ\theta\cos(\phi-\alpha)}\left\{ e^{-[A_1 J^2 + A_2 Jp\cos(\alpha-\beta)]} \cdot e^{-A_3 p^2/q}\right\} \tag{239}$$

where $(\theta,\phi),(J,\alpha)$ and (p,β) are the cylindrical equivalents of $(\theta_x,\theta_y),(J_x,J_y)$ and (p_x,p_y) respectively. We also used (196), (210) and

(214) on the right of (239). If we use the decomposition

$$e^{i b \rho \cos\alpha} = \sum_{m=-\infty}^{\infty} i^m e^{im\alpha} J_m(b\rho) \tag{240}$$

where J_m is a Bessel function of order m in both terms of this form that appear in (239), then the right hand side of (239) becomes

$$\frac{1}{2\pi}\int_0^{\infty} \tau d\tau \sum_{m=-\infty}^{+\infty} (-1)^m J_m(\tau\theta) e^{im\phi}\left[\frac{e}{\psi}^{-(A_1\tau^2+A_3\rho^2)} J_m(i\rho\tau A_2)\, e^{-im\beta}\right]$$

By comparing Bessel's equation for non-zero order against the associated Legendre equation, and using also the definition of spherical harmonics, we would be led to replace $(-1)^m J_m(\tau\theta) e^{im\phi} \to \left(\frac{4\pi}{2j+1}\right)^{1/2} Y_{jm}(\theta,\phi)$. Along with the replacement $\tau^2 \to j(j+1)$ so that $2\tau d\tau \to 2j+1$ which was used earlier, (239) becomes

$$\frac{1}{(2\pi)^2}\int\int d\tau_x\, d\tau_y\, e^{i\vec{\tau}\cdot\vec{\theta}} f(\ell,\tau_x,\tau_y,\rho_x,\rho_y,\gamma) \tag{241}$$

$$\longrightarrow \sum_{jm} \left(\frac{2j+1}{4\pi}\right)^{1/2} f_{jm}(\ell,\rho_x,\rho_y,\gamma)\, Y_{jm}(\theta,\phi)$$

where

$$f_{jm}(\ell,\rho_x,\rho_y,\gamma) = \left(f_{jm}(\ell,\rho,0,\gamma) \equiv f_{jm}(\ell,\rho,\gamma)\right) e^{-im\beta} \tag{242a}$$

$$f_{jm}(\ell,\rho,\gamma) \longleftarrow f_m(\ell,\tau,\rho,\gamma) = J_m(i\rho\tau A_2)\frac{e}{\psi}^{-(A_1\tau^2+A_3\rho^2)} \tag{242b}$$

The arrow in (242b) means that we still need to specify a rule for converting functions with continuous τ on the right into discrete j on the left. This rule will often mean $\tau^2 \to j(j+1)$ but it may also mean other expressions that are similar to it. We are allowing for those

other possibilities as well.

Only the small argument expansions of these Bessel functions will be needed. The small angle approximation, which was used to obtain (242b), could be used to show that $ip\mathcal{T}A_2$ is small. However, apart from that, a Taylor expansion in powers of p is a moments expansion of the lateral movement. The first term in this expansion, $p=0$, leaves only the longitudinal movement which is described by $\mathcal{T}_m(0) = \delta_{m0}$ and (231)-(234). We now continue this expansion to include expressions that are linear in p as $p \to 0$. The $f_{j,m=+1}^{(\ell,p,\beta)}$ are the only terms that have this behavior and they satisfy (237) with the first term on the right hand side discarded. It leads to order p^3 and higher. We then have

$$2(2j+1)\left[\frac{\partial f_{j,+1}^{(\ell,p,\beta)}}{\partial \ell} + j(j+1)\frac{K(\ell)}{4} f_{j,+1}\right] = -ip\sqrt{j(j+1)}\left(f_{j+1,0}^{(\ell,p=0,\beta)} - f_{j-1,0}\right)$$

$$-2i\beta\left((2j+1) f_{j,+1}^{(\ell,p,\beta)} - [(j+1)(j-1)]^{1/2} f_{j-1,+1} - [j(j+2)]^{1/2} f_{j+1,+1}\right) \qquad (243)$$

to first order in p. As a first step towards the solution of (243) we consider its $\beta \to 0$ limit. We already know that

$$f_{j,0}^{(\ell,p=0,\beta)}\Big|_{\beta=0} = \frac{e^{-j(j+1)A_1(\ell,\beta)}}{\psi(\ell,\beta)}\Big|_{\beta=0} \qquad (244)$$

from (231). We also have $\psi(\ell,0)=1$ from (234) while (232) and (234) give the differential equation for $A_1(\ell,\beta)$ from which we can easily obtain

$$A_1(\ell,0) = \int_0^\ell d\ell' \, \frac{K(\ell')}{4} \qquad (245)$$

With these remarks, the $\beta \to 0$ limit of (243) gives

$$f_{j,+1}(\ell,p,\beta=0) = \frac{ip\sqrt{j(j+1)}}{2(2j+1)} e^{-j(j+1)A_1(\ell,0)} \int_0^{\ell} d\ell' \left\{ e^{2jA_1(\ell',0)} - e^{-2(j+1)A_1(\ell',0)} \right\} \tag{246}$$

without difficulty. We now try to generalize this relation to $\beta \neq 0$ by writing

$$f_{j,+1}(\ell,p,\beta) = \frac{ip\sqrt{j(j+1)}}{2} \frac{e^{-j(j+1)A_1(\ell,\beta)}}{\psi(\ell,\beta)} A_2^j(\ell,\beta) \tag{247a}$$

where

$$A_2^j(\ell,\beta) \equiv \frac{1}{(2j+1)} \int_0^{\ell} \frac{d\ell'}{\psi(\ell',\beta)} \left\{ e^{2jA_1(\ell',\beta)} - e^{-2(j+1)A_1(\ell',\beta)} \right\} \tag{247b}$$

Here we have used the substitutions $A_1(\ell,0) \to A_1(\ell,\beta)$ and $\ell = \psi(\ell,0) \to \psi(\ell,\beta)$. Since $\psi(\ell,\beta)$ and $A_1(\ell,\beta)$ are connected by (232), to change one is to change the other. Setting $\beta = 0$ removes the longitudinal movement from the theory by integrating over it while allowing for arbitrary β returns it to the theory. However, at this stage, (247) should be regarded as a guess and so we check it against the small angle result that has continuous and non-zero values of β in it. The small angle expansion of these relations leads to

$$A_2^j(\ell,\beta) \to \int_0^{\ell} d\ell' \frac{2A_1(\ell',\beta)}{\psi(\ell',\beta)} = \int_{\psi_0}^{\psi} d\left(\frac{-1}{i\beta\psi}\right) = A_2(\ell,\beta) \tag{248}$$

where we have used (212) and (215) on the right side of (248). We compare (247) with (248) against the small angle result (242b), a result

that we know to be correct. With the first order expansion $J_{\nu,1}(i\rho_J A_2) \rightarrow i\rho_J A_2/2$ and the replacement $J \rightarrow \sqrt{j(j+1)}$, (242b) and (247) will agree if we use (248). At this stage, (247) would become a definition.

The expression (247) is an analogue of (231). What we could prove about one could be proved about the other, not more nor less. We could prove that (231) is correct at all times for $\xi = 0$ with a simple demonstration using (225). We would then discover the relation (245) if we were not already aware of it. We can also prove that (231) contains the correct small angle behavior within it and then use that to prove several other things. An alternate way of introducing the small angle approximation, which yields differential equations, is to take the small difference limit of difference equations. This method appears to have been introduced into a transport problem by G.C. Wick. Since we obtained (231) by solving a differential equation, we could use it in the reverse manner and show that (231) solves the difference equation (225), under the condition that the differences are small. A most important feature of the small angle analysis is that it contains the transform variable ξ as a continuous parameter and we get two conditions concerning it by considering when this analysis actually does apply. It clearly pertains whenever

$$A_1(\ell,\xi) = -\frac{1}{2}\ln\left(1+\frac{i}{\xi}\frac{1}{\psi}\frac{d\psi}{d\ell}\right) \rightarrow \frac{1}{2i\xi}\frac{1}{\psi(\ell,\xi)}\frac{d\psi(\ell,\xi)}{d\ell} << 1 \qquad (249)$$

so that (232) agrees with (212). At any time, even at a long time when it may well apply to only a few particles of a group, this condition can always be satisfied by choosing sufficiently high values of ξ, a

point also recognized by Wick[19]. At short times, when it will apply to all the particles of a group, this condition will be satisfied for all values of γ, extending down to and including the point $\gamma=0$. In the general case, a gap exists which separates the point $\gamma=0$ from the continuous high γ (small angle) region where (249) applies. In our approach, large angle expressions such as (231) and (247) are obtained by rearranging analogous small angle relations. We aim to insure that these amended (and more general) relations are always correct at the point $\gamma=0$ as well. This simultaneously defines distributions within the gap although it does not prove that our definitions are correct there.

