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WAVE PACKET SCATTERING AND TIME DELAY

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ABSTRACT

The scattering of a wave packet by a finite range potential may be described by a wave function in which the initial state is specified at time $t = 0$, and the time dependence appears in functions $M(r, k, t)$, first obtained by Moshinsky.

The $t = 0$ wave function is derived, following the treatment of Rosenfeld, but using the Green's function for the radial wave equation to simplify the calculation of the Laplace transform. The treatment is extended to include the case of a packet initially within the potential, and the wave function for a decaying wave packet is derived. This agrees in form with the wave function obtained by Jeukenne in another approach.

By using an alternative expression for the Green's function, it is shown that the $t = 0$ wave function is equivalent to an expansion in scattering states. The relationship between the $t = 0$ wave function and the $t \to -\infty$ wave function of standard scattering theory is examined, and the restrictions on the position and shape of the initial packet in the latter wave function are emphasized. On the question of transients in time-dependent scattering theory, it is pointed out that a distinction should be drawn between plane wave treatments and those using wave packets.

The second part of the thesis is concerned with the calculation of time delay for an arbitrary wave packet interacting with a finite range potential. The $t = 0$ wave function is used, and a new method of calculation developed, in which momentum coefficients in the wave function are written as transforms of the initial packet, and momentum integrals are expressed in terms of Green's functions. General expressions are obtained for the time spent within a sphere of finite radius by the wave packet, in the presence of the potential and with the potential removed. The idea of time delay for a scattered packet is extended to include the lifetime of a decaying wave packet, and corresponding expressions are obtained when the packet is initially within the region of the potential.

Previous expressions for time delay have been derived using the $t \to -\infty$ wave function, and it is found that the use of the $t = 0$ wave function gives new terms, which arise from the principal part integral of a $\delta^{(+)}$ function. Terms of the type $\frac{d\alpha}{dk}$, which appear in Ohmura's expression for time delay, are found only in the calculation of lifetime. A discussion in one dimension shows that these terms represent the mean arrival time of the packet at the origin, and that other terms appearing in the various expressions have simple physical interpretations.

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INTRODUCTION

Time-dependent scattering theory describes the development of the scattering system from the initial state to the final state under the action of the Hamiltonian $H = H_o + V$.

The scattering process is usually divided into three stages. Initially, the particles are free and propagate according to the Hamiltonian H_o. The collision occurs when the particles come within the range of interaction, and the potential V takes effect. After some time, the particles separate, and in the final state the propagation is again governed by H_o.

In the standard treatment of Lippmann and Schwinger (1950), the initial and final states are actually eigenstates of H_o (plane waves), and the interaction producing the scattering is switched on and off adiabatically,

$$V(\underset{\sim}{r},t) \quad = \quad V(\underset{\sim}{r})\ e^{-\varepsilon|t|/\hbar} \underset{t \to \pm\infty}{\longrightarrow} 0 \quad . \tag{I.1}$$

This procedure leads to the wave functions of formal scattering theory,

$$\Psi^{(\pm)} \quad = \quad \Phi + \frac{1}{E_o \pm i\varepsilon - H_o}\ V\ \Psi^{(\pm)} \quad , \tag{I.2}$$

where Φ is a plane wave state,

$$H_o\Phi \quad = \quad E_o\Phi \quad . \tag{I.3}$$

The use of plane waves is familiar from elementary (time-independent) scattering theory, but it introduces the complication that the wave functions are not readily normalised. Some artifice such as box normalisation must be used, and this in turn makes it necessary to treat the limiting procedures of time-dependent theory very carefully (Gell-Mann and Goldberger 1953). It is more satisfactory to treat scattering in terms of wave packets, since normalisation is then included automatically, and the variation of the interaction with time arises from the approach and separation of the localised particles, rather than switching of the potential.

Wave packet scattering has been treated by many authors (Sunakawa 1955, Moses 1955, Jauch 1958, Low 1959, Haag 1960, Green and Lanford 1960, Goldberger and Watson 1964) but it is generally the case that discussion is limited to obtaining plane wave results. The treatment may be such that it is valid only for long wave packets, or the restriction to a narrow momentum distribution may be applied at the end of a more general calculation. In either case, the cross section (or some other quantity) is derived for a fixed value of the momentum, and the use of wave packets in the derivation simply provides a reasonable physical picture, or permits a mathematically rigorous treatment.

The results thus obtained are sufficient to describe most current scattering experiments, but they do not exhaust the possibilities of wave packet scattering. The most obvious application of wave packet ideas is in the consideration of <u>time-dependent</u> experiments. If the time at which an interaction occurs is to be well defined, the particles involved must be strongly localised in space, and so must be described by wave packets with broad momentum distributions.

A model of a time-dependent scattering situation which has been studied by several authors (Nussenzveig 1961, Dodd and McCarthy 1964, Goebel and McVoy 1966) is that of a wave packet of resonance shape interacting with a scatterer which has a resonance of similar position and width. As the width of the packet is varied, the rise time and decay time for the compound system also vary. If the width of the packet, γ_o, is much less than that of the resonance, γ_1, the rise time is roughly $2\tau_1$ ($\tau_i \propto \frac{1}{\gamma_i}$) but the decay time is $2\tau_o$. This corresponds to exciting the resonance with a very long packet, so that the rate of decay is equal to the rate at which the incident packet dies away. If instead $\gamma_o >> \gamma_1$, the rise time is $2\tau_o$ and the decay time $2\tau_1$ - the resonance is excited rapidly by a sharp packet, and then decays at its natural rate.

It has been suggested that wave packet experiments would provide a means of separating direct and compound nucleus processes in nuclear reactions, and the model mentioned above is relevant to discussion of such experiments. In order that the direct and compound scattered packets may be well separated in time, the incident packet must have a very broad momentum distribution ($\gamma_o >> \gamma_1$). This produces a direct packet which leaves the scatterer almost immediately, and a compound packet which emerges after an appropriate time delay. If the momentum distribution is too narrow ($\gamma_o << \gamma_1$), the duration of the incident packet is so long that there is still a direct component present when the compound packet emerges, and it is not possible to separate the two by time resolution.

An important quantity in the consideration of such time-dependent experiments is the time delay suffered by the particle as it interacts with the scatterer. If the particle is captured in a resonance it is delayed for a long time before being emitted from the compound nucleus, whereas if it undergoes a direct reaction it is delayed very little relative to the corresponding free particle. The idea of separating compound nucleus and direct processes in a wave packet experiment depends, of course, on the fact that the two types of scattering give vastly different time delays.

This thesis is concerned with the question of time delay in scattering situations, and in particular, with the calculation of the time delay experienced by an arbitrary wave packet as it interacts with an arbitrary finite range potential.

It should be mentioned that the notion of time delay is closely linked with the idea of measuring the mean arrival time of the wave packet at a point or at a surface. The measurement of arrival times in quantum mechanics has recently been the subject of an intensive investigation by Allcock (1969), but the questions and problems raised by Allcock's paper are quite beyond the scope of our discussion. We shall be content rather to start from a generally accepted definition of time delay, and to compare our results with those of other authors who have used the same, or a similar, definition.

Previous discussions of wave packet scattering have generally been based on the wave function of standard scattering theory, which involves the asymptotic limit $t \to -\infty$. The initial state of the system is defined by a free wave packet, $\Phi(\underset{\sim}{r},t)$, such that the total wave function for the interacting system, $\Psi(\underset{\sim}{r},t)$, approaches $\Phi(\underset{\sim}{r},t)$ as $t \to -\infty$. The use of this wave function imposes certain restrictions on the position and shape of the initial packet, however, as may be seen by examining a free wave packet in one dimension.

Let us consider a free particle of mass μ, described by a wave packet

$$\Phi(x,t) = (2\pi)^{-\frac{1}{2}} \int_{-\infty}^{\infty} dk\, A(k)\, e^{ikx - \frac{i\hbar k^2 t}{2\mu}} , \qquad (I.4)$$

with the normalisation

$$\int_{-\infty}^{\infty} dk\ A^*(k)\ A(k) \quad = \quad 1 \qquad . \tag{I.5}$$

The mean position of the wave packet at time t is given by

$$\bar{x}(t) \quad = \quad \int_{-\infty}^{\infty} dx\ \Phi^*(x,t)\ x\ \Phi(x,t)$$

$$= \quad \int_{-\infty}^{\infty} dx\ (2\pi)^{-\frac{1}{2}} \int_{-\infty}^{\infty} dk\ A^*(k)\ e^{-ikx + \frac{i\hbar k^2 t}{2\mu}}$$

$$\cdot\ x\ (2\pi)^{-\frac{1}{2}} \int_{-\infty}^{\infty} dk'\ A(k')\ e^{ik'x - \frac{i\hbar k'^2 t}{2\mu}}$$

$$= \quad \int_{-\infty}^{\infty} dk\ A^*(k)\ i\ \frac{d}{dk}\ A(k) \quad + \quad \int_{-\infty}^{\infty} dk\ A^*(k)\ \frac{\hbar k}{\mu}\ A(k)\ .\ t$$

$$= \quad \bar{x}(o) \quad + \quad \bar{v}\ t \qquad . \tag{I.6}$$

In deriving Eq. (6) we have expressed $x\ e^{ik'x}$ in the second line as $-i \frac{d}{dk'}\ e^{ik'x}$, and used integration by parts within the k' integral to transfer the derivative to $A(k')\ e^{\frac{-i\hbar k'^2 t}{2\mu}}$. Since the integral (4) converges, the integrated part vanishes at the upper and lower limits. The expression for $\bar{x}(o)$ may be shown to be real by taking the complex conjugate, integrating by parts, and noting that Eq. (5) converges.

The mean value of $x^2(t)$ may be calculated similarly:

$$\overline{x^2}(t) = \int_{-\infty}^{\infty} dx\ \Phi^*(x,t)\ x^2\ \Phi(x,t)$$

$$= \int_{-\infty}^{\infty} dk\ A^*(k) \left[i \frac{d}{dk}\right]^2 A(k) + \int_{-\infty}^{\infty} dk\ A^*(k) \left[i \frac{d}{dk} \frac{\hbar k}{\mu} + \frac{\hbar k}{\mu} i \frac{d}{dk}\right] A(k)\ .\ t$$

$$+ \int_{-\infty}^{\infty} dk\ A^*(k) \left[\frac{\hbar k}{\mu}\right]^2 A(k)\ .\ t^2$$

$$= \overline{x^2}(o) + \left[\overline{x(o)v} + \overline{vx(o)}\right] t + \overline{v^2}\ t^2 \quad . \tag{I.7}$$

Then the mean square deviation of x is

$$\Delta_x^2(t) = \overline{x^2}(t) - \bar{x}^2(t)$$

$$= \Delta_x^2(o) + \left[\overline{x(o)v} + \overline{vx(o)} - 2\bar{x}(o)\bar{v}\right]t + \Delta_v^2 t^2 \quad . \tag{I.8}$$

From Eq.(6), if we assume $\bar{v}$ is positive it will be seen that $\bar{x}(t) \to -\infty$ as $t \to -\infty$, so the centre of the packet is situated at an infinite distance from the origin. From Eq.(8), since Δ_v^2 is positive, $\Delta_x^2(t) \to +\infty$ as $t \to -\infty$, so the width of the packet increases indefinitely in this limit. Since the wave packet remains normalised, as the width of the packet increases the amplitude at a given point decreases, and in the limit the packet is "thinly spread" over all space. In general, for a wave packet which contains no bound state components, the probability of finding the particle in any finite region goes to zero as t^{-3} in the limit $t \to \pm\infty$ (Haag 1960).

The sense in which the wave functions $\Phi(\underset{\sim}{r},t)$ and $\Psi(\underset{\sim}{r},t)$ approach each other in the initial state must be defined with some care, since the wave functions at any point $\underset{\sim}{r}$ go to zero individually as $t \to -\infty$. The notion of pointwise convergence is inadequate in this situation, and it must be shown instead that $\Psi(\underset{\sim}{r},t)$ converges strongly to $\Phi(\underset{\sim}{r},t)$, i.e.

$$\lim_{t \to -\infty} \int d\underset{\sim}{r} \left| \Psi(\underset{\sim}{r},t) - \Phi(\underset{\sim}{r},t) \right|^2 = 0 \quad . \tag{I.9}$$

The use of the asymptotic limit in scattering theory is usually justified on the grounds that scattering experiments involve distances and times which are large on the quantum scale - the initial packet is prepared in the source of an accelerator, and the time of travel down the accelerator tube is long compared to the time taken to cross a region of nuclear dimensions. However, scattering can be studied in situations which do not involve large distances and times. As an example we mention proximity scattering (Fox 1962), in which the incident and target particles are produced by sequential nuclear decay.

Proximity scattering occurs when the final state of a nuclear reaction contains three particles, and the kinematics are such that two of the particles may subsequently rescatter. In the reaction

$$a + b \to B^* \to c + D^* \to c + d + e \quad , \tag{I.10}$$

if the energy and angular distribution of (say) particle d are suitable, it is possible for d to catch up with c and produce the proximity scattering

$$c + d \underset{\text{prox}}{\to} c + d \quad . \tag{I.11}$$

The lifetime τ_D of D^* and the c-d scattering cross section may be related to the observed energy and angular correlation of c and d. Lifetimes of the order of 10^{-20} sec have been measured by this method (Lang et al 1966), and it also presents a way of obtaining cross sections when either c or d is unstable.

Since c and d are the products of decay processes, they do not have well defined momenta, but may be represented by exponentially decaying wave packets whose momentum widths are inversely proportional to the respective lifetimes. From the mean energies of c and d, and the order of magnitude of τ_D, it is possible to estimate the distance travelled by d before it interacts with c, and in the examples considered by Fox this is typically $\approx$400 fm. The initial state of the reaction (11) thus consists of two exponential wave packets, separated by a distance of several hundred fermis, and the proper treatment of such a reaction requires a scattering theory which is not limited to long wave packets or to infinite separation of the incident and target particles.

Wave packet scattering can in fact be treated as a simple initial-value problem, with the initial state specified at time t = 0. In such a treatment the initial packet, of arbitrary shape, may be localised in a finite region and situated at a finite distance from the scatterer. We shall use the t = 0 wave function in the calculation of time delay in order to obtain expressions valid for an arbitrary initial packet, without restriction on its position or shape.

Apart from allowing the initial packet to be quite general, the use of the t = 0 wave function opens up the possibility of carrying out a calculation in which transient effects in the scattering process are taken into account. In discussions of time-dependent scattering theory, mention is often made of "transients" in the wave function. Gell-Mann and Goldberger (1953), for instance, represent the initial state of the scattering system as a train of waves fed in over a period of time in order to avoid "undesirable transients", which would arise if the incident waves were released all at once. The method of adiabatic switching may also be viewed as a device for avoiding transients. It is understandable that transient effects should be removed or avoided if the system under consideration is essentially stationary, but this does not seem reasonable if we are dealing with a situation which is time-dependent. Transients usually reflect the rate at which an interaction is switched on, or an excitation produced, so a discussion of a time-dependent scattering situation should include a proper treatment of transient effects.

In the $t = 0$ wave function, transient effects are found to be described by certain functions $M(r,k,t)$ of position, momentum and time, whose form is known explicitly. By using this wave function in the calculation of time delay, therefore, we aim to obtain an expression for time delay containing terms representing transient effects, from which the importance of such effects in a particular scattering situation can be gauged.

Chapters 1 and 2 of the thesis are devoted to the derivation and discussion of the $t = 0$ wave function.

CHAPTER 1

THE $t = 0$ WAVE FUNCTION

1a. Introduction

In early treatments of scattering (Dirac 1926, 1927) the initial state of the system was specified at time $t = 0$. The wave function for subsequent times was obtained by time-dependent perturbation theory, however, and so was accurate only to some order in the perturbation. The first exact solution of a scattering problem with the initial state at $t = 0$ seems to have been given by Moshinsky (1951, 1952 a), who considered the situation of a scatterer suddenly inserted into a beam of particles. Moshinsky obtained the space and time dependence of the wave function for $t > 0$ in terms of functions $M(r,k,t)$ (in Moshinsky's notation $\chi(r,k,t)$) related to the complementary error function. In subsequent papers Lozano (1953, 1954) treated the scattering of an arbitrary wave packet by a finite range potential, and the transmission of a wave packet through a potential barrier, with the wave function in each case being expressed in terms of the functions $M(r,k,t)$. Sasakawa (1959) examined the s-wave scattering problem independently, and solved the time-dependent Schrödinger equation by the Laplace transform method. He obtained functions denoted by G which are essentially the M functions of Moshinsky.

A detailed exposition of initial-value problems in both classical and quantum physics has been given by Beck and Nussenzveig (1960). They show that the problem of the "exponential catastrophe", which arises in discussions of scattering and decay, is eliminated by taking into account the initial excitation of the system at time $t = 0$. In quantum mechanics, the exponentially increasing Gamow states are replaced by the functions M, and Beck and Nussenzveig discuss the properties of these functions in some detail.

With the initial packet specified at t = 0, it is no longer necessary to treat scattering and decay on different footings (cf Heitler 1954, pp 150, 163). A unified treatment is possible, in which the two processes differ only in the position of the initial packet. If the packet is completely outside the interaction region at t = 0, the wave function for subsequent times describes its scattering by the potential. If the packet is completely inside the potential at t = 0, the wave function describes the decay of the wave packet as it leaks through the potential. Nussenzveig (1961) has considered the interaction of an arbitrary wave packet with a partially transparent sphere, and followed the behaviour in time of the wave function in the cases when the packet is scattered by the sphere and when it is decaying from within the sphere.

All the previous work on the scattering problem is brought together in a paper by Rosenfeld (1965), and more recently Jeukenne (1967 a,b, 1968) has studied examples of scattering and decay. Our treatment is similar to that of Rosenfeld, though we shall make explicit use of the Green's function for the radial wave equation, since this simplifies the derivation of the Laplace transform. By allowing the initial wave packet to be non-zero within the potential, we shall be able to extend Rosenfeld's treatment, and derive the wave function for the decay problem in a form similar to his scattering wave function.

The wave functions for scattering and decay may be obtained in two different, but equivalent, forms. In the first, the initial packet is written as a function of the spatial co-ordinates $\underset{\sim}{r}$ only, and the wave function for $t > 0$ is expressed as an integral over $\underset{\sim}{r}$ of the product of the initial packet and a space-time propagator. The wave functions in the papers of Nussenzveig and Jeukenne are given in this form. Alternatively, the initial packet may be expanded in terms of plane waves, and then the wave functions are obtained as integrals over momentum, containing the coefficients of the expansion and functions of $\underset{\sim}{r}$, $\underset{\sim}{k}$ and t. This method has been used by Lozano, Sasakawa, and Rosenfeld.

We shall adopt the second approach, as this will allow us, in Chapter 2, to derive a simpler expression for the wave function and to relate it to the wave function of standard scattering theory, which is based on the asymptotic limit $t \to -\infty$. Since we are interested only in the general features of the wave function, we shall retain the Mittag - Leffler expansion used by Rosenfeld. In applications involving the single-level approximation, Jeukenne (1967a) has shown that a Cauchy expansion (Humblet and Jeukenne 1966), which avoids the infinite power series in the background term, is more useful.

1b. Derivation of the t = 0 Wave Function

We consider a wave packet, representing a spinless particle of mass μ, interacting with a real spherical potential $V(r)$, of finite range a,

$$V(r) = 0 \quad , \quad r > a \quad . \tag{1.1}$$

The initial packet is arbitrary, and in particular we shall allow it to overlap the region of the potential. The wave function for time $t > 0$ will be found to contain two components. The first represents the propagation of that part of the packet which is initially outside the potential, and is the wave function appropriate to the scattering problem. The second represents the propagation of that part of the packet initially inside the potential, and is the wave function for the decay problem.

The initial packet may be expanded in plane waves,

$$\Phi(\underset{\sim}{r}) = \int d\underset{\sim}{k}\; A(\underset{\sim}{k})\; e^{i\underset{\sim}{k}.\underset{\sim}{r}} \quad , \tag{1.2}$$

and in terms of partial waves

$$\Phi(\underset{\sim}{r}) = \sum_{\ell m} Y_{\ell m}(\Omega)\; \frac{1}{r}\; \Phi_{\ell m}(r) \quad , \tag{1.3}$$

where

$$\Phi_{\ell m}(r) = \int_0^\infty dk\; A_{\ell m}(k)\; J_\ell(kr) \quad . \tag{1.4}$$

The functions $Y_{\ell m}(\Omega)$ are spherical harmonics, with the normalisation

$$\int_{4\pi} d\Omega\; Y^*_{\ell m}(\Omega)\; Y_{\ell' m'}(\Omega) = \delta_{\ell\ell'}\delta_{mm'} \quad . \tag{1.5}$$

The $J_\ell(kr)$ are Riccatti - Bessel functions†, related to the usual spherical Bessel functions j_ℓ by

$$J_\ell(\rho) = \rho\; j_\ell(\rho) \quad , \tag{1.6}$$

and they satisfy the orthogonality relation

$$\int_0^\infty dr\; J_\ell(kr)\; J_\ell(k'r) = \frac{\pi}{2}\; \delta(k - k') \quad . \tag{1.7}$$

† In Rosenfeld's paper, and also in Humblet and Rosenfeld 1961, the Riccatti - Bessel functions are denoted by a script $\mathcal{J}_\ell$. Since this symbol was not available to us, we use J_ℓ for the Riccatti - Bessel functions.

Note that Bessel functions of the first kind, for which the symbol J_ℓ is normally reserved, do not appear anywhere in the thesis.

Using Eq.(7) in Eq.(4) we have

$$A_{\ell m}(k) = \frac{2}{\pi}\int_0^\infty dr\ \Phi_{\ell m}(r)\ J_\ell(kr) \quad , \tag{1.8}$$

and the packet is normalised so that

$$\frac{\pi}{2}\sum_{\ell m}\int_0^\infty dk\ A^*_{\ell m}(k)\ A_{\ell m}(k) = 1 \quad . \tag{1.9}$$

By retaining the factor $\frac{\pi}{2}$ in Eq.(9), we avoid the appearance of factors $\left(\frac{2}{\pi}\right)^{\frac{1}{2}}$ in the wave functions derived later.

We wish to solve the time-dependent Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}\Psi(\underset{\sim}{r},t) = \left[-\frac{\hbar^2}{2\mu}\nabla^2 + V(r)\right]\Psi(\underset{\sim}{r},t) \quad , \tag{1.10}$$

subject to the initial condition

$$\Psi(\underset{\sim}{r},0) = \Phi(\underset{\sim}{r}) \quad . \tag{1.11}$$

Let us define†

$$\tau = \frac{\hbar}{\mu}t \quad , \tag{1.12}$$

$$v(r) = \frac{2\mu}{\hbar^2}V(r) \quad , \tag{1.13}$$

† We shall make frequent use of the variable τ throughout the thesis, since this simplifies the appearance of the time factor $e^{\frac{-i\hbar k^2 t}{2\mu}} \rightarrow e^{\frac{-ik^2\tau}{2}}$. Integrals over τ in later chapters will be referred to loosely as "time integrals".

and expand the wave function $\Psi(\underset{\sim}{r},\tau)$ in partial waves,

$$\Psi(\underset{\sim}{r},\tau) = \sum_{\ell m} Y_{\ell m}(\Omega)\ \frac{1}{r}\ \psi_{\ell m}(r,\tau) \quad . \tag{1.14}$$

Then $\psi_{\ell m}(r,\tau)$ satisfies the radial wave equation

$$2i\ \frac{\partial}{\partial\tau}\ \psi_{\ell m}(r,\tau) = \left[-\frac{\partial^2}{\partial r^2} + \frac{\ell(\ell+1)}{r^2} + v(r)\right] \psi_{\ell m}(r,\tau) \quad , \tag{1.15}$$

subject to the boundary conditions

$$\psi_{\ell m}(0,\tau) = 0 \quad , \tag{1.16}$$

$$\lim_{r\to\infty} \psi_{\ell m}(r,\tau) = 0 \quad , \tag{1.17}$$

and the initial condition

$$\psi_{\ell m}(r,0) = \Phi_{\ell m}(r) \quad . \tag{1.18}$$

Eq.(16) is the condition that the wave function be regular at the origin, and Eq.(17) is necessary for the wave function to be normalised.

The solution of Eqs (15) to (18) may be obtained by means of the Laplace transform. Let

$$\overline{\psi}_{\ell m}(r,p) \equiv \int_0^\infty d\tau\ e^{-p\tau}\psi_{\ell m}(r,\tau) \tag{1.19}$$

be the Laplace transform of $\psi_{\ell m}(r,\tau)$, and let there be positive constants M, α and τ_o such that

$$\left|\psi_{\ell m}(r,\tau)\right| \leqslant M\ e^{\alpha\tau}$$

for $\tau \geqslant \tau_o$. Then $\overline{\psi}_{\ell m}(r,p)$ is an analytic function of the complex variable p in the half-plane Re $p > \alpha$. We know however that the wave function must remain finite for all times, so in fact $\alpha = 0$, and $\bar{\psi}_{\ell m}(r,p)$ is analytic for Re $p > 0$.

Applying the transform (19) to Eq.(15), and using Eqs (16) to (18), we have

$$-\frac{\partial^2}{\partial r^2}\bar{\psi}_{\ell m}(r,p) + \frac{\ell(\ell+1)}{r^2}\bar{\psi}_{\ell m}(r,p) + v(r)\,\bar{\psi}_{\ell m}(r,p) - 2ip\bar{\psi}_{\ell m}(r,p) = -2i\Phi_{\ell m}(r) \;, \tag{1.20}$$

with

$$\bar{\psi}_{\ell m}(0,p) = 0 \tag{1.21}$$

and

$$\lim_{r\to\infty} \bar{\psi}_{\ell m}(r,p) = 0 \quad . \tag{1.22}$$

The homogeneous part of Eq.(20) is just the radial wave equation with k^2 replaced by $2ip$. Let us define a complex wave number k_p by

$$k_p = \sqrt{2|p|}\; e^{i\left(\frac{\theta}{2} + \frac{\pi}{4}\right)} \quad , \qquad \theta \equiv \arg p \quad , \tag{1.23}$$

so that $k_p^2 = 2ip$, and let $G_\ell(k : r,r')$ denote the Green's function for the radial wave equation,

$$\left[-\frac{\partial^2}{\partial r^2} + \frac{\ell(\ell+1)}{r^2} + v(r) - k^2\right] G_\ell(k : r,r') = \delta(r - r') \quad . \tag{1.24}$$

Then the solution of Eq.(20) is

$$\bar{\psi}_{\ell m}(r,p) = -2i\int_0^\infty dr'\; G_\ell(k_p : r,r')\;\Phi_{\ell m}(r') \quad . \tag{1.25}$$

We define regular and irregular solutions, $\phi_\ell(k,r)$ and $f_\ell(k,r)$, of the radial wave equation by (Newton 1960)

$$\lim_{r \to o} \; (2\ell + 1)\,!!\; r^{-\ell-1}\, \phi_\ell(k,r) \;=\; 1 \qquad , \qquad (1.26)$$

$$\lim_{r \to \infty} \; e^{ikr}\, f_\ell(k,r) \;=\; i^\ell \qquad , \qquad (1.27)$$

and the Jost function $f_\ell(k)$ by

$$f_\ell(k) \;=\; \lim_{r \to o} \; (kr)^\ell\, f_\ell(k,r)/(2\ell - 1)\,!! \qquad . \qquad (1.28)$$

(The potential V(r) is assumed to satisfy the condition

$$\int_o^\infty dr\; r\, |V(r)| \;<\; \infty$$

in addition to (1), so that the regular solution $\phi_\ell(k,r)$ does in fact exist.) Then the Green's function appropriate to the boundary conditions (21) and (22) is

$$G_\ell(k_p : r,r') \;=\; \frac{(-)^\ell\, k_p^\ell\, \phi_\ell(k_p,r_<)\, f_\ell(-k_p,r_>)}{f_\ell(-k_p)} \qquad , \qquad (1.29)$$

where $r_<$ is the lesser, and $r_>$ the greater, of r and r'. Note that for Re p > 0, the argument of k_p lies between 0 and $\frac{\pi}{2}$, and Im k_p > 0.

We shall use the following relations, which may be derived from the differential equation for ϕ_ℓ and f_ℓ, and the corresponding equation with v(r) = 0 for J_ℓ :

$$\int_o^r dr'\; \phi_\ell(k_p,r')\; J_\ell(kr')$$

$$= \frac{1}{(k^2 - k_p^2)} \left\{ W\left[J_\ell(kr), \phi_\ell(k_p,r)\right] - \int_o^r dr'\; v(r')\phi_\ell(k_p,r')\; J_\ell(kr') \right\} \qquad , \qquad (1.30a)$$

$$\int_r^\infty dr' \, f_\ell(-k_p,r') \, J_\ell(kr')$$

$$= \frac{1}{(k^2 - k_p^2)} \left\{ -W\left[J_\ell(kr), f_\ell(-k_p,r)\right] - \int_r^\infty dr' \, v(r') f_\ell(-k_p,r') \, J_\ell(kr') \right\} \quad , \quad (1.30b)$$

where the Wronskian is defined as

$$W\left[g(r), \, h(r) \right] \equiv g(r) \frac{\partial}{\partial r} h(r) - \frac{\partial}{\partial r} g(r) \, h(r) \quad . \qquad (1.31)$$

By direct expansion of the Wronskians, and using Eq. (4.3) of Newton 1960, we also have

$$f_\ell(-k_p,r) \, W\left[J_\ell(kr), \phi_\ell(k_p,r)\right] - \phi_\ell(k_p,r) \, W\left[J_\ell(kr), \, f_\ell(-k_p,r)\right]$$

$$= W\left[f_\ell(-k_p,r), \phi_\ell(k_p,r)\right] J_\ell(kr)$$

$$= (-)^\ell \frac{f_\ell(-k_p)}{k_p^\ell} J_\ell(kr) \quad . \qquad (1.32)$$

Inserting (4) and (29) into Eq. (25), and using (30) and (32), we obtain for the Laplace transform

$$\overline{\psi}_{\ell m}(r,p)$$

$$= \int_0^\infty dk \, A_{\ell m}(k) \frac{2i}{(k_p^2 - k^2)} \left\{ J_\ell(kr) - (-)^\ell \frac{k_p^\ell}{f_\ell(-k_p)} f_\ell(-k_p,r) \int_0^r dr' \, v(r') \phi_\ell(k_p,r') J_\ell(kr') \right.$$

$$\left. - (-)^\ell \frac{k_p^\ell}{f_\ell(-k_p)} \phi_\ell(k_p,r) \int_r^a dr' \, v(r') \, f_\ell(-k_p,r') \, J_\ell(kr') \right\} \quad .$$

(1.33)

In the third term within the curly brackets, $\int_r^\infty dr'$ has been replaced by $\int_r^a dr'$, since $v(r')$ is zero for $r' > a$.

The derivation so far is valid for all values of r, so that we could, if we wished, calculate the wave function $\Psi(\underset{\sim}{r},\tau)$ for points <u>inside</u> the interaction region. Nussenzveig (1961) and Jeukenne (1967 b) have carried out such calculations for the scattering problem in order to follow the formation and decay of the "compound nucleus". We shall limit our discussion to the external region $r > a$, however, and in this case the first integral over r' in Eq. (33) becomes $\int_o^a$, and the second integral over r' vanishes. Using the relation

$$(-)^{\ell} f_{\ell}(-k,r) = O_{\ell}(kr) \quad , \quad r \geqslant a \quad , \tag{1.34}$$

where $O_\ell(kr)$ is the outgoing spherical Hankel function, and rewriting the r' integral by means of Eq. (30a), we obtain finally

$$\begin{aligned}\overline{\psi}_{\ell m}(r,p) \underset{r>a}{=} &\int_o^\infty dk\ A_{\ell m}(k) \frac{2i}{(k_p^2 - k^2)} \left\{ J_\ell(kr) - O_\ell(k_p r) \frac{W\left[J_\ell(ka),\phi_\ell(k_p,a)\right]}{W\left[O_\ell(k_p a),\phi_\ell(k_p,a)\right]} \right\} \\ &+ \int_o^\infty dk\ A_{\ell m}(k)\ (-2i)\ O_\ell(k_p r) \frac{\int_o^a dr'\ J_\ell(kr')\phi_\ell(k_p,r')}{W\left[O_\ell(k_p a),\phi_\ell(k_p,a)\right]} \quad . \end{aligned} \tag{1.35}$$

The specification $r > a$ will be omitted from subsequent equations, it being understood that the wave functions are those for the external region.

The first integral in Eq. (35) is given in Rosenfeld 1965, where the initial packet is assumed to be localised outside the potential, and the Laplace transform is derived by a different method. On taking the inverse Laplace transform of this term, Rosenfeld obtains the wave function for the scattering problem in the form

$$\psi_{\ell m}(r,\tau) = \int_0^\infty dk\ A_{\ell m}(k)\ J_\ell(kr)\ e^{\frac{-ik^2\tau}{2}}$$

$$- \int_0^\infty dk\ A_{\ell m}(k)\ D_\ell(r) \left\{ \left[\sum_n \frac{\rho_n(k)}{(k-k_n)} + \sum_{s=0}^\infty \alpha_s(k) \left(\frac{1}{i}\frac{\partial}{\partial r} \right)^s \right] M(r,k,\tau) \right.$$

$$+ \left[\sum_n \frac{\rho_n(k)}{(-k-k_n)} + \sum_{s=0}^\infty \alpha_s(k) \left(\frac{1}{i}\frac{\partial}{\partial r} \right)^s \right] M(r,-k,\tau)$$

$$\left. - \sum_n \frac{2k_n \rho_n(k)}{(k^2 - k_n^2)} M(r,k_n,\tau) \right\} . \qquad (1.36)$$

The operator $D_\ell(r)$ is given by

$$D_\ell(r) = \frac{1}{2i} (-r)^{\ell+1} \left(\frac{1}{r}\frac{\partial}{\partial r} \right)^\ell \frac{1}{r} , \qquad (1.37)$$

with

$$D_\ell(r)\ e^{ikr} = \frac{-k^\ell}{2i} O_\ell(kr) , \qquad (1.38)$$

and the M functions by

$$M(r,k_\nu,\tau) = \frac{1}{2} e^{ik_\nu r - \frac{ik_\nu^2\tau}{2}} \operatorname{erfc}\left(\frac{r - k_\nu\tau}{\sqrt{2i\tau}} \right) , \qquad (1.39)$$

where

$$\operatorname{erfc}(z) = \frac{2}{\sqrt{\pi}} \int_z^\infty e^{-u^2} du$$

for complex z.

