Rigorous Derivation of the Phase Shift Formula for the Hilbert Space Scattering Operator of a Single Particle

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For a single nonrelativistic particle moving in a spherically symmetric potential, the existence of the Hilbert space wave operators and S operator is proved and phase shift formulas for these operators are deduced. The probability, $P(\Omega)$, for scattering into the solid angle Ω is obtained from the time dependent theory. The relation between $P(\Omega)$ and the R matrix of the standard plane wave formulation of scattering theory is established. For collimated incoming packets, it is shown that $P(\Omega)$ can be expressed as an energy average of the differential cross section.

I. INTRODUCTION

THE importance of the asymptotic behavior of the field operators in quantum field theories has recently motivated mathematically rigorous studies of the asymptotic behavior of the solutions of the nonrelativistic Schroedinger equation.[1–5] In these studies the Hamiltonian operators of the free and interacting particle are defined as Hilbert space operators following Von Neumann[6] and Kato,[7] so that the kind of convergence involved in the asymptotic limits can be precisely specified. Suitable restrictions are placed on the scattering potential $V(\mathbf{x})$; for example, that $V(\mathbf{x})$ be square integrable over any finite region of three-dimensional space, and that as $r\rightarrow\infty$ $V(\mathbf{x})$ be $0(r^{-1-\epsilon})$, where r is the radial variable in spherical coordinates and $\epsilon>0$. It is then possible to prove that for every Hilbert space element u (i.e., for every normalizable wave function, $u(\mathbf{x})$), there are elements $u_\pm$ belonging to the continuum subspace of the total Hamiltonian H such that as the time t approaches $\mp\infty$,

$$\exp(-iH_0t)u\rightarrow\exp(-iHt)u_\pm \tag{1.1}$$

in the sense of strong convergence in Hilbert Space. In Eq. (1.1) H_0 is the kinetic energy operator and $H=H_0+V(\mathbf{x})$. Wave operators $\Omega_\pm$ are defined by the relations $u_\pm=\Omega_\pm u$, and it is shown that they and their adjoints $\Omega_\pm{}^*$ obey the relations

$$\Omega_\pm{}^*\Omega_\pm=1 \tag{1.2a}$$

and

$$\Omega_\pm\Omega_\pm{}^*=P_c, \tag{1.2b}$$

where 1 is the unit operator and P_c is the projection operator onto the continuum subspace of H. The S operator is defined as the operator, which connects the incoming and outgoing states associated through Eq. (1.1) with a given time-dependent continuum state. It follows that

$$S=\Omega_-{}^*\Omega_+ \tag{1.3}$$

and that S is unitary. Equations (1.1) to (1.3) thus provide a mathematically rigorous time-dependent basis for scattering theory.

The present paper adds to the foregoing considerations in three respects. First, Eq. (1.1) is proved for potentials which are effectively $0(r^{-2+\epsilon})$ rather than $0(r^{-\frac{3}{2}+\epsilon})$ as $r\rightarrow 0$. Second, explicit phase shift formulas for $\Omega_\pm$ and S are obtained. Third, the experimentally important formula for the scattering probability as an energy average over the usual differential cross section is deduced from the time-dependent Hilbert space formalism.

The material is presented as follows. In Sec. II a well-known eigenfunction expansion for the Schroedinger equation is stated so that it can be used to define the Hamiltonian operators. In Sec. III, the Hamiltonians are defined. In Sec. IV, Eq. (1.1) is proved and the formulas for $\Omega_\pm$ and S are obtained. In Sec. V the formula for the scattering probability is derived.