An alternate approach towards bridging this gap would begin by setting up Taylor-moment expansions about the point $\gamma=0$. The necessary coefficients would then be obtained by applying Lewis type moment relations to (193). This procedure would appear to be stronger than the method that we proposed above because all the coefficients would now be obtained directly from the transport equation and it would then be expected to provide us with a proof. This procedure would lead us to a mistake if we pursued it. The exact transport equation contains the correct boundary behavior at all of its boundaries while the small angle solution does not have this property. By avoiding this approach we avoid the second large A problem with moments that was noted in our final remarks at the end of Chapter IV. Since we can't use the exact transport equation to prove the correctness of our approach, we require an alternate method and we will rely on the correctness of its predictions to do this for us. What we need to demonstrate mainly is that

the passage from small to large angles is perfectly continuous and that the solutions are always developing towards spherical symmetry. Our work in the later parts of this chapter will illustrate that these features are correctly built into our method.

Spencer's work is worth mentioning again. In his 1955 paper, Spencer suggested that his method of constructing spatial distributions was equivalent to combining Lewis's moment relations (for its low q features) to a Wick type asymptotic behavior (for its high q features). Both had problems. Spencer did not uncover or investigate any further the problems connected with Lewis' moment relations. He was aware, however, that his argument concerning the asymptotic behavior had difficulties since he mentioned that he had found a much better argument which would be presented later. This led to the paper by Spencer and Coyne (1962) which considered the longitudinal part of the multiple scattering problem within the context of the small angle approximation. They made progress with it in their first calculation, their sections III and IV, but it was limited progress, well short of a breakthrough, and so Spencer and Coyne then turned their attention back towards eigenvalues, which is not what we want. Spencer and Coyne had missed very key ideas concerning Yang's analysis. They did not appreciate that first order in time is needed to derive the form of the solution and that Yang's method of handling the time development was the pivotal problem in his analysis. They did discover a second order differential equation but they missed the wave equation (213), the principal equation of the small angle theory and so did not recognize that in it we have another oscillator and a different oscillator from the one that

Yang was discussing. We will be developing this "other oscillator" idea in the later sections of this chapter.

We should have qualified the remark that (247) and (242b) agree. They agree only to within an exponential factor involving $\rho^2 A_3$ which is absent from (247). The first order argument that we used to obtain (247), linear in ρ as $\rho \to 0$, cannot see second order terms involving ρ^2 and we can say nothing new about $A_3(\ell,\beta)$ without going to the next order. On the other hand, we know everything about the small angle function $A_2(\ell,\beta)$. It splits into many functions that now need to be distinguished by an index j. The polar parts of the spherical harmonics $Y_{j,\pm 1}(\theta,\phi)$ involve $\sin\theta$, $\sin\theta\cos\theta$, ... for $j=1,2$, etc. In the small angle approximation that we used, which is valid up to second order, all could be replaced by the same expression θ. A consequence is that the $A_2^{\pm}(\ell,\beta)$ became degenerate for small angles and were represented by the same function $A_2(\ell,\beta)$. Further, in an argument which is valid up to order ρ^2, an argument that will not be given here, we would find that the association

$$J^2 \to \left[(j-1)\, j\, (j+1)(j+2) \right]^{1/2} \qquad (250)$$

automatically appears in our equations. This is necessary so that the coefficients $f_{j,\pm 2}(\ell,\rho,\beta)$ vanish for $j=0, j=1$. We would be using (250) in some parts of our equations while also using $J^2 \to j(j+1)$ in other places. The small angle analysis does not distinguish them.

The small angle analysis could be called the infinitesimally small angle analysis and its extension to large angles would then be called the extension to finite angles. Regardless of terminology, the role of this extension is to provide better definition, to separate what is indistinguishable in one analysis from what clearly is by another. We appear to have just enough structure to do that. Use of the $\rho \to 0$ transport relations, combined with the substitutions $\psi(\ell,0) \to \psi(\ell,\rho)$ $A_i(\ell,0) \longrightarrow A_i(\ell,\rho)$, and careful comparisons against the small angle equations should provide all the $f_{jm}(\ell,\rho,\beta)$ that we would ever need. We do not pursue this topic further.

It is evident that the A_i^j are in no way fundamental since we can express them as functions of ψ and its time derivative by using (232). The set of coefficients $f_{jm}(\ell,\rho,\beta)$, which provide a complete description of the system, are similar in that they are integrals and combinations of these more fundamental functions. What we have is a dynamical system, which requires a good deal of structure to describe it, but a system which is being driven by a dynamical differential equation, (234) now rather then (213). This underlying differential equation now becomes the object of our attention.

Large angle equations are difficult to work with and we will develop an approximate solution to them. Of the two terms in (234) that amend (213), the cubic correction is the smaller and the more difficult to handel. Rather than using the exact continuation (234), we will consider the approximation

$$\frac{d^2\psi}{d\ell^2} + \frac{K(\ell)}{2}\frac{d\psi}{d\ell} + \frac{\rho}{2i}K(\ell)\psi = 0 \qquad (251)$$

which retains the principal correction to the small angle theory. Rather than using an exact expression for $A_3(z,\beta)$, we would also choose the approximation

$$f(z,\rho,\beta) = \frac{1}{\psi(z,\beta)}\, e^{-\frac{\rho^2 z}{2i\beta}\left(1 - \frac{\psi(z,0)}{\psi(z,\beta)}\frac{\chi(z,\beta)}{\chi(z,0)}\right)} \qquad (252)$$

which is a generalization of (220). Here χ is defined as the second solution of (251) with its initial conditions reversed form ψ. We will use results from the exact expressions mainly to check the quality of these approximations.

C. Analysis

Regardless of the choice of $K(z)$, any solution of (213) or (251) satisfying $\psi(0,\beta)=1$, $\psi'(0,\beta)=0$ can be represented as an infinite product of the form

$$\psi(z,\beta) = \prod_{n=1}^{\infty}\left\{1 - \beta/\beta_n(z)\right\} \qquad (253)$$

where the β_n are the points where $\psi=0$. The second solution χ can also be represented this way if we normalize with $\chi(z,0)$. The zeros of these functions define the density by (220) or (252) and also contain the information that we require to invert the Fourier transforms by contour integration. Our problem reduces to finding a method which will locate the zeros of these functions in a useful way. We consider some cases of special interest here that develop and define our method.

The example of greatest interest to us concerns relativistic electrons penetrating a homogeneous low Z material. A reasonable model of this problem uses a constant mean free path, a constant rate of energy loss with distance of travel, and a mean square deflection angle per collision that is inversely porportional to the square of the energy of the penetrating particle. Combining these remarks then leads to a parameterization of the form

$$K(\ell) = K(0)/(1-(\ell/R+\alpha))^2 \qquad (254)$$

where $\alpha \simeq (mc^2/E_0)R$, E_0 is the initial electron energy, R is the corresponding range, the total particle path length from start to stop, and mc^2 is the electron rest energy.

We first consider the small angle problem

$$\frac{d^2\psi}{d\ell^2} + \frac{q}{2i}\frac{K(0)}{(1-\ell/(R+\alpha))^2}\psi = 0 \qquad (255)$$

which is (254) in (213). With a change of variable $F(\ell) = -\ln(1-\ell/R+\alpha)$ followed by $\psi = e^{-F/2}\Phi$ (255) becomes

$$\frac{d^2\Phi}{dF^2} + \omega^2\Phi = 0 \qquad (256)$$

where

$$\omega^2 = q\lambda/2i \quad ; \quad \lambda = K(0)(R+\alpha)^2 \qquad (257)$$

From the general solution of (256) we find that the two solutions of (255) with the correct initial conditions are

$$\psi(\ell,q) = e^{-F/2}\left(\cos\omega F + \frac{1}{2\omega}\sin\omega F\right) \qquad (258a)$$

$$\chi(\ell,q)/\ell = \frac{e^{-F/2}}{(1-e^{-F})}\left(\frac{\sin\omega F}{\omega}\right) \qquad (258b)$$

At any instant we know the value of $F(\ell)$. If we set $\psi = 0$ and use (258a), we are led to compute the intersection of the two curves

$$y_1(\omega F) = -\frac{2}{F(\ell)}(\omega F) \quad ; \quad y_2(\omega F) = \tan(\omega F) \qquad (259)$$

The solution is an infinite number of discrete points, a set of numerical values $(\omega\xi)_n$ from which we easily determine the β_n . Since $\xi(\ell)$ is time dependent, the inclination angle of the line $y_1(\omega\xi)$ changes with time causing it to rotate. The intersection is clearly a continously changing pattern of zeros. It is easily verified that the relation $(\omega\xi)_n = (2n+1)\pi/2$ is always true for large n and that for early times it is true for all n .

Despite the specific choice (254), the behavior just described is general since we can also arrive at it by the WKB approximation that uses arbitrary $K(\ell)$. The WKB method uses solutions to (213) in the form

$$\psi_{\pm}^{WKB}(\ell,\beta) = A_{\pm}(\beta)\, b^{-1/2}(\ell,\beta)\, e^{\pm i\int_0^{\ell} d\ell'\, b(\ell',\beta)} \qquad (260)$$

where b is the wave number $\left(\beta\frac{K(\ell)}{2i}\right)^{1/2}$. Our initial conditions require

$$\psi^{WKB}(\ell,\beta) = \left(\frac{b(0,\beta)}{b(\ell,\beta)}\right)^{1/2}\left\{\cos\phi(\ell,\beta) + \frac{1}{2}\left[\frac{1}{b^2(\ell,\beta)}\frac{db}{d\ell}(\ell,\beta)\right]_{\ell=0}\sin\phi(\ell,\beta)\right\} \qquad (261)$$

where $\phi(\ell,\beta)$ is the phase in the exponent of (260). The WKB approach is a short wavelength approximation that is applicable when

$$\left(\frac{1}{K(\ell)}\frac{dK(\ell)}{d\ell}\right)\frac{1}{\left(\beta\frac{K(\ell)}{2i}\right)^{1/2}} << 1 \qquad (262)$$

For $\beta \to \infty$, (261) and (262) show that

$$\left(\beta_n(\ell)\frac{}{2i}\right)^{1/2}\int_0^{\ell} d\ell'\,(K(\ell'))^{1/2} = (2n+1)\frac{\pi}{2} \quad ; n\to\infty \qquad (263)$$

will always locate the high β zeros of ψ. When energy loss is negligible, $K(\ell)\to K$, the derivatives in (261) and (262) vanish. We have pure oscillations for all β and (263) holds for all n .