In writing Eq.(36) we have combined S_1 and S_∞ of Rosenfeld's Eq.(42) into the term in $M(r,k,\tau)$, expressed S_2 in terms of $M(r,-k,\tau)$, and combined S_3 and S_4 into the term in $M(r,k_n,\tau)$. The sums over n and s arise from a Mittag - Leffler expansion of the Wronskian term in Eq.(35) :

$$-2i\, k_p^{-\ell} \frac{W\left[J_\ell(ka),\phi_\ell(k_p,a)\right]}{W\left[O_\ell(k_p a),\phi_\ell(k_p,a)\right]} = \sum_n \frac{\rho_n(k)}{k_p - k_n} + \sum_{s=o}^{\infty} \alpha_s(k)\, k_p^s \quad . \tag{1.40}$$

The poles k_n are at the zeros of the Wronskian in the denominator,

$$W\left[O_\ell(k_n a),\phi_\ell(k_n,a)\right] = 0 \quad , \tag{1.41}$$

and coincide with the poles of the S matrix (Humblet and Rosenfeld 1961). Comparing Eqs (4) and (36), it can be seen that the first integral in Eq.(36) is the wave function for the incident packet, and the second integral the wave function for the scattered packet.

Lozano (1953) has treated the scattering problem for arbitrary angular momentum by another method, and obtained a wave function similar to (36). Sasakawa (1959) has considered s-wave scattering, but he overlooks the poles of the S matrix in the evaluation of a contour integral, so that his expression for the wave function lacks the terms in $M(r,k_n,\tau)$.

The second integral in Eq.(35) represents the contribution from the part of the initial packet inside the potential, as may be seen by rearranging it into the form $-2i \int_0^a dr'\, G_\ell(k_p : r,r')\, \Phi_{\ell m}(r')$. We shall calculate the inverse Laplace transform of this term, and obtain the wave function for the decay problem.

The inverse Laplace transform is given by

$$\psi_{\ell m}(r,\tau) = \frac{1}{2\pi i} \int_{C_i} dp\ e^{p\tau}\ \bar{\psi}_{\ell m}(r,p) \quad , \tag{1.42}$$

where C_i is a line in the right half of the p plane, parallel to the imaginary axis and as close to it as we please, Fig.1.

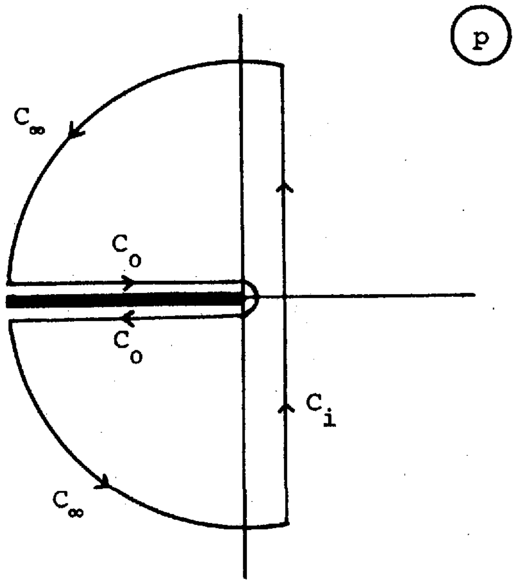

Fig. 1.1. Contour for Evaluation of the Inverse Laplace Transform.

Following Rosenfeld, we work within the k integral and calculate

$$\mathcal{J} \equiv \frac{1}{2\pi i} \int_{C_i} dp\ e^{p\tau}\ (-2i)\ O_\ell(k_p r) \frac{\int_o^a dr'\ J_\ell(kr')\ \phi_\ell(k_p,r')}{W\left[O_\ell(k_p a),\phi_\ell(k_p,a)\right]} \quad . \tag{1.43}$$

The integrand has a square root branch point at the origin, and we make a cut from the origin along the negative real axis to infinity. The contour may then be completed by a semicircle C_∞, of infinite radius, in the left half of the p plane, and an indentation C_o around the cut.

The poles of the integrand are again given by Eq.(41), and they are distributed in the k_p plane as shown in Fig.2.

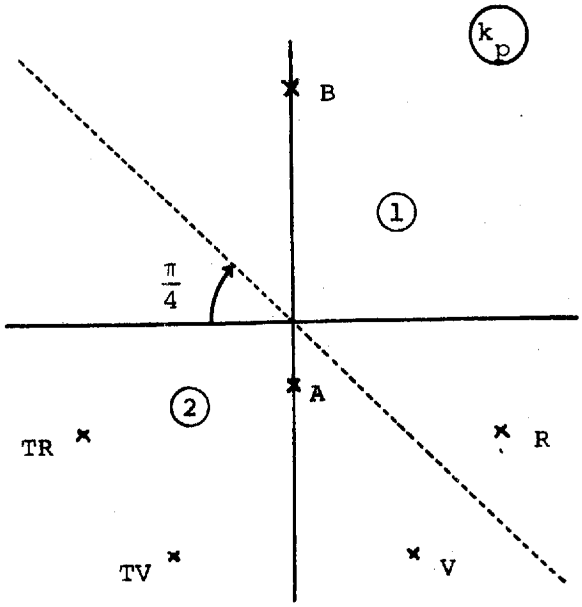

Fig.1.2 Zeros of $W[O_\ell,\phi_\ell]_a$, Eq.(41).

----------- Second bisector.

B	Bound state	R	Resonance	V	Virtual
A	Antibound state	TR	Time-reversed resonance	TV	Time-reversed virtual

We divide the k_p plane into two regions, labelled (1) and (2) , separated by the second bisector. From Eq.(23) we see that region (1) is mapped onto the first sheet $(-\pi < \theta < \pi)$ of the p plane, and region (2) is mapped onto the second sheet $(\pi < \theta < 3\pi)$. Accordingly, in integrating around the contour in Fig.1, we shall obtain contributions from the residues of the bound state and resonance poles in region (1) . The integral around C_∞ vanishes, so we have

$$\oint + \frac{1}{2\pi i}\int_{C_o} = \sum_{(1)} \text{res}_n \quad . \tag{1.44}$$

The integral around the indentation C_o may be evaluated by reverting to the k_p plane, where the path of integration coincides with the second bisector. Denoting the integral by $\mathcal{J}_o$, and using Eq.(38) to rewrite the Hankel function $O_\ell(k_p r)$, we have

$$\mathcal{J}_o = D_\ell(r) \frac{1}{2\pi i} \int_{-\infty+i\infty}^{+\infty-i\infty} dk_p \, e^{ik_p r - ik_p^2 \frac{\tau}{2}} \, 4ik_p^{-\ell+1} \frac{\int_0^a dr' \, J_\ell(kr')\phi_\ell(k_p,r')}{W\left[O_\ell(k_p a), \phi_\ell(k_p,a)\right]} \qquad (1.45)$$

Now

$$\phi_\ell(k,r) = \frac{f_\ell(-k)}{k^{\ell+1}} \chi_\ell(k,r) \quad ,$$

where $\chi_\ell(k,r)$ is the "physical" solution of the radial wave equation (Newton 1960), and

$$W\left[O_\ell(ka), \phi_\ell(k,a)\right] = \frac{f_\ell(-k)}{k^\ell}$$

(cf. Eqs (32), (34)), so we have

$$4i\, k_p^{-\ell+1} \frac{\int_0^a dr' \, J_\ell(kr')\phi_\ell(k_p,r')}{W\left[O_\ell(k_p a), \phi_\ell(k_p,a)\right]} = 4i\, k_p \int_0^a dr' \, J_\ell(kr') \frac{\chi_\ell(k_p,r')}{k_p^{\ell+1}} \, . \qquad (1.46)$$

We know that

$$\chi_\ell(k,r) = \mathcal{O}(k^{\ell+1}) \quad \text{as} \quad k \to 0 \quad ,$$

so the function on the LHS of Eq.(46) has a first order zero at $k_p = 0$. Removing a factor ik_p, we obtain a meromorphic function of k_p, with poles given by Eq.(41), which approaches a finite limit as $k_p \to 0$. The function may be expressed as a Mittag - Leffler expansion of the form

$$\frac{4k_p^{-\ell}\int_0^a dr'\; J_\ell(kr')\phi_\ell(k_p,r')}{W\left[O_\ell(k_pa),\phi_\ell(k_p,a)\right]} = \sum_n \frac{\rho_n'(k)}{k_p - k_n} + \sum_{s=o}^{\infty} \alpha_s'(k)\; k_p^s \quad , \tag{1.47}$$

where the sum over n includes all poles of regions (1) and (2) in Fig.2. The residues $\rho_n'(k)$ and coefficients $\alpha_s'(k)$ have been primed to distinguish them from similar quantities appearing in the expansion used by Rosenfeld, Eq.(40).

To prove that the sum over the poles in Eq.(47) converges, we compare the residue $\rho_n'(k)$ with the residue $\rho_n(k)$ of Eq.(40). If we denote by a further ρ_n the residue of the scattering amplitude

$$S_\ell(k_p) - 1 = -2i\;\frac{W\left[J_\ell(k_pa),\phi_\ell(k_p,a)\right]}{W\left[O_\ell(k_pa),\phi_\ell(k_p,a)\right]} \tag{1.48}$$

at the pole k_n, Rosenfeld has shown that

$$\frac{\rho_n(k)}{\rho_n} = \frac{-1}{k_n^{\ell+1}}\; W\left[J_\ell(ka),\; O_\ell(k_na)\right] \quad . \tag{1.49}$$

Now it can be seen from Eqs (47) and (48) that

$$\frac{\rho_n'(k)}{\rho_n} = 2i\;\frac{1}{k_n^{\ell}}\;\frac{\int_0^a dr'\; J_\ell(kr')\phi_\ell(k_n,r')}{W\left[J_\ell(k_na),\phi_\ell(k_n,a)\right]} \quad . \tag{1.50}$$

Using the fact that $W\left[O_\ell(k_n a), \phi_\ell(k_n, a)\right] = 0$, we can write

$$W\left[J_\ell(k_n a), \phi_\ell(k_n, a)\right] = W\left[J_\ell(k_n a), O_\ell(k_n a)\right] \frac{\phi_\ell(k_n, a)}{O_\ell(k_n a)}$$

$$= -k_n \frac{\phi_\ell(k_n, a)}{O_\ell(k_n a)} \quad . \qquad (1.51)$$

The function $\phi_\ell(k,r)$ is given by (Newton 1960)

$$\phi_\ell(k,r) = \frac{i}{2} \frac{1}{k^{\ell+1}} \left[f_\ell(-k) f_\ell(k,r) - (-)^\ell f_\ell(k) f_\ell(-k,r)\right] ,$$

but

$$f_\ell(-k_n) = 0 ,$$

so

$$\phi_\ell(k_n, r) = \frac{i}{2} \frac{1}{k_n^{\ell+1}} (-)^{\ell+1} f_\ell(k_n) f_\ell(-k_n, r) \quad . \qquad (1.52)$$

Then from Eqs (50),(51) and (52)

$$\frac{\rho_n'(k)}{\rho_n} = \frac{-2i}{k_n^{\ell+1}} \frac{\int_0^a dr' \, J_\ell(kr') \, f_\ell(-k_n, r')}{f_\ell(-k_n, a)} O_\ell(k_n a) \quad . \qquad (1.53)$$

Comparing Eqs (49) and (53) we have

$$\frac{\rho_n'(k)}{\rho_n(k)} = 2i \frac{\int_0^a dr' \, J_\ell(kr') \, f_\ell(-k_n, r')}{f_\ell(-k_n, a)} \times \frac{O_\ell(k_n a)}{W\left[J_\ell(ka), O_\ell(k_n a)\right]} \quad . \qquad (1.54)$$

Now

$$f_\ell(-k_n,r) \underset{|k_n|\to\infty}{\sim} i^\ell e^{ik_n r} ,$$

and except for a finite number of bound states, the pole k_n is given by $k_n = \kappa_n - i\gamma_n$, $\gamma_n > 0$, so for $|k_n|$ sufficiently large, the integrand in the first term of Eq.(54) contains a factor $e^{\gamma_n r'}$. Thus as $|k_n| \to \infty$, the integral is $\mathcal{O}(e^{ik_n a})$, and

$$\frac{\int_0^a dr' \, J_\ell(kr') \, f_\ell(-k_n,r')}{f_\ell(-k_n,a)} = \mathcal{O}(1) \quad \text{as} \quad |k_n| \to \infty \quad . \tag{1.55}$$

Further,

$$O_\ell(k_n a) \underset{|k_n|\to\infty}{\sim} i^{-\ell} e^{ik_n a} ,$$

so

$$\frac{O_\ell(k_n a)}{W\left[J_\ell(ka),\, O_\ell(k_n a)\right]} = \mathcal{O}\left(\frac{1}{k_n}\right) \quad \text{as} \quad |k_n| \to \infty \quad . \tag{1.56}$$

Combining Eqs (54), (55) and (56),

$$\frac{\rho_n'(k)}{\rho_n(k)} = \mathcal{O}\left(\frac{1}{k_n}\right) \quad \text{as} \quad |k_n| \to \infty \quad , \tag{1.57}$$

and the series in Eq.(47) converges by comparison with the corresponding series in Eq.(40).

On inserting the expansion (47) into Eq.(45), we obtain two types of integrals. The first is related to the function $F(k_n)$ appearing in Rosenfeld's paper, defined by

$$F(k_n) = \frac{1}{2\pi i}\int_{-\infty+i\infty}^{+\infty-i\infty} dk\; \frac{e^{ikr-ik^2\frac{\tau}{2}}}{k-k_n} \quad . \tag{1.58}$$

Then

$$\frac{1}{2\pi i}\int_{-\infty+i\infty}^{+\infty-i\infty} dk_p\; ik_p\; \frac{e^{ik_p r-ik_p^2\frac{\tau}{2}}}{k_p-k_n} = \frac{\partial}{\partial r} F(k_n) \quad . \tag{1.59}$$

The second type of integral may be expressed in terms of the point source propagator $U(r,\tau)$. Using the change of variable $u = \frac{r - k\tau}{\sqrt{2i\tau}}$ we have

$$\frac{1}{2\pi i}\int_{-\infty+i\infty}^{+\infty-i\infty} dk\; e^{ikr-ik^2\frac{\tau}{2}} = \frac{-1}{2\pi i}\,\frac{\sqrt{2i}}{\sqrt{\tau}}\; e^{\frac{-r^2}{2i\tau}}\int_{-i\infty}^{i\infty} du\; e^{u^2}$$

$$= -i\,\frac{e^{\frac{-r^2}{2i\tau}}}{\sqrt{2\pi i\tau}}$$

$$= \frac{1}{i}\,U(r,\tau) \quad . \tag{1.60}$$

Then

$$\frac{1}{2\pi i}\int_{-\infty+i\infty}^{+\infty-i\infty} dk_p\; ik_p\; e^{ik_p r-ik_p^2\frac{\tau}{2}}\, k_p^s = \frac{\partial}{\partial r}\left(\frac{1}{i}\frac{\partial}{\partial r}\right)^s \frac{1}{i}\,U(r,\tau) \quad . \tag{1.61}$$

Finally, from Eqs (45), (47), (59) and (61), the integral around the cut is

$$\oint_o = D_\ell(r)\;\frac{\partial}{\partial r}\left\{\sum_n \rho_n'(k)\; F(k_n) + \sum_{s=o}^{\infty} \alpha_s'(k)\left(\frac{1}{i}\frac{\partial}{\partial r}\right)^s \frac{1}{i}\;U(r,\tau)\right\} \quad . \tag{1.62}$$

Returning to Eq.(44), the residue at a pole in region (1) may be obtained by inspection from Eqs (45) and (47) :

$$\mathrm{res}_n = D_\ell(r)\, e^{ik_n r - \frac{ik_n^2\tau}{2}}\, ik_n\, \rho_n'(k)$$

$$= D_\ell(r)\, \frac{\partial}{\partial r}\left\{ \rho_n'(k)\, e^{ik_n r - \frac{ik_n^2\tau}{2}} \right\} . \qquad (1.63)$$

In combining Eqs (62) and (63), we use the following expressions for $F(k_n)$ (Rosenfeld 1965, Eq.(49)) :

$$F(k_n) = e^{ik_n r - \frac{ik_n^2 t}{2}} - M(r,k_n,\tau) \quad , \quad k_n \text{ in } (1) \quad ,$$

$$\qquad (1.64)$$

$$= - M(r,k_n,\tau) \quad , \quad k_n \text{ in } (2) \quad ,$$

where $M(r,k_n,\tau)$ is defined by Eq.(39). Then from Eqs (44), (62) and (63),

$$\oint = D_\ell(r)\, \frac{\partial}{\partial r}\left\{ \sum_n \rho_n'(k)\, M(r,k_n,\tau) - \sum_{s=o}^{\infty} \alpha_s'(k) \left(\frac{1}{i}\frac{\partial}{\partial r}\right)^s \frac{1}{i}\; U(r,\tau)\right\}$$

$$= D_\ell(r) \left\{ \sum_n \rho_n'(k)\; ik_n\; M(r,k_n,\tau) \right.$$

$$\left. - \left[\sum_n \rho_n'(k) + \sum_{s=o}^{\infty} \alpha_s'(k) \left(\frac{1}{i}\frac{\partial}{\partial r}\right)^{s+1}\right] U(r,\tau) \right\} , \qquad (1.65)$$

where we have used

$$\frac{\partial}{\partial r} M(r,k_n,\tau) = ik_n\, M(r,k_n,\tau) - U(r,\tau) .$$

Finally, placing Eq. (65) within the momentum integral we obtain the wave function for the decay problem

$$\psi_{\ell m}(r,\tau) = \int_0^\infty dk\ A_{\ell m}(k)\ D_\ell(r) \left\{ i \sum_n k_n\ \rho_n'(k)\ M(r,k_n,\tau) - \left[\sum_n \rho_n'(k) + \sum_{s=o}^\infty \alpha_s'(k) \left(\frac{1}{i}\frac{\partial}{\partial r}\right)^{s+1} \right] U(r,\tau) \right\} . \qquad (1.66)$$

The wave function (66) is similar in form to the scattering wave function (36), though we may note certain differences. In Eq. (36) the first integral represents the wave function of the unscattered packet, and the second the wave function of the scattered packet. Eq. (66) does not contain a term $\int_0^\infty dk\ A_{\ell m}(k)\ J_\ell(kr)\ e^{\frac{-ik^2\tau}{2}}$. In the decay problem, of course, the whole of the initial packet interacts with the potential, and no part of it experiences free propagation. Both wave functions contain the functions $M(r,k_n,\tau)$ summed over all the poles, but the terms in $M(r,k,\tau)$ and $M(r,-k,\tau)$ in Eq. (36) have been replaced by the term in $U(r,\tau)$ in Eq. (66). It is a general feature of this type of calculation that the functions $M(r,k,\tau)$ and $M(r,-k,\tau)$ appear only in the wave function for the scattering problem (cf Moshinsky 1951, Lozano 1953, 1954).

Wave functions for decay situations have been obtained by Lozano (1954), Nussenzveig (1961), and Jeukenne (1968). It is difficult to compare our result with those of Lozano and Nussenzveig, however, since there are considerable differences in approach - Lozano expands the initial packet in a Fourier sine series and obtains the wave function as a sum over the terms of the series, while Nussenzveig considers a partially transparent sphere, $V(r) = \frac{1}{2}\ \frac{A}{a}\ \delta(r-a)$, rather than a general potential.

Jeukenne has treated the s-wave case for an arbitrary potential, and obtained a wave function in terms of a propagator

$$\psi(r,\tau) = 2i \int_0^a G(r,r',\tau)\, f(r')\, dr' \qquad , \qquad (1.67)$$

where f(r) (= 0 for r > a) is the initial packet. The propagator contains coefficients $c_s(r')$ and $C_n(r')$, and on setting

$$h_s(a) = 2i \int_0^a f(r')\, c_s(r')\, dr' \qquad ,$$

and

$$g_n(a) = 2i \int_0^a f(r')\, C_n(r')\, dr' \qquad ,$$

the wave function is obtained in the form

$$\psi(r,\tau) = -i \sum_n k_n\, g_n(a)\, M(r-a,\, k_n,\tau)$$

$$+ \left[\sum_n g_n(a)\, k_n^{-m-2} \sum_{s=o}^{m+2} k_n^s \left(\frac{1}{i}\frac{\partial}{\partial r}\right)^{m+2-s} + \sum_{s=o}^{m+1} h_s(a)\, \frac{1}{s!} \left(\frac{1}{i}\frac{\partial}{\partial r}\right)^{s+1} \right] U(r-a,\tau) \; , \qquad (1.68)$$

where the sum over n is over all poles of the scattering matrix.

After making allowance for the use of the space-time propagator rather than the momentum expansion, this wave function may be compared with Eq. (66). The main difference arises from the fact that Jeukenne has used a Cauchy expansion rather than a Mittag - Leffler expansion in his derivation, so the infinite series $\sum_{s=o}^{\infty}$ in Eq. (66) is replaced by a polynomial $\sum_{s=o}^{m+1}$. The parameter m is determined by the potential V(r), and is the smallest integer for which

$$\frac{d^m}{dr^m} V(r) \Big|_{a-o} \neq 0 \quad .$$

In order to write the scattering matrix as a Cauchy expansion (Humblet and Jeukenne 1966) it is necessary to separate out the hard sphere scattering term. A similar separation has been carried out in the propagator G(r,r',t), and this accounts for the presence of the radial variable r-a in Eq.(68). The double sum in the first term within square brackets has its origin in the pole terms of the Cauchy expansion, which are of the form $\frac{C_n(r')}{k - k_n} \left(\frac{k}{k_n} \right)^{m+2}$.

It is quite difficult to say anything about the relative importance of individual terms in a wave function such as (66) or (36), and we shall not attempt to do so. Rosenfeld, Nussenzveig, and Jeukenne have examined different aspects of this problem and in fact Jeukenne's use of the Cauchy expansion is aimed at simplifying the separation of background and resonance terms. Our interest, however, lies more in the overall appearance of the wave function, and we shall be able to say something further about this in Chapter 2.

1c. The M Functions

A well known difficulty in stationary scattering theory arises in connection with the wave function for a decaying resonance state. The "Gamow state" wave functions, which increase exponentially with distance, cannot be normalised in the usual way, and require the introduction of special techniques (Berggren 1968, Romo 1968, Huby 1969, Fuller 1969). The problem of the "exponential catastrophe" is not unique to quantum mechanics however (Beck and Nussenzveig 1960), and its origin lies in the assumption that the exponentially decaying state has been in existence for an indefinite time. The difficulty may be removed by taking into account the excitation of the system at some initial instant.

In the wave function (36) the place of the Gamow states is taken by the functions $M(r,k_n,\tau)$ for poles k_n, and these ensure that no exponential catastrophe occurs. To see this, let us study the behaviour of the M function for an arbitrary pole, $k_n = \kappa_n - i\gamma_n$, of the S matrix. From Fig.2, $\kappa_n = 0$ and $\gamma_n < 0$ for a bound state pole, but otherwise $\gamma_n > 0$, and the pole lies in the lower half of the k plane.

We define

$$\omega_n = \frac{r - k_n\tau}{\sqrt{2i\tau}} , \qquad (1.69)$$

with

$$|\omega_n|^2 = \frac{r^2}{2\tau} - \kappa_n r + \frac{(\kappa_n^2 + \gamma_n^2)\tau}{2} \qquad (1.70)$$

and

$$\mathrm{Re}\ \omega_n = \frac{r - (\kappa_n - \gamma_n)\tau}{2\sqrt{\tau}} . \qquad (1.71)$$

From the asymptotic behaviour of the complementary error function (Abramowitz and Stegun 1964) we have

$M(r,k_n,\tau)$

$$\underset{\substack{|\omega_n| \to \infty \\ \mathrm{Re}\,\omega_n < 0}}{\sim} \quad e^{ik_n r - \frac{ik_n^2\tau}{2}} + \frac{e^{\frac{-r^2}{2i\tau}}}{2\sqrt{\pi}\,\omega_n}\left[1 - \frac{1}{2\omega_n^2} + \ldots + (-)^m \frac{(2m-1)!!}{(2\omega_n^2)^m} + \ldots\right], \tag{1.72a}$$

$$\underset{\substack{|\omega_n| \to \infty \\ \mathrm{Re}\,\omega_n > 0}}{\sim} \quad \frac{e^{\frac{-r^2}{2i\tau}}}{2\sqrt{\pi}\,\omega_n}\left[1 - \frac{1}{2\omega_n^2} + \ldots + (-)^m \frac{(2m-1)!!}{(2\omega_n^2)^m} + \ldots\right]. \tag{1.72b}$$

The term $e^{ik_n r - \frac{ik_n^2\tau}{2}} \propto e^{\gamma_n r}$ in Eq. (72a) corresponds to the Gamow state in stationary theory. From Eq. (71) this term can occur if k_n is a bound state or a resonance ($\kappa_n > \gamma_n > 0$) pole, but only the latter need be considered since γ_n is negative for a bound state.

For a given value of τ, $M(r,k_n,\tau)$ behaves according to (72a) for $r < (\kappa_n - \gamma_n)\tau$, and the term proportional to $e^{\gamma_n r}$ is present in the wave function. As r increases beyond the value $(\kappa_n - \gamma_n)\tau$, however, Re ω_n becomes positive, and for r large $M(r,k_n,\tau)$ decreases smoothly in accordance with (72b). The properties of the M function are such that the Gamow state term is cut off in the region $r \approx (\kappa_n - \gamma_n)\tau$, and the exponential catastrophe is avoided. Roughly speaking, we may think of $(\kappa_n - \gamma_n)\tau$ as the point which the exponential wave front has reached at time τ.

Moshinsky (1952b) has shown that the function $M(x,k,\tau)$, k real, describes transient effects which arise when a steady beam of particles (of momentum k) is disturbed. If the beam is confined to the region

$x \leqslant 0$ by a perfect absorber placed at the origin, and the absorber is suddenly removed at $t = 0$, the wave function for subsequent times is just $M(x,k,\tau)$.

Classically, the current detected at a point $x > 0$ would be zero until $t = \frac{x}{v}$, where v is the velocity of the particles, and constant thereafter. In quantum mechanics, however, the current exhibits oscillations, and the stationary value is attained only in the limit $t \to \infty$, as the transient terms die away. The mathematical form of the transient current is closely related to an expression arising in optics, in connection with Fresnel diffraction by a straight edge, and Moshinsky has labelled the quantum - mechanical effect "diffraction in time".

In scattering situations, such as the scattering of a plane wave by a hard sphere (Moshinsky 1952 a), the functions $M(r,k,\tau)$ and $M(r,-k,\tau)$ again represent the transient behaviour of the system as it changes from the initial state (plane wave) to the final state (plane wave plus scattered wave). The correspondence between the interrupted beam experiment and scattering is made more obvious if the absorber at the origin is replaced by a perfect reflector, when the wave function for $t > 0$ becomes $M(x,k,\tau) - M(x,-k,\tau)$.

Sasakawa and Rosenfeld have separated out the transient and asymptotic parts of the scattering wave function (36) using the behaviour of the M functions as $\tau \to \infty$. From Eq.(72),

$$M(r,k,\tau) \underset{\tau \to \infty}{\sim} e^{ikr-\frac{ik^2\tau}{2}}$$

$$\lim_{\tau \to \infty} M(r,-k,\tau) = 0$$

and $$\lim_{\tau \to \infty} M(r,k_n,\tau) = 0 \quad \text{for all } k_n \quad .$$

Then with the relations

$$\sum_n \frac{\rho_n(k)}{(k-k_n)} \quad + \quad \sum_{s=o}^{\infty} \alpha_s(k)\ k^s \quad = \quad k^{-\ell}\left[S_\ell(k) - 1\right] \qquad ,$$

and

$$k^{-\ell} D_\ell(r)\ e^{ikr} \quad = \quad \frac{-1}{2i}\ O_\ell(kr) \qquad ,$$

where $S_\ell(k)$ is the S matrix for the ℓ'th partial wave, the asymptotic part is

$$\psi_{\ell m}^{asym}(r,\tau) \quad = \quad \int_0^\infty dk\ A_{\ell m}(k)\ \left\{ J_\ell(kr) + \frac{1}{2i}\left[S_\ell(k) - 1\right]\ O_\ell(kr)\right\} e^{\frac{-ik^2\tau}{2}} \quad .$$

(1.73)

If we note that (Eq.(48))

$$\frac{W\left[J_\ell(ka), \phi_\ell(k,a)\right]}{W\left[O_\ell(ka), \phi_\ell(k,a)\right]} \quad = \quad \frac{-1}{2i}\left[S_\ell(k) - 1\right] \qquad ,$$

it may be seen that in the calculation of the inverse Laplace transform for the scattering wave function (cf Eqs (35) and (42)), the term (73) is just the residue at the pole $p = \frac{-ik^2}{2}$. The term within curly brackets in Eq.(73) is familiar as the ℓ'th partial wave component of the total wave function in stationary scattering theory - $J_\ell(kr)$ is the component of the incident plane wave, and $\frac{1}{2i}\left[S_\ell(k) - 1\right] O_\ell(kr)$ the component of the outgoing scattered wave.

CHAPTER 2

SCATTERING STATE EXPANSION OF THE WAVE FUNCTION

2a. The t = 0 Wave Function

In the derivation of the wave function in Chapter 1, the first step was to obtain an expression for the Laplace transform $\bar{\psi}_{\ell m}(r,p)$ in terms of the initial packet $\Phi_{\ell m}(r)$ and the Green's function $G_{\ell}(k_p : r,r')$, Eq.(1.25). We then wrote the Green's function in terms of the regular and irregular solutions of the radial wave equation, Eq.(1.29), and proceeded to the calculation of the inverse Laplace transform, which eventually gave us the wave function in the form (1.36) and (1.66), containing the functions $M(r,k_{\nu},\tau)$ and $U(r,\tau)$.

We shall now show that the wave function can be obtained in a much simpler form by using an alternative expression for the Green's function. Let us define scattering states $\chi_{\ell}(k,r)$ and bound states $\chi_{\ell}^{(n)}(r)$ by the relations

$$\chi_{\ell}(k,r) = \frac{k^{\ell+1}}{f_{\ell}(-k)} \phi_{\ell}(k,r) , \qquad (2.1)$$

$$\chi_{\ell}^{(n)}(r) = \frac{\phi_{\ell}(-i\gamma_n,r)}{N_n} , \qquad (2.2)$$

where $k_n = -i\gamma_n$, $\gamma_n < 0$, is a bound state pole of the S matrix, and N_n is a normalisation constant. The functions $\chi_{\ell}(k,r)$ and $\chi_{\ell}^{(n)}(r)$ satisfy the orthogonality relations

$$\int_0^\infty dr\ \chi_\ell(k,r)\ \chi_\ell^*(k',r) \quad = \quad \frac{\pi}{2}\ \delta(k - k') \quad , \qquad (2.3a)$$

$$\int_0^\infty dr\ \chi_\ell^{(n)}(r)\ \chi_\ell^{(n')}(r) \quad = \quad \delta_{nn'} \quad , \qquad (2.3b)$$

$$\int_0^\infty dr\ \chi_\ell(k,r)\ \chi_\ell^{(n)}(r) \quad = \quad 0 \quad , \qquad (2.3c)$$

and the completeness relation

$$\frac{2}{\pi}\int_0^\infty dk\ \chi_\ell(k,r)\ \chi_\ell^*(k,r') + \sum_n \chi_\ell^{(n)}(r)\ \chi_\ell^{(n)}(r') \quad = \quad \delta(r - r') \quad . \qquad (2.4)$$

Then the Green's function $G_\ell(k_p: r,r')$ is given by (Newton 1960)

$$G_\ell(k_p: r,r') \quad = \quad \frac{2}{\pi}\int_0^\infty dk\ \frac{\chi_\ell(k,r)\ \chi_\ell^*(k,r')}{k^2 - k_p^2} \quad + \quad \sum_n \frac{\chi_\ell^{(n)}(r)\ \chi_\ell^{(n)}(r')}{k_n^2 - k_p^2} \quad , \qquad (2.5)$$

where the sum over n refers to bound state poles only.†

Now let us use Eq.(5) in the expression for the Laplace transform, Eq.(1.25):

† Our notation differs from Newton's in two respects. In the definition of the bound state wave function, Eq.(2), γ_n is negative, whereas Newton uses $\phi_\ell(-i\kappa_n,r)$ with κ_n positive. Since $\phi_\ell(k,r)$ is a function of k^2 only, the same wave function is obtained in each case. The Green's function used in the thesis differs by a sign from that of Newton - compare Eq.(6.1) of Newton 1960 with our Eq.(1.24).

$$\overline{\psi}_{\ell m}(r,p) = -2i \int_0^\infty dr' \, G_\ell(k_p : r,r') \, \Phi_{\ell m}(r')$$

$$= -2i \left\{ \int_0^\infty dr' \, \frac{2}{\pi} \int_0^\infty dk \, \frac{\chi_\ell(k,r) \, \chi_\ell^*(k,r')}{k^2 - k_p^2} \, \Phi_{\ell m}(r') \right.$$

$$\left. + \int_0^\infty dr' \sum_n \frac{\chi_\ell^{(n)}(r) \, \chi_\ell^{(n)}(r')}{k_n^2 - k_p^2} \, \Phi_{\ell m}(r') \right\}$$

$$= 2i \int_0^\infty dk \, B_{\ell m}(k) \, \frac{\chi_\ell(k,r)}{k_p^2 - k^2} + 2i \sum_n B_{\ell m}^{(n)} \, \frac{\chi_\ell^{(n)}(r)}{k_p^2 - k_n^2} \, , \qquad (2.6)$$

where

$$B_{\ell m}(k) = \frac{2}{\pi} \int_0^\infty dr' \, \Phi_{\ell m}(r') \, \chi_\ell^*(k,r') \qquad (2.7)$$

and

$$B_{\ell m}^{(n)} = \int_0^\infty dr' \, \Phi_{\ell m}(r') \, \chi_\ell^{(n)}(r') \, . \qquad (2.8)$$

The $B_{\ell m}$ are the coefficients in the expansion of $\Phi_{\ell m}(r)$ in terms of the complete set $\chi_\ell(k,r)$, $\chi_\ell^{(n)}(r)$,

$$\Phi_{\ell m}(r) = \int_0^\infty dk \, B_{\ell m}(k) \, \chi_\ell(k,r) + \sum_n B_{\ell m}^{(n)} \, \chi_\ell^{(n)}(r) \, , \qquad (2.9)$$

as may be seen by applying the orthogonality relations (3) to Eq.(9).