This section will be concluded with a statement of the precise conditions imposed on $V(r)$. It is assumed that $V(r)$ is Lebesgue integrable over any finite interval not including the origin, that for $0<R<\infty$

$$\int_0^R rV(r)dr<\infty, \tag{1.4a}$$

$$\int_R^\infty V(r)dr<\infty, \tag{1.4b}$$

and that either

$$\int_r^\infty V(s)ds \text{ belongs to } L^2(R,\infty), \tag{1.5a}$$

or as $r\rightarrow\infty$,

$$V(r)=0(r^{-1-\epsilon}). \tag{1.5b}$$

The notation $L^2(a,b)$ designates the class of functions, which are Lebesgue measurable and square integrable

[1] J. M. Cook, J. Math. Phys. **36**, 82 (1957).
[2] J. M. Jauch, Helv. Phys. Acta **31**, 127 and 661 (1958).
[3] J. M. Jauch and I. I. Zinnes, Nuovo cimento **11**, 553 (1959).
[4] M. N. Hack, Nuovo cimento **9**, 731 (1958).
[5] S. T. Kuroda, Nuovo cimento **12**, 431 (1959).
[6] J. Von Neumann, *Mathematical Foundations of Quantum mechanics*, translated by R. T. Beyer (Princeton University Press, Princeton, New Jersey, 1955).
[7] Tosio Kato, Trans. Am. Math. Soc. **70**, 195 (1951).

on the interval (a,b). Equations (1.4) are used to establish the eigenfunction expansion; one or the other of Eqs. (1.5) is joined to Eqs. (1.4) in the proof of Eq. (1.1).

II. EIGENFUNCTION EXPANSION

In this section, the bound state and continuum solutions, $Y_{ml}(\theta,\phi)r^{-1}\psi_l(r)$, of the Schroedinger equation are used to generate a mean-square eigenfunction expansion of the Hilbert space elements, u, which is used in Sec. III for the definition of H and H_0. The expansion theorem could be obtained as a special case of a general theorem of Titchmarsh[8] by adapting his proof to the conditions of Eq. (1.4). However, for the simple problem under discussion, the elementary approach used here serves its purpose in a direct way in terms of formulas which the physicist will find familiar. For ease in reference in later sections, the angular and radial parts of the expansion theorem are treated separately.

Let L^2 designate the Hilbert space of complex-valued Lebesgue measurable functions, $u(x_1,x_2,x_3)$, which are square integrable on $-\infty<x_i<\infty$, $i=1, 2, 3$. Let $u(r,\theta,\phi)$ be an abbreviation for $u(r\sin\theta\cos\phi, r\sin\theta\sin\phi, r\cos\theta)$. Then $r(\sin\theta)^{\frac{1}{2}}u(r,\theta,\phi)$ is measurable and square integrable on $(0\leqslant r<\infty, 0\leqslant\theta\leqslant\pi, 0\leqslant\phi<2\pi)$. Let $Y_{ml}(\theta,\phi)$ designate the normalized spherical harmonics. As is well known, it can be shown that[9]

$$r(\sin\theta)^{\frac{1}{2}}u(r,\theta,\phi)=\underset{L\to\infty}{\text{l.i.m.}}\Sigma_L(\sin\theta)^{\frac{1}{2}}Y_{ml}(\theta,\phi)\alpha_{ml}(r), \quad (2.1)$$

where

$$\alpha_{ml}(r)=\int_{4\pi}\bar{Y}_{ml}(\theta,\phi)ru(r,\theta,\phi)d\Omega. \quad (2.2)$$

In Eq. (2.1) the notation $\sum_L$ stands for

$$\sum_{l=0}^{L}\sum_{m=-l}^{l}.$$

The notation l.i.m. means the limit in mean square on the interval $(0\leqslant r<\infty, 0\leqslant\theta\leqslant\pi, 0\leqslant\phi<2\pi)$. In Eq. (2.2), $d\Omega$ stands for $\sin\theta d\theta d\phi$ and $\int_{4\pi}$ indicates integration over $(0\leqslant\theta\leqslant\pi, 0\leqslant\phi<2\pi)$. The functions $\alpha_{ml}(r)$ belong to $L^2(0,\infty)$ and have the property that

$$\|u\|^2\equiv\int_{-\infty}^{\infty}dx_1\int_{-\infty}^{\infty}dx_2\int_{-\infty}^{\infty}dx_3|u(x_1,x_2,x_3)|^2$$
$$=\Sigma_\infty\int_0^\infty|\alpha_{ml}(r)|^2dr. \quad (2.3)$$