As the second case of special interest we use the large angle problem

$$\frac{d^2\psi}{dl^2} + \frac{K}{2}\frac{d\psi}{dl} + \frac{s}{2i}K\psi = 0 \qquad (264)$$

which is the energy independent version of (251). Most readers of this text would be able to find its solutions for themselves, so it is the method by which we solve it that is under discussion. Our method will be applicable to (251) itself where $K(l)$ is arbitrary.

We first note that any ψ that can be represented by an infinite product of the form (253) can also be represented by a Taylor series

$$\psi(l,s) = \sum_{m=0}^{\infty} \frac{\partial^m}{\partial s^m}\psi(l,s)\Big|_{s=0} \frac{s^m}{m!} \qquad (265)$$

since it is the more general form. The differential equation that defines also defines the coefficients in (265) and we are especially interested in the first derivative. Since $\psi(l,s=0) = 1$ is an immediate consequence of the initial conditions, (265) in (251) gives

$$\frac{\partial\psi}{\partial s}(l,s=0) = i\int_0^l dl' \left\{1 - e^{-\int_0^{l'} dl'' \frac{K(l'')}{2}}\right\} \qquad (266)$$

without difficulty. Using (253), we also have

$$\frac{\partial\psi}{\partial s}(l,s=0) = -\sum_n \frac{1}{s_n(l)} \qquad (267)$$

The numerical value of this derivative, given by (266), is continually changing with time because the zeros are moving. By (267), the important contributions to it always come from the zeros which are closest to the point $s=0$. Those which are most distant, near $s\to\infty$, will hardly contribute at all.

Our method of solving (251) begins with the function (258a). We aim to construct the large angle solution by continuously deforming this small angle result. The first step in the procedure is to allow $\mathcal{F}$ and λ to become two arbitrary time dependent parameters. These could be determined by any two pieces of independent information. As the first, we choose the asymptotic relations (263). The second is a low condition, that the first derivative, given by (266), always be computed correctly.

As an illustration of the procedure in a simple case, we now apply it to (264). The functional form (258a) has asymptotic zeros at

$$\left(\frac{\mathcal{E}_n(\ell)\lambda(\ell)}{2i}\right)^{1/2}\mathcal{F}(\ell) = (2n+1)\frac{\pi}{2} \qquad ; n\to\infty \tag{268a}$$

while the condition (263) locates them at

$$\left(\frac{\mathcal{E}_n(\ell)}{2i}\right)^{1/2} K^{1/2}\ell = (2n+1)\frac{\pi}{2} \qquad ; n\to\infty \tag{268b}$$

The first derivative of the function (258a) is

$$\frac{\partial\psi}{\partial\mathcal{E}}(\ell,\mathcal{E}=0) = i\frac{\lambda(\ell)}{2}\left[\mathcal{F}(\ell) - \left(1-e^{-\mathcal{F}(\ell)}\right)\right] \tag{269a}$$

while, in the energy independent case, (266) becomes

$$\frac{\partial\psi}{\partial\mathcal{E}}(\ell,\mathcal{E}=0) = i\left[\ell - \frac{2}{K}\left(1-e^{-K\ell/2}\right)\right] \tag{269b}$$

Inspection shows that $\mathcal{F} = K\ell/2$ and $\lambda = 4/K$. It is easy to verify that the function (258a), with these parameters, has been transformed into the exact solution of (264). At the same time, the function (258b) will also transform into the second normalized solution of (264), $\chi(\ell,\mathcal{E})/\chi(\ell,0)$.

D. Sample Calculations

We analyze a charged particle multiple scattering problem from beginning to end and construct a few of the relevant distributions.

We continue with the relativistic electron example defined by

$$\frac{d^2\psi}{dl^2} + \frac{K(0)}{2(1-l/R+\alpha)^2}\frac{d\psi}{dl} + \frac{g}{2i}\frac{K(0)}{(1-l/R+\alpha)^2}\psi = 0 \qquad (270)$$

The functions (258a,b) become solutions when we determine the parameters ξ, λ by applying the conditions (263) and (266) with (254). Matching the locations of the asymptotic zeros gives

$$\lambda\,\xi^2(l) = \left\{\int_0^l dl'\,(K(l'))^{1/2}\right\}^2 \qquad (271)$$

from (263) and (268). Doing this integral with (254) gives

$$\lambda\,\xi^2(l) = K(0)(R+\alpha)^2\,\ln^2(1-l/R+\alpha) \qquad (272)$$

as our first condition. The integral (266) using (254) may be written

$$\frac{\partial\psi(l,g=0)}{\partial g} = i(R+\alpha)t_0\,e^{t_0}\left\{\left(E_1(t_0)-\frac{e^{-t_0}}{t}\right)-\left(E_1(t)-\frac{e^{-t}}{t}\right)\right\} \qquad (273)$$

where

$$t(l) = \frac{K(0)(R+\alpha)}{2(1-l/R+\alpha)} \quad ; \quad E_1(t) = \int_t^\infty dy\,\frac{e^{-y}}{y} \qquad (274)$$

and $t_0 = t(0)$. Once we specify the numerical values of $K(0)$, R and α we can simply look up the value of this derivative since E_1, is a tabul-

ated function[20]. We equate (268) and (273) to obtain our second condition and then solve easily for $\Sigma(\ell), \lambda(\ell)$ by using (272) as well. The numerical behavior of Σ, λ determined this way is plotted in Fig. (7a,7b) for the case of electrons, with initial energies of 5 and 20 MeV, penetrating water. The numerical values of $K(o), R, u$ that were used will be given in Fig. (9).

The zeros of ψ are the calculable from (259) and the first several are plotted in Fig. (7c) for the 20 MeV electron case. For $\rho \to \infty$ we can approximate terms in the infinite product (253) as

$$\left(1 - \frac{\rho}{\rho_n(\ell)}\right) \simeq -\frac{\rho}{\rho_n(\ell)} \simeq \frac{\rho_n^{WKB}(\ell)}{\rho_n(\ell)} \left(1 - \frac{\rho}{\rho^{WKB}(\ell)}\right) \qquad (275)$$

and then use it to show that

$$e^{-\Sigma(\ell)/2} = \prod_{n=1}^{\infty} \left\{ \frac{\rho_n^{WKB}(\ell)}{\rho_n(\ell)} \right\} \qquad (276)$$

In the initial stages of the problem, all the zeros may be computed by (263) and $\Sigma = 0$ identically, as was the case in Yang's problem. Scattering deforms distributions by moving the zeros around and the ratio (276) can give a measure of how much rearrangement there has been from very early times to some later time that we might be interested in. The suggestion is that $\Sigma/2 = 1$ will allow us to estimate when rearrangement due to scattering is beginning to become noticable or significant. This occurs at about $\ell = .8R$ in both the 5 and 20 MeV electron examples.

To construct a distribution we invert the Fourier transform by

closing a contour in the upper half complex ξ plane. The longitudinal density

$$f(\ell,\Delta) = \frac{1}{2\pi}\oint d\xi \, \frac{e^{i\xi\Delta}}{\psi(\ell,\xi)} \tag{277}$$

then becomes

$$f(\ell,\Delta) = \sum \frac{i}{\phi_n(\ell)}\, e^{i\xi_n(\ell)\Delta} \tag{278}$$

for $\Delta>0$, where the slope of the wave at its n^{th} zero is defined by

$$\phi_n(\ell) = \left.\frac{\partial\psi(\ell,\xi)}{\partial\xi}\right|_{\xi=\xi_n(\ell)} \tag{279}$$

For $\Delta<0$ we close contours in the lower half plane. Since ψ^{-1} is never singular there, we always have $f(\ell, \Delta<0)=0$. Along with the zero locations, we also need the derivative of (258a) to evaluate (279). This is given by

$$\frac{\partial\psi}{\partial\xi}(\ell,\xi) = e^{-F/2}\left[-F\sin\omega F - \frac{1}{2}\frac{\sin\omega F}{\omega^2} + \frac{F}{2}\frac{\cos\omega F}{\omega^2}\right] \tag{280}$$

where $\omega = (\xi\lambda/2i)^{1/2}$.

Sample results are shown in Fig. (7d)for the 20 MeV electron case. The number of terms in the series (278) that are required to adequately represent a result depends on Δ. Large Δ, $\Delta/\bar{\Delta} \gtrsim 2$ requires only the first term, small Δ, $\Delta/\bar{\Delta} \simeq .2$ requires the first five.

Up to now we have used the time dependent picture exclusively, a picture which considers particle distributions at any given instant.

Some of the most important and familiar results are steady state or time independent calculations which are obtained by integrating over many instants.