The inverse Laplace transform of Eq.(6) may be calculated by completing the contour around an infinite semicircle in the left half of the p plane, Fig.1.

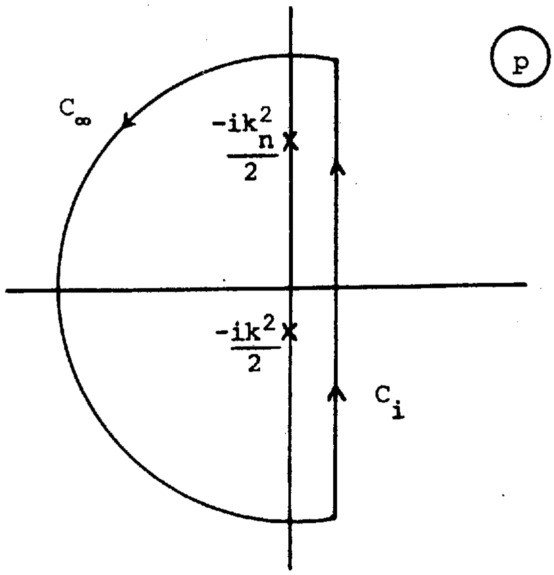

Fig.2.1 Contour for Evaluation of the Inverse Laplace Transform of Eq.(6)

The integral around C_∞ vanishes, and we are left with the pole contributions:

$$\frac{1}{2\pi i}\int_{C_i} dp\; e^{p\tau}\,\frac{2i}{k_p^2 - k_\nu^2} = e^{\frac{-ik_\nu^2\tau}{2}}, \qquad (2.10)$$

where $k_\nu = k$ or k_n, and $k_p^2 = 2ip$. Then the time-dependent wave function is

$$\psi_{\ell m}(r,\tau) = \int_0^\infty dk\; B_{\ell m}(k)\,\chi_\ell(k,r)\,e^{\frac{-ik^2\tau}{2}} + \sum_n B_{\ell m}^{(n)}\,\chi_\ell^{(n)}(r)\,e^{\frac{-ik_n^2\tau}{2}}. \qquad (2.11)$$

The wave function (11) has a simple interpretation, since it is just the form obtained by expanding the initial packet in terms of scattering and bound states, Eq. (9), and applying the operator e^{-iHt}, where H is the total Hamiltonian. It is clear from the derivation that the wave functions (1.36), or (1.66), and (2.11) are completely equivalent, and differ only in the expansion of the initial packet. If the packet is expanded in terms of plane waves, which are not eigenstates of H, it is not possible to apply the operator e^{-iHt} directly, and the Laplace transform method of Chapter 1 must be used to derive the wave function. If, instead, the packet is expanded in terms of scattering states, the operator e^{-iHt} may be used, and the wave function is obtained in the form (2.11).

The scattering state expansion is actually the starting point for the derivations of Moshinsky and Lozano. In the wave packet treatment, Lozano expresses the coefficient $B_{\ell m}$ as an integral containing $A_{\ell m}$ and the functions χ_ℓ and J_ℓ. The wave function (11) is then converted to the form (1.36) by means of contour integration, when the M functions arise at poles $k - i\varepsilon$, $-k-i\varepsilon$, and the poles of the S matrix. A similar method of obtaining the wave function of Chapter 1 from the scattering state expansion has been suggested by Beck and Nussenzveig (1960), but they do not actually carry out the calculation. In the present discussion the use of the Green's function provides a particularly simple means of proving the equivalence of the wave function (1.36) and the expansion in scattering states. We shall use the form (2.11) in discussing the relationship between the t = 0 wave function and the standard wave function for scattering problems, which involves the asymptotic limit $t \to -\infty$.

It will be noted from Eq. (9) that the initial packet contains, in general, a bound state component $B_{\ell m}^{(n)}$. This means that in the scattering (or decay) process, some fraction of the packet is left behind in the interaction region, even as $\tau \to +\infty$. It is usual to avoid this situation by assuming that the initial packet is orthogonal to all bound states, i.e.

$$B_{\ell m}^{(n)} \quad = \quad 0 \qquad \text{for all } n\ . \tag{2.12}$$

At this point, we shall make a brief diversion to mention a method of treating wave packet scattering which is used in several text books (Merzbacher 1961, Rodberg & Thaler 1967). The method is due to Low (1959), and may be applied only to "long" wave packets containing a narrow range of momenta. It is normally discussed in terms of the three-dimensional form of the wave function, $\Psi(\underset{\sim}{r},t)$, but we shall consider the corresponding partial wave components in order to show its relationship to the present work.

The initial packet is specified at $t = 0$, and expanded in terms of plane waves, with the radial component of the ℓ'th partial wave given by (Eq. (1.4))

$$\Phi_{\ell m}(r) \quad = \quad \int_0^\infty dk\ A_{\ell m}(k)\ J_\ell(kr) \quad . \tag{2.13}$$

The packet is situated at a distance L from the scatterer, and has a mean momentum $\underset{\sim}{p}_o$ directed towards the scatterer and a spread in momentum $\Delta p << p_o$. The width of the packet, Δx, is chosen to satisfy the conditions $\Delta p\ \Delta x \approx \hbar$, so that Δx is actually a minimum, $\Delta x << L$, so that the initial overlap between packet and scatterer is negligible, and $\Delta x >> b$, where b is the radius of the scatterer. Finally, it is assumed that Δx does not change appreciably in the course of the experiment, and this yields the "constant shape" condition $\frac{(\Delta p)^2 T}{\mu} << 1$, where μ is the mass of the particle, and T a characteristic time $\left(\approx \frac{2L}{p_o/\mu} \right)$.

With these restrictions on the position and shape of the initial packet, it is proved that the plane waves may be replaced by scattering states in the initial expansion without affecting the form of the packet, i.e.

$$\Phi_{\ell m}(r) \approx \int_{0}^{\infty} dk \; A_{\ell m}(k) \; \chi_{\ell}(k,r) \quad . \tag{2.14}$$

Then the time-dependent wave function for the interacting packet is obtained by applying e^{-iHt} to the expansion (14), and the wave function for the unscattered packet by applying $e^{-iH_o t}$ to the expansion (13). The wave function for the scattered packet may be separated out from the total wave function, and it is found to consist of an outgoing packet of width Δx in the radial direction, which reaches a radius r at time $t = \dfrac{(L + r)}{p_o/\mu}$. The shape of the scattered packet in the radial direction is similar to the shape of the initial packet in the incident direction. (The differential cross section for scattering into an angle θ may be calculated quite easily, and it has the usual form $|f_{\underset{\sim}{p}_o}(\theta)|^2$, where $f_{\underset{\sim}{p}_o}(\theta)$ is the scattering amplitude for a plane wave of momentum $\underset{\sim}{p}_o$.)

The treatment of scattering by Goldberger and Watson (1964, Chap.3) is similarly restricted to wave packets with a narrow momentum distribution, which propagate without changing shape. The initial packet is specified at a finite time t_o, and the method of deriving the wave function for subsequent times differs from that of Low. However, by extrapolating their Eq.(70) back to time t_o, and comparing with their Eqs (28b) and (33), it may be seen that the initial packet satisfies Low's condition of having the same coefficients whether expanded in plane waves or scattering states. Messiah (1965) uses the basic idea of Low's derivation, but his proof of the equivalence of the two expansions involves the limit $t \to -\infty$.

We can see from Eqs (9), (13) and (14) that for packets which are almost monochromatic, much larger than the scatterer, and situated at a long distance from the scatterer, the coefficients $A_{\ell m}(k)$ and $B_{\ell m}(k)$ are approximately equal. In experiments involving accelerators, the incident packets will usually satisfy these three conditions, and the scattering may be treated by Low's method. In more general scattering situations, however, the coefficients $A_{\ell m}(k)$ and $B_{\ell m}(k)$ are not equal, and the exact wave functions (1.36) or (2.11) must be used.

2b. The $t \to -\infty$ Wave Function and the Asymptotic Limit

Treatments of wave packet scattering using the asymptotic limit have been given by several authors, notably Moses (1955), Jauch (1958) and Haag (1960). The notation used in these papers is rather abstract, however, and we shall refer instead to the paper by Green and Lanford (1960), in which the correspondence between the Hilbert space notation and the more familiar partial wave expansion is made clear.

The central theorem in the usual treatment of wave packet scattering is the following (Green and Lanford 1960, Eq.(1.1)): For every element u belonging to the Hilbert space of the free Hamiltonian H_o, there are elements $u_\pm$ belonging to the continuum subspace of the total Hamiltonian H, such that

$$\lim_{t \to -\infty} \left\| e^{-iHt} u_+ - e^{-iH_o t} u \right\| = 0 \tag{2.15a}$$

and

$$\lim_{t \to +\infty} \left\| e^{-iHt} u_- - e^{-iH_o t} u \right\| = 0 \quad . \tag{2.15b}$$

The Hilbert space elements are just normalised wave packets, and the restriction on $u_{\pm}$ to the continuum subspace of H means that these packets contain no bound state components. The double bars in Eqs (15) signify the norm,

$$\| u \| \equiv \int d\underset{\sim}{r} \, | \, u(\underset{\sim}{r}) \, |^2 \quad , \tag{2.16}$$

and the functions in Eqs (15) thus approach each other in the sense of strong convergence.

The elements $u_{\pm}$ are related to u by the Møller wave matrices, $u_{\pm} = \Omega_{\pm} u$, and the S matrix is given by $S = \Omega_{-}^{*} \Omega_{+}$. Green and Lanford find the following expressions for $\Omega_{\pm}$ and S :

$$\Omega_{\pm} = F^{-1} \left[\exp(\pm \, i\delta_{\ell}(k) \,) \right] F_o \quad ,$$

$$S = F_o^{-1} \left[\exp(2i\delta_{\ell}(k) \,) \right] F_o \quad .$$

The operators F_o and F transform an element u into the partial wave expansion appropriate to the space of H_o and the continuum subspace of H respectively; $\delta_{\ell}(k)$ is the phase shift for the ℓ'th partial wave.

In partial wave notation, if

$$u_{\ell m}(r,\tau) = \int_0^{\infty} dk \, A_{\ell m}(k) \left(\frac{2}{\pi}\right)^{\frac{1}{2}} J_{\ell}(kr) \, e^{\frac{-ik^2\tau}{2}} \quad , \tag{2.17}$$

then

$$u^{+}_{\ell m}(r,\tau) = \int_0^{\infty} dk \, A_{\ell m}(k) \, e^{i\delta_{\ell}(k)} \, \psi_{\ell}(r,k) \, e^{\frac{-ik^2\tau}{2}} \tag{2.18}$$

and

$$u^{-}_{\ell m}(r,\tau) = \int_0^{\infty} dk \, A_{\ell m}(k) \, e^{-i\delta_{\ell}(k)} \, \psi_{\ell}(r,k) \, e^{\frac{-ik^2\tau}{2}} \quad . \tag{2.19}$$

Equations (17) to (19) correspond to Eq. (4.31) of Green and Lanford 1960, with the notation u retained instead of g. To avoid confusion with our scattering state $\chi_\ell(k,r)$, we have replaced the coefficients $\chi_{m\ell}(k)$ of Green and Lanford by $A_{\ell m}(k)$. Green and Lanford's scattering state $\psi_\ell(r,k)$, which appears in Eqs (18) and (19), is related to ours by

$$\psi_\ell(r,k) \quad = \quad \left(\frac{2}{\pi}\right)^{\frac{1}{2}} e^{-i\delta_\ell(k)} \chi_\ell(k,r) \qquad , \tag{2.20}$$

and this is the origin of the factor $\left(\frac{2}{\pi}\right)^{\frac{1}{2}}$ in Eq. (17).

If we were asked to specify the <u>position</u> and <u>shape</u> of the initial packet in this version of scattering theory, we might try to re-express the theorem (15) in the following way: Let the wave function for the scattering system at finite time τ be given by†

$$\psi_{\ell m}(r,\tau) \quad = \quad \int_0^\infty dk\ A_{\ell m}(k)\ \chi_\ell(k,r)\ e^{\frac{-ik^2\tau}{2}} \quad . \tag{2.21}$$

Then the initial state of the system is

$$\Phi_{\ell m}(r) \quad = \quad \lim_{\tau \to -\infty} \int_0^\infty dk\ A_{\ell m}(k)\ J_\ell(kr)\ e^{\frac{-ik^2\tau}{2}} \quad , \tag{2.22}$$

and the final state

$$\Phi'_{\ell m}(r) \quad = \quad \lim_{\tau \to +\infty} \int_0^\infty dk\ A_{\ell m}(k)\ e^{2i\delta_\ell(k)}\ J_\ell(kr)\ e^{\frac{-ik^2\tau}{2}} . \tag{2.23}$$

† The factor $\left(\frac{2}{\pi}\right)^{\frac{1}{2}}$ in Eqs (17) and (20) has been absorbed in the definition of $A_{\ell m}(k)$.

The equations (21) and (22) highlight the essential differences between the usual treatment of scattering, and that in which the initial state is given at $t = 0$. Although we have arranged that the same coefficients $A_{\ell m}(k)$ appear in Eqs (22) and (1.4), the initial packets represented by these equations are of quite different appearance in co-ordinate space. The packet (1.4) may be of any shape, and may be situated at any finite distance from the scatterer. The packet (22) is necessarily "thinly spread" over all space, with its centre at an infinite distance from the scatterer. The functions $\Phi_{\ell m}(r)$ and $\Phi'_{\ell m}(r)$ in Eqs (22) and (23) are actually symbolic, since the limit on the RHS of each equation is zero for all r.

The wave functions (11) and (21) are similar in appearance, if we assume the bound state terms to be omitted from Eq.(11), but they have rather different significance. At time $t = 0$, the wave function (11) represents the incident packet alone, with no scattered waves yet present. The wave function (21) at time $t = 0$ contains both incident and scattered packets, since the scattering has already been in progress for an infinite time.

The use of the asymptotic limit $t \to -\infty$ is often justified on the grounds that the incident packet is initially a long distance from the target, or that a long time elapses between formation of the packet and its interaction with the scatterer. In most scattering experiments, the packet must travel the length of the accelerator tube before striking the target, and the distances and times involved in this journey are long on the quantum scale. However we have seen in the discussion of Low's method that a packet specified at $t = 0$ may still be situated a long way from the target. If the scattering takes place in the interval $t = 0$ to $t = +\infty$, the packet may take an arbitrarily long time to reach the scatterer. There does not seem to be any conflict, therefore, between the use of the initial condition $t = 0$ and the occurrence of large distances and times in normal scattering experiments.

A more general argument for the limits $t \to \pm\infty$ is based on the idea that the incident and scattered particles are "asymptotically free" (Jauch 1958, Haag 1960). Since wave packets in non-relativistic quantum mechanics cannot propagate with sharp wave fronts (Van Kampen 1953), the wave packets must always have some overlap with the potential, and strictly speaking their propagation is always governed by the full Hamiltonian H. However as $|t| \to \infty$, and provided the wave packets have no bound state components, the probability density at any point within the potential goes to zero as t^{-3}. In this limit, the incident and scattered packets have negligible overlap with the potential, and their propagation is essentially free.

Now a packet specified at $t = 0$ may also have negligible overlap with the potential. If the parameters of the packet are suitably chosen, the overlap will remain negligible until the main body of the packet reaches the interaction region at some collision time t_c . The packet propagates "freely" from $t = 0$ to $t = t_c$. It seems, therefore, that the requirements usually associated with the asymptotic limit may also be satisfied by a treatment in which the initial packet is given at $t = 0$. Such a treatment has the additional advantage that it is directly applicable to scattering situations, such as proximity scattering, which involve small distances and times.

2c. Transients

Our initial interest in the t = 0 wave function arose partly from the possibility of investigating transient effects. We might expect that in a general expression for time delay, the transient and asymptotic parts of the scattering wave function in Chapter 1 would give rise to separate terms, from which one could draw conclusions about the significance of transient effects in a given situation. However on the general question of transients in time-dependent scattering theory, a distinction may be made between plane wave derivations and those using wave packets.

In the plane wave approach, the particle is initially and finally in a stationary state, with the transition from one state to the other produced by an interaction which varies with time. The early treatment of scattering by Dirac (1927), for example, starts with an initial state ψ_o which is an eigenstate of the free Hamiltonian H_o, and to this applies a perturbation V, switched on at time $t = 0$. The method of variation of constants is used to calculate the probability, $|a_n(t)|^2$, that the system is afterwards in the state ψ_n, also an eigenstate of H_o. The derivation of formal scattering theory by Lippmann and Schwinger (1950) similarly uses plane waves for the initial and final state, but in this case the interaction is switched on and off adiabatically. Cross sections are calculated from ω_{ba}, the probability per unit time of transitions from stationary state a to stationary state b. In derivations of this type, components of the wave function which decay to zero as $t \to +\infty$, i.e. as stationary conditions are re-established, may properly be labelled "transient".

In the wave packet treatment of scattering, the final state of the system contains the scattered and unscattered packets, both of which undergo spreading as they move away from the region of interaction. As a consequence of the spreading, the <u>total</u> wave function in any finite region decays to zero as $t \to +\infty$. Stationary conditions are <u>not</u> established, and in a sense the whole wave function is "transient".

Moshinsky's discussion of scattering uses a plane wave for the initial state, and after the scatterer is inserted into the beam of particles the wave function contains transient components, described by the functions M. The transient terms go to zero as the system approaches a new stationary state in the limit $t \to +\infty$. In the corresponding wave packet treatment, however, the situation is rather different, as may be seen by examining the "asymptotic" part of the wave function separated out by Sasakawa and Rosenfeld. This term is (Eq.(1.73))

$$\psi_{\ell m}^{asym}(r,\tau) = \int_0^\infty dk\, A_{\ell m}(k)\left\{ J_\ell(kr) + \frac{1}{2i}\Big[S_\ell(k) - 1\Big] O_\ell(kr)\right\} e^{\frac{-ik^2\tau}{2}} . \tag{2.24}$$

We may use the relation

$$\chi_\ell(k,r) = J_\ell(kr) + \frac{1}{2i}\Big[S_\ell(k) - 1\Big] O_\ell(kr) \quad , \quad r \geqslant a \, , \tag{2.25}$$

to write it in the form

$$\psi_{\ell m}^{asym}(r,\tau) = \int_0^\infty dk\, A_{\ell m}(k)\, \chi_\ell(k,r)\, e^{\frac{-ik^2\tau}{2}} . \tag{2.26}$$

It is now identical with the expression (21), and by the discussion following that equation we see that as $\tau \to +\infty$, the limit of the RHS of Eq.(26) is zero for all r. Thus the whole of the wave function (1.36), including the asymptotic part, goes to zero as $\tau \to +\infty$.[†]

It is interesting to note that a direct connection exists between Dirac's perturbation treatment of scattering, and the M functions of Chapter 1. Moshinsky (1952a) has considered the problem of a plane wave, $e^{ik_o x}$, which is disturbed at time t = 0 by the sudden insertion of a hard sphere scatterer at the origin. As $t \to +\infty$, the system gradually reverts to a new stationary state, with the transient behaviour being described by the functions M. Moshinsky calculates the probability that the scattered particles have energy E at time t (the probability amplitude involves Fourier transforms of M functions, $\int_0^\infty dr\, M(r, k_o, t) \sin kr$), and obtains the result $\dfrac{\sin^2 \frac{1}{2}(E-E_o)t}{(E-E_o)^2}$, where E_o is the energy of the original plane wave. In Dirac's calculation, the probability $|a_n(t)|^2$ that the system is in the eigenstate ψ_n with energy E_n at time t is proportional to $\dfrac{\sin^2 \frac{1}{2}(E_n - E_o)t}{(E_n - E_o)^2}$. The similarity of these results arises from the fact that in both cases a stationary state is disturbed at time t = 0.

The function $\dfrac{\sin^2 \frac{1}{2}(E_n - E_o)t}{(E_n - E_o)^2}$ is related, by a well known argument, to the problem of conservation of energy (Dirac 1927). For finite times the function is peaked around E_o, and there is a finite probability of finding the particle with energy $E_n \neq E_o$. As t increases, however, the width of the peak decreases, and in the limit $t \to +\infty$ the function becomes a δ function, and ensures that the scattered particles have exactly the same energy as the incident particles. We may note here another difference between the plane wave and wave packet treatments of scattering, since particles described by wave packets do not have a definite energy.

† It should perhaps be mentioned that Sasakawa, who is interested mainly in long wave packets, describes as "transient" effects which arise as the front or rear of the packet moves across the scatterer. This suggests that when the scatterer is submerged in the body of the wave packet, stationary conditions prevail, and although this is a good approximation for long wave packets, it is not true in general.

Our original calculation of time delay used the $t = 0$ wave function in the form (1.36), since it was hoped to obtain contributions from the M functions representing transient effects. While the calculation could be carried out with the wave function of Chapter 1, it is much easier to use the scattering state expansion (2.11), and this we shall do in subsequent chapters. It will be found that the calculation and the results still contain new features, and these arise from specifying the initial packet at $t = 0$ rather than in the limit $t \to -\infty$.

CHAPTER 3

TIME DELAY OF A SCATTERED WAVE PACKET

3a. Introduction

The idea of time delay in quantum scattering processes is familiar from nuclear reaction theory, where it provides the basis for the distinction between compound nucleus and direct reactions. In a compound nucleus reaction, the incident particle excites many degrees of freedom in the target nucleus, so that its energy is rapidly spread amongst all the target nucleons. After a considerable number of energy exchanges, and a long time delay, sufficient energy is concentrated in the final state particle for it to be emitted from the compound nucleus. In a direct reaction, on the other hand, the energy of the incident particle is transferred to the final state particle almost immediately, and the particle is emitted with very little delay. Of course, it is usual to think in terms of level widths, rather than lifetimes, and so compound nucleus processes are characterised by very narrow resonances, direct processes by broad resonances.

An expression relating the time delay for elastic scattering to the phase shift was first obtained by Eisenbud (1948), who considered the scattering of a wave packet with a narrow momentum distribution, and followed the motion of the "centre" of the packet (see also Bohm 1951). Let the scattered packet have the asymptotic wave function

$$\psi_{sc}(\underset{\sim}{r},t) \underset{r \to \infty}{\sim} \int_0^\infty dk\ A(k)\ f(k,\theta)\ \frac{e^{ikr-\frac{i\hbar k^2 t}{2\mu}}}{r} \quad , \qquad (3.1)$$

where $$f(k,\theta) = |f(k,\theta)|\, e^{i\eta(k)}$$

is the scattering amplitude, and $A(k)$ is strongly peaked around $k = k_o$. At time t, the centre of the scattered packet is at that value of r which makes the phase of the integrand in (1) stationary, i.e. at

$$\frac{d}{dk}\left(kr + \eta - \frac{\hbar k^2}{2\mu} t\right)_{k=k_o} = 0 ,$$

or $$r = \frac{\hbar k_o}{\mu}(t - t_d) ,$$

where $$t_d = \frac{\mu}{\hbar k_o}\left(\frac{d\eta}{dk}\right)_{k_o} . \qquad (3.2)$$

The time t_d is the amount by which the scattered packet (at angle θ) is delayed over the corresponding free packet. If the scattering amplitude is expanded in partial waves,

$$f(k,\theta) = \frac{1}{2ik}\sum_{\ell}(2\ell + 1)\left[e^{2i\delta_\ell(k)} - 1\right] P_\ell(\cos\theta) ,$$

and only one partial wave has appreciable phase shift, then

$$t_d = \frac{\mu}{\hbar k_o}\left(\frac{d\delta_\ell}{dk}\right)_{k_o} . \qquad (3.3)$$

It can be seen that the expression (3) has the behaviour we would expect of the time delay by considering the nature of $\delta_\ell(k)$ at a resonance. The phase shift increases sharply by π at a resonance, so $\frac{d\delta_\ell}{dk}$, and therefore the time delay t_d, is large and positive. Away from the resonance region, where direct processes are more important, δ_ℓ changes slowly with energy, so that the time delay is small. It is possible for $\frac{d\delta_\ell}{dk}$ to be negative, and in this case t_d is to be interpreted as a time advance. If the potential is repulsive, for instance, the scattered particle may appear at a point r sooner than in the case of free propagation.

It was pointed out by Wigner (1955) that, for potentials of finite range a, there is a lower limit on $\frac{d\delta_\ell}{dk}$ - the greatest time advance occurs if the particles are completely excluded from the region $r < a$, i.e. in hard sphere scattering. This qualitative argument suggests

$$\frac{d\delta_\ell}{dk} \geqslant -a \quad , \tag{3.4}$$

and Wigner showed that in fact

$$\frac{d\delta_\ell}{dk} \geqslant \mathrm{Re}\left\{\frac{1}{2k} W\left[I_\ell, \frac{\partial}{\partial k} O_\ell\right]_a - \frac{1}{2k} e^{2i\delta_\ell} W\left[O_\ell, \frac{\partial}{\partial k} O_\ell\right]_a\right\} , \tag{3.5}$$

where I_ℓ and O_ℓ denote the incoming and outgoing spherical Hankel functions, $W[\ldots]_a$ is a Wronskian evaluated at $r = a$, and Re signifies the real part. This relation was derived by differentiating the expression relating δ_ℓ to the R matrix,

$$e^{2i\delta_\ell} = \frac{I_\ell - I'_\ell R_\ell}{O_\ell - O'_\ell R_\ell}$$

(prime denotes differentiation with respect to r), and omitting a positive term $k \frac{dR_\ell}{dk} \left|I_\ell - I'_\ell R_\ell\right|^2$. In the case of s waves the inequality is

$$\frac{d\delta_o}{dk} \geqslant -a + \frac{1}{2k} \sin(2ka + 2\delta_o) \quad . \tag{3.6}$$

A more general definition of time delay was given by Smith (1960), who considered the average time spent by the particle in a large sphere surrounding the scatterer. If this "residence time" or "occupation time" is calculated with the scatterer present, and again with the scatterer removed, the difference of the two times is a measure of the time delay due to the interaction. Smith's calculation uses stationary state wave functions rather than wave packets, and the occupation time is defined as the number of particles within the sphere, divided by the number of particles entering the sphere per unit time. (The notation Q for the time delay is used because of the analogy with the Q value of an electrical system.)

For elastic scattering, Smith finds the occupation time for the ℓ'th partial wave to be

$$\int^{|r| < R} d\underset{\sim}{r}\ \psi_\ell^* \psi_\ell = 2\hbar \frac{d\delta_\ell}{dE} + \frac{2R}{v} - \frac{\hbar}{2E} \sin\left(2kR + 2\delta_\ell + \frac{\ell\pi}{2}\right) + G_\ell/R \quad , \tag{3.7}$$

where R is the radius of the observer's sphere, v the velocity of the incident particles, δ_ℓ the usual phase shift, and G_ℓ/R a remainder term which goes to zero as $R \to \infty$. The functions ψ_ℓ are normalised to unit incident flux.

The occupation time with the potential removed is just $\frac{2R}{v}$, and this is subtracted from (7) to obtain the time delay. The oscillatory term is removed by averaging over R and taking the limit $R \to \infty$. The term G_ℓ/R then vanishes, and a result independent of the size of the observer's sphere is obtained. The time delay for the ℓ'th partial wave is

$$Q_{\ell\ell} = 2\hbar \frac{d\delta_\ell}{dE} \quad , \qquad (3.8)$$

which is similar to the result obtained by Eisenbud, Eq.(3). (There is a difference of a factor of 2, which arises from different definitions of the outgoing wave. If the total outgoing wave is used, the phase is $e^{2i\delta_\ell}$, whereas if only the scattered outgoing wave is considered, the phase is altered to $e^{2i\delta_\ell} - 1 \propto e^{i\delta_\ell} \sin \delta_\ell$.)

The aim of Smith's paper was to obtain a time delay or lifetime <u>operator</u>, and with this in mind, Eq.(8) may be written as

$$Q_{\ell\ell} = -i\hbar\, S_\ell^* \frac{d}{dE} S_\ell \quad , \qquad (3.9)$$

where $S_\ell = e^{2i\delta_\ell}$ is the S matrix for the ℓ'th partial wave. This establishes a formal relation between the Q matrix (or operator) and the S matrix for elastic scattering. Smith extended his treatment to the case of inelastic scattering, and obtained a similar relation,

$$Q_{ij} = -i\hbar \sum_n S_{jn}^* \frac{d}{dE} S_{in} \quad , \qquad (3.10)$$

where S_{ij} are elements of the general scattering matrix, and Q is a generalised lifetime matrix. A diagonal element of Q, say Q_{ii}, represents the average time delay in a collision in which the initial channel is i.

Lippmann (1966) has suggested that a time operator be defined as

$$t = -i\hbar \frac{d}{dE} \qquad (3.11)$$

and then Eqs (9) and (10) may be written in the general form

$$Q = -S\ t\ S^{\dagger} \quad , \tag{3.12}$$

where † denotes the Hermitian adjoint. Gien (1965, 1969, 1970) has carried out calculations of time delay starting from the operator t, rather than the idea of occupation time, and he obtains results which agree with those of Smith. Razavy (1967, 1969) has investigated the problem of deriving such a time operator by quantising the operator conjugate to the Hamiltonian in classical theory.

A calculation of time delay for a general wave packet, as distinct from one with a narrow momentum distribution, has been given by Ohmura (1964). We shall discuss Ohmura's results in some detail, since the questions raised by Ohmura's paper stimulated the present investigation. (In what follows, Ohmura's notation is retained to facilitate reference to the original paper.)

The scattering process is described by a time-dependent wave function with the asymptotic form (Ohmura 1964, Eq.(26))

$$\psi(\underset{\sim}{r},t) \underset{r\to\infty}{\sim} \int_{-\infty}^{\infty} G(\nu)\ e^{i\alpha(\nu)} \left\{ e^{ikz} + g(\nu)\ e^{i\beta(\nu)}\ \frac{e^{ikr}}{r} \right\}\ e^{-i\nu t}\ d\nu \quad , \tag{3.13}$$

where ν is a frequency and k the corresponding wave number (i.e. $E = \hbar\nu = \frac{\hbar^2 k^2}{2\mu}$). The functions G, α, g and β are real, with the last two related to the scattering amplitude by

$$f_\nu(\theta) = g(\nu)\, e^{i\beta(\nu)} \tag{3.14}$$

(g and β are therefore functions of θ also). The lower integration limit in Eq.(13) is formal, since G(ν) vanishes for ν negative.

The wave function (13) may be split into incident and scattered packets,

$$\psi(\underset{\sim}{r},t) = \psi_{in}(\underset{\sim}{r},t) + \frac{1}{r}\psi_{sc}(\underset{\sim}{r},t) \quad , \tag{3.15}$$

where $$\psi_{in}(\underset{\sim}{r},t) = \int_{-\infty}^{\infty} G(\nu)\, e^{i\alpha(\nu)}\, e^{ikz-i\nu t}\, d\nu \tag{3.16}$$

and $$\psi_{sc}(\underset{\sim}{r},t) \underset{r\to\infty}{\sim} \int_{-\infty}^{\infty} G(\nu)\, e^{i\alpha(\nu)}\, g(\nu) e^{i\beta(\nu)}\, e^{ikr-i\nu t}\, d\nu \quad . \tag{3.17}$$

Note that the incident packet depends only on z , and is therefore of infinite extent in the x and y directions.