Conversely, given any set $\{\beta_{ml}(r)\}$ of functions belonging to $L^2(0,\infty)$ and such that the right-hand side of Eq. (2.3) is finite, the right-hand side of Eq. (2.1) exists and defines a function $g(x_1,x_2,x_3)$ belonging to L^2. Moreover, if $\gamma_{ml}(r)$ is the function calculated for $g(x_1,x_2,x_3)$ from Eq. (2.2), $\gamma_{ml}(r)$ equals $\beta_{ml}(r)$ almost everywhere. Equations (2.1) and (2.2) thus establish a one to one correspondence between the elements of L^2 and the sets, $\{\alpha_{ml}(r)\}$, of functions for which the right-hand side of Eq. (2.3) is finite.

Since each $\alpha_{ml}(r)$ belongs to $L^2(0,\infty)$, it can itself be expanded in mean square on $(0,\infty)$ according to

$$\alpha_{ml}(r)=\underset{N\to\infty}{\text{l.i.m.}}\sum_{n=0}^{N}\alpha_{mln}\psi_{ln}(r)$$
$$+\underset{\omega\to\infty}{\text{l.i.m.}}\int_0^\omega\phi_{ml}(k)\psi_l(r,k)dk, \quad (2.4)$$

where

$$\alpha_{mln}=\int_0^\infty\alpha_{ml}(r)\psi_{ln}(r)dr, \quad (2.5a)$$

and

$$\phi_{ml}(k)=\underset{\omega\to\infty}{\text{l.i.m.}}\int_0^\omega\alpha_{ml}(r)\psi_l(r,k)dr. \quad (2.5b)$$

Furthermore, for each (ml),

$$\int_0^\infty|\alpha_{ml}(r)|^2dr=\sum_{n=0}^{\infty}|\alpha_{mln}|^2+\int_0^\infty|\phi_{ml}(k)|^2dk. \quad (2.6)$$

The $\psi_{ln}(r)$, $n=0, 1, \cdots$, are the normalized eigensolutions of the radial equation

$$-u''+(l(l+1)r^{-2}+2\mu V(r))u(r)=k^2u(r), \quad (2.7)$$

for $k^2\leqslant0$. The function $\psi_l(r,k)$ is the solution for $k>0$, which is normalized so that

$$\psi_l(r,k)\to(2/\pi)(\sin(kr-l\pi/2+\delta_l(k))$$

as $r\to\infty$; $\delta_l(k)$ is the phase shift. For all k the solutions are $0(r^{l+1})$ as $r\to0$. The scattered particle's mass is μ; its total energy is $k^2/2\mu$.

With each $\alpha_{ml}(r)$ belonging to $L^2(0,\infty)$, Eqs. (2.4) and (2.5) associate a function $\phi_{ml}(k)$ belonging to $L^2(0,\infty)$ and a set of constants α_{mln} such that the right-hand side of Eq. (2.6) is finite. Conversely, given a function $x_{ml}(k)$ and a set of constants β_{mln} with the above properties, Eq. (2.4) defines a function $\beta_{ml}(r)$ belonging to $L^2(0,\infty)$. If $\xi_{ml}(k)$ and γ_{mln} are calculated for $\beta_{ml}(r)$ from Eqs. (2.5), $\beta_{mln}=\gamma_{mln}$ for all n and $\xi_{ml}(k)=x_{ml}(k)$, almost everywhere. Thus Eqs. (2.4) and (2.5) establish a one to one correspondence between the $\alpha_{ml}(r)$ belonging to $L^2(0,\infty)$ and the sets $\{\phi_{ml}(k),\alpha_{mln}\}$ for which the right hand side of Eq. (2.6) is finite.

A proof of the radial expansion theorem stated above has been given by Kodaira.[10] In this proof it was assumed that $V(r)$ is continuous on $(0,\infty)$, that $V(r)=0(r^{-2+\epsilon})$ as $r\to0$, and that $V(r)=0(r^{-1-\epsilon})$ as $r\to\infty$. These conditions are equivalent to those of Eq. (1.4) for physical applications, except that Eq. (1.4) allows discontinuous potential wells of the kind which are

[8] E. C. Titchmarsh, *Eigenfunction Expansions, Part II* (Oxford University Press, New York, 1958), Chaps. 12 and 15.