The longitudinal steady state density defined by

$$f(z) = \int_0^\ell d\ell\, f(\ell, \ell - z) = \int_0^{R-z} d\Delta\, f(z+\Delta, \Delta) \qquad (281)$$

sweeps a pulse across a plane at depth and counts the number of particles between $z, z+dz$ over the duration of a particle's lifetime. The normalized distribution $f(z)/R$ corresponds to injecting a continuous current of particles where the current strength is adjusted so that there is always one particle somewhere within the material at all times. Expanding the integrand about the time $\ell = z$

$$f(z+\Delta, \Delta) = f(z, \Delta) + \frac{\partial f(z,\Delta)}{\partial z}\Delta + \ldots \qquad (282)$$

develops (281) into a series of time derivatives of space integrals

$$f(z) = \sum_{K=0}^{\infty} \frac{1}{K!} \frac{\partial^K}{\partial z^K} \left(\int_0^\delta d\Delta\, f(z,\Delta)\, \Delta^K \right) = \sum_{K=0}^{\infty} f^{(K)}(z) \qquad (283)$$

where the upper limit remains fixed $\delta = R - z$. The first term in the series is the largest and is given explicitly by

$$f^{(0)}(z) = \sum_n \frac{e^{i g_n(z)\Delta}}{g_n(z)\,\phi_n(z)} \Bigg|_{\Delta=0}^{\Delta=\delta} \qquad (284)$$

using (278). Since

$$\int_{-\infty}^{\infty} d\Delta\, f(z,\Delta) = \int_0^\infty d\Delta \sum_n \frac{i\, e^{i g_n(z)\Delta}}{\phi_n(z)} = \sum_n \frac{-1}{g_n(z)\,\phi_n(z)} \qquad (285)$$

by (278), and since

$$\int_{-\infty}^{\infty} d\Delta\, f(z,\Delta) = \int_{-\infty}^{\infty} d\Delta \left(\frac{1}{2\pi} \int_{-\infty}^{\infty} d\beta\, \frac{e^{i\beta\Delta}}{\psi(\lambda,\beta)} \Big|_{\lambda=z} \right) = 1$$

we can write (284) simply as

$$f^{(0)}(z) = 1 + \sum_n \frac{e^{i\beta_n(z)\delta}}{\beta_n(z)\,\phi_n(z)} \qquad (287)$$

Analogous expressions can be given for the higher $f^{(\kappa)}(z)$ as well. The numerical behavior of the first several $f^{(\kappa)}(z)$ is shown in Fig. (8a) for the 20 MeV electron example. Their summation into $f(z)$ is Fig. (8b).

Spatial distributions indicating the release or absorption of energy within a material are also quite important in applications and are very closely related to density calculations. For example, the energy dissipated between the layers $z, z+dz$ by a penetrating primary beam would be given by

$$D(z) = \int_0^R d\lambda\, S(E(\lambda))\, f(\lambda, \lambda - z) \qquad (288)$$

where S represents an appropriate stopping power. If we continue with the 20 MeV electron example, then the nearly constant behavior of allows us to write

$$D(z) \simeq S(E(\lambda = z))\, f(z) \qquad (289)$$

which will realize a good estimate easily. Combining the collision part of the stopping power, which accounts for ionization losses only and $f(z)$ according to (289) gives our estimate of $D_c(z)$. This is plotted in Fig. (8c). The short horizontal lines on that plot are Berger's 20

MeV electron result[21] obtained by a variation of the Monte Carlo method. The agreement is reasonable and there probably should be some disagreement in these results because of differences in the way the electron scattering was parameterized, e.g., Berger did not use (254).

Berger and Seltzer[22] gave a much more extensive presentation of their results in their 1969 work and followed later with further calculations also based on Monte Carlo methods[23]. These works also provide some worthwhile background information and perspective on the electron penetration problem.

E. The Linear Approximation

The replacement of (234) by (251) was a key simplicity that was incorporated into the results of sections VC, VD. We check the sense and quality of that approximation here.

Consider first a more extended use of the functions (258a,b) in which we aim to construct the complete spatial density. We again need two conditions to determine the parameters ξ, λ but this time we use the first two longitudinal moments to do it. The moment series for the longitudinal distribution is obtained by comparing the exponential expansion

$$f(t,\beta) = \sum_{m=0}^{\infty} \frac{(-i\beta)^m}{m!} \overline{\Delta^m(t)} \qquad (124)$$

against the Taylor expansion of

$$f(t,\beta) = 1/\psi(t,\beta) = \left(\sum_{m=0}^{\infty} \frac{\partial^m}{\partial \beta^m} \psi(t,\beta=0) \frac{\beta^m}{m!} \right)^{-1} \qquad (265)$$

from which we obtain

$$\psi(\ell,\beta)\Big|_{\beta=0} = 1 \qquad (290a)$$

$$\frac{1}{i}\frac{\partial \psi(\ell,\beta)}{\partial \beta}\Big|_{\beta=0} = \overline{\Delta(\ell)} \qquad (290b)$$

$$\left\{\frac{\partial^2 \psi}{\partial \beta^2} - \left(\frac{\partial \psi}{\partial \beta}\right)^2\right\} = \overline{\Delta^2} - (\bar{\Delta})^2 = \sigma^2 \qquad (290c)$$

without much difficulty. Expressions which will give the numerical values of these derivatives are obtained directly from the differential equation for ψ, which in this case would be (234). If we also have a specific function in mind, in this case (258a), we simply take its derivatives and evaluate them at $\beta = 0$, giving expressions which involve only F, λ. We then set these expressions equal to their numerical values that were obtained from the transport equation to determine the numerical values of F, λ.

This procedure defines the parameters of the second function, (258b), simultaneously. We could then use both of them and write the complete density as

$$f(\ell,\rho,\beta) = \frac{1}{\psi(\ell,\beta)}\, e^{-\rho^2 \frac{\eta(\ell)}{2i\beta}} \left(1 - \frac{\psi(\ell,0)}{\psi(\ell,\beta)}\,\frac{\chi(\ell,\beta)}{\chi(\ell,0)}\right) \qquad (291)$$

which generalizes on (252) by introducing a third parameter η. We would determine this third parameter by requiring that

$$\eta(\ell)\left\{\frac{1}{2i\beta}\left(1 - \frac{\psi(\ell,0)}{\psi(\ell,\beta)}\,\frac{\chi(\ell,\beta)}{\chi(\ell,0)}\right)\right\}_{\beta\to 0} = A_3(\ell,\beta=0) \qquad (292)$$

where $A_3(\ell,0)$ would be computed from (237) and a calculation valid to order ρ^2.

The quantity $A_3(\ell,0)$ gives a measure of the lateral spread of the beam. From the definition

$$\overline{\eta^2(\ell)} = \iiint dx\, dy\, d\Delta\, (x^2+y^2)\, f(\ell,x,y,\Delta) \tag{293}$$

spatial Fourier transforms of the type (218) give

$$\overline{\eta^2(\ell)} = -\left(\frac{\partial^2}{\partial p_x^2} + \frac{\partial^2}{\partial p_y^2}\right) f(\ell,p_x,p_y,\beta)\Big|_{\substack{p=0\\ \beta=0}} \tag{294}$$

regardless of the form of the distribution. Since we also know the form of the (Fourier transform of) the density, we obtain

$$\overline{\eta^2(\ell)} = 4\, A_3(\ell,\beta=0) \tag{295}$$

The method just outlined is a moments approach in which the first three moments, the average depth of penetration $\overline{\Delta}$, the lateral and longitudinal widths, $\overline{\eta^2}$ and σ^2, are used to construct the complete density. This approach is more general and allows us to produce results of greater accuracy than the procedure discussed in section VC because we can apply it to (234) without the approximation (251). This improved accuracy is not free because the moments procedure is considerably more laborious. Our remaining remarks are intended to illustrate that we achieve very little improvement for this extra effort and that the procedures discussed in sections VC,D are perfectly adequate to handle the electron penetration problem.

Let us first note that the transport equations (193), (234), and (251) all agree exactly on the first moment, $\overline{\Delta}$. Our method of solving (251) used the condition (266). Because we incorporated that step into our method of solution, we are guaranteed, by relation (290b), that distributions constructed by that method will always have an aver-

age value that is in exact agreement with the transport equation. To see differences between (234) and (251) and the corresponding densities that they produce, we need to look at the next moments, $\overline{n^3}(\ell)$ and $\sigma^2(\ell)$, which describe the widths of the particle distributions.

Let us further note that the equations of motion (213), (251), (234) are progressively more accurate descriptions of the diffusion process and would be used to describe small angle behavior, a transition region, spherical symmetry. In the electron problems that we have been using, the charged particles are relativistic over most of their path length and are rather difficult to deflect under these conditions. Once they do lose enough energy so that they are more easily deflected, they won't go very far. They soon run out of energy and stop well short of the diffusion limit, spherical symmetry, while still in the transition region. This is the physical reason why we would try to apply (251).

Since the differences between these equations develop with increasing time, the case of energy independent scattering is worth considering first. We can easily compute all the relevant moment expressions and then project them to indefinitely long times, allowing a worst case comparison. We find that $\sigma_{251}/\sigma_{234} = \sqrt{3}$ as $\ell \to \infty$ and that there is an analogous disagreement in the lateral width by a factor of $\sqrt{3/2}$. The differences will be smaller in actual problems because particles don't scatter forever.