The incident flux is

$$\frac{\hbar}{2i\mu}\left(\frac{\partial\psi_{in}}{\partial z}\psi_{in}^* - \frac{\partial\psi_{in}^*}{\partial z}\psi_{in}\right)$$

and the total number of incident particles

$$S = \frac{\hbar}{2i\mu}\int_{-\infty}^{\infty} \left(\frac{\partial\psi_{in}}{\partial z}\psi_{in}^{*} - \frac{\partial\psi_{in}^{*}}{\partial z}\psi_{in}\right) dt$$

$$= 2\pi \int_{-\infty}^{\infty} G^2(\nu)\ v\ d\nu \qquad , \tag{3.18}$$

where $v = \frac{\hbar k}{\mu}$ is a velocity. (The notation S is Ohmura's - it does not denote the scattering matrix.) The incident particles arrive at a point z at a mean time

$$t_{in} = \frac{1}{S}\frac{\hbar}{2i\mu}\int_{-\infty}^{\infty} \left(\frac{\partial\psi_{in}}{\partial z}\psi_{in}^{*} - \frac{\partial\psi_{in}^{*}}{\partial z}\psi_{in}\right) t\ dt$$

$$= \frac{1}{S}\left\{2\pi\int_{-\infty}^{\infty} G^2(\nu)\ d\nu\ .\ z + 2\pi\int_{-\infty}^{\infty} G^2(\nu)\ \frac{d\alpha'}{d\nu}(\nu)\ v\ d\nu\right\} . \tag{3.19}$$

The total number of scattered particles in a direction θ is equal to the mean cross section $\langle\sigma\ (\theta)\rangle$ multiplied by S of Eq.(18), so that

$$\langle\sigma\ (\theta)\rangle\ S = \frac{\hbar}{2i\mu}\int_{-\infty}^{\infty} \left(\frac{\partial\psi_{sc}}{\partial r}\psi_{sc}^{*} - \frac{\partial\psi_{sc}^{*}}{\partial r}\psi_{sc}\right) dt$$

$$= 2\pi\int_{-\infty}^{\infty} G^2(\nu)\ g^2(\nu)\ v\ d\nu \quad . \tag{3.20}$$

The scattered particles arrive at a point r at a mean time

$$t_{sc} = \frac{1}{\langle\sigma\ (\theta)\rangle S} \frac{\hbar}{2i\mu} \int_{-\infty}^{\infty} \left(\frac{\partial\psi_{sc}}{\partial r} \psi^{*}_{sc} - \frac{\partial\psi^{*}_{sc}}{\partial r} \psi_{sc} \right) t\ dt$$

$$= \frac{1}{\langle\sigma\ (\theta)\rangle S} \left\{ 2\pi \int_{-\infty}^{\infty} G^2(\nu) g^2(\nu) d\nu\ .\ r\ +\ 2\pi \int_{-\infty}^{\infty} G^2(\nu) g^2(\nu) \frac{d}{d\nu}\left[\alpha(\nu) + \beta(\nu)\right] v\ d\nu \right\}. \tag{3.21}$$

The time delay is to be found by comparing (19) and (21), but since t_{in} is a function of z, and t_{sc} a function of r and θ, some care is needed in making this comparison. This point is not mentioned by Ohmura, however we can obtain his result if we assume θ = 0, and set z = r = R. Then the time delay is

$$\langle\Delta\ t\rangle = \frac{\int G^2 g^2 \frac{d\beta}{d\nu}\ v\ d\nu}{\int G^2 g^2\ v\ d\nu} + \left[\frac{\int G^2 g^2\ \frac{d\alpha}{d\nu}\ v\ d\nu}{\int G^2 g^2\ v\ d\nu} - \frac{\int G^2\ \frac{d\alpha}{d\nu}\ v\ d\nu}{\int G^2\ v\ d\nu} \right]$$

$$+ \quad R \left[\frac{\int G^2 g^2 d\nu}{\int G^2 g^2\ v\ d\nu} - \frac{\int G^2\ d\nu}{\int G^2\ v\ d\nu} \right] , \tag{3.22}$$

which corresponds to Ohmura's Eq.(33).

The first term in Eq.(22) represents a wave packet average of the derivative of the phase shift, and is the generalisation to an arbitrary wave packet of the expressions obtained by Eisenbud and Smith. Since Ohmura does not use partial waves, β(ν) is the phase of the total scattering amplitude, and the term in $\frac{d\beta}{d\nu}$ corresponds directly to Eq.(2).

The second term in Eq.(22) suggests that the time delay depends on the phase of the momentum distribution of the initial packet. By using a simple model, Ohmura shows that this term can have a considerable effect on the value of $\langle \Delta t \rangle$. For a wave packet of decaying resonance shape, with width $\hbar\Delta$ and mean energy $\hbar\nu_o$, the phase α is given by $\tan \alpha = \frac{\Delta}{\nu_o - \nu}$. If such a packet is scattered from a resonance of the same width, but centred at energy $\hbar\nu_r$, the time delay depends on the separation $\hbar\nu_o - \hbar\nu_r$ between the packet and resonance energies. Setting $|\hbar\nu_o - \hbar\nu_r|$ equal to $m\Gamma$, where $\Gamma = 2\hbar\Delta$, Ohmura finds that the time delay is $\frac{2\hbar}{\Gamma}$, $\frac{\hbar}{\Gamma}$ and zero for $m = 0$, 1 and ∞ respectively, and in each case the second term in Eq.(22) is of the same order of magnitude as the first.

Fong (1965) has extended the wave packet calculations to the case of inelastic scattering, and he also finds a term depending on $\frac{d\alpha}{d\nu}$. In this case the term is significant only near the threshold of a channel, but it is of the same general form as that obtained by Ohmura. Gien (1970) has investigated the problem using the time operator approach, and concludes that the time delay does not depend on the phase of the momentum distribution. He suggests that the term arises because Ohmura has used only the scattered part of the interacting packet to calculate the time delay.

The term proportional to R in Eq.(22) is omitted by Ohmura. In an earlier part of the paper he assumes separate normalisation of the incident and scattered packets, and this may have led to the term being overlooked. It has the form $R\left[\frac{1}{\bar{v}_{sc}} - \frac{1}{\bar{v}_{in}}\right]$, where the $\bar{v}$ are average velocities, and suggests a kinematic contribution to time delay arising from different average velocities of the incident and scattered packets.

While the operator expression for time delay derived by Smith, Eq.(9), has considerable formal appeal, it is obtained from stationary theory, and could not be expected to contain terms representing wave packet effects. Ohmura's paper suggests that if an arbitrary wave packet is considered, the expression for time delay will include terms in which the shape of the packet, and in particular the phase of its momentum distribution, is important.

We have carried out a new calculation of time delay, for an arbitrary wave packet, in order to examine the questions raised by Ohmura. Although our approach differs from Ohmura's in several respects, we shall be able to shed light on the physical significance of the $\frac{d\alpha}{d\nu}$ term appearing in Eq.(22). Our results will also be compared with those obtained by Kilian (1968) in a paper which appeared during the course of the present work.

3b. Definition of Time Delay

A general definition of time delay has been given by Goldberger and Watson (1964, Chap.8). We shall use this definition in our calculation, with the difference that the initial packet is specified at time $t = 0$, rather than in the limit $t \to -\infty$.

Let us consider a spherical potential $V(r)$, of finite range a, centred at the origin and surrounded by a sphere of radius R, with an arbitrary wave packet situated outside the sphere at $t = 0$, Fig. 1.

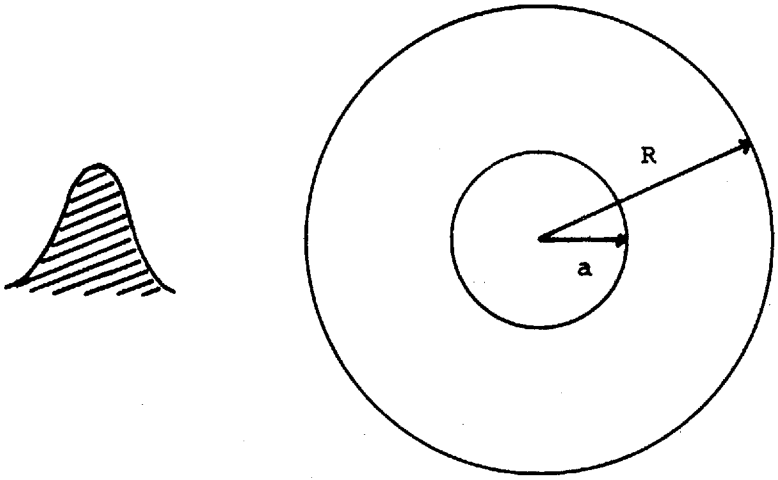

Fig.3.1 Initial Configuration
for Time Delay Calculation

Let the wave function for the propagation of the packet as it interacts with the potential be $\Psi(\underset{\sim}{r},t)$. Then the mean time spent within the sphere by the wave packet is defined as

$$T_{int}(R) \equiv \int_0^\infty dt \int_{V_R} d\underset{\sim}{r}\ \Psi^*(\underset{\sim}{r},t)\Psi(\underset{\sim}{r},t) \quad , \qquad (3.23)$$

where V_R is the volume of the sphere of radius R.

Similarly, let the wave function for free propagation of the packet be $\Phi(\underset{\sim}{r},t)$. Then the free packet spends a time

$$T_{fr}(R) \equiv \int_0^\infty dt \int_{V_R} d\underset{\sim}{r}\ \Phi^*(\underset{\sim}{r},t)\Phi(\underset{\sim}{r},t) \qquad (3.24)$$

within the observer's sphere.

The time delay due to the interaction with the potential V is given by

$$Q(R) = T_{int}(R) - T_{fr}(R) \quad . \tag{3.25}$$

This definition of time delay is similar to that used by Smith, but the occupation times are now defined in terms of time-dependent wave functions, rather than stationary states. Roughly speaking, the volume integral in Eqs (23) and (24) is equal to unity if the packet is within the sphere, and zero if it is outside the sphere. The time integral then gives the mean time spent within the sphere.

To see how the definition is related to the current integrals used in Ohmura's calculation, let us integrate Eq.(23) by parts:

$$\int_0^\infty dt \int_{V_R} d\underset{\sim}{r}\ \Psi^*(\underset{\sim}{r},t)\Psi(\underset{\sim}{r},t) = -\int_0^\infty dt\ t \frac{\partial}{\partial t}\int_{V_R} d\underset{\sim}{r}\ \Psi^*(\underset{\sim}{r},t)\Psi(\underset{\sim}{r},t) \quad .$$

The integrated part vanishes, since the volume integral is zero at $t = 0$, and it goes to zero as t^{-3} in the limit $t \to +\infty$. Using the continuity equation and Gauss' theorem we have

$$\begin{aligned} T_{int}(R) &= \int_0^\infty dt\ t \int_{V_R} d\underset{\sim}{r}\ \underset{\sim}{\nabla} \cdot \underset{\sim}{J}(\underset{\sim}{r},t) \\ &= \int_0^\infty dt\ t \int_{S_R} d\underset{\sim}{S} \cdot \underset{\sim}{J}(\underset{\sim}{R},t) \quad , \end{aligned} \tag{3.26}$$

where S_R is the surface of the observer's sphere, and the current $\underset{\sim}{J}(\underset{\sim}{r},t)$ is defined as

$$\underset{\sim}{J}(\underset{\sim}{r},t) = \frac{\hbar}{2i\mu}\left[\Psi^*(\underset{\sim}{r},t)\underset{\sim}{\nabla}\Psi(\underset{\sim}{r},t) - \Psi(\underset{\sim}{r},t)\underset{\sim}{\nabla}\Psi^*(\underset{\sim}{r},t)\right] \quad .$$

Eq.(26) may be compared with the definitions (19) and (21) used by Ohmura.

For a packet which is strongly localised, the surface integral in (26) will consist of two δ functions of opposite sign,

$$\int_{S_R} d\underset{\sim}{S} \cdot \underset{\sim}{J}(\underset{\sim}{R},t) = -\delta(t-t_1) + \delta(t-t_2) \quad ,$$

since $d\underset{\sim}{S} \cdot \underset{\sim}{J}$ is positive if the current is outwards, negative if the current is inwards. Then

$$T_{int}(R) = \int_0^\infty dt\ t \left[-\delta(t-t_1) + \delta(t-t_2)\right]$$

$$= t_2 - t_1 \quad ,$$

and the occupation time is just the difference of the entrance and exit times measured at the surface S_R.

The initial packet $\Phi(\underset{\sim}{r})$ is expanded in terms of partial waves,

$$\Phi(\underset{\sim}{r}) = \sum_{\ell m} Y_{\ell m}(\Omega)\ \frac{1}{r}\ \Phi_{\ell m}(r) \quad , \tag{3.27}$$

where $\Phi_{\ell m}(r)$ is the radial wave function for the m'th component of the ℓ'th partial wave. To obtain the wave function $\Psi(\underset{\sim}{r},t)$ for the interacting packet, we expand $\Phi_{\ell m}(r)$ in terms of scattering states:

$$\Phi_{\ell m}(r) = \int_0^\infty dk\ B_{\ell m}(k)\chi_\ell(k,r) \quad , \tag{3.28}$$

and then $\Psi(\underset{\sim}{r},t) = e^{-iHt}\ \Phi(\underset{\sim}{r})$

$$= \sum_{\ell m} Y_{\ell m}(\Omega)\ \frac{1}{r}\int_0^\infty dk\ B_{\ell m}(k)\chi_\ell(k,r)\ e^{\frac{-i\hbar k^2 t}{2\mu}} \quad . \tag{3.29}$$

Similarly, the wave function for the free packet is obtained by expanding $\Phi_{\ell m}(r)$ in terms of Riccatti - Bessel functions:

$$\Phi_{\ell m}(r) = \int_0^\infty dk\ A_{\ell m}(k)\ J_\ell(kr) \quad , \tag{3.30}$$

$$\Phi(\underset{\sim}{r},t) = e^{-iH_o t}\ \Phi(\underset{\sim}{r})$$

$$= \sum_{\ell m} Y_{\ell m}(\Omega)\ \frac{1}{r} \int_0^\infty dk\ A_{\ell m}(k)\ J_\ell(kr)\ e^{\frac{-i\hbar k^2 t}{2\mu}} \quad . \tag{3.31}$$

Note that in Eq.(28) we have assumed that the packet contains no bound state components. If this were not so, the integral (23) would diverge, due to the bound state part of the packet remaining in the sphere for all times.

The calculations of T_{int} and T_{fr} are quite similar. We shall calculate T_{fr} first, since the Bessel and Hankel functions are more familiar than the scattering states, and it is thus rather easier to follow the method of the calculation.

3c. Calculation of $T_{fr}(R)$

Inserting the wave function (31) into the definition (24) we have

$$T_{fr}(R) \equiv \int_0^\infty dt \int_{V_R} d\underset{\sim}{r}\ \Phi^*(\underset{\sim}{r},t)\ \Phi\ (\underset{\sim}{r},t)$$

$$= \frac{\mu}{\hbar} \int_0^\infty d\tau \int_0^R dr\ r^2 \int_{4\pi} d\Omega \sum_{\ell m} Y^*_{\ell m}(\Omega)\ \frac{1}{r} \int_0^\infty dk\ A^*_{\ell m}(k)\ J_\ell(kr) e^{\frac{ik^2\tau}{2}}$$

$$\times \sum_{\ell' m'} Y_{\ell' m'}(\Omega)\ \frac{1}{r} \int_0^\infty dk'\ A_{\ell' m'}(k')\ J_{\ell'}(k'r) e^{\frac{-ik'^2\tau}{2}}$$

$$= \frac{\mu}{\hbar}\int_0^\infty d\tau \int_0^R dr \sum_{\ell m} \int_0^\infty dk \int_0^\infty dk' \, A^*_{\ell m}(k)\, A_{\ell m}(k')\, J_\ell(kr)\, J_\ell(k'r)\, e^{\frac{i(k^2-k'^2)\tau}{2}} \,. \tag{3.32}$$

The time integral in Eq.(32) may be calculated in the usual way by inserting a factor $e^{-\varepsilon\tau}$ in the integrand, where the limit $\varepsilon \to 0$ is to be taken later in the calculation:

$$\int_0^\infty d\tau \, e^{\frac{i(k^2-k'^2)\tau}{2}} \, e^{-\varepsilon\tau} = \int_0^\infty d\tau \, e^{\frac{i(k^2-k'^2+2i\varepsilon)\tau}{2}}$$

$$= \frac{2i}{k^2 - k'^2 + 2i\varepsilon} \,. \tag{3.33}$$

Then

$$T_{fr}(R) = \frac{\mu}{\hbar}\int_0^R dr \sum_{\ell m} \int_0^\infty dk \int_0^\infty dk' \, A^*_{\ell m}(k)\, A_{\ell m}(k')\, J_\ell(kr)\, J_\ell(k'r) \, \frac{2i}{k^2 - k'^2 + 2i\varepsilon} \,. \tag{3.34}$$

At this point we may make use of the fact that the coefficients $A_{\ell m}(k)$ are defined in terms of the radial component $\Phi_{\ell m}(r)$ of the initial packet. Using the orthogonality relation (1.7) for the Bessel functions in Eq.(30) we have, formally,

$$A_{\ell m}(k) = \frac{2}{\pi}\int_0^\infty dr \, \Phi_{\ell m}(r)\, J_\ell(kr) \,. \tag{3.35}$$

However the initial packet is localised outside the sphere of radius R, so

$$\Phi_{\ell m}(r) = 0 \quad , \quad r < R_1 \quad , \tag{3.36}$$

where R_1 is some radius greater than R. Then

$$A_{\ell m}(k) = \frac{2}{\pi}\int_{R_1}^\infty dr \, \Phi_{\ell m}(r)\, J_\ell(kr) \,. \tag{3.37}$$

We shall introduce a special notation in connection with relations of the type (37). Let $\tilde{\Phi}_{\ell m}(k,J)$ denote the transform of the function $\Phi_{\ell m}(r)$ with respect to the function $J_\ell(kr)$, evaluated at the momentum k :

$$\tilde{\Phi}_{\ell m}(k,J) \equiv \int_{R_1}^{\infty} dr\ \Phi_{\ell m}(r)\ J_\ell(kr) \quad . \tag{3.38}$$

Then $$A_{\ell m}(k) = \frac{2}{\pi}\tilde{\Phi}_{\ell m}(k,J) \quad . \tag{3.39}$$

The coefficients $B_{\ell m}(k)$ in the interacting wave function (29) may be expressed similarly as transforms of $\Phi_{\ell m}(r)$ with respect to the scattering states $\chi_\ell(k,r)$. From Eq.(28) and the orthogonality relation (2.3a),

$$B_{\ell m}(k) = \frac{2}{\pi}\tilde{\Phi}_{\ell m}(k,\chi^*) \quad , \tag{3.40}$$

where $$\tilde{\Phi}_{\ell m}(k,\chi^*) \equiv \int_{R_1}^{\infty} dr\ \Phi_{\ell m}(r)\ \chi_\ell^*(k,r) \quad . \tag{3.41}$$

To see how the transform notation is to be used in the calculation, let us consider the relation

$$J_\ell(kr) = \frac{1}{2i}\left[O_\ell(kr) - I_\ell(kr)\right] \quad , \tag{3.42}$$

where $I_\ell(kr)$ and $O_\ell(kr)$ are the incoming and outgoing spherical Hankel functions. Inserting (42) into the definition (38) gives

$$\tilde{\Phi}_{\ell m}(k,J) = \frac{1}{2i}\int_{R_1}^{\infty} dr\ \Phi_{\ell m}(r)\ O_\ell(kr) - \frac{1}{2i}\int_{R_1}^{\infty} dr\ \Phi_{\ell m}(r)\ I_\ell(kr)$$

$$= \frac{1}{2i}\tilde{\Phi}_{\ell m}(k,O) - \frac{1}{2i}\tilde{\Phi}_{\ell m}(k,I) \quad , \tag{3.43}$$

where $\widetilde{\Phi}_{\ell m}(k,O)$ and $\widetilde{\Phi}_{\ell m}(k,I)$ are the transforms of $\Phi_{\ell m}(r)$ with respect to the functions $O_\ell(kr)$ and $I_\ell(kr)$.

Since $\Phi_{\ell m}(r)$ is not in general real, we must distinguish between the transforms of $\Phi_{\ell m}(r)$ and $\Phi^*_{\ell m}(r)$. We shall use an asterisk placed at the extreme right of a transform, $\widetilde{\Phi}_{\ell m}(k, \ldots)^*$, to denote the complex conjugate of the complete transform, and an asterisk placed beside the tilde, $\widetilde{\Phi}^*_{\ell m}(k, \ldots)$, to denote a transform of $\Phi^*_{\ell m}(r)$.

Taking the complex conjugate in Eq.(43), and using the relation

$$O^*_\ell(kr) = I_\ell(kr) \quad , \quad k \text{ real} \quad , \tag{3.44}$$

we have

$$\widetilde{\Phi}_{\ell m}(k,J)^* = \frac{-1}{2i}\int_{R_1}^{\infty} dr\, \Phi^*_{\ell m}(r)\, O^*_\ell(kr) + \frac{1}{2i}\int_{R_1}^{\infty} dr\, \Phi^*_{\ell m}(r)\, I^*_\ell(kr)$$

$$= \frac{-1}{2i}\int_{R_1}^{\infty} dr\, \Phi^*_{\ell m}(r)\, I_\ell(kr) + \frac{1}{2i}\int_{R_1}^{\infty} dr\, \Phi^*_{\ell m}(r)\, O_\ell(kr)$$

$$= \frac{-1}{2i}\widetilde{\Phi}^*_{\ell m}(k,I) + \frac{1}{2i}\widetilde{\Phi}^*_{\ell m}(k,O) \quad , \tag{3.45}$$

or, using Eq.(42),

$$\widetilde{\Phi}_{\ell m}(k,J)^* = \widetilde{\Phi}^*_{\ell m}(k,J) \quad . \tag{3.46}$$

It can be seen that in taking complex conjugates of the various transforms, we must pay attention mainly to the behaviour under conjugation of the function inside the brackets.

Returning to Eq.(34), we may now evaluate the integral over k' by writing $A_{\ell m}(k')$ in terms of $\Phi_{\ell m}$ and J_ℓ :

$$\int_0^\infty dk' \; A_{\ell m}(k') \; J_\ell(k'r) \; \frac{2i}{k^2 - k'^2 + 2i\varepsilon}$$

$$= \int_0^\infty dk' \; \frac{2}{\pi} \int_{R_1}^\infty dr' \; \Phi_{\ell m}(r') \; J_\ell(k'r') \; J_\ell(k'r) \; \frac{2i}{k^2 - k'^2 + 2i\varepsilon}$$

$$= -2i \int_{R_1}^\infty dr' \; \Phi_{\ell m}(r') \; \frac{2}{\pi} \int_0^\infty dk' \; \frac{J_\ell(k'r) \; J_\ell(k'r')}{k'^2 - (k + i\varepsilon)^2} \quad , \tag{3.47}$$

where we have used $k^2 + 2i\varepsilon \approx (k + i\varepsilon)^2$ for k positive and ε small.

The k' integral in Eq.(47) is just the free Green's function for the ℓ'th partial wave, and is evaluated in Appendix A. The value of the integral depends on the relationship between r and r' , and on the sign of the imaginary part of the second term in the denominator. From Eq.(34) we have $0 \leqslant r \leqslant R$, and from Eq.(47) $R < R_1 \leqslant r' < \infty$, so $r < r'$. Since Im $(k + i\varepsilon) > 0$, the integral is given by Eq.(A.6),

$$\frac{2}{\pi} \int_0^\infty dk' \; \frac{J_\ell(k'r) \; J_\ell(k'r')}{k'^2 - (k + i\varepsilon)^2} = \frac{1}{k} J_\ell(kr) \; O_\ell(kr') \quad , \quad r < r'. \tag{3.48}$$

We have allowed ε to go to zero on the RHS of Eq.(48) since it serves to select the asymptotic behaviour of the Green's function, and this is incorporated in the factor $O_\ell(kr')$.

Combining Eqs (47) and (48) gives

$$\int_0^\infty dk' A_{\ell m}(k')\ J_\ell(k'r)\ \frac{2i}{k^2 - k'^2 + 2i\varepsilon} = -2i \int_{R_1}^\infty dr' \Phi_{\ell m}(r')\ \frac{1}{k} J_\ell(kr)\ O_\ell(kr')$$

$$= \frac{-2i}{k} J_\ell(kr)\ \tilde{\Phi}_{\ell m}(k,0) \quad , \qquad (3.49)$$

and then in Eq.(34)

$$T_{fr}(R) = \frac{\mu}{\hbar} \sum_{\ell m} \int_0^\infty dk\ A^*_{\ell m}(k)\ \tilde{\Phi}_{\ell m}(k,0)\ \left(\frac{-2i}{k}\right) \int_0^R dr\ J_\ell(kr)\ J_\ell(kr) \quad . \quad (3.50)$$

The integral over r in Eq.(50) is of the type calculated in Appendix B, and may be written in terms of Wronskians evaluated at the upper and lower limits. We define a Wronskian containing a derivative with respect to k :

$$W\left[g(k,r),\ \frac{\partial}{\partial k} h(k,r)\right] \equiv g \frac{\partial^2}{\partial r \partial k} h - \frac{\partial g}{\partial r} \frac{\partial h}{\partial k} \quad ,$$

where g and h are arbitrary functions of k and r. Then

$$\int_a^b dr\ J_\ell(kr)\ J_\ell(kr) = \frac{-1}{2k} \left\{ W\left[J_\ell(kr),\ \frac{\partial}{\partial k} J_\ell(kr)\right]_b - W\left[J_\ell(kr),\ \frac{\partial}{\partial k} J_\ell(kr)\right]_a \right\} \quad . \qquad (3.51)$$

Now

$$J_\ell(\rho) \underset{\rho \to 0}{\sim} \frac{\rho^{\ell+1}}{(2\ell+1)!!} \quad ,$$

so

$$\lim_{r \to 0} W\left[J_\ell(kr),\ \frac{\partial}{\partial k} J_\ell(kr)\right] = 0 \quad ,$$

and

$$\int_0^R dr\; J_\ell(kr)\; J_\ell(kr) \quad = \quad \frac{-1}{2k}\, W\left[J_\ell,\ \frac{\partial}{\partial k} J_\ell\right]_R \quad . \tag{3.52}$$

In future we shall omit the arguments of the functions within the Wronskian (as has been done in Eq.(52)) in order to simplify the appearance of the results.

Inserting (52) into Eq.(50), and using the relation

$$A^*_{\ell m}(k) \quad = \quad \frac{2}{\pi}\, \tilde{\Phi}^*_{\ell m}(k,J) \quad , \tag{3.53}$$

we obtain

$$T_{fr}(R) \quad = \quad \frac{2i}{\pi}\,\frac{\mu}{\hbar} \sum_{\ell m} \int_0^\infty dk\; \tilde{\Phi}^*_{\ell m}(k,J)\; \tilde{\Phi}_{\ell m}(k,O)\; \frac{1}{k^2}\; W\left[J_\ell,\ \frac{\partial}{\partial k} J_\ell\right]_R \quad . \tag{3.54}$$

We now have an expression for $T_{fr}(R)$ which consists of a single integral over k for each partial wave, with the properties of the incident wave packet contained in the transforms $\tilde{\Phi}^*_{\ell m}(k,J)$ and $\tilde{\Phi}_{\ell m}(k,O)$, and the dependence on the radius of the observer's sphere contained in the Wronskian $W\left[J_\ell,\ \frac{\partial}{\partial k} J_\ell\right]_R$. However, before we can be satisfied with the form of the expression, a further point must be discussed. The occupation time $T_{fr}(R)$ is necessarily real, so we must prove that the expression we have obtained is real.

Let us consider the imaginary part of Eq.(54) :

$$\text{Im}\; T_{fr}(R) \quad = \quad \frac{1}{2i} \left\{ T_{fr}(R) \quad - \quad T^*_{fr}(R) \right\}$$

$$= \quad \frac{1}{\pi}\,\frac{\mu}{\hbar} \sum_{\ell m} \int_0^\infty dk \left\{ \tilde{\Phi}^*_{\ell m}(k,J)\; \tilde{\Phi}_{\ell m}(k,O) \;+\; \tilde{\Phi}_{\ell m}(k,J)\; \tilde{\Phi}^*_{\ell m}(k,I) \right\} \frac{1}{k^2}\; W\left[J_\ell,\ \frac{\partial}{\partial k} J_\ell\right]_R \quad .$$

(3.55)

Using the relation (42) we have

$$\tilde{\Phi}^*_{\ell m}(k,J)\ \tilde{\Phi}_{\ell m}(k,O) \ + \ \tilde{\Phi}_{\ell m}(k,J)\ \tilde{\Phi}^*_{\ell m}(k,I)$$

$$= \frac{1}{2i}\left\{\tilde{\Phi}^*_{\ell m}(k,O)\ \tilde{\Phi}_{\ell m}(k,O) - \tilde{\Phi}^*_{\ell m}(k,I)\tilde{\Phi}_{\ell m}(k,O) + \tilde{\Phi}_{\ell m}(k,O)\ \tilde{\Phi}^*_{\ell m}(k,I) - \tilde{\Phi}_{\ell m}(k,I)\ \tilde{\Phi}^*_{\ell m}(k,I)\right\}$$

$$= \frac{1}{2i}\left\{\tilde{\Phi}^*_{\ell m}(k,O)\ \tilde{\Phi}_{\ell m}(k,O) \ - \ \tilde{\Phi}^*_{\ell m}(k,I)\ \tilde{\Phi}_{\ell m}(k,I)\right\} \quad , \tag{3.56}$$

and using the further relations

$$I_\ell(kr) \quad = \quad (-)^\ell\ O_\ell(-kr) \tag{3.57}$$

$$J_\ell(kr) \quad = \quad (-)^{\ell+1}\ J_\ell(-kr) \quad , \tag{3.58}$$

we may write the contribution to (55) from the second term in (56) as

$$\int_0^\infty dk\ \tilde{\Phi}^*_{\ell m}(k,I)\ \tilde{\Phi}_{\ell m}(k,I)\ \frac{1}{k^2}\ W\left[J_\ell,\ \frac{\partial}{\partial k}J_\ell\right]_R$$

$$= \ -\int_{-\infty}^{0} dk\ \tilde{\Phi}^*_{\ell m}(k,O)\ \tilde{\Phi}_{\ell m}(k,O)\ \frac{1}{k^2}\ W\left[J_\ell,\ \frac{\partial}{\partial k}J_\ell\right]_R \quad .$$

Then the integral in Eq.(55) is equal to

$$\mathcal{I}_{fr} \ \equiv \ \frac{1}{2i}\int_{-\infty}^{\infty} dk\ \tilde{\Phi}^*_{\ell m}(k,O)\ \tilde{\Phi}_{\ell m}(k,O)\ \frac{1}{k^2}\ W\left[J_\ell,\ \frac{\partial}{\partial k}J_\ell\right]_R \quad . \tag{3.59}$$

We evaluate (59) by contour integration. Now

$$\tilde{\Phi}_{\ell m}(k,O) \ = \ \int_{R_1}^{\infty} dr\ \Phi_{\ell m}(r)\ O_\ell(kr) \tag{3.60}$$

and

$$O_\ell(kr) \ \underset{|k|\to\infty}{\sim} \ i^{-\ell}\ e^{ikr} \quad ,$$

so for $|k|$ sufficiently large and $\gamma \equiv \text{Im } k > 0$, the integrand (60) contains a factor $e^{-\gamma r}$. Thus

$$\tilde{\Phi}_{\ell m}(k,0) = \mathcal{O}(e^{ikR_1}) \quad \text{as } |k| \to \infty \quad , \quad \text{Im } k > 0 \quad .$$

Further, $$J_\ell(kr) \underset{|k| \to \infty}{\sim} \sin\left(kr - \frac{\ell\pi}{2}\right)$$

so $$W\left[J_\ell, \frac{\partial}{\partial k} J_\ell\right]_R = \mathcal{O}(e^{-2ikR}) \quad \text{as } |k| \to \infty \quad , \text{Im } k > 0 \quad .$$

The contour for the integral (59) may therefore be completed by an infinite semicircle in the upper half plane, Fig.2, where for $|k|$ sufficiently large the integrand behaves as $\frac{1}{k^2} e^{2ik(R_1 - R)}$, with $R_1 > R$.

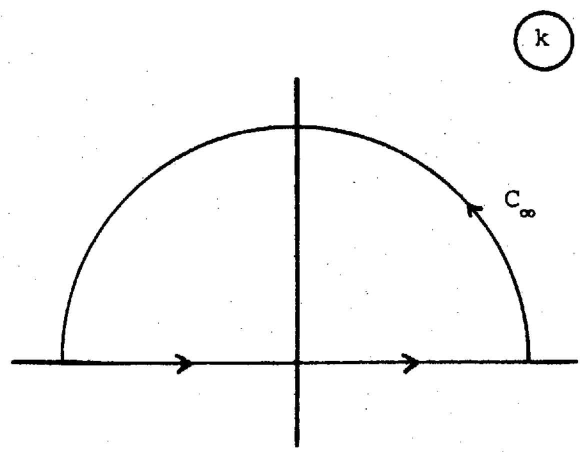

Fig.3.2 Contour for the Evaluation of Im $T_{fr}(R)$

The integrand has no poles, and the integral around C_∞ vanishes,

so

$$\int_{-\infty}^{\infty} dk \; \tilde{\Phi}^*_{\ell m}(k,0) \; \tilde{\Phi}_{\ell m}(k,0) \; \frac{1}{k^2} \; W\left[J_\ell, \frac{\partial}{\partial k} J_\ell\right]_R = 0 \quad , \qquad (3.61)$$

and the imaginary part of Eq.(54) is in fact zero.