[9] A proof is given in O. E. Lanford III, Thesis, Wesleyan University, 1959, Chap. II. This paper henceforth will be referred to as I.

[10] K. Kodaira, Am. J. Math. **71**, 921 (1949).

frequently convenient in practice. One of the authors (T.A.G.) has proved the expansion theorem using Eq. (1.4). The proof will be omitted.

Equations (2.1)–(2.6) jointly establish a one to one correspondence between functions $u(x_1,x_2,x_3)$ belonging to L^2 and the sets of functions and constants $\{\phi_{ml}(k),\alpha_{mln}\}$ such that

$$\sum_{l=0}^{\infty}\sum_{m=-l}^{l}\left\{\int_0^{\infty}|\phi_{ml}(k)|^2dk+\sum_{n=0}^{\infty}|\alpha_{mln}|^2\right\}<\infty. \quad (2.8)$$

Moreover, by Eqs. (2.3) and (2.6)

$$\|u\|^2=\sum_{l=0}^{\infty}\sum_{m=-l}^{l}\left\{\int_0^{\infty}|\phi_{ml}(k)|^2dk+\sum_{n=0}^{\infty}|\alpha_{mln}|^2\right\}. \quad (2.9)$$

The set $\{\phi_{ml}(k),\alpha_{mln}\}$ will be referred to as the transform, Fu, of the Hilbert space element, u. This element is then the inverse transform, $F^{-1}\{\phi_{ml}(k),\alpha_{mln}\}$, of $\{\phi_{ml}(k),\alpha_{mln}\}$. It is easy to verify that the elements $\{\phi_{ml}(k),\alpha_{mln}\}$ such that the right-hand side of Eq. (2.9) is finite constitute a Hilbert space with a norm given by the right-hand side of Eq. (2.9) and self-evident rules for addition, etc. The transform depends on the potential. It will be convenient to denote by F_0u the transform calculated with $V(r)\equiv 0$. In this case, there are no bound states so no coefficients α_{mln} appear.

III. OPERATORS H AND H_0

The transforms introduced in Sec. II are defined in terms of the solutions of the Schroedinger equation. Hence, it is physically clear that H must be the operator multiplication by $(k^2/2\mu)$ in the space of the transforms $\{\phi_{ml}(k),\alpha_{mln}\}$ and that H_0 must be the corresponding operator for $V(r)=0$, provided that the operators thus defined are unique and self-adjoint.

For a given $V(r)$ and $l=0$, however, it is well known that Eq. (2.7) belongs to the limit circle case at $r=0$. This implies that $\psi_0(r,k)$ (and, thus, the transform) is not unique; it also implies that $\psi_0(r,k)$ is not necessarily $0(r)$ as $r\rightarrow 0$. Hence, a boundary condition must be imposed to fix $\psi_0(r,k)$ uniquely. That the boundary condition $\psi_0(r,k)=0(r)$ as $r\rightarrow 0$ is the correct one is suggested by physical considerations. It is required by the physical interpretation of the quantum theory that the free particle Hamiltonian H_0 be the self-adjoint operator multiplication by $|\mathbf{k}|^2/2\mu$ in the space of Fourier-Plancherel transforms $\hat{u}(k_1,k_2,k_3)$ of the functions $u(x_1,x_2,x_3)$ belonging to L^2. This follows from the interpretation of $|\hat{u}(k_1,k_2,k_3)|^2$ as the probability density for momentum. It may be shown[11] that the operator multiplication by $k^2/2\mu$ in the space of transforms with $V(r)=0$ is identical with H_0 if and only if $\psi_0(r,k)=0(r)$ as $r\rightarrow 0$.