We consider again the example of electrons penetrating water and summarize the situation in Figure (9). The scattering parameters that

were used were obtained from the large angle version of (56) and also (160). Using reasonable approximation, they yield the simpler form (254), which allows convenient manipulation, as well as the values of $K(0)$ and α that are given in this table. The particle ranges, R, are obtained by evaluating integrals (42). This was done by Berger and Seltzer and it is their values that were used.

The results of interest are the longitudinal moments evaluated at $t=R$. The average value, $\bar{A}$, is the same whether computed by (234) or (251) but they differ on the second moment by ratios of 1.17, 1.12, 1.10. These ratios are all smaller than the upper limit of $\sqrt{3} = 1.73$ set by the energy independent example.

The greatest disagreement is in the 5 Mev case and a comparison of the two associated longitudinal densities is shown in Fig. (10). The improvement in accuracy is minor, almost negligible, and not worth the significant extra effort that it takes to achieve it. Since the lateral disagreement would be even smaller, as the energy independent example indicates, the replacement of (234) by (251) should be perfectly adequate to handle the electron penetration problem.

VI. Concluding Remarks

Theory and experiment work well together to promote genuine progress because each aims to accomplish something different. From experiment we can expect to produce accurate and reliable numbers. The primary purpose of a theory is to explain and predict these numbers, not to generate them. In the nearly four decades that medical physicists have used megavoltage electron beams, theory remained neglected and unattended to, with exceptional and undue emphasis placed on experiment. The one sided character of their effort seriously arrested their progress.

Part of the problem was medical physicists themselves. They chose to probe the charged particle penetration problem by using tools that they felt comfortable with, e.g., ionization chambers, but avoided the use of tools that they were unfamiliar with, e.g., differential equations. A more significant part of the problem was that the theory itself appeared not to be able to accomplish anything of value. The material that was generally being presented to them under the label of theory was actually numerical analysis. A successful numerical analysis will produce accurate numbers. Since medical physicists were already able to produce accurate numbers by experiment, and more reliably than by calculator, they found that "theory" was ignorable.

Theories should be developed analytically and the key word in a theory is structure. The mathematical structure that comes from the solution of a differential equation can be expected to provide an organization, connections and relations, that can reduce a tremendous

quantity of numbers down to a very few. That simplicity and understanding is what we mean by a solved problem. The structure that does this is not only valuable as theory but is also exploitable in applications. We cannot get it from a numerical analysis nor from an experiment.

That theories should be developed analytically is certainly the case in other successful theories with which we are familiar, e.g., Schrodinger's quantum mechanics or Maxwell's electrodynamics. That transport theory is no exception is a message that should have come through clearly in the works of Fermi and Yang. Moreover, as these works also illustrate, problem solving is accomplished by precision of thinking, by finding the right idea, not by reliance on brute force approaches, such as Monte Carlo methods.

It should not be surprising then that the first real breakthrough for medical physicists came about rather recently, after they ignored the last few decades of theoretical non-development and went back to use Fermi's analytic theory. Extending this success inevitably leads to Yang's theory, a much more complicated theory which engages a number of other topics, i.e., moments, the complex plane, wave equations and eigenvalues.

Chapters II, III and IV of this work may be considered to be background sections, of some interest to medical physicists. Chapter V contains the material that they will find most worthwhile. Parts of it will be essential to applications of this theory. Our development ended once we showed that we had a well defined theory, with its equa-

tions working, and that we could extract its predictions so that they could be compared against experiment. The actual comparisons with experiment, modeling with inhomogeneous configurations, the writing of treatment planning computer programs, are all topics that remain to be pursued.

Figures

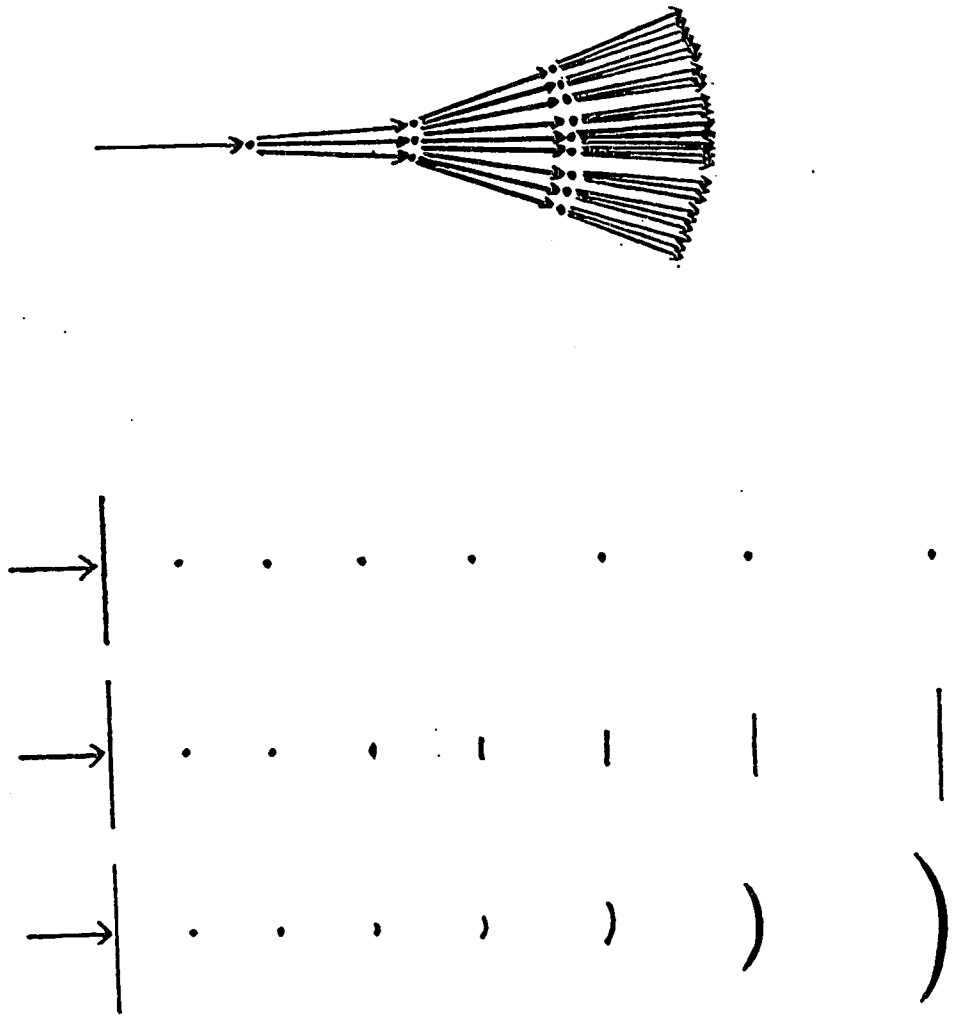


Fig. 1 Schematic transport diagrams. Top, Fermi's identification of multiple scatter as a shower or multiplication problem. The length of each arrow is the infinitesimal distance, dl. Proceeding downwards, (a) the ray, or scatterless picture, (b) Fermi's lateral transport model, (c) a second order picture which is equivalent to Yang's theory.

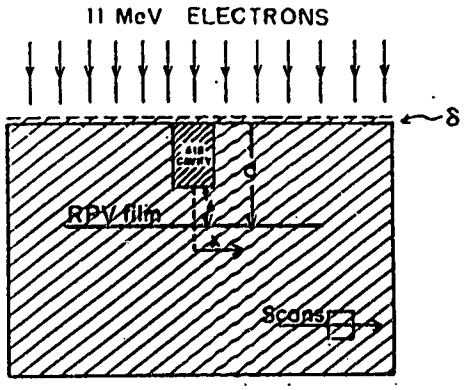


Fig. 2a. Schematic showing the experimental arrangement for determing the dose behind a small inhomogeneity. A 1x1x2 cm air cavity was cut into a solid polystyrene phanton. From Fig. 7 Perry and Holt.

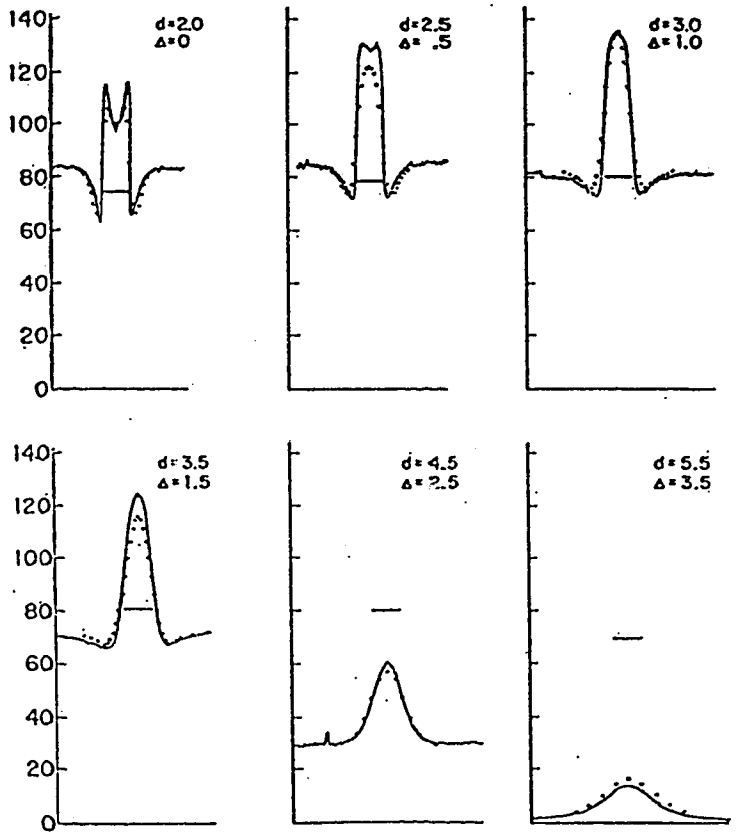


Fig. 2b. The agreement between measured and predicted dose distributions at various depths behind the test cavity. The continuous line is the measured film density; the points are our calculated values; the short horizontal line is the ray model prediction. From Fig. 8 Perry and Holt.