We may now rewrite the expression for T_{fr} as

$$T_{fr}(R) = \text{Re } T_{fr}(R)$$

$$= \frac{i}{\pi}\frac{\mu}{\hbar}\sum_{\ell m}\int_0^\infty dk \left\{ \tilde{\Phi}^*_{\ell m}(k,J)\ \tilde{\Phi}_{\ell m}(k,O) - \tilde{\Phi}_{\ell m}(k,J)\ \tilde{\Phi}^*_{\ell m}(k,I) \right\} \frac{1}{k^2}\ W\left[J_\ell, \frac{\partial}{\partial k} J_\ell\right]_R \quad ,$$

and by a calculation similar to (56),

$$\tilde{\Phi}^*_{\ell m}(k,J)\ \tilde{\Phi}_{\ell m}(k,O) \quad - \quad \tilde{\Phi}_{\ell m}(k,J)\ \tilde{\Phi}^*_{\ell m}(k,I)$$

$$= 2i\ \tilde{\Phi}^*_{\ell m}(k,J)\ \tilde{\Phi}_{\ell m}(k,J) \quad - \quad \frac{1}{2i}\left\{ \tilde{\Phi}^*_{\ell m}(k,I)\ \tilde{\Phi}_{\ell m}(k,O) - \tilde{\Phi}_{\ell m}(k,I)\ \tilde{\Phi}^*_{\ell m}(k,O) \right\} \quad .$$

Finally, writing the J transforms in terms of the coefficients $A_{\ell m}$, we have

$$T_{fr}(R) = \pi \sum_{\ell m}\int_0^\infty dk\ A^*_{\ell m}(k)\ A_{\ell m}(k)\ \frac{\mu}{\hbar k}\left(\frac{-1}{2k}\right) W\left[J_\ell, \frac{\partial}{\partial k} J_\ell\right]_R$$

$$+ \frac{1}{\pi}\sum_{\ell m}\int_0^\infty dk \left\{ \tilde{\Phi}^*_{\ell m}(k,I)\ \tilde{\Phi}_{\ell m}(k,O) - \tilde{\Phi}_{\ell m}(k,I)\ \tilde{\Phi}^*_{\ell m}(k,O) \right\} \frac{\mu}{\hbar k}\left(\frac{-1}{2k}\right) W\left[J_\ell, \frac{\partial}{\partial k} J_\ell\right]_R \quad . \tag{3.62}$$

The factor $\frac{-1}{2k}$ has been separated out and placed beside the Wronskian since these two terms arise from the radial integral (52).

We conclude this section with an observation regarding the real and imaginary parts of the expression for the occupation time. Returning to Eq.(34), it may be seen by taking the complex conjugate and interchanging k and k' that the expression at that point is real. After the evaluation of the Green's function, however, the form (50) or (54) is obtained, and it is no longer obvious that the expression for T_{fr} is real. The asymmetry of the transforms in Eq.(54) arises directly from the Green's function Eq.(48).

Comparison with Appendix A shows that the calculation of Im T_{fr} (Eqs (55) to (61)) bears a strong resemblance to the evaluation of the Green's function by contour integration. The similarities include the use of relations such as (57) and (58) to obtain an integral along the complete real axis, and the use of inequalities in the radial variables to justify completion of the contour in the upper half plane. Thus the proof that Im T_{fr} is zero involves the same type of integration as gives rise to the asymmetry in Eq.(54), and the derivation of the final expression Eq.(62) is seen to be internally consistent.

3d. Calculation of $T_{int}(R)$

The occupation time for the interacting packet may be calculated in a similar way to the occupation time for the free packet, with the coefficients $A_{\ell m}$ replaced by $B_{\ell m}$, the Bessel functions J_ℓ replaced by scattering states χ_ℓ, and so on. We shall not give all the details of the calculation here, but rather mention the points at which it differs from the calculation in the previous section.

The occupation time is, from Eqs (23) and (29),

$$
\begin{aligned}
T_{int}(R) &\equiv \int_0^\infty dt \int_{V_R} d\underset{\sim}{r}\ \Psi^*(\underset{\sim}{r},t)\ \Psi(\underset{\sim}{r},t) \\
&= \frac{\mu}{\hbar} \int_0^\infty d\tau \int_0^R dr \sum_{\ell m} \int_0^\infty dk \int_0^\infty dk' B^*_{\ell m}(k)\ B_{\ell m}(k')\ \chi^*_\ell(k,r)\chi_\ell(k',r)\ e^{\frac{i(k^2-k'^2)\tau}{2}} \\
&= \frac{\mu}{\hbar} \int_0^R dr \sum_{\ell m} \int_0^\infty dk \int_0^\infty dk' B^*_{\ell m}(k)\ B_{\ell m}(k')\ \chi^*_\ell(k,r)\chi_\ell(k',r)\ \frac{2i}{k^2 - k'^2 + 2i\varepsilon} .
\end{aligned}
\tag{3.63}
$$

Using the relation

$$B_{\ell m}(k) \quad = \quad \frac{2}{\pi}\,\tilde{\Phi}_{\ell m}(k,\chi^*) \qquad ,$$

the k' integral in Eq.(63) is

$$\int_0^\infty dk'\; B_{\ell m}(k')\chi_\ell(k',r) \quad \frac{2i}{k^2 - k'^2 + 2i\varepsilon}$$

$$= \quad -2i \int_{R_1}^\infty dr'\Phi_{\ell m}(r') \quad \frac{2}{\pi}\int_0^\infty dk' \;\frac{\chi_\ell(k',r)\chi_\ell^*(k',r')}{k'^2 - (k + i\varepsilon)^2} \qquad . \tag{3.64}$$

The Green's function integral is given in Appendix A :

$$\frac{2}{\pi}\int_0^\infty dk' \;\frac{\chi_\ell(k',r)\chi_\ell^*(k',r')}{k'^2 - (k + i\varepsilon)^2}$$

$$= \quad \frac{1}{k}\,\chi_\ell(k,r)\;\;(-)^\ell f_\ell(-k,r') - \sum_n \frac{\chi_\ell^{(n)}(r)\chi_\ell^{(n)}(r')}{k_n^2 - k^2} \qquad , \qquad r < r' \qquad , \tag{3.65}$$

where the sum is over all bound states.

On inserting (65) into Eq.(64) we obtain two integrals over r', the first containing $f_\ell(-k,r')$ and the second $\chi_\ell^{(n)}(r')$. Now

$$(-)^\ell\; f_\ell(-k,r') \quad = \quad O_\ell(kr') \qquad , \qquad r' \geqslant a \quad , \tag{3.66}$$

so

$$\int_{R_1}^\infty dr'\;\Phi_{\ell m}(r')\;\;(-)^\ell\; f_\ell(-k,r') \quad = \quad \int_{R_1}^\infty dr'\;\Phi_{\ell m}(r')\;O_\ell(kr')$$

$$= \quad \tilde{\Phi}_{\ell m}(k,O) \qquad . \tag{3.67}$$

The second integral is the overlap integral between the component $\Phi_{\ell m}(r)$ of the initial packet, and a bound state. Since we have assumed that the initial packet is orthogonal to all bound states, this integral is identically zero :

$$\int_{R_1}^{\infty} dr' \; \Phi_{\ell m}(r') \; \chi_\ell^{(n)}(r') \;=\; 0 \qquad \text{for all } n \quad . \tag{3.68}$$

Then from (64) and (65),

$$\int_0^{\infty} dk' \; B_{\ell m}(k') \; \chi_\ell(k',r) \; \frac{2i}{k^2 - k'^2 + 2i\varepsilon} \;=\; -\frac{2i}{k}\chi_\ell(k,r) \; \tilde{\Phi}_{\ell m}(k,0) \quad . \tag{3.69}$$

We are left with the radial integral in Eq.(63), and this is evaluated in Appendix B :

$$\int_0^{R} dr \; \chi_\ell^*(k,r) \; \chi_\ell(k,r) \;=\; -\frac{1}{2k} \; W\left[\chi_\ell^*, \frac{\partial}{\partial k}\chi_\ell\right]_R \quad , \tag{3.70}$$

since $\lim\limits_{r \to 0} \; W\left[\chi_\ell^* \, , \, \frac{\partial}{\partial k}\chi_\ell\right]_r \;=\; 0 \quad .$

Then from (63), (69) and (70), together with the relation

$$B_{\ell m}^*(k) \;=\; \frac{2}{\pi} \, \tilde{\Phi}_{\ell m}^*(k,\chi) \quad ,$$

we have

$$T_{int}(R) \;=\; \frac{2i}{\pi} \frac{\mu}{\hbar} \sum_{\ell m} \int_0^{\infty} dk \; \tilde{\Phi}_{\ell m}^*(k,\chi) \; \tilde{\Phi}_{\ell m}(k,0) \; \frac{1}{k^2} \; W\left[\chi_\ell^*, \frac{\partial}{\partial k}\chi_\ell\right]_R \quad . \tag{3.71}$$

This corresponds to the expression (54) for $T_{fr}(R)$.

Following the procedure of the previous section, we now calculate the imaginary part of (71). It can be seen from Eq.(70) that the Wronskian appearing in (71) is real, so

$$\mathrm{Im}\ T_{int}(R) = \frac{1}{\pi}\frac{\mu}{\hbar}\sum_{\ell m}\int_0^\infty dk\ \left\{\tilde{\Phi}^*_{\ell m}(k,\chi)\ \tilde{\Phi}_{\ell m}(k,O) + \tilde{\Phi}_{\ell m}(k,\chi^*)\ \tilde{\Phi}^*_{\ell m}(k,I)\right\}$$

$$\times\ \frac{1}{k^2}\ W\left[\chi^*_\ell,\ \frac{\partial}{\partial k}\chi_\ell\right]_R \quad . \qquad (3.72)$$

The initial packet is outside the potential, so we may use the relation

$$\chi_\ell(k,r) = \frac{-1}{2i}\left[I_\ell(kr) - S_\ell(k)\ O_\ell(kr)\right] \quad , \quad r \geqslant a \quad , \qquad (3.73)$$

to write

$$\tilde{\Phi}^*_{\ell m}(k,\chi) = \frac{-1}{2i}\left\{\tilde{\Phi}^*_{\ell m}(k,I) - S_\ell(k)\ \tilde{\Phi}^*_{\ell m}(k,O)\right\} \quad , \qquad (3.74)$$

where $S_\ell(k)$ is the scattering matrix for the ℓ'th partial wave. Taking the conjugate of (74) we find

$$\tilde{\Phi}^*_{\ell m}(k,\chi)\ \tilde{\Phi}_{\ell m}(k,O) + \tilde{\Phi}_{\ell m}(k,\chi^*)\ \tilde{\Phi}^*_{\ell m}(k,I)$$

$$= \frac{1}{2i}\left\{S_\ell(k)\ \tilde{\Phi}^*_{\ell m}(k,O)\ \tilde{\Phi}_{\ell m}(k,O) - S^*_\ell(k)\ \tilde{\Phi}^*_{\ell m}(k,I)\ \tilde{\Phi}_{\ell m}(k,I)\right\} \quad . \qquad (3.75)$$

Then, with the relations

$$W\left[\chi^*_\ell,\ \frac{\partial}{\partial k}\chi_\ell\right]_R = W\left[\chi_\ell,\ \frac{\partial}{\partial k}\chi^*_\ell\right]_R \quad ,$$

$$\chi_\ell(k,r) = S_\ell(k)\ \chi^*_\ell(k,r) \quad , \quad k \text{ real} \quad ,$$

and
$$\chi^*_\ell(k,r) = (-)^{\ell+1}\ \chi_\ell(-k,r) \quad , \quad k \text{ real} \quad ,$$

the integral appearing in (72) may be written as an integral along the complete real axis,

$$\mathcal{J}_{int} \cong \frac{1}{2i} \int_{-\infty}^{\infty} dk\ \tilde{\Phi}^*_{\ell m}(k,0)\ \tilde{\Phi}_{\ell m}(k,0)\ \frac{1}{k^2}\ W\left[\chi_\ell ,\ \frac{\partial}{\partial k}\chi_\ell\right]_R \quad . \tag{3.76}$$

As with (59), the integral (76) may be evaluated by completing the contour around an infinite semicircle in the upper half of the k plane. The integral around the semicircle vanishes, but now the integrand has poles in the upper half plane corresponding to the bound state poles of $S_\ell(k)$, which is contained in the Wronskian $W\left[\chi_\ell ,\ \frac{\partial}{\partial k}\chi_\ell\right]_R$ (cf. Eq.(73)).

At a bound state pole k_n, the residue of the integrand (76) contains the factor $\tilde{\Phi}^*_{\ell m}(k_n,0)\ \tilde{\Phi}_{\ell m}(k_n,0)$. However the bound state wave function $\chi_\ell^{(n)}(r)$ may be written as (Eq.(A.14))

$$\chi_\ell^{(n)}(r) = e^{\frac{i\pi}{4}}\ \mathrm{Res}_n^{\frac{1}{2}}\ f_\ell(-k_n,r) \quad ,$$

where Res_n is the residue of the S matrix at the bound state pole. We know that

$$(-)^\ell\ f_\ell(-k,r) = O_\ell(kr) \quad , \qquad r \geqslant a \quad ,$$

so

$$\tilde{\Phi}_{\ell m}(k_n,0) = \int_{R_1}^{\infty} dr\ \Phi_{\ell m}(r)\ O_\ell(k_n r)$$

$$\propto \int_{R_1}^{\infty} dr\ \Phi_{\ell m}(r)\ \chi_\ell^{(n)}(r) \quad ,$$

and by our assumption that the initial packet is orthogonal to all bound states, the residue of (76) at each bound state pole is zero. Then

$$\int_{-\infty}^{\infty} dk\ \tilde{\Phi}^*_{\ell m}(k,0)\ \tilde{\Phi}_{\ell m}(k,0)\ \frac{1}{k^2}\ W\left[\chi_\ell ,\ \frac{\partial}{\partial k}\chi_\ell\right]_R = 0 \quad , \tag{3.77}$$

and the imaginary part of $T_{int}(R)$ vanishes.

From Eq. (71),

$$T_{int}(R) = \mathrm{Re}\, T_{int}(R)$$

$$= \frac{i}{\pi}\frac{\mu}{\hbar}\sum_{\ell m}\int_0^\infty dk \left\{ \tilde{\Phi}^*_{\ell m}(k,\chi)\ \tilde{\Phi}_{\ell m}(k,O) - \tilde{\Phi}_{\ell m}(k,\chi^*)\ \tilde{\Phi}^*_{\ell m}(k,I)\right\}$$

$$\times \frac{1}{k^2}\ W\left[\chi^*_\ell,\ \frac{\partial}{\partial k}\chi_\ell\right]_R ,$$

and by using (74) and its conjugate we have

$$\tilde{\Phi}^*_{\ell m}(k,\chi)\ \tilde{\Phi}_{\ell m}(k,O) \quad - \quad \tilde{\Phi}_{\ell m}(k,\chi^*)\ \tilde{\Phi}^*_{\ell m}(k,I)$$

$$= 2i\ \tilde{\Phi}^*_{\ell m}(k,\chi)\ \tilde{\Phi}_{\ell m}(k,\chi^*) - \frac{1}{2i}\left\{\tilde{\Phi}^*_{\ell m}(k,I)\ \tilde{\Phi}_{\ell m}(k,O) - \tilde{\Phi}_{\ell m}(k,I)\ \tilde{\Phi}^*_{\ell m}(k,O)\right\} .$$

Then, writing the χ transforms in terms of the $B_{\ell m}$,

$$T_{int}(R) = \pi\sum_{\ell m}\int_0^\infty dk\ B^*_{\ell m}(k)\ B_{\ell m}(k)\ \frac{\mu}{\hbar k}\left(\frac{-1}{2k}\right)\ W\left[\chi^*_\ell,\ \frac{\partial}{\partial k}\chi_\ell\right]_R$$

$$+ \frac{1}{\pi}\sum_{\ell m}\int_0^\infty dk\left\{\tilde{\Phi}^*_{\ell m}(k,I)\ \tilde{\Phi}_{\ell m}(k,O) - \tilde{\Phi}_{\ell m}(k,I)\ \tilde{\Phi}^*_{\ell m}(k,O)\right\}\frac{\mu}{\hbar k}\ \left(\frac{-1}{2k}\right)\ W\left[\chi^*_\ell,\frac{\partial}{\partial k}\chi_\ell\right]_R . \tag{3.78}$$

The expression (78) for $T_{int}(R)$ corresponds to Eq. (62) for $T_{fr}(R)$, with the coefficients $A_{\ell m}$ replaced by $B_{\ell m}$ and the functions J_ℓ replaced by scattering states χ_ℓ. The time delay $Q(R)$ is the difference of the occupation times $T_{int}(R)$ and $T_{fr}(R)$. However it does not seem possible to obtain a simple expression for Q by combining (62) and (78), so the results of the calculation are best left in the form of occupation times.

We shall postpone discussion of these results until Chapter 5, where we will be able to compare them with similar expressions relating to the decay of a wave packet initially inside the potential.

CHAPTER 4

LIFETIME OF A DECAYING WAVE PACKET

4a. Introduction

In the early treatment of decay by Weisskopf and Wigner (1930), the wave function for the decaying system was expanded in terms of eigenstates of the unperturbed Hamiltonian, with the coefficients of the expansion depending on the time t. If the perturbed system satisfies the wave equation

$$i\hbar \frac{\partial \psi}{\partial t} = (H_o + V)\,\psi \quad , \qquad (4.1)$$

where H_o is the unperturbed Hamiltonian and V the perturbation producing the decay, the wave function ψ may be written in the form

$$\psi = \sum_n b_n(t)\, e^{\frac{-iE_n t}{\hbar}}\, \psi_n \quad , \qquad (4.2)$$

where $$H_o\psi_n = E_n\psi_n \quad , \qquad (4.3)$$

and the time dependence of ψ is contained in the coefficients $b_n(t)$.

On substituting the expansion (2) into Eq.(1), a set of equations for the coefficients b_n is obtained:

$$i\hbar \frac{db_n}{dt} = \sum_m V_{nm}\, e^{\frac{i(E_n-E_m)t}{\hbar}}\, b_m \quad , \qquad (4.4)$$

where V_{nm} is a matrix element of the perturbation between eigenstates of H_o,

$$V_{nm} = \int \psi_n^* V \psi_m \quad . \tag{4.5}$$

If the system is assumed to be in the unperturbed eigenstate ψ_o at time $t = 0$, the equations (4) are subject to the initial conditions

$$\begin{aligned} b_o(0) &= 1 \\ b_n(0) &= 0 \qquad n \neq 0 \quad . \end{aligned} \tag{4.6}$$

Weisskopf and Wigner assumed a form for the coefficient b_o,

$$b_o(t) = e^{\frac{-\Gamma_o t}{2\hbar}} \quad , \tag{4.7}$$

expressed the coefficients b_n ($n \neq 0$) as combinations of similar exponentials, and then verified that these assumptions gave consistent results.

The treatment of Weisskopf and Wigner was extended by Heitler and Ma (1949), who expressed the coefficients b as Fourier transforms, e.g.

$$b_o(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dE \; a_o(E) \; e^{\frac{i(E_o - E)t}{\hbar}} \quad , \tag{4.8}$$

where E_o is the energy of the unperturbed eigenstate ψ_o. They derived general expressions for the coefficients a, in particular

$$a_o(E) = \frac{i}{E - E_o + i\Gamma(E)/2} \quad , \tag{4.9}$$

where $\Gamma(E)$ represents the coupling of the state ψ_o to all the other states ψ_n through the perturbation V. Then in the particular case that $\Gamma(E)$ is a slowly varying function of E, they showed that the result (7) is regained,

$$b_o(t) = \frac{-1}{2\pi i}\int_{-\infty}^{\infty} dE \frac{e^{\frac{i(E_o - E)t}{\hbar}}}{E - E_o + i\Gamma_o/2}$$

$$= e^{\frac{-\Gamma_o t}{2\hbar}} \qquad , \qquad (4.10)$$

where $\Gamma_o = \Gamma(E_o)$ and the integral is evaluated by contour integration. From Eq.(7) or (10), the probability that the system is still in the eigenstate ψ_o at time t is

$$|b_o(t)|^2 = e^{\frac{-\Gamma_o t}{\hbar}} \qquad , \qquad (4.11)$$

which is the well known exponential decay law.

A general theory of decay in which the initial state is described by a wave packet rather than an eigenstate of H_o has been given by Krylov and Fock (1947). In outlining the details of their approach we shall follow a paper by Khalfin (1958).† Let the state of the system at time t = 0 be

$$\psi(x, 0) = \int_0^{\infty} dE \; c(E) \; \psi_E(x) \qquad , \qquad (4.12)$$

† Goldberger and Watson (1964, Chap.8) give a general treatment of decay with the initial state of the system described by a wave packet. However it is assumed that the wave packet contains only a narrow range of momenta, and in the evaluation of transition probabilities this condition is used to remove the wave packet dependence - cf their Eqs (53) and (54a). The final expression for the probability of finding the system in the initial state is (Eq.(117))

$$P(t) = e^{\frac{-\Gamma t}{\hbar}} \qquad ,$$

which is just the result obtained by Weisskopf and Wigner.

where $\psi_E(x)$ is an eigenstate of the total Hamiltonian, and x represents the set of variables on which the wave function depends, apart from the time t. At later times, the state of the system is given by

$$\psi(x,t) = \int_0^\infty dE\ c(E)\ \psi_E(x)\ e^{\frac{-iEt}{\hbar}} . \tag{4.13}$$

The probability amplitude that the system is still in the initial (wave packet) state at time t is

$$p(t) \equiv (\ \psi(x,0),\ \psi(x,t)\ ) \tag{4.14}$$

or
$$p(t) = \int_0^\infty dE\ e^{\frac{-iEt}{\hbar}}\ \omega(E) , \tag{4.15}$$

where
$$\omega(E) = c^*(E)\ c(E) \tag{4.16}$$

is the energy distribution of the initial packet. Then the probability that the system has not decayed is defined as

$$P(t) = |p(t)|^2 , \tag{4.17}$$

and the decay law is seen to be determined entirely by the energy distribution $\omega(E)$.

If $\omega(E)$, considered as a function of the complex variable E, has poles only at $E = E_o \pm i\Gamma_o/2$, then the probability amplitude is

$$p(t) = \frac{1}{\pi}\int_0^\infty dE\ e^{\frac{-iEt}{\hbar}} \frac{\Gamma_o/2}{(E - E_o)^2 + \Gamma_o^2/4} . \tag{4.18}$$

It is usual to assume that $\Gamma_o << E_o$ and $E_o >> 0$, and then the lower limit in the integral is changed to $-\infty$, giving

$$p(t) \approx \frac{1}{\pi} \int_{-\infty}^{\infty} dE\, e^{\frac{-iEt}{\hbar}} \frac{\Gamma_o/2}{(E - E_o)^2 + \Gamma_o^2/4}$$

$$= e^{\frac{-iE_o t}{\hbar}} e^{\frac{-\Gamma_o t}{2\hbar}}$$

and $$P(t) = e^{\frac{-\Gamma_o t}{\hbar}} , \tag{4.19}$$

which is the same as Eq.(11). However Khalfin shows that by a more careful evaluation of Eq.(18), retaining the lower limit 0 and integrating around a quadrant in the E plane, the result

$$p(t) = e^{\frac{-iE_o t}{\hbar} - \frac{\Gamma_o t}{2\hbar}} - \frac{i}{\pi} \frac{\hbar\Gamma_o/2}{(E_o^2 + \Gamma_o^2/4)t} \tag{4.20}$$

is obtained for $t >> \hbar\left[\sqrt{E_o^2 + \Gamma_o^2/4}\right]^{-1}$. Thus, as is well known, the exponential decay law is eventually replaced by decay as an inverse power of t.

The definition (17) of Krylov and Fock has been criticised by Nussenzveig (1961) on the grounds that it gives a "decay law" in situations where decay, in the usual sense of the word, does not occur. If a wave packet is placed inside an impenetrable sphere, for instance, the probability $|(\psi(x,o), \psi(x,t))|^2$ of finding the system in the initial state will certainly change with time, but the system would not normally be described as "decaying". In studying the time behaviour of a (spherical) wave packet placed inside a partially transparent sphere, Nussenzveig defines the decay law as the probability that the particle is still within the sphere at time t :

$$P(t) = \frac{\int_0^a dr \; | \; \phi(r,t)|^2}{\int_0^a dr \; | \; f(r) \; |^2} \quad , \tag{4.21}$$

where f(r) (=0 for r > a) is the initial packet and $\phi(r,t)$ the wave function describing its propagation for t > 0. Thus the probability of finding the particle in a particular <u>state</u> (eigenstate or wave packet) is replaced by the probability of finding the particle in a particular <u>region</u>. In the example considered by Nussenzveig, the decay law (21) is found to contain the usual terms having exponential and inverse power dependence on the time.

With the decay law defined by Eq.(21), the mean <u>lifetime</u> of the decaying wave packet might be defined as

$$L = \int_0^\infty dt \; P(t)$$

$$= \int_0^\infty dt \int_0^a dr \; | \; \phi(r,t)|^2 \quad , \tag{4.22}$$

where we have assumed the initial packet to be normalised to unity. If the decay were purely exponential, for example, the mean lifetime would be

$$\int_0^\infty dt \; e^{\frac{-\Gamma_o t}{\hbar}} = \frac{\hbar}{\Gamma_o} \quad . \tag{4.23}$$

There is however an important difference between wave packets and the eigenstates considered in earlier discussions of decay. If the system is initially in an eigenstate of H_o , and the perturbation is not applied, the system will remain in the eigenstate and not decay. If the initial state of the system is described by a wave packet, decay will always occur due to the spreading of the wave packet, whether the interaction is switched on or not. This is true even if the mean velocity of the packet is zero.† Thus a better measure of the lifetime of the wave packet, as determined by the interaction, is obtained by subtracting from Eq.(22) the corresponding expression for the free packet. The mean lifetime of the decaying system then appears (Kilian 1968) as a time delay in the arrival of the decay products at the point of observation, relative to the case of the corresponding free particles.

Let us again consider a spherical potential V(r), of finite range a, surrounded by a sphere of radius R, but with an arbitrary wave packet situated <u>inside</u> the potential at t = 0, Fig.1.

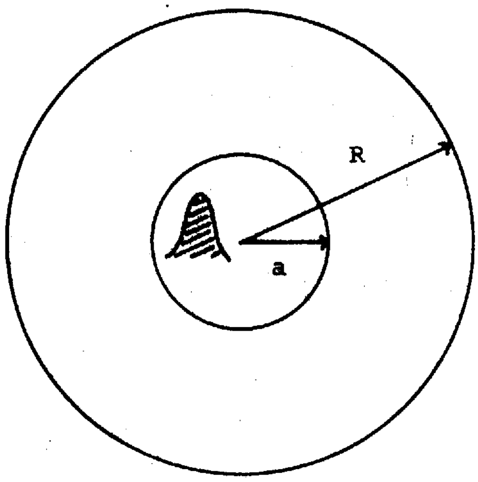

Fig.4.1 Initial Configuration
for Lifetime Calculation

† An exception occurs in the case of a Gaussian wave packet within an harmonic oscillator potential - see Furry 1962.

Let the wave function for the propagation of the packet in the presence of the potential be $\Psi(\underset{\sim}{r},t)$. Then the mean time spent within the sphere by the wave packet is

$$T_{int}(R) \equiv \int_0^\infty dt \int_{V_R} d\underset{\sim}{r}\ \Psi^*(\underset{\sim}{r},t)\ \Psi(\underset{\sim}{r},t) \quad , \tag{4.24}$$

where V_R is the volume of the sphere of radius R.

Similarly, let the wave function for free propagation of the packet be $\Phi(\underset{\sim}{r},t)$. Then the free packet spends a time

$$T_{fr}(R) \equiv \int_0^\infty dt \int_{V_R} d\underset{\sim}{r}\ \Phi^*(\underset{\sim}{r},t)\ \Phi(\underset{\sim}{r},t) \tag{4.25}$$

within the observer's sphere.

We shall define the <u>lifetime</u> of the decaying wave packet, as observed at the surface of the sphere, to be

$$L(R) = T_{int}(R) - T_{fr}(R) \quad . \tag{4.26}$$

The wave functions $\Psi(\underset{\sim}{r},t)$ and $\Phi(\underset{\sim}{r},t)$ have the same form as the wave functions in Chapter 3, but the coefficients $A_{\ell m}$ and $B_{\ell m}$ are different, as the packet is now inside the potential. Thus

$$\Phi(\underset{\sim}{r}) = \sum_{\ell m} Y_{\ell m}(\Omega)\ \frac{1}{r}\ \Phi_{\ell m}(r) \quad , \tag{4.27}$$

$$\Psi(\underset{\sim}{r},t) = \sum_{\ell m} Y_{\ell m}(\Omega)\ \frac{1}{r}\int_0^\infty dk\ B_{\ell m}(k)\chi_\ell(k,r)\ e^{\frac{-i\hbar k^2 t}{2\mu}} \quad , \tag{4.28}$$

where

$$\begin{aligned} B_{\ell m}(k) &= \frac{2}{\pi}\tilde{\Phi}_{\ell m}(k,\chi^*) \\ &= \frac{2}{\pi}\int_0^a dr\ \Phi_{\ell m}(r)\ \chi_\ell^*(k,r) \quad , \end{aligned} \tag{4.29}$$

and

$$\Phi(\underset{\sim}{r},t) = \sum_{\ell m} Y_{\ell m}(\Omega)\ \frac{1}{r}\int_0^\infty dk\ A_{\ell m}(k)\ J_\ell(kr)\ e^{\frac{-i\hbar k^2 t}{2\mu}} \quad , \tag{4.30}$$

where

$$\begin{aligned} A_{\ell m}(k) &= \frac{2}{\pi}\tilde{\Phi}_{\ell m}(k,J) \\ &= \frac{2}{\pi}\int_0^a dr\ \Phi_{\ell m}(r)\ J_\ell(kr) \quad . \end{aligned} \tag{4.31}$$

We again assume that the initial packet is orthogonal to all bound states in order to ensure the convergence of the integral (24).