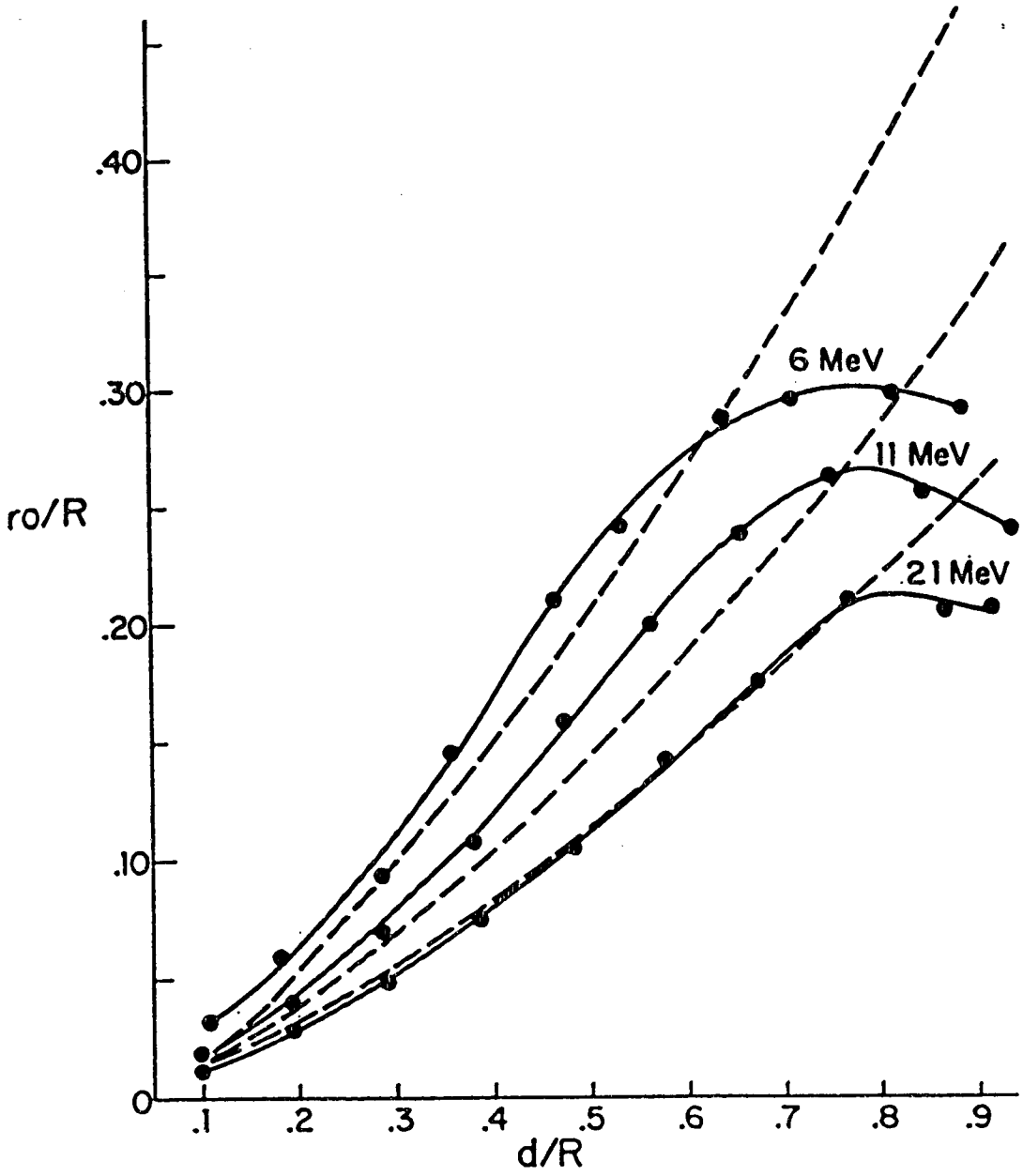
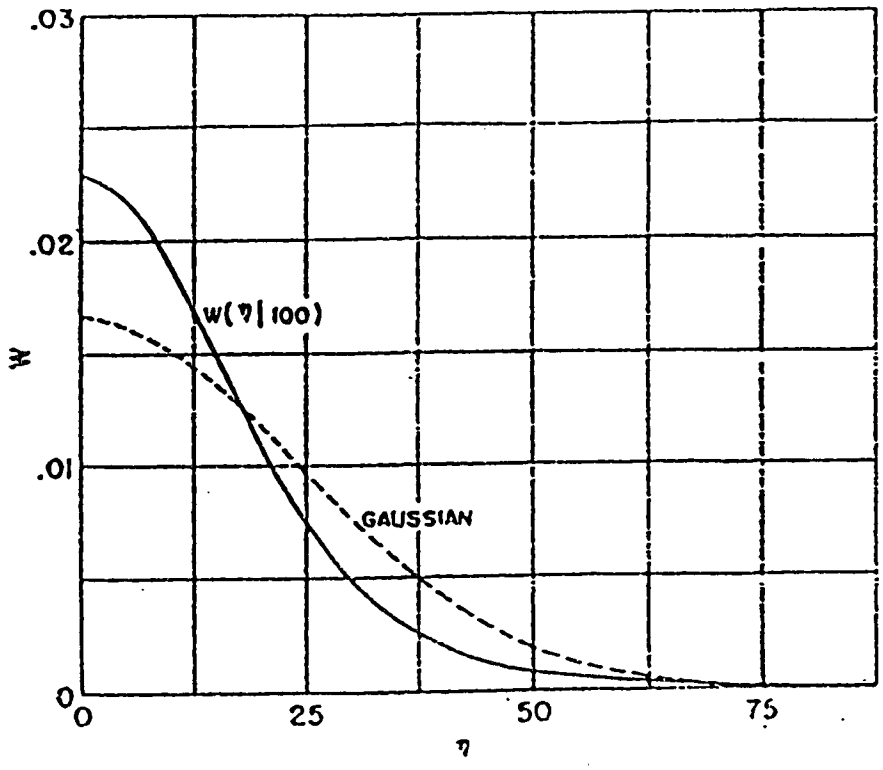


Fig. 3 Lateral width as a function of depth in polystyrene. Measured values (solid lines) are compared against predicted values (dashed lines) for electron beams with various incident energies. From Fig. 5 of Perry and Holt.



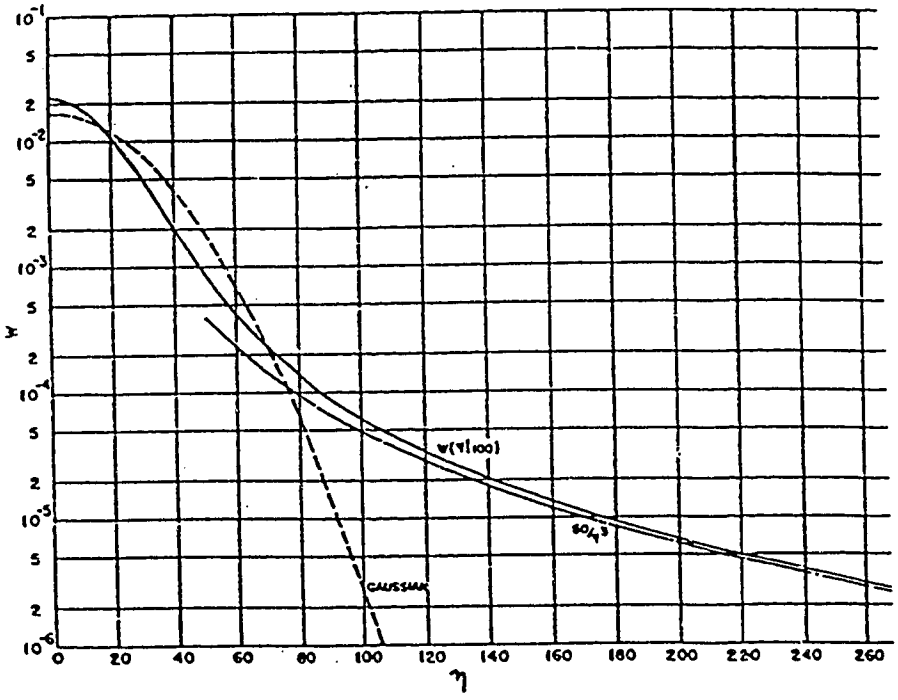


Fig. 4. The angular distribution after 100 collisions is compared against the Gaussian approximation and the single scattering Rutherford result which it approaches for larger angles. From Figs. 5 & 6 Snyder and Scott.