4b. Calculation of $T_{fr}(R)$

From Eqs (25) and (30),

$$T_{fr}(R) \equiv \int_0^\infty dt \int_{V_R} d\underset{\sim}{r}\ \Phi^*(\underset{\sim}{r},t)\ \Phi(\underset{\sim}{r},t)$$

$$= \frac{\mu}{\hbar}\int_0^\infty d\tau \int_0^R dr\ r^2 \int_{4\pi} d\Omega \sum_{\ell m} Y_{\ell m}^*(\Omega)\ \frac{1}{r}\int_0^\infty dk\ A_{\ell m}^*(k)\ J_\ell(kr)\ e^{\frac{ik^2\tau}{2}}$$

$$\times \sum_{\ell' m'} Y_{\ell' m'}(\Omega)\ \frac{1}{r}\int_0^\infty dk'\ A_{\ell' m'}(k')\ J_{\ell'}(k'r)\ e^{\frac{-ik'^2\tau}{2}}$$

$$= \frac{\mu}{\hbar} \int_0^\infty d\tau \int_0^R dr \sum_{\ell m} \int_0^\infty dk \int_0^\infty dk' \; A^*_{\ell m}(k) \; A_{\ell m}(k') \; J_\ell(kr) \; J_\ell(k'r) \; e^{\frac{i(k^2-k'^2)\tau}{2}} ,$$

i.e.

$$T_{fr}(R) = \frac{\mu}{\hbar} \int_0^R dr \sum_{\ell m} \int_0^\infty dk \int_0^\infty dk' \; A^*_{\ell m}(k) \; A_{\ell m}(k') \; J_\ell(kr) \; J_\ell(k'r) \; \frac{2i}{k^2 - k'^2 + 2i\varepsilon} . \tag{4.32}$$

As in the calculation of time delay, we may evaluate the integral over k' by expressing $A_{\ell m}(k')$ as a transform of the initial packet, and making use of the Green's function integral. The procedure is a little more complicated in the present case, however, since the initial packet is now within the region of the observer's sphere, and the range of the radial integral in the transform lies within the range of the radial integral in Eq.(32). Thus from Eq.(31),

$$\int_0^\infty dk' \; A_{\ell m}(k') \; J_\ell(k'r) \; \frac{2i}{k^2 - k'^2 + 2i\varepsilon}$$

$$= -2i \int_0^a dr' \; \Phi_{\ell m}(r') \; \frac{2}{\pi} \int_0^\infty dk' \; \frac{J_\ell(k'r) \; J_\ell(k'r')}{k'^2 - (k + i\varepsilon)^2} , \tag{4.33}$$

where $0 \leqslant r \leqslant R$. Using Eq.(A.6) we have

$$\int_0^\infty dk' \; A_{\ell m}(k') \; J_\ell(k'r) \; \frac{2i}{k^2 - k'^2 + 2i\varepsilon}$$

$$= \frac{-2i}{k} O_\ell(kr) \int_0^r dr' \; \Phi_{\ell m}(r') \; J_\ell(kr') \quad - \frac{2i}{k} J_\ell(kr) \int_r^a dr' \; \Phi_{\ell m}(r') \; O_\ell(kr') \quad . \tag{4.34}$$

Now let us consider the radial integral which arises when Eq.(34) is inserted into Eq.(32) :

$$\mathcal{R}_{fr} \equiv \int_0^R dr\, J_\ell(kr) \left(\frac{-2i}{k} \right) \left\{ O_\ell(kr) \int_0^r dr'\, \Phi_{\ell m}(r')\, J_\ell(kr') + J_\ell(kr) \int_r^a dr'\, \Phi_{\ell m}(r')\, O_\ell(kr') \right\} . \tag{4.35}$$

Since $\Phi_{\ell m}(r)$ is zero for $r > a$, we may alter the integral over r' in the second term within curly brackets to $\int_r^R dr' \ldots$. Then the r and r' integrals may be interchanged in each term (cf Fig.2) to obtain

$$\mathcal{R}_{fr} = \frac{-2i}{k} \left\{ \int_0^R dr'\, \Phi_{\ell m}(r')\, J_\ell(kr') \int_{r'}^R dr\, J_\ell(kr)\, O_\ell(kr) + \int_0^R dr'\, \Phi_{\ell m}(r')\, O_\ell(kr') \int_0^{r'} dr\, J_\ell(kr)\, J_\ell(kr) \right\} . \tag{4.36}$$

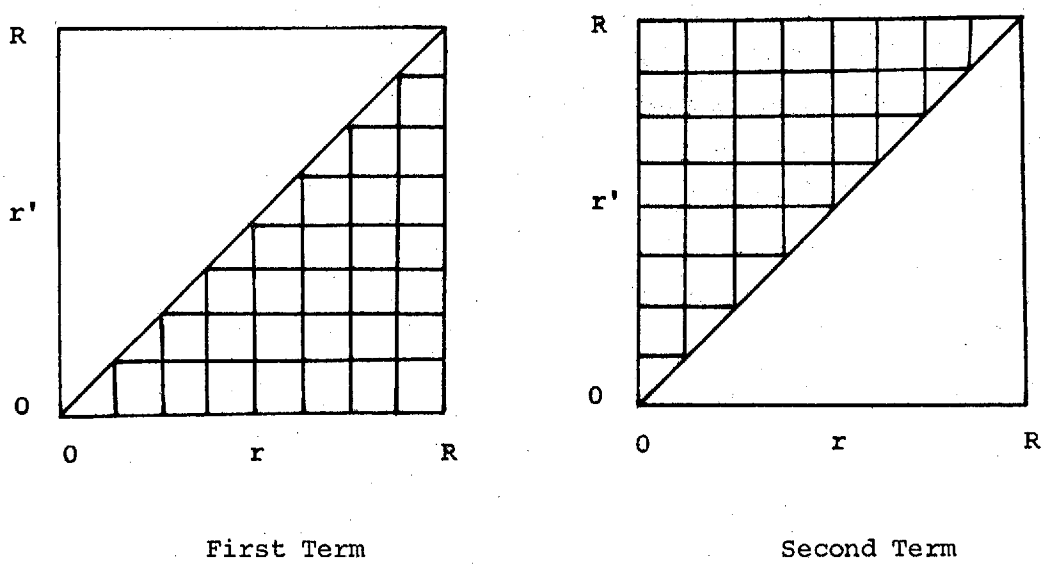

Fig.4.2 Ranges of Integration for Terms in Eq.(35)

The integrals over r in Eq.(36) are of the type evaluated in Appendix B:

$$\int_{r'}^{R} dr\, J_\ell(kr)\, O_\ell(kr) = \frac{-1}{2k}\left\{ W\left[J_\ell, \frac{\partial}{\partial k} O_\ell\right]_R - W\left[J_\ell, \frac{\partial}{\partial k} O_\ell\right]_{r'} \right\} , \quad (4.37)$$

$$\int_{0}^{r'} dr\, J_\ell(kr)\, J_\ell(kr) = \frac{-1}{2k}\, W\left[J_\ell, \frac{\partial}{\partial k} J_\ell\right]_{r'} , \quad (4.38)$$

where the Wronskian at the lower limit in Eq.(38) vanishes. On inserting (37) and (38) into Eq.(36), we have

$$\mathcal{R}_{fr} = \frac{i}{k^2} \int_0^R dr'\, \Phi_{\ell m}(r')\, J_\ell(kr')\; W\left[J_\ell, \frac{\partial}{\partial k} O_\ell\right]_R$$

$$+ \frac{i}{k^2} \int_0^R dr'\, \Phi_{\ell m}(r') \left\{ O_\ell(kr')\, W\left[J_\ell, \frac{\partial}{\partial k} J_\ell\right]_{r'} - J_\ell(kr')\, W\left[J_\ell, \frac{\partial}{\partial k} O_\ell\right]_{r'} \right\} .$$

(4.39)

In order to evaluate the expression within curly brackets in Eq.(39), we shall make use of several identities which follow directly from the definition of the Wronskian:

$$W\left[g(r), h(r)\right] \equiv g \cdot \frac{\partial}{\partial r} h - \frac{\partial}{\partial r} g \cdot h .$$

Thus $$W[g,h] = -W[h,g] , \quad (4.40a)$$

$$f\, W[g,h] - h\, W[g,f] = g\, W[f,h] , \quad (4.40b)$$

and $$\frac{\partial}{\partial k} W\left[g(k,r), h(k,r)\right] = W\left[\frac{\partial g}{\partial k}, h\right] + W\left[g, \frac{\partial h}{\partial k}\right] . \quad (4.40c)$$

Then $\quad O_\ell \, W\left[J_\ell, \frac{\partial}{\partial k} J_\ell\right] \; - \; J_\ell \, W\left[J_\ell, \frac{\partial}{\partial k} O_\ell\right]$

$$= O_\ell \, W\left[J_\ell, \frac{\partial}{\partial k} J_\ell\right] - J_\ell \frac{\partial}{\partial k} W\left[J_\ell, O_\ell\right] + J_\ell \, W\left[\frac{\partial}{\partial k} J_\ell, O_\ell\right]$$

$$= J_\ell \frac{\partial}{\partial k} \frac{1}{2i} W\left[I_\ell, O_\ell\right] + J_\ell \, W\left[\frac{\partial}{\partial k} J_\ell, O_\ell\right] - O_\ell \, W\left[\frac{\partial}{\partial k} J_\ell, J_\ell\right]$$

$$= J_\ell + W\left[J_\ell, O_\ell\right] \frac{\partial}{\partial k} J_\ell$$

$$= J_\ell - k \frac{\partial}{\partial k} J_\ell \quad , \tag{4.41}$$

since $W\left[I_\ell, O_\ell\right] = 2ik$. Using (41) in Eq.(39) we have

$$\mathcal{R}_{fr} = \frac{i}{k^2} \int_0^R dr' \, \Phi_{\ell m}(r') \, J_\ell(kr') \, W\left[J_\ell, \frac{\partial}{\partial k} O_\ell\right]_R$$

$$+ \frac{i}{k^2} \int_0^R dr' \, \Phi_{\ell m}(r') \, J_\ell(kr') - \frac{i}{k} \int_0^R dr' \, \Phi_{\ell m}(r') \frac{\partial}{\partial k} J_\ell(kr') \quad .$$

Finally, the upper limit in each integral may be changed to a, and the integrals written as transforms of the initial packet, to obtain

$$\mathcal{R}_{fr} = \frac{i}{k^2} \tilde{\Phi}_{\ell m}(k,J) \, W\left[J_\ell, \frac{\partial}{\partial k} O_\ell\right]_R + \frac{i}{k^2} \tilde{\Phi}_{\ell m}(k,J) - \frac{i}{k} \frac{d}{dk} \tilde{\Phi}_{\ell m}(k,J) \quad . \tag{4.42}$$

On placing the radial integral (42) into the expression (32) for $T_{fr}(R)$ and writing $A^*_{\ell m}(k)$ as a transform, we find

$$T_{fr}(R) = \frac{2i}{\pi}\frac{\mu}{\hbar}\sum_{\ell m}\int_0^\infty dk\, \tilde{\Phi}^*_{\ell m}(k,J)\left\{\frac{1}{k^2} - \frac{1}{k}\frac{d}{dk}\right\}\tilde{\Phi}_{\ell m}(k,J)$$

$$+ \frac{2i}{\pi}\frac{\mu}{\hbar}\sum_{\ell m}\int_0^\infty dk\, \tilde{\Phi}^*_{\ell m}(k,J)\, \tilde{\Phi}_{\ell m}(k,J)\, \frac{1}{k^2}\, W\Big[J_\ell, \frac{\partial}{\partial k} O_\ell\Big]_R \quad . \tag{4.43}$$

It is interesting to compare Eq.(43) with the expression obtained at the corresponding stage in the time delay calculation, Eq.(3.54). We see that the J_ℓ functions in the Wronskian in Eq.(3.54) appear within the transforms in the second line of Eq.(43), and the functions J_ℓ and O_ℓ have moved from the transforms into the Wronskian. The origin of this interchanging is the Green's function, in which the function O_ℓ is always associated with the larger of the two radii. If the packet is outside the sphere, O_ℓ appears in the transforms, and if the packet is inside the sphere, O_ℓ appears in the Wronskian. In addition to an integral similar to (3.54), Eq.(43) contains a new term which does not involve a Wronskian, and is in fact independent of the radius R.

Following the method of the time delay calculation, we shall prove that the expression for the occupation time T_{fr} is real by calculating the imaginary part of Eq.(43) explicitly. In taking the complex conjugate of the first line, we momentarily revert from the transform notation to the coefficients $A_{\ell m}(k)$, i.e.

$$\tilde{\Phi}_{\ell m}(k,J) = \frac{\pi}{2} A_{\ell m}(k) \quad ,$$

$$\tilde{\Phi}^*_{\ell m}(k,J) = \frac{\pi}{2} A^*_{\ell m}(k) \quad .$$

Then the complex conjugate of the first line in Eq.(43) contains the integral

$$\int_0^\infty dk\ A_{\ell m}(k) \left\{\frac{1}{k^2} - \frac{1}{k}\frac{d}{dk}\right\} A^*_{\ell m}(k)$$

$$= \int_0^\infty dk\ A_{\ell m}(k)\ \frac{1}{k^2}\ A^*_{\ell m}(k) + A_{\ell m}(k)\left(\frac{-1}{k}\right) A^*_{\ell m}(k)\Big|_0^\infty - \int_0^\infty dk\ A^*_{\ell m}(k)\ \frac{d}{dk}\left\{\frac{-1}{k}\ A_{\ell m}(k)\right\}$$

$$= \int_0^\infty dk\ A^*_{\ell m}(k)\ \frac{1}{k}\frac{d}{dk}\ A_{\ell m}(k) \quad , \qquad (4.44)$$

where we have used integration by parts to transfer the derivative from $A^*_{\ell m}(k)$ to $A_{\ell m}(k)$. In evaluating the integrated part, we note that the normalisation of the packet, Eq.(1.9), requires that the integral $\int_0^\infty dk\ A^*_{\ell m}(k)\ A_{\ell m}(k)$ converge. The integrated part therefore certainly vanishes at the upper limit. At the lower limit we have

$$A_{\ell m}(k) = \frac{2}{\pi}\int_0^a dr\ \Phi_{\ell m}(r)\ J_\ell(kr) \quad ,$$

but $$J_\ell(kr) \sim \frac{(kr)^{\ell+1}}{(2\ell+1)\,!!} \qquad \text{as} \quad k \to 0 \quad ,$$

so $$A_{\ell m}(k) = \mathcal{O}\,(k^{\ell+1}) \qquad \text{as} \quad k \to 0 \quad ,$$

and the integrated part again vanishes.

The imaginary part of the complete expression (43) is

$$\mathrm{Im}\ T_{fr}(R) = \frac{1}{\pi}\frac{\mu}{\hbar}\sum_{\ell m}\int_0^\infty dk\ \tilde{\Phi}^*_{\ell m}(k,J)\tilde{\Phi}_{\ell m}(k,J)\ \frac{1}{k^2}\left\{W\left[J_\ell,\frac{\partial}{\partial k}\ O_\ell\right]_R + W\left[J_\ell,\frac{\partial}{\partial k}\ I_\ell\right]_R + 1\right\} \ .$$

$$(4.45)$$

Using the relation

$$W\left[\frac{\partial I_\ell}{\partial k}, O_\ell\right] + W\left[I_\ell, \frac{\partial}{\partial k} O_\ell\right] = 2i \quad , \tag{4.46}$$

we have

$$W\left[J_\ell, \frac{\partial}{\partial k} O_\ell\right]_R + W\left[J_\ell, \frac{\partial}{\partial k} I_\ell\right]_R + 1 = \frac{1}{2i}\left\{W\left[O_\ell, \frac{\partial}{\partial k} O_\ell\right]_R - W\left[I_\ell, \frac{\partial}{\partial k} I_\ell\right]_R\right\} \quad . \tag{4.47}$$

By Eqs (3.57) and (3.58),

$$I_\ell(kr) = (-)^\ell \, O_\ell(-kr) \quad ,$$

$$J_\ell(kr) = (-)^{\ell+1} J_\ell(-kr) \quad ,$$

so the contribution from the second Wronskian in Eq.(47) may be converted to an integral along the negative real axis:

$$\int_0^\infty dk \; \tilde{\Phi}^*_{\ell m}(k,J) \; \tilde{\Phi}_{\ell m}(k,J) \; \frac{1}{k^2} \; W\left[I_\ell, \frac{\partial}{\partial k} I_\ell\right]_R$$

$$= - \int_{-\infty}^0 dk \; \tilde{\Phi}^*_{\ell m}(k,J) \; \tilde{\Phi}_{\ell m}(k,J) \; \frac{1}{k^2} \; W\left[O_\ell, \frac{\partial}{\partial k} O_\ell\right]_R \quad .$$

Then the integral in Eq.(45) is

$$\oint_{fr} \equiv \frac{1}{2i} \int_{-\infty}^{\infty} dk \; \tilde{\Phi}^*_{\ell m}(k,J) \; \tilde{\Phi}_{\ell m}(k,J) \; \frac{1}{k^2} \; W\left[O_\ell, \frac{\partial}{\partial k} O_\ell\right]_R \quad , \tag{4.48}$$

which we shall evaluate by contour integration.

Now

$$\tilde{\Phi}_{\ell m}(k,J) \;=\; \int_{o}^{a} dr\ \Phi_{\ell m}(r)\ J_{\ell}(kr)$$

and $$J_{\ell}(kr) \underset{|k|\to\infty}{\sim} \frac{1}{2i}\left(i^{-\ell}\, e^{ikr} \;-\; i^{\ell}\, e^{-ikr}\right)$$

so for Im $k > o$, $\tilde{\Phi}_{\ell m}(k,J) = \mathcal{O}(e^{-ika})$ as $|k| \to \infty$.

We know that $$O_{\ell}(kr) \underset{|k|\to\infty}{\sim} i^{-\ell}\, e^{ikr}$$

so $$W\left[O_{\ell},\, \frac{\partial}{\partial k} O_{\ell}\right]_R \underset{|k|\to\infty}{\sim} (-)^{\ell}\, i\, e^{2ikR} \quad .$$

Thus the contour for the integral (48) may be completed by a semicircle of infinite radius in the upper half plane, Fig.3, where for $|k|$ sufficiently large the integrand behaves as $\frac{1}{k^2}\, e^{2ik(R-a)}$ with $R > a$.

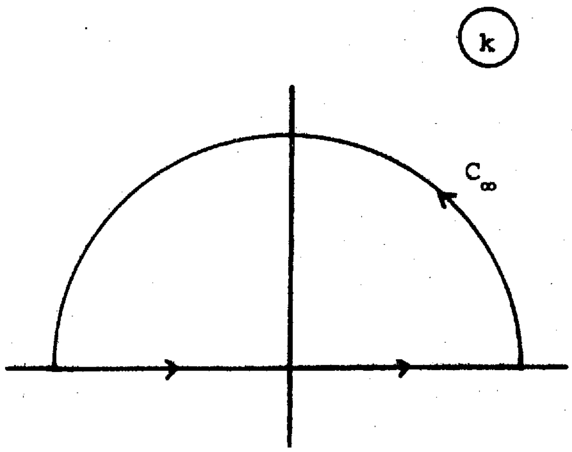

Fig.4.3 Contour for the Evaluation of Im $T_{fr}(R)$

The integrand has no poles, and the integral around C_∞ vanishes, so

$$\int_{-\infty}^{\infty} dk\ \tilde{\Phi}^{*}_{\ell m}(k,J)\ \tilde{\Phi}_{\ell m}(k,J)\ \frac{1}{k^2}\ W\left[O_\ell,\ \frac{\partial}{\partial k}\ O_\ell\right]_R \quad = \quad 0 \quad , \tag{4.49}$$

and the imaginary part of $T_{fr}(R)$ is zero.

Returning to Eq.(43) we may now take the real part of this expression to obtain the final form for $T_{fr}(R)$. We note that

$$W\left[J_\ell,\ \frac{\partial}{\partial k}\ O_\ell\right]_R \ - \ W\left[J_\ell,\ \frac{\partial}{\partial k}\ I_\ell\right]_R \ = \ 2i\ W\left[J_\ell,\ \frac{\partial}{\partial k}\ J_\ell\right]_R \quad .$$

Then writing the J transforms in terms of the coefficients $A_{\ell m}$ we find

$$T_{fr}(R) \ = \ \frac{\pi}{4} \sum_{\ell m} \int_0^{\infty} dk \left\{ A_{\ell m}(k)\ \frac{\mu}{\hbar k}\ i\ \frac{d}{dk}\ A^{*}_{\ell m}(k) \ - \ A^{*}_{\ell m}(k)\ \frac{\mu}{\hbar k}\ i\ \frac{d}{dk}\ A_{\ell m}(k) \right\}$$

$$+ \ \pi \sum_{\ell m} \int_0^{\infty} dk\ A^{*}_{\ell m}(k)\ A_{\ell m}(k)\ \frac{\mu}{\hbar k} \left(\frac{-1}{2k}\right) \ W\left[J_\ell,\ \frac{\partial}{\partial k}\ J_\ell\right]_R \quad . \tag{4.50}$$

4c. Calculation of $T_{int}(R)$

In the derivation of the expression corresponding to Eq.(50) for the interacting packet, we shall find that the function $f_\ell(-k,r)$ appears, and this will always be written with a factor $(-)^\ell$ beside it. Although this makes the mathematics appear a little more cumbersome, it has the effect of preserving the parallel with the calculation of the previous section, since $(-)^\ell\ f_\ell(-k,r)$ corresponds to the $O_\ell(kr)$ appearing there.

From the definition (24) and the expression (28) for the wave function with the potential present,

$$T_{int}(R) \equiv \int_0^\infty dt \int_{V_R} d\underset{\sim}{r}\, \Psi^*(\underset{\sim}{r},t)\, \Psi(\underset{\sim}{r},t)$$

$$= \frac{\mu}{\hbar} \int_0^\infty d\tau \int_0^R dr \sum_{\ell m} \int_0^\infty dk \int_0^\infty dk'\, B^*_{\ell m}(k) B_{\ell m}(k')\, \chi^*_\ell(k,r)\chi_\ell(k',r)\, e^{\frac{i(k^2-k'^2)\tau}{2}}$$

$$= \frac{\mu}{\hbar} \int_0^R dr \sum_{\ell m} \int_0^\infty dk \int_0^\infty dk'\, B^*_{\ell m}(k)\, B_{\ell m}(k')\, \chi^*_\ell(k,r)\, \chi_\ell(k',r)\, \frac{2i}{k^2 - k'^2 + 2i\varepsilon} \quad . \tag{4.51}$$

The integral over k' is (Eqs (29) and (A.7))

$$\int_0^\infty dk'\, B_{\ell m}(k')\, \chi_\ell(k',r)\, \frac{2i}{k^2 - k'^2 + 2i\varepsilon}$$

$$= -2i \int_0^a dr'\, \Phi_{\ell m}(r')\, \frac{2}{\pi} \int_0^\infty dk'\, \frac{\chi_\ell(k',r)\, \chi^*_\ell(k',r')}{k'^2 - (k + i\varepsilon)^2}$$

$$= \frac{-2i}{k} (-)^\ell f_\ell(-k,r) \int_0^r dr'\, \Phi_{\ell m}(r')\, \chi_\ell(k,r') + 2i \sum_n \frac{\chi_\ell^{(n)}(r)}{k_n^2 - k^2} \int_0^r dr'\, \Phi_{\ell m}(r')\, \chi_\ell^{(n)}(r')$$

$$\frac{-2i}{k} \chi_\ell(k,r) \int_r^a dr'\, \Phi_{\ell m}(r')\, (-)^\ell f_\ell(-k,r') + 2i \sum_n \frac{\chi_\ell^{(n)}(r)}{k_n^2 - k^2} \int_r^a dr'\, \Phi_{\ell m}(r')\, \chi_\ell^{(n)}(r')$$

$$= -\frac{2i}{k} (-)^\ell f_\ell(-k,r) \int_0^r dr'\, \Phi_{\ell m}(r')\, \chi_\ell(k,r') \quad \frac{-2i}{k} \chi_\ell(k,r) \int_r^a dr'\, \Phi_{\ell m}(r') (-)^\ell f_\ell(-k,r')$$

$$+ 2i \sum_n \frac{\chi_\ell^{(n)}(r)}{k_n^2 - k^2} \int_0^a dr'\, \Phi_{\ell m}(r')\, \chi_\ell^{(n)}(r') \quad , \tag{4.52}$$

where the sum is over all bound states. The integral in the third term of Eq.(52) is just the overlap between the initial packet and a bound state, and by the assumption that the packet is orthogonal to all bound states, it vanishes for each n:

$$\int_0^a dr' \; \Phi_{\ell m}(r') \; \chi_\ell^{(n)}(r') \;=\; 0 \qquad . \tag{4.53}$$

The radial integral obtained by inserting (52) into Eq.(51) may be calculated in a similar way to the integral (35). Corresponding to Eq.(39) we have

$$\mathcal{R}_{\text{int}} = \frac{i}{k^2}\int_0^R dr' \; \Phi_{\ell m}(r') \; \chi_\ell(k,r') \;\; W\Big[\chi_\ell^*, \frac{\partial}{\partial k} \; (-)^\ell \; f_\ell(-k,r)\Big]_R$$

$$+ \frac{i}{k^2}\int_0^R dr' \; \Phi_{\ell m}(r')\Big\{(-)^\ell f_\ell(-k,r') \; W\Big[\chi_\ell^*, \frac{\partial}{\partial k} \; \chi_\ell\Big]_{r'}$$

$$- \chi_\ell(k,r') \; W\Big[\chi_\ell^*, \frac{\partial}{\partial k} \; (-)^\ell f_\ell(-k,r)\Big]_{r'}\Big\} \qquad . \tag{4.54}$$

The expression within curly brackets in Eq.(54) is evaluated by using the Wronskian identities (40) and the following expressions for the scattering states:

$$\chi_\ell(k,r) \;=\; \frac{-1}{2i}\Big[f_\ell(k,r) - S_\ell(k) \;\; (-)^\ell \; f_\ell(-k,r)\Big] \qquad , \tag{4.55a}$$

$$\chi_\ell^*(k,r) \;=\; \frac{1}{2i}\Big[(-)^\ell \; f_\ell(-k,r) - S_\ell^*(k) \; f_\ell(k,r)\Big] \quad , \; k \text{ real} \; , \tag{4.55b}$$

$$\chi_\ell^*(k,r) \;=\; S_\ell^*(k) \;\; \chi_\ell(k,r) \qquad , \; k \text{ real} \; , \tag{4.55c}$$

and

$$W\Big[\, f_\ell(k,r) \;,\; (-)^\ell \; f_\ell(-k,r)\,\Big] \;=\; 2ik \qquad . \tag{4.55d}$$

Then $(-)^{\ell} f_{\ell}(-k,r)\, W\left[\chi_{\ell}^{*}, \frac{\partial}{\partial k}\chi_{\ell}\right] - \chi_{\ell}\, W\left[\chi_{\ell}^{*}, \frac{\partial}{\partial k}(-)^{\ell} f_{\ell}(-k,r)\right]$

$$= S_{\ell}^{*}\left\{(-)^{\ell} f_{\ell}(-k,r)\, W\left[\chi_{\ell}, \frac{\partial}{\partial k}\chi_{\ell}\right] - \chi_{\ell}\, W\left[\chi_{\ell}, \frac{\partial}{\partial k}(-)^{\ell} f_{\ell}(-k,r)\right]\right\}$$

$$= S_{\ell}^{*}\left\{\chi_{\ell} + W\left[\chi_{\ell}, (-)^{\ell} f_{\ell}(-k,r)\right]\frac{\partial}{\partial k}\chi_{\ell}\right\}$$

or

$$(-)^{\ell} f_{\ell}(-k,r)\, W\left[\chi_{\ell}^{*}, \frac{\partial}{\partial k}\chi_{\ell}\right] - \chi_{\ell}\, W\left[\chi_{\ell}^{*}, \frac{\partial}{\partial k}(-)^{\ell} f_{\ell}(-k,r)\right] = \chi_{\ell}^{*} - S_{\ell}^{*}\, k\,\frac{\partial}{\partial k}\chi_{\ell} \quad . \tag{4.56}$$

The intermediate steps in the calculation are similar to those used to derive Eq.(41). Using (56) in Eq.(54), and writing the integrals over r' as transforms of the initial packet, we obtain

$$\mathcal{R}_{int} = \frac{i}{k^2}\tilde{\Phi}_{\ell m}(k,\chi)\, W\left[\chi_{\ell}^{*}, \frac{\partial}{\partial k}(-)^{\ell} f_{\ell}(-k,r)\right]_R + \frac{i}{k^2}\tilde{\Phi}_{\ell m}(k,\chi^{*}) - S_{\ell}^{*}\frac{i}{k}\frac{d}{dk}\tilde{\Phi}_{\ell m}(k,\chi) \tag{4.57}$$

which corresponds to the expression (42) in the calculation of T_{fr}.

Inserting the radial integral (57) into Eq.(51), and using Eq.(29) to express $B_{\ell m}^{*}(k)$ as a transform, we obtain for the occupation time

$$T_{int}(R) = \frac{2i}{\pi}\frac{\mu}{\hbar}\sum_{\ell m}\int_0^{\infty} dk\, \tilde{\Phi}_{\ell m}^{*}(k,\chi^{*})\left\{\frac{1}{k^2} - \frac{1}{k}\frac{d}{dk}\right\}\tilde{\Phi}_{\ell m}(k,\chi) + \frac{2i}{\pi}\frac{\mu}{\hbar}\sum_{\ell m}\int_0^{\infty} dk\, \tilde{\Phi}_{\ell m}^{*}(k,\chi^{*})\,\tilde{\Phi}_{\ell m}(k,\chi)\,\frac{1}{k^2}\, W\left[\chi_{\ell}, \frac{\partial}{\partial k} O_{\ell}\right]_R \quad . \tag{4.58}$$

In writing Eq.(58) we have used Eq.(55c) to transfer a factor S_{ℓ}^{*} between transforms, and from the Wronskian to a transform, e.g.

$$\tilde{\Phi}^{*}_{\ell m}(k,\chi)\ \tilde{\Phi}_{\ell m}(k,\chi^{*}) \;=\; \tilde{\Phi}^{*}_{\ell m}(k,\chi^{*})\ \tilde{\Phi}_{\ell m}(k,\chi) \quad . \tag{4.59}$$

We shall now examine the imaginary part of Eq.(58). Taking the complex conjugate of the first line gives the integral

$$\int_{0}^{\infty} dk\ \tilde{\Phi}_{\ell m}(k,\chi)\left\{\frac{1}{k^{2}} - \frac{1}{k}\frac{d}{dk}\right\}\tilde{\Phi}^{*}_{\ell m}(k,\chi^{*})$$

$$= \int_{0}^{\infty} dk\ \tilde{\Phi}_{\ell m}(k,\chi)\ \frac{1}{k^{2}}\ \tilde{\Phi}^{*}_{\ell m}(k,\chi^{*}) \;+\; \tilde{\Phi}_{\ell m}(k,\chi)\left(\frac{-1}{k}\right)\tilde{\Phi}^{*}_{\ell m}(k,\chi^{*})\Big|_{0}^{\infty}$$

$$- \int_{0}^{\infty} dk\ \tilde{\Phi}^{*}_{\ell m}(k,\chi^{*})\ \frac{d}{dk}\left\{\frac{-1}{k}\ \tilde{\Phi}_{\ell m}(k,\chi)\right\}$$

$$= \int_{0}^{\infty} dk\ \tilde{\Phi}^{*}_{\ell m}(k,\chi^{*})\ \frac{1}{k}\ \frac{d}{dk}\ \tilde{\Phi}_{\ell m}(k,\chi) \quad , \tag{4.60}$$

where we have used integration by parts, as was done in Eq.(44) for the free packet. The evaluation of the integrated part follows the argument given below Eq.(44) if we note that (cf Eqs (29) and (59))

$$\tilde{\Phi}_{\ell m}(k,\chi)\left(\frac{-1}{k}\right)\tilde{\Phi}^{*}_{\ell m}(k,\chi^{*}) \;=\; B_{\ell m}(k)\left(\frac{-1}{k}\right)B^{*}_{\ell m}(k) \quad . \tag{4.61}$$

The normalisation of the wave function (28) for the interacting packet is

$$\frac{\pi}{2}\sum_{\ell m}\int_{0}^{\infty} dk\ B^{*}_{\ell m}(k)\ B_{\ell m}(k) \;=\; 1 \quad , \tag{4.62}$$

so the integrated part (61) vanishes at the upper limit. At the lower limit,

$$B_{\ell m}(k) = \frac{2}{\pi}\int_0^a dr\ \Phi_{\ell m}(r)\ \chi_\ell^*(k,r)$$

and $\chi_\ell(k,r) = \mathcal{O}(k^{\ell+1}) \qquad \text{as} \quad k \to o ,$

so $B_{\ell m}(k) = \mathcal{O}(k^{\ell+1}) \qquad \text{as} \quad k \to o ,$

and the integrated part again vanishes.

From Eqs (58) and (60),

$$\text{Im}\ T_{\text{int}}(R) = \frac{1}{\pi}\frac{\mu}{\hbar}\sum_{\ell m}\int_0^\infty dk\ \tilde{\Phi}^*_{\ell m}(k,\chi^*)\ \tilde{\Phi}_{\ell m}(k,\chi)$$

$$\times\ \frac{1}{k^2}\left\{W\left[\chi_\ell,\ \frac{\partial}{\partial k}O_\ell\right]_R + W\left[\chi_\ell^*,\ \frac{\partial}{\partial k}I_\ell\right]_R + 1\right\} .$$

(4.63)

The Wronskian expression may be evaluated by using Eq.(46) and the relations (55) for the scattering states, with $f_\ell(k,r) = I_\ell(kr)$ for $r \geqslant a$:

$$W\left[\chi_\ell,\ \frac{\partial}{\partial k}O_\ell\right]_R + W\left[\chi_\ell^*,\ \frac{\partial}{\partial k}I_\ell\right]_R + 1$$

$$= \frac{1}{2i}\left\{S_\ell\ W\left[O_\ell,\ \frac{\partial}{\partial k}O_\ell\right]_R - S_\ell^*\ W\left[I_\ell,\ \frac{\partial}{\partial k}I_\ell\right]_R\right\} .$$

(4.64)

The contribution to the integral in Eq.(63) from the second term on the RHS of Eq.(64) may be converted into an integral along the negative real axis:

$$\int_0^\infty dk\ \tilde{\Phi}^*_{\ell m}(k,\chi^*)\ \tilde{\Phi}_{\ell m}(k,\chi)\ \frac{1}{k^2}\ S^*_\ell\ W\left[I_\ell,\ \frac{\partial}{\partial k}\ I_\ell\right]_R$$

$$= -\int_{-\infty}^0 dk\ \tilde{\Phi}^*_{\ell m}(k,\chi)\ \tilde{\Phi}_{\ell m}(k,\chi)\ \frac{1}{k^2}\ W\left[O_\ell,\ \frac{\partial}{\partial k}\ O_\ell\right]_R \tag{4.65}$$

where we have used Eq.(55c) and the relation

$$\chi^*_\ell(k,r) \quad = \quad (-)^{\ell+1}\ \chi_\ell(-k,r) \quad , \quad k\ \text{real} \quad . \tag{4.66}$$

Then the integral appearing in Eq.(63) is

$$\mathcal{J}_{\text{int}} \equiv \frac{1}{2i}\int_{-\infty}^\infty dk\ \tilde{\Phi}^*_{\ell m}(k,\chi)\ \tilde{\Phi}_{\ell m}(k,\chi)\ \frac{1}{k^2}\ W\left[O_\ell,\ \frac{\partial}{\partial k}\ O_\ell\right]_R \quad . \tag{4.67}$$

Now $\quad \tilde{\Phi}_{\ell m}(k,\chi) \quad = \quad \int_0^a dr\ \Phi_{\ell m}(r)\ \chi_\ell(k,r)$

and $\quad \chi_\ell(k,r) \quad = \quad \dfrac{k^{\ell+1}}{f_\ell(-k)}\ \phi_\ell(k,r)$

where $\phi_\ell(k,r)$ is the regular solution of the radial wave equation defined in Chapter 1, and $f_\ell(-k)$ the Jost function. By Eq.(4.16) of Newton 1960 we have

$$\lim_{|k|\to\infty} \quad f_\ell(-k) \quad = \quad 1 \quad , \quad \text{Im}\ k \geqslant 0$$

and by Eq.(3.13) of the same reference

$$\phi_\ell(k,r) = \frac{1}{k^{\ell+1}} \sin\left(kr - \frac{\ell\pi}{2}\right) + o\left(\frac{1}{|k|^{\ell+1}} e^{|\nu| r}\right) \quad \text{as } |k| \to \infty ,$$

where $\nu \equiv \text{Im } k$. Combining these results we see that

$$\tilde{\Phi}_{\ell m}(k,\chi) = \mathcal{O}(e^{-ika}) \quad \text{as } |k| \to \infty , \quad \text{Im } k > 0 .$$

The asymptotic behaviour of the Wronskian was given in the previous section:

$$W\left[O_\ell, \frac{\partial}{\partial k} O_\ell\right]_R \underset{|k| \to \infty}{\sim} (-)^\ell \, i \, e^{2ikR} .$$

Thus the integral (67) may be evaluated by completing the contour around an infinite semicircle in the upper half plane, Fig.3, where for $|k|$ sufficiently large the integrand behaves as $\frac{1}{k^2} e^{2ik(R-a)}$ with $R > a$.

The integral around C_∞ vanishes, but the integrand now has poles in the upper half plane, since the transform $\tilde{\Phi}_{\ell m}(k,\chi)$ contains the scattering matrix $S_\ell(k)$, with bound state poles at $k = -i\gamma_n$, $\gamma_n < 0$. It can be seen from Eq.(55a) that the residue at a bound state pole k_n contains the factor $\int_0^a dr\, \Phi_{\ell m}(r)\, f_\ell(-k_n,r)$. By Eq.(14) of Appendix A this integral is proportional to $\int_0^a dr\, \Phi_{\ell m}(r)\, \chi_\ell^{(n)}(r)$, where $\chi_\ell^{(n)}(r)$ is the bound state wave function. As the initial packet is orthogonal to all bound states, the integral vanishes, and the residue of the integrand (67) at each bound state pole is zero. Then

$$\int_{-\infty}^{\infty} dk\, \tilde{\Phi}^*_{\ell m}(k,\chi)\, \tilde{\Phi}_{\ell m}(k,\chi)\, \frac{1}{k^2}\, W\left[O_\ell, \frac{\partial}{\partial k} O_\ell\right]_R = 0 ,$$

and the imaginary part of the occupation time (58) is zero.