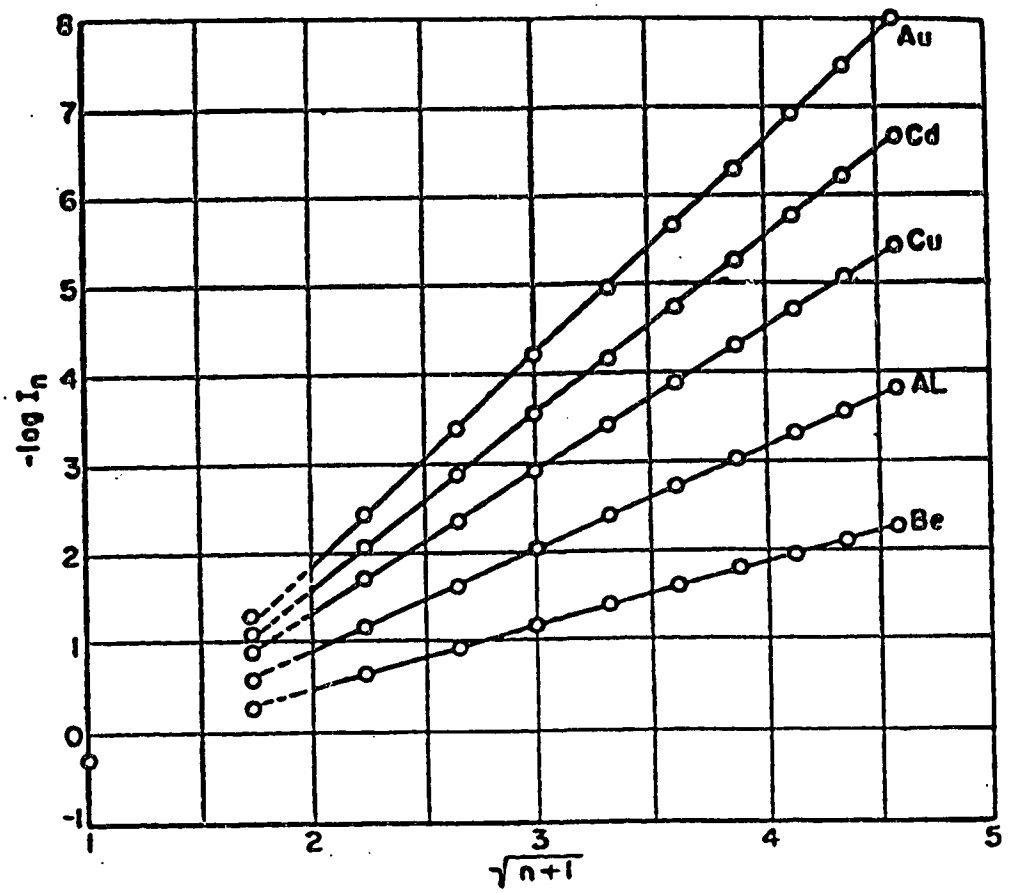


Fig. 5. Numerical values of moments plotted into straight lines. From Fig. 2 Spencer.

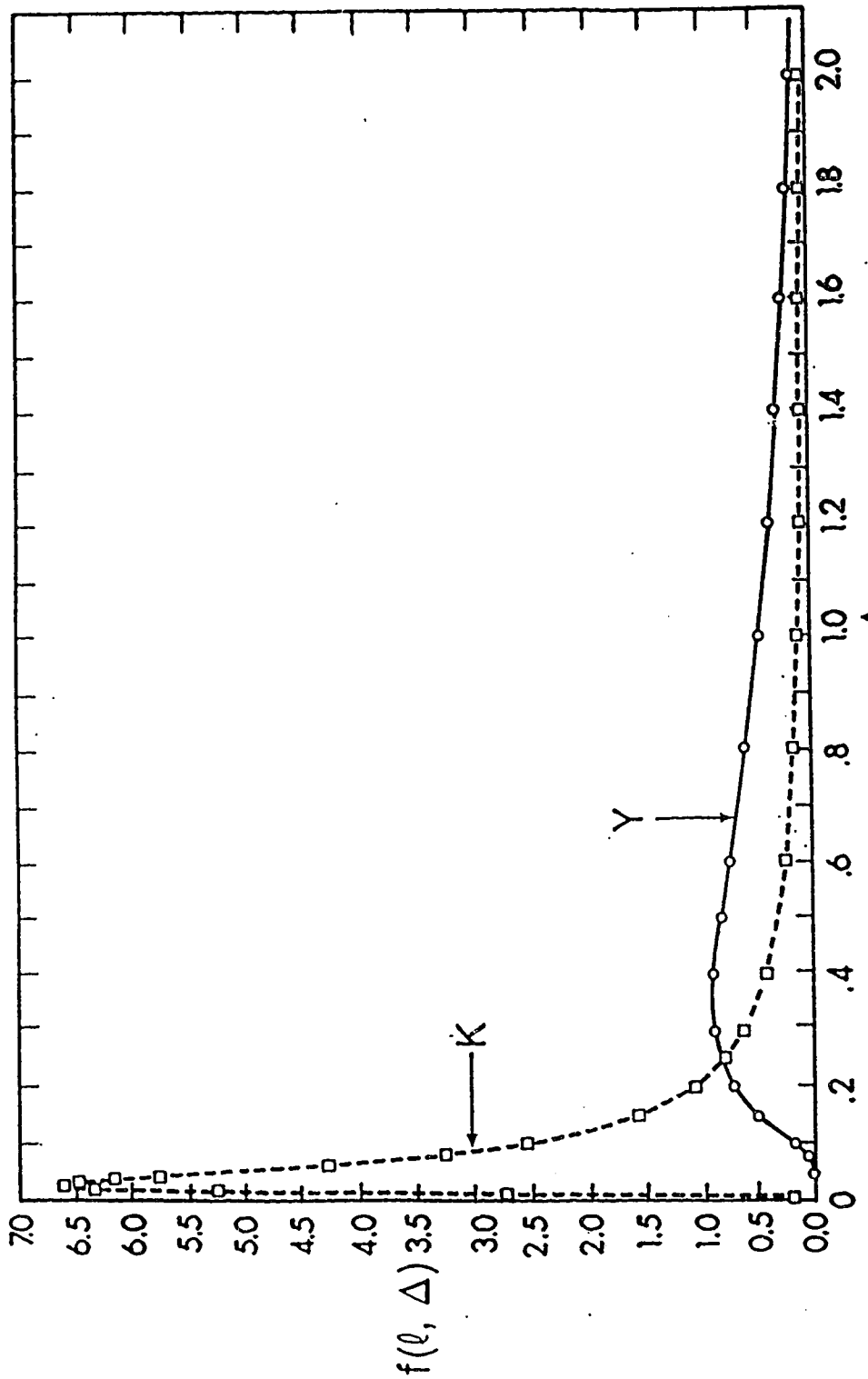


Fig. 6. Comparison of Kessaris' and Yang's calculations after 1.0 cm. of water.

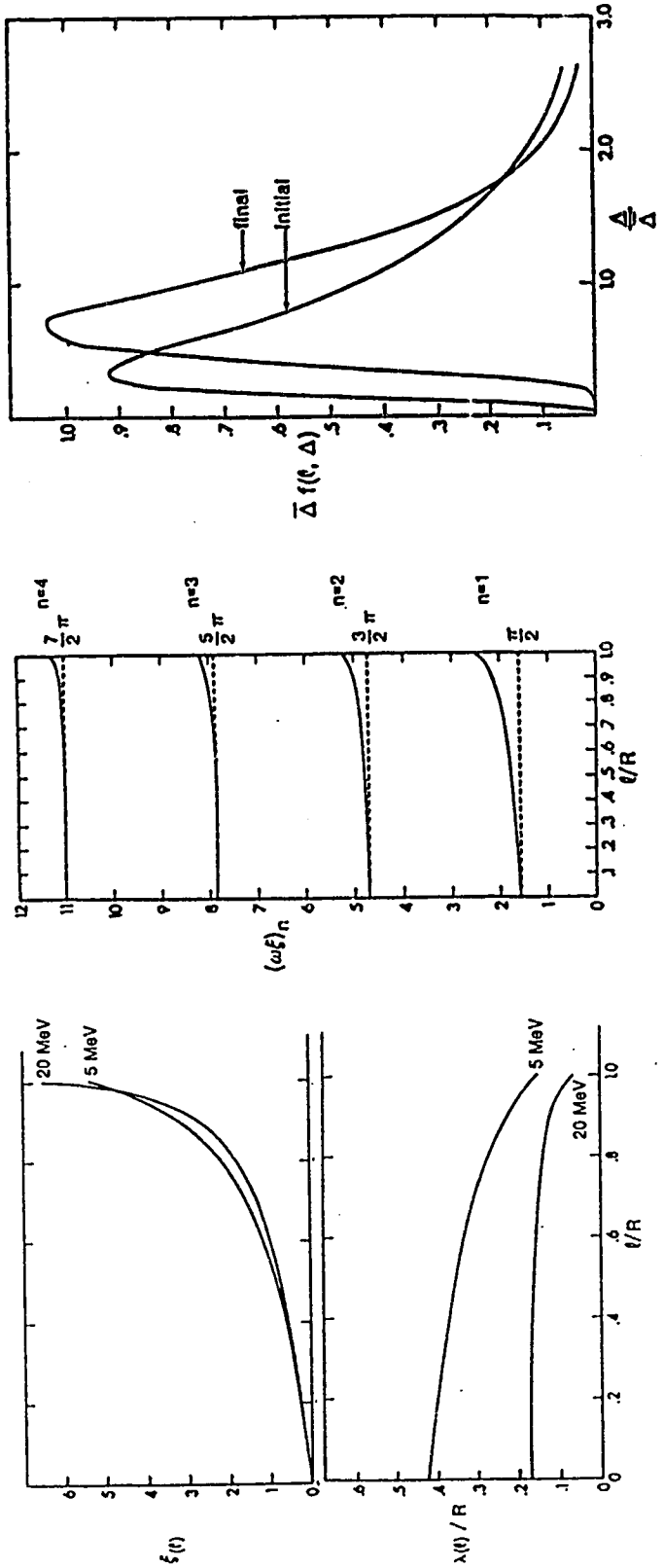


Fig. 7. The behavior of the parameters ξ, λ is shown for electrons with initial energies of 5 and 20 MeV penetrating water (a,b). The movement of zeros and corresponding longitudinal densities are illustrated (c,d) for the 20 MeV electron case.

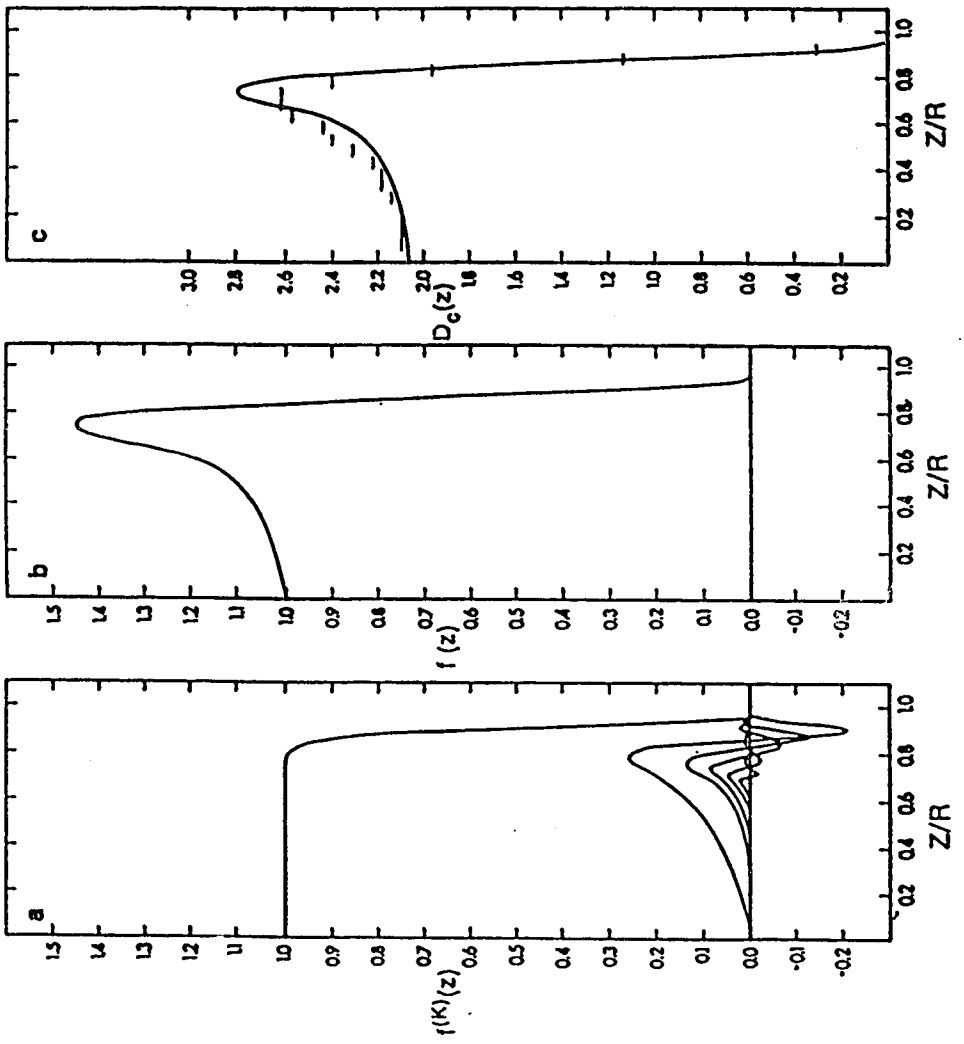


Fig. 8. Steady state results for the 20 MeV electron example. The numerical behavior of the first several $f^{(K)}(z)$ is shown on (a) and their sum into the density is (b). The energy loss by ionization (c) is compared against Berger's 20 MeV calculation, the short horizontal lines.

Model Parameters Used for Electrons Penetrating Water				First and Second Moments of the Longitudinal Distribution Computed at the End of Range			
E_o(MeV)	K(0) rad$^{\&}$/cm	R (cm)	$\propto$	$\bar{\Delta}$(234 or 251)	$(\sigma/\bar{\Delta})_{251}$	$(\sigma/\bar{\Delta})_{234}$	$\sigma_{251}/\sigma_{234}$
5	.255	2.50	.102 R	.334 R	.554	.475	1.17
10	.0761	4.88	.051 R	.259 R	.530	.472	1.12
20	.0217	9.18	.026 R	.184 R	.515	.469	1.10

Fig. 9. Parameters that were used in association with the energy dependent form (254).
The first and second moments of the longitudinal distribution computed by equation (251) and the more accurate (234) are then compared at the end of range using 5, 10, 20 MeV electrons penetrating water.

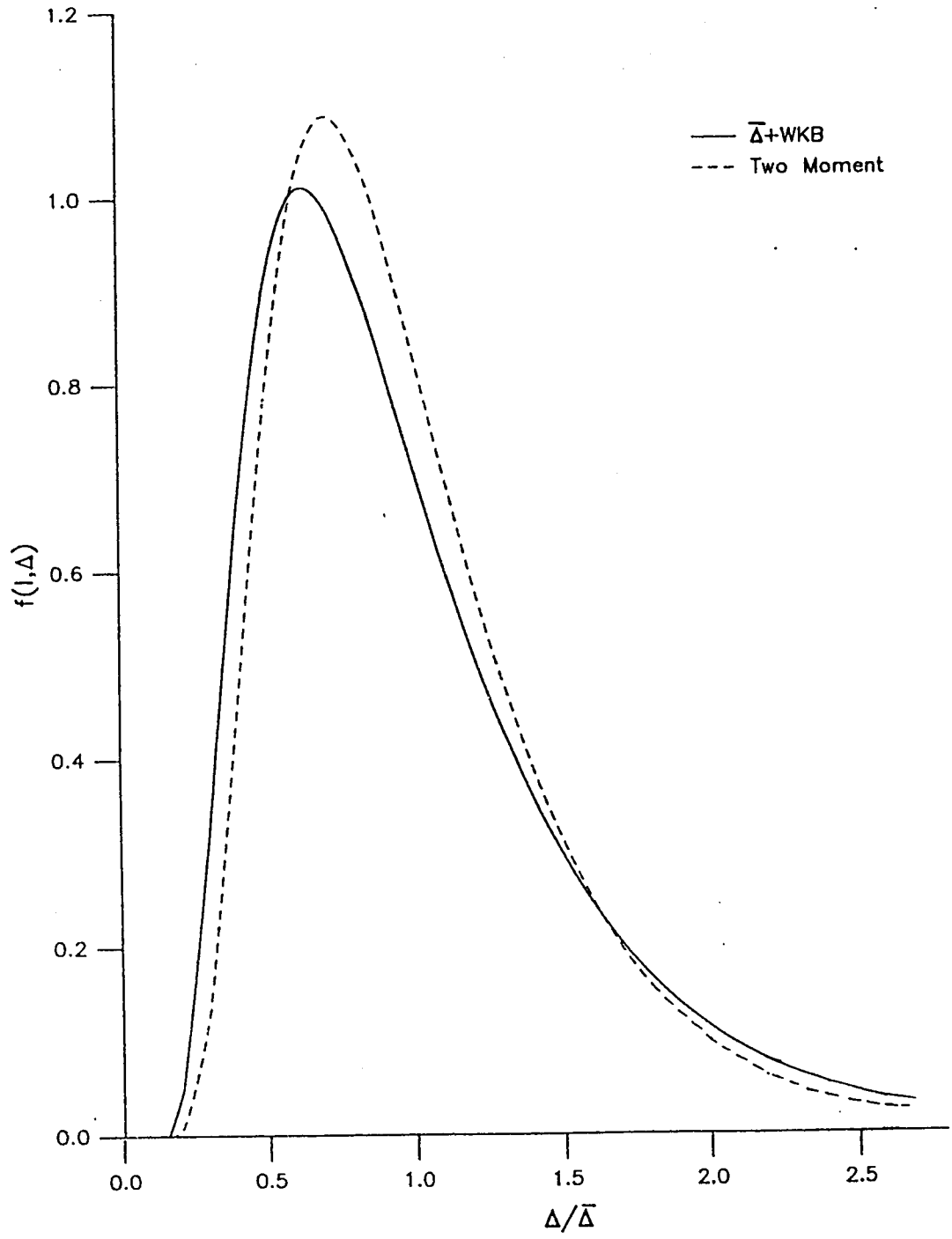


Fig. 10. The longitudinal distribution at the end of range for the case of 5 MeV initial energy electrons penetrating water. Two computations are compared. The curve labeled $\bar{\Delta}$ + WKB uses the method discussed in sections VC,D and equation (251). The more accurate two moment approach uses the method discussed in section VE and eqn. (234). The numbers used in both calculations are given in Figure 9. This comparison checks the quality of the linear approximation.

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