We may now take the real part of Eq.(58) and obtain an expression for $T_{int}(R)$ in terms of the coefficients $B_{\ell m}(k)$. From Eqs (29) and (55c),

$$\tilde{\Phi}^{*}_{\ell m}(k,\chi^{*})\ \frac{1}{k}\ \frac{d}{dk}\ \tilde{\Phi}_{\ell m}(k,\chi)$$

$$= \frac{\pi^2}{4}\ S^{*}_{\ell}\ B^{*}_{\ell m}(k)\ \frac{1}{k}\ \frac{d}{dk}\left\{ S_{\ell}\ B_{\ell m}(k) \right\}$$

$$= \frac{\pi^2}{4}\left\{B^{*}_{\ell m}(k)\ B_{\ell m}(k)\ S^{*}_{\ell}\ \frac{1}{k}\ \frac{d}{dk}\ S_{\ell} \quad + \quad B^{*}_{\ell m}(k)\ \frac{1}{k}\ \frac{d}{dk}\ B_{\ell m}(k)\right\} \tag{4.68}$$

where we have used $S^{*}_{\ell}(k)\ S_{\ell}(k) = 1$, for k real. From Eq.(55b),

$$W\left[\chi_{\ell},\ \frac{\partial}{\partial k}\ O_{\ell}\right]_R \quad - \quad W\left[\chi^{*}_{\ell},\ \frac{\partial}{\partial k}\ I_{\ell}\right]_R$$

$$= 2i\ W\left[\chi_{\ell},\ \frac{\partial}{\partial k}\ \chi^{*}_{\ell}\right]_R + \frac{\partial}{\partial k}\ S^{*}_{\ell}\ \cdot\ W\left[\chi_{\ell},\ I_{\ell}\right]_R + S^{*}_{\ell}\ W\left[\chi_{\ell},\ \frac{\partial}{\partial k}\ I_{\ell}\right]_R$$

$$- S^{*}_{\ell}\ W\left[\chi_{\ell},\ \frac{\partial}{\partial k}\ I_{\ell}\right]_R$$

$$= 2i\ W\left[\chi_{\ell},\ \frac{\partial}{\partial k}\ \chi^{*}_{\ell}\ \right]_R - k\ S_{\ell}\ \frac{\partial}{\partial k}\ S^{*}_{\ell} \quad . \tag{4.69}$$

Using Eqs (68) and (69), and the relation

$$S_{\ell}\ \frac{\partial}{\partial k}\ S^{*}_{\ell} = -S^{*}_{\ell}\ \frac{\partial}{\partial k}\ S_{\ell} \quad , \quad k \text{ real} \quad ,$$

we obtain finally

$$T_{int}(R) = \frac{\pi}{4} \sum_{\ell m} \int_0^\infty dk \left\{ B_{\ell m}(k) \frac{\mu}{\hbar k} i \frac{d}{dk} B^*_{\ell m}(k) - B^*_{\ell m}(k) \frac{\mu}{\hbar k} i \frac{d}{dk} B_{\ell m}(k) \right\}$$

$$- \frac{\pi}{4} \sum_{\ell m} \int_0^\infty dk \, B^*_{\ell m}(k) \, B_{\ell m}(k) \, S^*_\ell(k) \frac{\mu}{\hbar k} i \frac{d}{dk} S_\ell(k)$$

$$+ \pi \sum_{\ell m} \int_0^\infty dk \, B^*_{\ell m}(k) \, B_{\ell m}(k) \frac{\mu}{\hbar k} \left(\frac{-1}{2k} \right) W\left[\chi^*_\ell, \frac{\partial}{\partial k} \chi_\ell \right]_R \quad . \tag{4.70}$$

CHAPTER 5

DISCUSSION OF RESULTS

We have obtained expressions for the occupation times $T_{fr}(R)$ and $T_{int}(R)$ in the cases: (i) when the initial packet is outside the observer's sphere, $T_{int} - T_{fr}$ being the time delay for the interacting wave packet; (ii) when the initial packet is within the region of the potential, $T_{int} - T_{fr}$ being the lifetime of the decaying wave packet. The expressions contain the effects of the packet shape in the coefficients $A_{\ell m}$, $B_{\ell m}$, and the transforms $\tilde{\Phi}_{\ell m}$, and the dependence on the size of the observer's sphere in the Wronskians evaluated at the surface. Our results cannot be compared immediately with those of Ohmura, since his calculation is carried out with the three-dimensional form of the wave function, while we have used partial waves. We can, however, make a comparison with the calculation of time delay for an arbitrary wave packet given by Kilian (1968).

We shall give brief details of Kilian's calculation, since this will help in relating the various expressions to our own results. Kilian uses the $t \to -\infty$ wave function in the form given by Green and Lanford (1960), and discussed in Chapter 2. It will simplify matters if we retain the coefficients $A_{\ell m}$ used in Chapter 2, and note that these are related to Kilian's $\Phi_{m\ell}(k)$ by

$$A_{\ell m}(k) = \left(\frac{2}{\pi}\right)^{\frac{1}{2}} \Phi_{m\ell}(k) \quad . \tag{5.1}$$

Then the wave function for the free packet is (Eq.(2.22))

$$\Phi(\underset{\sim}{r},\tau) = \sum_{\ell m} Y_{\ell m}(\Omega)\ \frac{1}{r}\int_0^\infty dk\ A_{\ell m}(k)\ J_\ell(kr)\ e^{\frac{-ik^2\tau}{2}} , \tag{5.2}$$

and for the interacting packet

$$\Psi(\underset{\sim}{r},\tau) = \sum_{\ell m} Y_{\ell m}(\Omega)\ \frac{1}{r}\int_0^\infty dk\ A_{\ell m}(k)\ \chi_\ell(k,r)\ e^{\frac{-ik^2\tau}{2}} , \tag{5.3}$$

with

$$\lim_{\tau\to-\infty} \int d\underset{\sim}{r} \left| \Psi(\underset{\sim}{r},\tau) - \Phi(\underset{\sim}{r},\tau)\right|^2 = 0 . \tag{5.4}$$

The occupation times are as defined in Chapter 3, but the time integral is now $\int_{-\infty}^{\infty} dt$. Thus

$$T_{fr}(R) \equiv \int_{-\infty}^{\infty} dt \int_{V_R} d\underset{\sim}{r}\ \Phi^*(\underset{\sim}{r},t)\ \Phi(\underset{\sim}{r},t)$$

$$= \frac{\mu}{\hbar}\int_0^R dr \sum_{\ell m}\int_0^\infty dk \int_0^\infty dk'\ A^*_{\ell m}(k)\ A_{\ell m}(k')\ J_\ell(kr)\ J_\ell(k'r) \int_{-\infty}^{\infty} d\tau\ e^{\frac{i(k^2-k'^2)\tau}{2}}$$

$$= 2\pi \sum_{\ell m}\int_0^\infty dk\ A^*_{\ell m}(k)\ A_{\ell m}(k)\ \frac{\mu}{\hbar k}\int_0^R dr\ J_\ell(kr)\ J_\ell(kr)$$

i.e.

$$T_{fr}(R) = 2\pi \sum_{\ell m}\int_0^\infty dk\ A^*_{\ell m}(k)\ A_{\ell m}(k)\ \frac{\mu}{\hbar k}\left(\frac{-1}{2k}\right) W\left[J_\ell, \frac{\partial}{\partial k} J_\ell\right]_R , \tag{5.5}$$

where we have used

$$\int_{-\infty}^{\infty} d\tau\ e^{\frac{i(k^2 - k'^2)\tau}{2}} = \frac{2\pi}{k}\ \delta(k - k') . \tag{5.6}$$

Similarly,

$$T_{int}(R) \quad = \quad 2\pi \sum_{\ell m} \int_0^\infty dk \; A^*_{\ell m}(k) \; A_{\ell m}(k) \; \frac{\mu}{\hbar k} \left(\frac{-1}{2k}\right) W\left[\chi^*_\ell, \frac{\partial}{\partial k} \chi_\ell\right]_R \quad . \qquad (5.7)$$

Kilian uses the asymptotic forms of the Wronskians in Eqs (5) and (7):

$$-\frac{1}{2k} W\left[J_\ell, \frac{\partial}{\partial k} J_\ell\right]_R \quad \underset{R \to \infty}{\sim} \quad \frac{1}{2}\left\{R + \frac{(-)^{\ell+1}}{2k} \sin 2kR\right\} \quad , \qquad (5.8)$$

$$-\frac{1}{2k} W\left[\chi^*_\ell, \frac{\partial}{\partial k} \chi_\ell\right]_R \quad \underset{R \to \infty}{\sim} \quad \frac{1}{2}\left\{R + \frac{d\delta_\ell}{dk} + \frac{(-)^{\ell+1}}{2k} \sin\,(2kR + 2\delta_\ell)\right\} , \qquad (5.9)$$

to obtain

$$Q \quad = \quad \lim_{R \to \infty} \left[T_{int}(R) - T_{fr}(R)\right]$$

$$= \quad \pi \sum_{\ell m} \int_0^\infty dk \; A^*_{\ell m}(k) \; A_{\ell m}(k) \; \frac{\mu}{\hbar k} \frac{d\delta_\ell}{dk} \quad . \qquad (5.10)$$

Eq.(10) corresponds to Eq.(6.5) of Kilian 1968, and is a simple wave packet average of the time delay $\frac{\mu}{\hbar k} \frac{d\delta_\ell}{dk}$ obtained by Eisenbud and Smith. Expressions similar to Eq.(10), but restricted to the case of spherical wave packets, have been derived by Goldberger and Watson (1964, Chap.8) and Nussenzveig (1969).

When the Wronskians (8) and (9) are placed within the wave packet integrals, and the limit $R \to \infty$ taken, the oscillatory terms $\sin 2kR$ and $\sin\,(2kR + 2\delta_\ell)$ vanish by the Riemann - Lebesgue lemma.

Such terms also occur in Smith's calculation of time delay, and there they are removed by applying the averaging procedure

$$\langle Q \rangle \quad = \quad \lim_{R \to \infty} \frac{1}{R} \int_{R}^{2R} Q(R')\, dR' \quad . \qquad (5.11)$$

The limit $R \to \infty$ may, of course, be used quite freely in calculations involving the $t \to -\infty$ wave function, since the centre of the initial packet is at infinity, and the packet is not localised in any region. In Smith's treatment the particles are described by plane waves, so the expressions obtained cannot depend on the position of the particles in any way. In our calculation, however, the initial packet is localised outside the observer's sphere, at a finite distance from the scatterer, and we are not at liberty to make R infinite. We shall therefore consider the expressions arising in Kilian's calculation for finite R in making comparison with our own.

In the $t \to -\infty$ wave function, the free and interacting packets contain the same coefficients $A_{\ell m}$, and this leads to the simple expression (10) for the time delay. The wave functions $\Phi(\underset{\sim}{r},\tau)$ and $\Psi(\underset{\sim}{r},\tau)$ in the present calculation contain different coefficients $A_{\ell m}$ and $B_{\ell m}$, and it does not seem possible to obtain a simple expression for the time delay (or lifetime) by actually subtracting T_{fr} from T_{int}. When the packet is outside the region of the potential, the coefficient $B_{\ell m}$ can be expressed in terms of $A_{\ell m}$ as follows:

$$B_{\ell m}(k) \quad = \quad \frac{2}{\pi}\, \tilde{\Phi}_{\ell m}(k,\chi^{*}) \qquad ,$$

$$\chi^{*}_{\ell}(k,r) \underset{r \geqslant a}{=} J_{\ell}(kr) \; - \; \frac{1}{2i}\left[S^{*}_{\ell}(k) \; - \; 1\right] I_{\ell}(kr) \qquad , \qquad (5.12)$$

$$\therefore \quad B_{\ell m}(k) = \frac{2}{\pi}\,\tilde{\Phi}_{\ell m}(k,J) - \frac{1}{\pi i}\left[S_\ell^*(k) - 1\right]\,\tilde{\Phi}_{\ell m}(k,I)$$

$$= A_{\ell m}(k) - \frac{1}{\pi i}\left[S_\ell^*(k) - 1\right]\,\tilde{\Phi}_{\ell m}(k,I) \quad . \qquad (5.13)$$

From Eq.(12) and its conjugate, the Wronskian appearing in our expression for $T_{int}(R)$ (Eq.(3.78)) can be written as

$$W\left[\chi_\ell^*, \frac{\partial}{\partial k}\chi_\ell\right]_R = W\left[J_\ell, \frac{\partial}{\partial k} J_\ell\right]_R - \frac{1}{4}\left\{(S_\ell - 1)\; W\left[O_\ell, \frac{\partial}{\partial k} O_\ell\right]_R + (S_\ell^* - 1)\; W\left[I_\ell, \frac{\partial}{\partial k} I_\ell\right]_R\right\}$$

$$+ \frac{i}{2}\, k\, S_\ell^* \frac{\partial}{\partial k} S_\ell \quad . \qquad (5.14)$$

However when these results are used in the expression (3.78), and the occupation time T_{fr} is subtracted out, a very complicated expression for the time delay Q ensues, which does not seem particularly useful. Accordingly we shall leave the results of the calculations of time delay and lifetime in the form of occupation times.

Let us, then, compare the expression (5) for $T_{fr}(R)$ with the result obtained in Chapter 3, Eq.(3.62):

$$T_{fr}(R) = \pi \sum_{\ell m} \int_0^\infty dk\; A_{\ell m}^*(k)\; A_{\ell m}(k)\; \frac{\mu}{\hbar k}\left(\frac{-1}{2k}\right) W\left[J_\ell, \frac{\partial}{\partial k} J_\ell\right]_R$$

$$+ \frac{1}{\pi}\sum_{\ell m}\int_0^\infty dk \left\{\tilde{\Phi}_{\ell m}^*(k,I)\;\tilde{\Phi}_{\ell m}(k,O) - \tilde{\Phi}_{\ell m}(k,I)\;\tilde{\Phi}_{\ell m}^*(k,O)\right\}\frac{\mu}{\hbar k}\left(\frac{-1}{2k}\right) W\left[J_\ell, \frac{\partial}{\partial k} J_\ell\right]_R .$$

(5.15)

Our expression contains the term (5) (apart from a factor of 2) plus an extra term involving the I and O transforms. If we note that

$$\tilde{\Phi}_{\ell m}(k,O)^* = \tilde{\Phi}^*_{\ell m}(k,I) \quad ,$$

$$\tilde{\Phi}_{\ell m}(k,I)^* = \tilde{\Phi}^*_{\ell m}(k,O) \quad ,$$

the second line of Eq.(15) can be written in the form

$$\frac{1}{\pi}\sum_{\ell m}\int_0^\infty dk \left\{\left|\tilde{\Phi}_{\ell m}(k,O)\right|^2 - \left|\tilde{\Phi}_{\ell m}(k,I)\right|^2\right\} \frac{\mu}{\hbar k}\left(\frac{-1}{2k}\right) W\left[J_\ell, \frac{\partial}{\partial k} J_\ell\right]_R \quad . \tag{5.16}$$

Now $|\tilde{\Phi}_{\ell m}(k,O)|^2$ is just the fraction of the initial packet with momentum k in the outward direction, and $|\tilde{\Phi}_{\ell m}(k,I)|^2$ is the fraction with momentum k directed inwards. The new term thus suggests a contribution to the occupation time which varies according to whether the overall motion of the packet is towards or away from the observer's sphere.

The source of the extra term can be seen by going back to the time integrals. In Kilian's calculation the time integral gives a simple δ function,

$$\int_{-\infty}^{\infty} d\tau \; e^{\frac{i(k^2 - k'^2)\tau}{2}} = \frac{2\pi}{k}\,\delta(k - k') \quad , \tag{5.17}$$

and in our calculation the integral gives a $\delta^{(+)}$ function,

$$\int_0^\infty d\tau \; e^{\frac{i(k^2 - k'^2)\tau}{2}} = \frac{2i}{k^2 - k'^2 + 2i\varepsilon}$$

$$= \frac{\pi}{k}\,\delta(k - k') + 2i \, PP\left(\frac{1}{k^2 - k'^2}\right) , \tag{5.18}$$

where PP denotes the principal part. Clearly the new term in Eq.(15) arises from the principal part integral in Eq.(18).

Previous calculations of time delay (Ohmura 1964, Goldberger and Watson 1964, Fong 1965, Nussenzveig 1969) have all used the time integral (17), so in this respect our calculation is quite new. We have shown that the expressions arising from the time integral (18) may be handled by writing the momentum coefficients in the wave functions as transforms over the initial packet, and making use of the Green's function integrals. The transform notation plays an important part in this approach, and it allows the orthogonality of the initial packet to all bound states to be taken into account quite readily. Since we have not otherwise placed any restrictions on the initial packet, it seems reasonable to suggest that the method we have used in the calculations of time delay and lifetime might provide a general basis for future calculations involving the t = 0 wave function.

The occupation time with the potential present is (Eq.(3.78))

$$T_{int}(R) = \pi \sum_{\ell m} \int_0^\infty dk\; B^*_{\ell m}(k)\; B_{\ell m}(k)\; \frac{\mu}{\hbar k}\left(\frac{-1}{2k}\right) W\left[\chi^*_\ell, \frac{\partial}{\partial k}\chi_\ell\right]_R$$

$$+ \frac{1}{\pi}\sum_{\ell m}\int_0^\infty dk \left\{\tilde{\Phi}^*_{\ell m}(k,I)\;\tilde{\Phi}_{\ell m}(k,O) - \tilde{\Phi}_{\ell m}(k,I)\;\tilde{\Phi}^*_{\ell m}(k,O)\right\}\frac{\mu}{\hbar k}\left(\frac{-1}{2k}\right) W\left[\chi^*_\ell, \frac{\partial}{\partial k}\chi_\ell\right]_R , \qquad (5.19)$$

and this is to be compared with Eq.(7). The term containing the coefficients $B_{\ell m}$ in Eq.(19) corresponds to the expression (7) because of the different wave functions used in the two calculations, and again there is an extra term containing I and O transforms. In the scattering wave function, the total outgoing wave is $S_\ell(k)\; O_\ell(kr)$, where $S_\ell(k)$ is the scattering matrix for the ℓ'th partial wave, and it will be seen that $S_\ell(k)$ does not appear in Eq.(19). However $S_\ell(k)$ is unitary, so we could write the outgoing term in the second line of (19) as

$$\left|S_\ell(k)\ \tilde{\Phi}_{\ell m}(k,O)\right|^2 = \tilde{\Phi}^*_{\ell m}(k,I)\ S^*_\ell(k)\ S_\ell(k)\ \tilde{\Phi}_{\ell m}(k,O)$$

$$= \tilde{\Phi}^*_{\ell m}(k,I)\ \tilde{\Phi}_{\ell m}(k,O) \quad , \tag{5.20}$$

without affecting the final expression.

Our results contain Wigner's inequality in the Wronskian $W\left[\chi^*_\ell, \frac{\partial}{\partial k}\chi_\ell\right]_R$ appearing in Eq.(19). If we use

$$\chi_\ell(k,r) \underset{r\geqslant a}{=} \frac{i}{2}\left[I_\ell(kr) - S_\ell(k)\ O_\ell(kr)\right] \tag{5.21}$$

and its conjugate, we may expand the Wronskian into the form

$$W\left[\chi^*_\ell,\frac{\partial}{\partial k}\chi_\ell\right]_R = \frac{i}{2}\, k\, S^*_\ell \frac{\partial}{\partial k} S_\ell + \frac{1}{2}\, \mathrm{Re}\left\{W\left[I_\ell,\frac{\partial}{\partial k}O_\ell\right]_R - S_\ell W\left[O_\ell,\frac{\partial}{\partial k}O_\ell\right]_R\right\} \quad , \tag{5.22}$$

where Re denotes the real part of the expression within brackets. The Wronskian is also equal to a radial integral:

$$W\left[\chi^*_\ell, \frac{\partial}{\partial k}\chi_\ell\right]_R = -2k\int_0^R dr\ \chi^*_\ell(k,r)\ \chi_\ell(k,r)$$

so, noting that

$$S^*_\ell \frac{\partial}{\partial k} S_\ell = 2i\ \frac{d\delta_\ell}{dk} \quad ,$$

we have

$$\frac{d\delta_\ell}{dk} = \frac{1}{2k} \operatorname{Re} \left\{ W\left[I_\ell, \frac{\partial}{\partial k} O_\ell\right]_R - S_\ell W\left[O_\ell, \frac{\partial}{\partial k} O_\ell\right]_R \right\} + 2 \int_0^R dr\, \chi_\ell^*(k,r)\, \chi_\ell(k,r) \ . \tag{5.23}$$

The integral is necessarily non-negative, and if it is omitted from Eq.(23) an inequality for $\frac{d\delta_\ell}{dk}$ is obtained. By first letting the radius R decrease to the value a (the radius of the potential), we find Wigner's result (Eq.(3.5)):

$$\frac{d\delta_\ell}{dk} \geqslant \frac{1}{2k} \operatorname{Re} \left\{ W\left[I_\ell, \frac{\partial}{\partial k} O_\ell\right]_a - S_\ell W\left[O_\ell, \frac{\partial}{\partial k} O_\ell\right]_a \right\} \ . \tag{5.24}$$

The equality sign holds when $\int_0^a dr\, \chi_\ell^*\, \chi_\ell$ is actually zero, i.e. for hard sphere scattering. Wigner (1955) derived the inequality (24) by differentiation of the expression relating the S matrix to the R matrix, but it was shown soon afterwards by Martin (1956), and Corinaldesi and Zienau (1956), that the same result could be obtained by the radial integral method given here.

If we now consider the results of the lifetime calculation, we see that another type of term arises when the packet is initially inside the observer's sphere. The occupation times are (Eqs (4.50) and (4.70)):

$$T_{fr}(R) = \frac{\pi}{4} \sum_{\ell m} \int_0^\infty dk \left\{ A_{\ell m}(k) \frac{\mu}{\hbar k}\, i \frac{d}{dk} A_{\ell m}^*(k) - A_{\ell m}^*(k) \frac{\mu}{\hbar k}\, i \frac{d}{dk} A_{\ell m}(k) \right\}$$

$$+ \ \pi \sum_{\ell m} \int_0^\infty dk\, A_{\ell m}^*(k)\, A_{\ell m}(k) \frac{\mu}{\hbar k} \left(\frac{-1}{2k}\right) W\left[J_\ell, \frac{\partial}{\partial k} J_\ell\right]_R \ , \tag{5.25}$$

and

$$T_{int}(R) = \frac{\pi}{4}\sum_{\ell m}\int_0^\infty dk \left\{B_{\ell m}(k)\,\frac{\mu}{\hbar k}\, i\frac{d}{dk}\, B^*_{\ell m}(k) - B^*_{\ell m}(k)\,\frac{\mu}{\hbar k}\, i\frac{d}{dk}\, B_{\ell m}(k)\right\}$$

$$- \frac{\pi}{4}\sum_{\ell m}\int_0^\infty dk\, B^*_{\ell m}(k)\, B_{\ell m}(k)\, S^*_\ell(k)\,\frac{\mu}{\hbar k}\, i\frac{d}{dk}\, S_\ell(k)$$

$$+ \pi\sum_{\ell m}\int_0^\infty dk\, B^*_{\ell m}(k)\, B_{\ell m}(k)\,\frac{\mu}{\hbar k}\left(\frac{-1}{2k}\right) W\left[\chi^*_\ell\, ,\, \frac{\partial}{\partial k}\chi_\ell\right]_R \quad . \tag{5.26}$$

In each expression, the last line is identical with a term in the corresponding expression for the time delay problem. These terms depend on the size of the observer's sphere through the Wronskians $W\left[\,\ldots.\,\right]_R$. The remaining terms, however, are quite different, and do not depend on R at all.

Let us write the complex coefficient $A_{\ell m}(k)$ as

$$A_{\ell m}(k) = \left|A_{\ell m}(k)\right|\, e^{i\alpha_{\ell m}(k)} \quad . \tag{5.27}$$

Then by a simple calculation

$$A_{\ell m}(k)\,\frac{\mu}{\hbar k}\, i\frac{d}{dk}\, A^*_{\ell m}(k) - A^*_{\ell m}(k)\,\frac{\mu}{\hbar k}\, i\frac{d}{dk}\, A_{\ell m}(k) = 2\left|A_{\ell m}\right|^2\frac{\mu}{\hbar k}\,\frac{d\alpha_{\ell m}}{dk} \quad . \tag{5.28}$$

The first line of Eq.(25) is thus of the form

$$\frac{\pi}{2}\sum_{\ell m}\int_0^\infty dk\, \left|A_{\ell m}(k)\right|^2\frac{\mu}{\hbar k}\,\frac{d\alpha_{\ell m}(k)}{dk} \quad , \tag{5.29}$$

and it may be seen by comparing with Eqs (3.16) and (3.19) that this is the partial wave version of the term

$$\frac{2\pi}{S}\int_{-\infty}^{\infty} G^2(\nu)\ \frac{d\alpha}{d\nu}(\nu)\ v\ d\nu \tag{5.30}$$

obtained by Ohmura. If we express the coefficient $B_{\ell m}(k)$ as $|B_{\ell m}(k)|\ e^{i\beta_{\ell m}(k)}$, then the first line of Eq.(26) has a similar form

$$\frac{\pi}{2}\sum_{\ell m}\int_0^{\infty} dk\ |B_{\ell m}(k)|^2\ \frac{\mu}{\hbar k}\ \frac{d\beta_{\ell m}(k)}{dk} \quad . \tag{5.31}$$

Gien (1970) has suggested that the term $\frac{d\alpha}{d\nu}$ arises in Ohmura's calculation because the scattered part of the wave function has been separated out and used to calculate arrival times. In general, the incident and scattered parts of the wave function can only be separated if the initial packet is well collimated - in a wave packet experiment using an arbitrary initial packet, it is not possible to distinguish between scattered and unscattered particles.† For this reason we have been careful to refer to the occupation times and time delay of the "interacting" wave packet, rather than the "scattered" wave packet. It is clear, however, that this is not the source of the dependence on $\frac{d\alpha}{d\nu}$, since no separation of incident and scattered packets has been made in the derivation of Eq.(26), and in any case such a term occurs in the occupation time for the free packet, Eq.(25). It may be noted that the

† Gien's point is actually related to a somewhat different problem, namely that the scattered parts of the scattering states do not form a linear space in which the time operator $i\hbar\frac{\partial}{\partial E}$ may be defined.

terms (29) and (31) have been obtained in the calculation of lifetime, when the initial packet is inside the potential, and not in the calculation of time delay. Since the terms are independent of the radius R, one may guess that they are in some way related to the origin of the co-ordinate system, and this will become clearer in the one-dimensional calculation to be discussed in a few moments.

The second line of Eq.(26) is again independent of R, and if we use $S_\ell(k) = e^{2i\delta_\ell(k)}$, we see that it is equal to

$$\frac{\pi}{2} \sum_{\ell m} \int_0^\infty dk \; B^*_{\ell m}(k) \; B_{\ell m}(k) \; \frac{\mu}{\hbar k} \frac{d\delta_\ell}{dk} \qquad , \tag{5.32}$$

which is very similar to Kilian's expression, Eq.(10), for the time delay. The appearance of this term is rather unexpected, since the term $\frac{d\delta_\ell}{dk}$ in calculations of time delay is only obtained after an averaging procedure, or the Riemann - Lebesgue lemma, has been used to remove oscillatory terms sin $(2kR + 2\delta_\ell)$ etc. (Smith 1960, Kilian 1968, Nussenzveig 1969). It may be that the first two lines of Eq.(26) can be rearranged in some more natural way so that the term (32) does not appear by itself, but we have not been able to see this.

Having derived the general expressions (15), (19), (25) and (26) for the occupation times, one would naturally like to consider models in which the effect of the wave packet shape on the time delay or lifetime could be explored in detail. Previous treatments of wave packet scattering (Low 1959, Goldberger and Watson 1964, Chap.3) have often made use of the "constant shape" approximation, in which the parameters of the initial packet are so chosen that it does not spread or change shape appreciably before reaching the scatterer. Our calculation, however, is not limited in this way, so one could select a particular shape for the incident packet and then vary the initial distance between packet and scatterer in order to study the effect of spreading on the occupation time or time delay. The model of an exponential wave packet interacting with a resonance in the scatterer (Nussenzveig 1961, Dodd and McCarthy 1964, Goebel and McVoy 1966) would also be of interest, since experiments involving such packets have already been carried out (Lynch et al 1960).

The expressions we have obtained are, however, considerably more complicated than those derived with the $t \to -\infty$ wave function, and the problem of setting up a model is correspondingly more difficult. Kilian, for instance, has studied the time delay, Eq.(10), for two models in which the initial packet is specified simply by choosing a convenient form for the momentum distribution $A_{\ell m}(k)$. An important point in the derivation of Eq.(10) is, of course, that the wave functions for the free and interacting packets contain the same momentum coefficients. In our results the coefficients $A_{\ell m}$ and $B_{\ell m}$ are not equal, so in constructing a model one would have to start from the spatial form of the wave packet, $\Phi_{\ell m}(r)$, calculate $A_{\ell m}$ and $B_{\ell m}$ separately as transforms of $\Phi_{\ell m}$ with respect to J_ℓ and χ_ℓ^* , and then attempt to derive simple expressions for the time delay or lifetime from the appropriate occupation times.

Instead of considering model wave packets, we have found it easier to investigate the physical significance of our results by carrying out a similar calculation in one dimension. While it is natural to use partial waves in a topic which has close links with scattering experiments in nuclear physics, it must be admitted that the partial wave formalism can obscure quite simple points of interpretation. We shall therefore study the motion of a free wave packet in one dimension, with the aim of gaining more insight into the various expressions for occupation times.

Let us consider a one-dimensional wave packet describing the motion of a free particle of mass μ ,

$$\Phi(x,t) = (2\pi)^{-\frac{1}{2}} \int_{-\infty}^{\infty} dk\; A(k)\; e^{ikx - \frac{i\hbar k^2 t}{2\mu}} , \qquad (5.33)$$

where the wave function is normalised so that

$$\int_{-\infty}^{\infty} dk\; A^*(k)\; A(k) = 1 . \qquad (5.34)$$

We shall first calculate the time spent by the packet in the region $-R \leqslant x \leqslant +R$, if the motion of the packet is assumed to occur over the time interval $-\infty < t < +\infty$. Thus

$$T\;(-R, +R) \equiv \int_{-\infty}^{\infty} dt \int_{-R}^{R} dx\; \Phi^*(x,t)\; \Phi(x,t)$$

$$= \frac{\mu}{\hbar} \int_{-\infty}^{\infty} d\tau \int_{-R}^{R} dx\; (2\pi)^{-1} \int_{-\infty}^{\infty} dk \int_{-\infty}^{\infty} dk'\; A^*(k)\; A(k')\; e^{-ikx+ik'x}\; e^{\frac{i(k^2-k'^2)\tau}{2}}$$

$$= \frac{\mu}{\hbar} \int_{-R}^{R} dx \int_{-\infty}^{\infty} dk \int_{-\infty}^{\infty} dk'\; A^*(k)\; A(k')\; e^{-ikx+ik'x}\; \delta\left(\frac{k^2}{2} - \frac{k'^2}{2}\right) . \qquad (5.35)$$

The δ function in Eq. (35) gives rise to pairs of terms, since k and k' may now be positive or negative. We may use the general relation

$$\delta\left[f(x)\right] = \sum_n \frac{1}{\left|f'(x_n)\right|}\; \delta(x - x_n) , \qquad (5.36)$$

where the prime denotes differentiation with respect to x, and the sum is over all zeros of the function such that $f(x_n) = 0$, $f'(x_n) \neq 0$.

Then

$$\delta\left(\frac{k^2}{2} - \frac{k'^2}{2}\right) \underset{k>o}{=} \frac{1}{k}\,\delta(k - k') + \frac{1}{k}\,\delta(k + k')$$

$$\underset{k<o}{=} \frac{-1}{k}\,\delta(k - k') - \frac{1}{k}\,\delta(k + k') \quad . \tag{5.37}$$

The occupation time is thus

$$T\ (-R, +R) = \frac{\mu}{\hbar}\int_{-R}^{R} dx \left\{ \int_{0}^{\infty} dk\ A^*(k)\ A(k)\ \frac{1}{k} + \int_{0}^{\infty} dk\ A^*(k)\ A(-k)\ \frac{1}{k}\ e^{-2ikx} \right\}$$

$$- \frac{\mu}{\hbar}\int_{-R}^{R} dx \left\{ \int_{-\infty}^{0} dk\ A^*(k)\ A(k)\ \frac{1}{k} + \int_{-\infty}^{0} dk\ A^*(k)\ A(-k)\ \frac{1}{k}\ e^{-2ikx} \right\} ,$$

or

$$T\ (-R, +R) = \int_{0}^{\infty} dk\ A^*(k)\ A(k)\ \frac{\mu}{\hbar k}\ .\ 2R \ + \int_{0}^{\infty} dk\ A^*(-k)\ A(-k)\ \frac{\mu}{\hbar k}\ .\ 2R$$

$$+ \int_{0}^{\infty} dk \left\{A^*(k)\ A(-k) \ + \ A(k)\ A^*(-k)\right\} \frac{\mu}{\hbar k}\,\frac{1}{k}\,\sin 2kR \quad . \tag{5.38}$$

Let us now calculate the same quantity for a wave packet which is released at time t = 0. In this case we have

$$\left[\Phi(x,0) = \right] \qquad \Phi(x) = (2\pi)^{-\frac{1}{2}} \int_{-\infty}^{\infty} dk\ A(k)\ e^{ikx} \tag{5.39}$$

and

$$A(k) = (2\pi)^{-\frac{1}{2}} \int_{-\infty}^{\infty} dx\ \Phi(x)\ e^{-ikx} \quad . \tag{5.40}$$

Then

$$T\ (-R, +R) \equiv \int_{0}^{\infty} dt \int_{-R}^{R} dx\ \Phi^*(x,t)\ \Phi(x,t)$$

$$= \frac{\mu}{\hbar} \int_{0}^{\infty} d\tau \int_{-R}^{R} dx\ (2\pi)^{-1} \int_{-\infty}^{\infty} dk \int_{-\infty}^{\infty} dk'\ A^*(k)\ A(k')\ e^{-ikx+ik'x}\ e^{\frac{i(k^2 - k'^2)\tau}{2}}$$

$$= \frac{\mu}{\hbar} \int_{-R}^{R} dx\ (2\pi)^{-1} \int_{-\infty}^{\infty} dk \int_{-\infty}^{\infty} dk'\ A^*(k)\ A(k') e^{-ikx+ik'x}\ \frac{2i}{k^2 - k'^2 + 2i\varepsilon} \quad . \tag{5.41}$$

Following the method of the three-dimensional calculation, we may use Eq.(40) to express the integral over k' in Eq.(41) in terms of a Green's function:

$$\int_{-\infty}^{\infty} dk'\ A(k')\ e^{ik'x}\ \frac{2i}{k^2 - k'^2 + 2i\varepsilon}$$

$$= \int_{-\infty}^{\infty} dk'\ (2\pi)^{-\frac{1}{2}} \int_{-\infty}^{\infty} dx'\ \Phi(x')\ e^{-ik'x'}\ e^{ik'x}\ \frac{2i}{k^2 - k'^2 + 2i\varepsilon}$$

$$= \frac{-2i}{(2\pi)^{\frac{1}{2}}} \int_{-\infty}^{\infty} dx'\ \Phi(x') \int_{-\infty}^{\infty} dk'\ \frac{e^{ik'(x - x')}}{k'^2 - (k^2 + 2i\varepsilon)} \quad . \tag{5.42}$$

The Green's function may be evaluated by contour integration, with the result

$$\int_{-\infty}^{\infty} dk' \frac{e^{ik'(x-x')}}{k'^2 - (k^2 + 2i\varepsilon)} \underset{k>o}{=} \pi i \, \frac{e^{ik(x-x')}}{k} \, , \qquad x > x' \, ,$$

$$\underset{k<o}{=} -\pi i \, \frac{e^{-ik(x-x')}}{k} \, , \qquad x > x' \, . \tag{5.43}$$

Then combining Eqs (42) and (43),

$$\int_{-\infty}^{\infty} dk' \; A(k') \; e^{ik'x} \; \frac{2i}{k^2 - k'^2 + 2i\varepsilon}$$

$$\underset{k>o}{=} (2\pi)^{\frac{1}{2}} \left\{ \int_{-\infty}^{x} dx' \; \Phi(x') \; \frac{e^{ik(x-x')}}{k} + \int_{x}^{\infty} dx' \; \Phi(x') \; \frac{e^{-ik(x-x')}}{k} \right\}$$

$$\underset{k<o}{=} -(2\pi)^{\frac{1}{2}} \left\{ \int_{-\infty}^{x} dx' \; \Phi(x') \; \frac{e^{-ik(x-x')}}{k} + \int_{x}^{\infty} dx' \; \Phi(x') \; \frac{e^{ik(x-x')}}{k} \right\} \, . \tag{5.44}$$

We shall find that the occupation time depends on the position of the initial packet (39), so let us assume that the packet is to the left of the region (-R, +R), that is

$$\Phi(x) = 0 \quad , \quad x > -R_1 \tag{5.45}$$

where $R_1 > R$, Fig.5.1(a). Then, noting the range of the x integral in Eq.(41), we have from Eqs (44) and (40),

$$\int_{-\infty}^{\infty} dk' \; A(k') \; e^{ik'x} \; \frac{2i}{k^2 - k'^2 + 2i\varepsilon}$$

$$\underset{k>o}{=} \quad (2\pi)^{\frac{1}{2}} \int_{-\infty}^{-R_1} dx' \; \Phi(x') \; \frac{e^{ik(x-x')}}{k} \quad = \quad 2\pi \; A(k) \; \frac{e^{ikx}}{k} \tag{5.46a}$$

$$\underset{k<o}{=} \; -(2\pi)^{\frac{1}{2}} \int_{-\infty}^{-R_1} dx' \; \Phi(x') \; \frac{e^{-ik(x-x')}}{k} = -2\pi \; A(-k) \; \frac{e^{-ikx}}{k} \quad . \tag{5.46b}$$

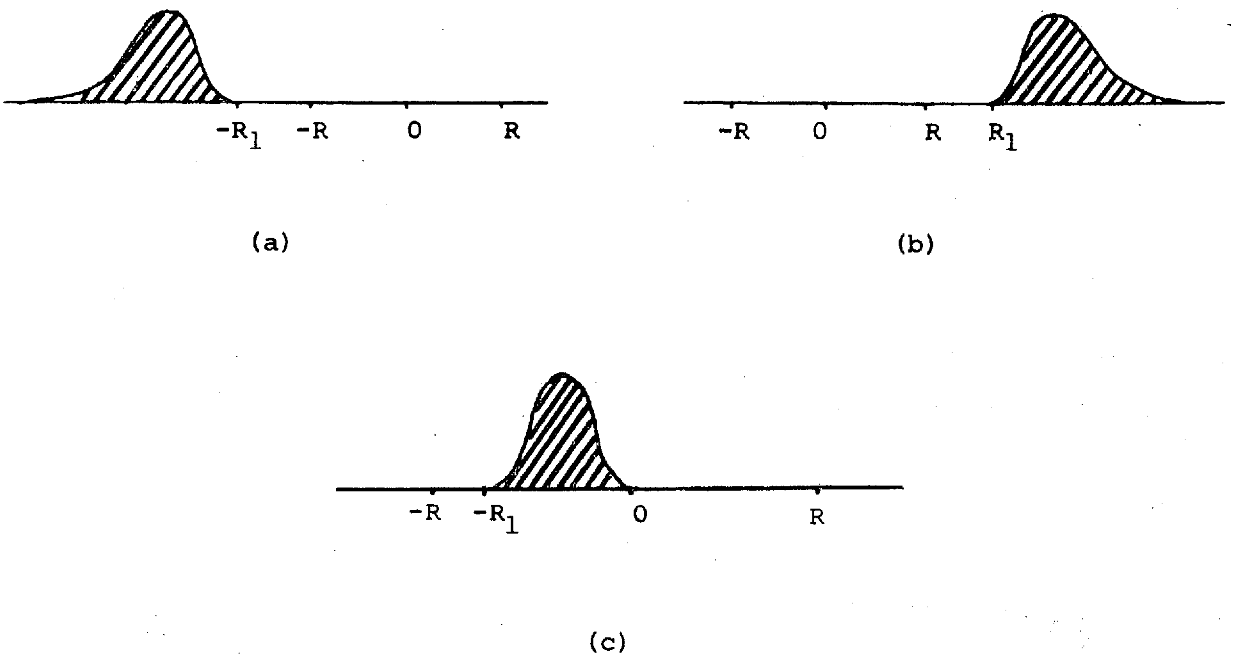

Fig.5.1 Initial Positions
of Wave Packet in One Dimension

Inserting Eqs (46) into Eq.(41) and carrying out the integration over x we obtain for the occupation time

$$T\;(-R,\,+R) \;=\; \int_{0}^{\infty} dk \; A^{*}(k) \; A(k) \; \frac{\mu}{\hbar k} \; . \; 2R \;+\; \int_{0}^{\infty} dk \; A^{*}(-k) \; A(k) \; \frac{\mu}{\hbar k} \, \frac{1}{k} \sin 2kR \; . \tag{5.47}$$

The first term of Eq.(47) is real, and it can be shown by means of contour integration that the imaginary part of the second term is zero, so we may take the real part of the second term to obtain finally

$$T\ (-R,\ +R) \;=\; \int_0^\infty dk\ A^*(k)\ A(k)\ \frac{\mu}{\hbar k}\ .\ 2R$$

$$+\ \frac{1}{2}\int_0^\infty dk\ \left\{A^*(k)\ A(-k)\ +\ A(k)\ A^*(-k)\right\} \frac{\mu}{\hbar k}\ \frac{1}{k}\sin 2kR \quad . \qquad (5.48)$$

A similar calculation may be carried out for a packet which is initially to the right of the region (-R, +R):

$$\Phi(x) \;=\; 0 \quad , \qquad x < R_1 \qquad\qquad (5.49)$$

where $R_1 > R$, Fig.5.1(b). The occupation time in this case is

$$T\ (-R,\ +R) \;=\; \int_0^\infty dk\ A^*(-k)\ A(-k)\ \frac{\mu}{\hbar k}\ .\ 2R$$

$$+\ \frac{1}{2}\int_0^\infty dk\ \left\{A^*(k)\ A(-k)\ +\ A(k)\ A^*(-k)\right\} \frac{\mu}{\hbar k}\ \frac{1}{k}\sin 2kR \quad . \qquad (5.50)$$

Comparing Eqs (38), (48) and (50), we see firstly that the occupation times contain terms which have the simple form of a distance, 2R, multiplied by the average of an inverse velocity, $\int_0^\infty dk\ A^*A\ \frac{\mu}{\hbar k}$. In Eqs (48) and (50) such a term is present only for that part of the initial packet which is directed towards the region (-R, +R) - the positive momentum component of the wave packet (45), and the negative momentum component of the wave packet (49). In Eq.(38), the term arises for both the positive and negative momentum components of the packet.

The difference between the results obtained from the initial conditions $t = 0$ and $t \to -\infty$ may be understood if we split the wave function (33) into two parts:

$$\Phi(x,t) = \Phi^{+}(x,t) + \Phi^{-}(x,t) \qquad , \tag{5.51}$$

where
$$\Phi^{+}(x,t) = (2\pi)^{-\frac{1}{2}} \int_{0}^{\infty} dk\ A(k)\ e^{ikx - \frac{ik^2\tau}{2}} \tag{5.52}$$

is the positive momentum component, and

$$\Phi^{-}(x,t) = (2\pi)^{-\frac{1}{2}} \int_{0}^{\infty} dk\ A(-k)\ e^{-ikx - \frac{ik^2\tau}{2}} \tag{5.53}$$

is the negative momentum component. In the limit $t \to -\infty$, the centre of the wave packet Φ^{+} moves to $x = -\infty$ (since the average velocity $\bar{v}$ is positive, cf Eq.(I.6)) and the centre of the wave packet Φ^{-} moves to $x = +\infty$. As $t \to +\infty$, each packet moves to the opposite end of the real axis, and in so doing passes through the region $(-R, +R)$, spending a time $2R\ \overline{v^{-1}}$ within it. If the wave packet is specified at $t = 0$, only one of the components Φ^{+} , Φ^{-} will pass through the region, which one being determined by the initial position of the packet.

In addition to the terms having a simple kinematic interpretation, each occupation time contains a term with the factor $\sin 2kR$. These are the oscillatory terms which are usually removed in calculations of time delay by averaging over R. They have generally been described as representing simply a "quantum effect" (Smith 1960, Nussenzveig 1969), but the expressions (38), (48) and (50) make it quite clear that they arise from interference between the positive and negative momentum components of the wave function.

It is interesting to note that the terms of the form $2R\,\overline{v^{-1}}$ give finite non-zero contributions to the occupation time, even if the packet has zero mean velocity. The mean velocity

$$\bar{v} = \int_{-\infty}^{\infty} dk\ A^*(k)\ A(k)\ \frac{\hbar k}{\mu}$$

$$= \int_{0}^{\infty} dk\ A^*(k)\ A(k)\ \frac{\hbar k}{\mu} - \int_{0}^{\infty} dk\ A^*(-k)\ A(-k)\ \frac{\hbar k}{\mu} \qquad (5.54)$$

is zero if $A(k) = \pm A(-k)$ or $A(k) = \pm A^*(-k)$, but in all cases the sum of the terms

$$\left\{ \int_{0}^{\infty} dk\ A^*(k)\ A(k)\ \frac{\mu}{\hbar k} + \int_{0}^{\infty} dk\ A^*(-k)\ A(-k)\ \frac{\mu}{\hbar k} \right\} 2R$$

in Eq.(38) is finite and non-zero. The packet cannot have a sharp wave front, so no matter where its centre is, part of the packet will be found in any given region, and the occupation time for that region is non-zero. Although the packet's mean velocity is zero, it nevertheless spreads and dies away, so the time spent within a region remains finite.

The discussion in one dimension makes it easier to understand the appearance of the various terms in the three-dimensional results, but it is rather difficult to show in detail the correspondence between the two calculations. The one-dimensional analysis has been carried out using travelling waves, whereas the partial wave decomposition is in terms of standing waves. This has the effect that the kinematic and interference terms, which have been separated in Eqs (48) and (50), are mixed together in a rather complicated way in Eqs (15) and (19). The Wronskian $W\left[J_o, \frac{\partial}{\partial k} J_o\right]_R$, for instance, may be evaluated to obtain the form

$$-\frac{1}{2k}\, W\left[J_o, \frac{\partial}{\partial k} J_o\right]_R = \frac{R}{2} - \frac{1}{4k} \sin 2kR \quad , \tag{5.55}$$

and this expression gives rise to both kinematic and interference terms. The coefficients $A_{\ell m}$ occur in an expansion in terms of $J_\ell = \frac{1}{2i}\left[O_\ell - I_\ell\right]$, and so are equivalent to a combination of the A(k) and A(-k) appearing in Eqs (48) and (50). The one-dimensional treatment does, however, make it plausible that the occupation times (15) and (19) should contain terms which depend on the motion of the packet towards or away from the scatterer.

If the wave packet is initially within the region (-R, +R), the calculation of the occupation time is considerably more complicated, and we shall not give all the details of the derivation here. Let us assume that the packet lies to the left of the origin,

$$\Phi(x) = 0 \text{ for } x < -R_1 \; , \quad x > 0 \tag{5.56}$$

where $R_1 < R$, Fig.5.1 (c). Then the integral over k' (Eq.(44)) becomes

$$\int_{-\infty}^{\infty} dk'\, A(k')\, e^{ik'x} \frac{2i}{k^2 - k'^2 + 2i\varepsilon}$$

$$\underset{k>o}{=} (2\pi)^{\frac{1}{2}} \left\{ \int_{-R_1}^{x} dx'\, \Phi(x')\, \frac{e^{ik(x-x')}}{k} + \int_{x}^{0} dx'\, \Phi(x')\, \frac{e^{-ik(x-x')}}{k} \right\}$$

(5.57)

$$\underset{k<o}{=} -(2\pi)^{\frac{1}{2}} \left\{ \int_{-R_1}^{x} dx'\, \Phi(x')\, \frac{e^{-ik(x-x')}}{k} + \int_{x}^{0} dx'\, \Phi(x')\, \frac{e^{ik(x-x')}}{k} \right\} .$$

On inserting the expressions (57) into Eq.(41), we obtain double integrals over x and x' which are analogous to the radial integrals $\mathcal{R}_{fr}$ and $\mathcal{R}_{int}$ appearing in Chapter 4. Thus from the first term in the first line of Eq.(57):

$$\int_{-R}^{R} dx\ e^{-ikx} \int_{-R_1}^{x} dx'\ \Phi(x')\ e^{ik(x-x')}$$

$$= \int_{-R}^{R} dx \int_{-R}^{x} dx'\ \Phi(x')\ e^{-ikx'}$$

$$= \int_{-R}^{o} dx \int_{-R}^{x} dx'\ \Phi(x')\ e^{-ikx'} + \int_{o}^{R} dx \int_{-R}^{o} dx'\ \Phi(x')\ e^{-ikx'}$$

$$= \int_{-R}^{o} dx' \int_{x'}^{o} dx\ \Phi(x')\ e^{-ikx'} + \int_{o}^{R} dx \int_{-R}^{o} dx'\ \Phi(x')\ e^{-ikx'}$$

$$= \int_{-R}^{o} dx'\ \Phi(x')\ (-x')\ e^{-ikx'} + R \int_{-R}^{o} dx'\ \Phi(x')\ e^{-ikx'}$$

$$= (2\pi)^{\frac{1}{2}} \left\{ -i \frac{\partial}{\partial k} A(k) + A(k)\ R \right\} \quad , \tag{5.58}$$

and from the second term, by a similar calculation,

$$\int_{-R}^{R} dx\ e^{-ikx} \int_{x}^{o} dx'\ \Phi(x')\ e^{-ik(x-x')}$$

$$= (2\pi)^{\frac{1}{2}} \left\{ -\frac{1}{2ik} A(k) + \frac{e^{2ikR}}{2ik} A(-k) \right\} \quad . \tag{5.59}$$

When the integrals over x and x' have been evaluated, the expression for T (-R, +R) contains eight terms, two of which are real by inspection. The imaginary part of the remaining terms may be shown to be zero by a method similar to that used in Chapters 3 and 4. On taking the real part of these terms, the final expression for the occupation time is

$$
\begin{aligned}
T\,(-R,\,+R) \\
&= \frac{1}{2}\int_0^\infty dk \left\{A(k)\,\frac{\mu}{\hbar k}\,i\,\frac{d}{dk}\,A^*(k) - A^*(k)\,\frac{\mu}{\hbar k}\,i\,\frac{d}{dk}\,A(k)\right\} + \int_0^\infty dk\, A^*(k)\,A(k)\,\frac{\mu}{\hbar k}\,.\,R \\
&+ \frac{1}{2}\int_0^\infty dk \left\{A(-k)\,\frac{\mu}{\hbar k}\,i\,\frac{d}{dk}\,A^*(-k) - A^*(-k)\,\frac{\mu}{\hbar k}\,i\,\frac{d}{dk}\,A(-k)\right\} \\
&\qquad + \int_0^\infty dk\, A^*(-k)\,A(-k)\,\frac{\mu}{\hbar k}\,.\,R \\
&+ \frac{1}{2}\int_0^\infty dk \left\{A^*(k)\,A(-k) + A(k)\,A^*(-k)\right\}\frac{\mu}{\hbar k}\,\frac{1}{k}\sin 2kR \quad . \qquad (5.60)
\end{aligned}
$$

Eq.(60) may be compared with Eqs (25) and (28), and it will be seen that we have again obtained terms of the form $\frac{d\alpha}{dk}$, where α is the phase of the momentum distribution.

In the first line of Eq.(60), there is a kinematic term $R\,\overline{v^{-1}}$, which represents the time taken by the positive momentum component of the wave packet (56) to cross the region (0, +R). Since the packet lies initially in the interval (-R, 0), it is clear that the first term represents the mean arrival time of the positive momentum component at the origin. The terms in the second line of Eq.(60) may be interpreted in a similar way if we note that the negative momentum component does not have to travel the full distance R to leave the region (-R, 0), since it is already within the region. The term containing $\frac{d}{dk}$ is therefore a "correction" to the kinematic term $R\,\overline{v^{-1}}$, and represents the time taken to travel from the origin to the initial position.

This interpretation of the $\frac{d\alpha}{dk}$ (or $\frac{d\alpha}{d\nu}$) term is verified if we return to the expression (3.19) derived by Ohmura. Choosing z = 0 we find the arrival time for the free packet is

$$t_{in} = 2\pi \int_{-\infty}^{\infty} G^2(\nu) \frac{d\alpha}{d\nu}(\nu)\; v\, d\nu \quad . \tag{5.61}$$

The reason such a term does not appear in our expressions (15) and (19) is, of course, that we have calculated the difference of two arrival times (see the discussion following Eq. (3.26)), and the term in $\frac{d\alpha}{dk}$ has cancelled out.

We have obtained kinematic terms analogous to those in Ohmura's expression (third term of Eq. (3.22)), but one may wonder if these make any contribution to the time delay $T_{int} - T_{fr}$. Since the wave packet is scattered elastically, it might seem that the mean (inverse) velocities of the free and interacting packets should be the same, and the kinematic terms should cancel each other. Although we have not been able to explore this question in detail, it seems that the kinematic term in T_{int} should reflect the fact that the particle travels faster within the potential, even though its velocity outside may be the same as that of the corresponding unscattered particle. On this basis, one would not expect the kinematic terms to cancel out.

The expression for time delay $\frac{\mu}{\hbar k}\frac{d\delta_\ell}{dk}$ is usually thought of as relating the scattering matrix $S_\ell = e^{2i\delta_\ell}$ to the time operator

$$-\frac{\mu}{\hbar k}\, i \frac{d}{dk} = -i\hbar \frac{d}{dE} \quad . \tag{5.62}$$

However the LHS of Eq.(62) can be put in another form if we remember that $i\frac{d}{dk}$ is just the position operator in the momentum representation (Furry 1962)

$$x_{op} = i\frac{d}{dk} \quad . \tag{5.63}$$

Then $$\frac{\mu}{\hbar k}\, i\frac{d}{dk} = v^{-1}\, x_{op} \quad , \tag{5.64}$$

where v is the velocity corresponding to the momentum $\hbar k$, and one is led to interpret the $\frac{d}{dk}$ terms in Eq.(60) not as derivatives of phases, but rather as expectation values involving combinations of the operators x and v. This becomes clearer if one uses partial integration to rearrange the terms as follows:

$$\int_0^\infty dk \left\{ A(k)\, \frac{\mu}{\hbar k}\, i\frac{d}{dk}\, A^*(k) - A^*(k)\, \frac{\mu}{\hbar k}\, i\frac{d}{dk}\, A(k) \right\}$$

$$= -\int_0^\infty dk\, A^*(k) \left\{ i\frac{d}{dk}\frac{\mu}{\hbar k} + \frac{\mu}{\hbar k}\, i\frac{d}{dk} \right\} A(k)$$

$$= -\left[\overline{x(o)\; v^{-1}} + \overline{v^{-1}\; x(o)} \right] \quad . \tag{5.65}$$

Eq.(65) may be compared with the term in t in Eq.(I.7). Furry points out that symmetrised products of operators, such as (65), are typical of quantum-mechanical expressions, and arise from the necessity of working only with Hermitian operators, which give pure real expectation values. The form on the LHS of Eq.(65) has its origin, of course, in our taking the real part of T (-R, +R), after proving the imaginary part to be zero.

The one-dimensional treatment has shown that terms obtained in the calculation of time delay and lifetime often have quite a simple interpretation in terms of distances, velocities and so on. These points are generally not considered in discussions based on formal relations between the time delay Q and the S matrix. If wave packet experiments involving small distances and times are to be performed and analysed, it may prove fruitful to return to such simple ideas.

APPENDIX A

GREEN'S FUNCTION INTEGRALS

The integrals for the free and interacting Green's functions appearing in the text may be evaluated by contour integration. The method is quite standard, but we include it here so that the similarity to the calculation of Im T in Chapters 3 and 4 may be seen.

We shall consider the free Green's function only, and evaluate the integral

$$\mathcal{J} \equiv \frac{2}{\pi}\int_0^\infty dk\, \frac{J_\ell(kr)\, J_\ell(kr')}{k^2 - k'^2} \tag{A.1}$$

for the case $r < r'$ and $\mathrm{Im}\, k' > 0$. Using the relations

$$J_\ell(kr) = \frac{1}{2i}\left[O_\ell(kr) - I_\ell(kr)\right] , \tag{A.2a}$$

$$J_\ell(-kr) = (-)^{\ell+1}\, J_\ell(kr) , \tag{A.2b}$$

and

$$O_\ell(-kr) = (-)^{\ell}\, I_\ell(kr) , \tag{A.2c}$$

we have

$$\mathcal{J} = \frac{2}{\pi}\frac{1}{2i}\int_0^\infty dk\, \frac{J_\ell(kr)\, O_\ell(kr')}{k^2 - k'^2} - \frac{2}{\pi}\frac{1}{2i}\int_0^\infty dk\, \frac{J_\ell(kr)\, I_\ell(kr')}{k^2 - k'^2}$$

$$= \frac{1}{\pi i}\int_{-\infty}^\infty dk\, \frac{J_\ell(kr)\, O_\ell(kr')}{k^2 - k'^2} . \tag{A.3}$$

Now $$J_\ell(kr) \underset{|k| \to \infty}{\sim} \frac{1}{2i}\left[i^{-\ell} e^{ikr} - i^{\ell} e^{-ikr}\right] ,$$

and $$O_\ell(kr') \underset{|k| \to \infty}{\sim} i^{-\ell} e^{ikr'} ,$$

so $$J_\ell(kr)\ O_\ell(kr') \underset{|k| \to \infty}{\sim} \frac{1}{2i}\left[(-)^{\ell} e^{ik(r+r')} - e^{ik(r'-r)}\right] . \tag{A.4}$$

Since $r < r'$, the integral (3) may be evaluated by completing the contour in the upper half plane, Fig.1.

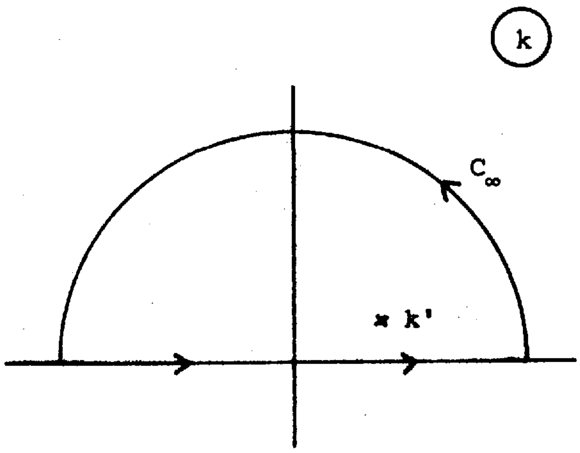

Fig.A.1 Contour for Evaluation of the Green's Function Integral, Eq.(3)

The integral around C_∞ is zero, and the integrand has a pole at $k = k'$, so

$$\frac{1}{\pi i}\int_{-\infty}^{\infty} dk\ \frac{J_\ell(kr)\ O_\ell(kr')}{k^2 - k'^2} = \frac{1}{k'}\ J_\ell(k'r)\ O_\ell(k'r') . \tag{A.5}$$

Finally,

$$\frac{2}{\pi}\int_0^\infty dk\ \frac{J_\ell(kr)\ J_\ell(kr')}{k^2 - k'^2}$$

$$= \frac{1}{k'}\ J_\ell(k'r)\ O_\ell(k'r') \quad , \quad r < r' \quad , \quad \text{Im } k' > 0 \quad . \tag{A.6}$$

The integral for the interacting Green's function may be evaluated in a similar way, though in this case the integrand also has poles at the bound states $k_n = -i\gamma_n$, $\gamma_n < 0$. The final result is

$$\frac{2}{\pi}\int_0^\infty dk\ \frac{\chi_\ell(k,r)\ \chi_\ell^*(k,r')}{k^2 - k'^2}$$

$$= \frac{1}{k'}\ \chi_\ell(k',r)\ (-)^\ell\ f_\ell(-k',r') - \sum_n \frac{\chi_\ell^{(n)}(r)\ \chi_\ell^{(n)}(r')}{k_n^2 - k'^2} \quad , \quad r < r' \quad , \quad \text{Im } k' > 0 \ , \tag{A.7}$$

where the functions $f_\ell(k,r)$ have been defined in Chapter 1, and the scattering and bound states, $\chi_\ell(k,r)$ and $\chi_\ell^{(n)}(r)$, in Chapter 2.

The expressions corresponding to Eqs (6) and (7) for Im $k' < 0$ may be obtained by noting that in this case the integrand has a pole at $k = -k'$ in the upper half plane. The relations (2b) and (2c) may be used to rewrite the result for the free Green's function in terms of $I_\ell(k'r')$, and a similar procedure may be applied to the interacting Green's function.

We conclude this Appendix with a note regarding the bound state wave functions $\chi_\ell^{(n)}(r)$. The wave function corresponding to the bound state pole $k_n = -i\gamma_n$, $\gamma_n < 0$, is defined as

$$\chi_\ell^{(n)}(r) = \frac{1}{N_n}\,\phi_\ell(-i\gamma_n,r) \quad , \tag{A.8}$$

where $\phi_\ell(k,r)$ is the regular solution of the radial wave equation,

$$\phi_\ell(k,r) = \frac{i}{2}\,\frac{1}{k^{\ell+1}}\left[f_\ell(-k)\ f_\ell(k,r) - (-)^\ell\ f_\ell(k)\ f_\ell(-k,r)\right] \quad , \tag{A.9}$$

and N_n is a normalisation constant ,

$$N_n^2 = \int_0^\infty dr\ \left[\phi_\ell(-i\gamma_n,r)\right]^2 \quad . \tag{A.10}$$

At the pole k_n we have $f_\ell(-k_n) = 0$, so

$$\left[\phi_\ell(-i\gamma_n,r) = \right] \quad \phi_\ell(k_n,r) = \frac{i}{2}\,\frac{(-)^{\ell+1}}{k_n^{\ell+1}}\ f_\ell(k_n)\ f_\ell(-k_n,r) \quad . \tag{A.11}$$

Further, if we denote by Res_n the residue of the S matrix at the bound state pole, this may be expressed as (Newton 1960, Eq.(5.2))

$$Res_n = \frac{(-)^{\ell+1}\ i\ \left[f_\ell(k_n)\right]^2}{4\gamma_n^{2\ell+2}\int_0^\infty dr\ \left[\phi_\ell(-i\gamma_n,r)\right]^2} \quad , \tag{A.12}$$

so that

$$N_n^2 = \frac{(-)^{\ell+1}\ i\ \left[f_\ell(k_n)\right]^2}{4\gamma_n^{2\ell+2}\ Res_n} \quad . \tag{A.13}$$

Combining Eqs (8), (11) and (13), the bound state wave function may be written as

$$\chi_{\ell}^{(n)}(r) = e^{\frac{i\pi}{4}} \, \mathrm{Res}_n^{\frac{1}{2}} \, f_{\ell}(-k_n,r) \quad . \tag{A.14}$$

The sign of the wave function is undetermined in Eq.(14), but this is not important since the purpose of deriving the relation is simply to show that $\chi_{\ell}^{(n)}(r)$ is proportional to $f_{\ell}(-k_n,r)$. It should perhaps be mentioned that the residue of the S matrix at a bound state pole is pure imaginary, and the properties of Res_n and $f_{\ell}(-k_n,r)$ under complex conjugation are such that $\chi_{\ell}^{(n)}(r)$ is in fact real.

APPENDIX B

RADIAL INTEGRALS

As an example of the radial integrals occurring in Chapters 3 and 4, we calculate

$$\int_a^b dr\ \chi_\ell^*(k,r)\ \chi_\ell(k,r) \qquad , \qquad\qquad (B.1)$$

where $\chi_\ell(k,r)$ are the scattering states defined in Chapter 2. The method has been given by Martin (1956), and Corinaldesi and Zienau (1956).

Consider the radial wave equation for two different energies:

$$-\frac{\partial^2}{\partial r^2}\chi_\ell^*(k,r) + \frac{\ell(\ell+1)}{r^2}\chi_\ell^*(k,r) + v(r)\ \chi_\ell^*(k,r) - k^2\chi_\ell^*(k,r) = 0 \quad ,$$

$$-\frac{\partial^2}{\partial r^2}\chi_\ell(k',r) + \frac{\ell(\ell+1)}{r^2}\chi_\ell(k',r) + v(r)\ \chi_\ell(k',r) - k'^2\chi_\ell(k',r) = 0 \quad .$$

Multiplying the first by $\chi_\ell(k',r)$, the second by $\chi_\ell^*(k,r)$, and subtracting the second from the first, we obtain

$$\frac{d}{dr}\ W\left[\chi_\ell^*(k,r),\ \chi_\ell(k',r)\right] \quad + \quad (k'^2 - k^2)\ \chi_\ell^*(k,r)\ \chi_\ell(k',r) \quad = \quad 0 \quad .$$

Then

$$\int_a^b dr\ \chi_\ell^*(k,r)\ \chi_\ell(k',r)$$

$$= \frac{1}{(k^2 - k'^2)}\left\{W\left[\chi_\ell^*(k,r),\chi_\ell(k',r)\right]_b - W\left[\chi_\ell^*(k,r),\chi_\ell(k',r)\right]_a\right\} .$$

(B.2)

The integral (1) is to be evaluated as

$$\lim_{k' \to k} \int_a^b dr\ \chi_\ell^*(k,r)\ \chi_\ell(k',r) \qquad .$$

Now $\qquad W\left[\chi_\ell^*(k,r), \chi_\ell(k',r)\right]$

$$= \chi_\ell^*(k,r)\ \frac{\partial}{\partial r}\chi_\ell(k',r) - \frac{\partial}{\partial r}\chi_\ell^*(k,r)\ \chi_\ell(k',r)$$

$$= \chi_\ell^*(k,r)\ \frac{\partial}{\partial r}\left[\chi_\ell(k,r) + (k'-k)\ \frac{\partial}{\partial k}\chi_\ell(k,r)\right]$$

$$- \frac{\partial}{\partial r}\chi_\ell^*(k,r)\left[\chi_\ell(k,r) + (k'-k)\ \frac{\partial}{\partial k}\chi_\ell(k,r)\right] + \mathcal{O}(\ (k'-k)^2)$$

$$= (k'-k)\ W\left[\chi_\ell^*(k,r),\ \frac{\partial}{\partial k}\chi_\ell(k,r)\right] + \mathcal{O}(\ (k'-k)^2) \qquad , \quad \text{(B.3)}$$

where we have used $\chi_\ell^*(k,r) = S_\ell^*(k)\chi_\ell(k,r)$, k real .

Using Eq. (3) in Eq. (2), and taking the limit $k' \to k$ we obtain

$$\int_a^b dr\ \chi_\ell^*(k,r)\ \chi_\ell(k,r)$$

$$= -\frac{1}{2k}\left\{W\left[\chi_\ell^*(k,r), \frac{\partial}{\partial k}\chi_\ell(k,r)\right]_b - W\left[\chi_\ell^*(k,r), \frac{\partial}{\partial k}\chi_\ell(k,r)\right]_a\right\} \qquad . \quad \text{(B.4)}$$

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