The boundary condition being thus determined, the operator H is defined as follows: The element, u, whose transform is $\{\phi_{ml}(k),\alpha_{mln}\}$ is in the domain $D(H)$ of H if and only if

$$\sum_{l=0}^{\infty}\sum_{m=-l}^{l}\left\{\int_0^{\infty}|k^2\phi_{ml}(k)|^2dk+\sum_{n=0}^{\infty}|k_{ln}{}^2\alpha_{mln}|^2\right\}<\infty. \quad (3.1)$$

Then, by definition,

$$Hu=F^{-1}\{(k^2/2\mu)\phi_{ml}(k),(k_{ln}{}^2/2\mu)\alpha_{mln}\}, \quad (3.2)$$

where $k_{ln}{}^2$ is the eigenvalue of the eigenfunction $\psi_{ln}(r)$ of Eq. (2.7). H_0 is defined analogously for $V(r)=0$. It is readily verified that H and H_0 are self-adjoint operators.[12]

Having defined H and H_0, it is a straightforward matter to define the unitary operators $\exp(-iHt)$ and $\exp(-iH_0t)$, which determine the time dependence of the scattered wave packet. This is done in Chap. III of I with the expected result that if $Fu=\{\phi_{ml}(k),\alpha_{mln}\}$,

$$\exp(-iHt)f=F^{-1}\{\phi_{ml}(k)\exp(-ik^2t/2\mu),\ \alpha_{mln}\exp(-ik_{ln}{}^2t/2\mu)\} \quad (3.3)$$

A corresponding formula is valid for H_0. Equation (3.3) is the starting point in the derivation of Eq. (1.1), which is carried out in the next section.

This section will be concluded with a few remarks about the use of the eigenfunction transform as a means of defining H. The method just presented can be generalized to non spherically symmetrical potentials and to an arbitrary number of particles. The essential steps in such a program have been carried out in Chapters XII and XIII of reference 8 where the existence of a unique[13] eigenfunction transform is established on the basis of physically reasonable assumptions. The transform established by Titchmarsh can be reduced in the problem under consideration to the one established directly in Sec. II.

The eigenfunction transform method of defining H differs from that used by Kato[7] although the two methods must of course lead to the same final result. In order to point up the difference, Kato's method will be briefly described.

The kinetic energy operator is defined as the closure of the differential operator T_1, which is defined to be $-\nabla^2/2\mu$ on a suitably chosen linear manifold D_1. It is then proved that H_0 is equal to the operator, multiplication by $|\mathbf{k}|^2/2\mu$, in the space of Fourier-Plancherel transforms. With H_0 thus defined, the potential $V(x_1,x_2,x_3)$ is restricted sufficiently that Vu is defined everywhere on the domain of H_0. The total Hamiltonian, H, is defined as the closure of an operator H_1, which itself is taken to be $-\nabla^2/2\mu+V$ for elements of D_1. It is proved that $H=H_0+V$, the domain of H being

[11] See Appendix A.

[12] See Chap. III of I.

[13] In footnote 8, the requirement that for $V(r)=0$ the Green's function $G_0(\mathbf{x},\mathbf{y},E)$ be singular only at $\mathbf{x}=\mathbf{y}$ accomplishes the same result as regards uniqueness as the kinetic energy argument used above.

the same as that of H_0. Kato's simple and elegant method, which he has formulated for the many particle problem, has the merit of guaranteeing a self-adjoint Hamiltonian without requiring the introduction of eigenfunction transforms.

Because in the problem under consideration $V(r)$ is more singular than the potentials envisaged in Kato's proof, and because for a partial wave analysis the existence of the eigenfunction transform is essential to begin with, the authors found it simplest to employ the definition of H given in Eqs. (3.1) and (3.2). When Kato's conditions on $V(r)$ are joined to those in Eq. (1.4), the two definitions of H yield the same operator.

IV. ASYMPTOTIC LIMITS

The purpose of this section is to prove Eq. (1.1). Let u belong to L^2 and be such that $Fu=\{\phi_{ml}(k),0\}$ so that u is orthogonal to the subspace spanned by the bound states.[14] Let $u_t=\exp(-iHt)u$. By the expansion theorems of Sec. II and Eq. (3.3),

$$r(\sin\theta)^{\frac{1}{2}}u_t(r,\theta,\phi)=\underset{L\to\infty}{\text{l.i.m.}}\sum_L(\sin\theta)^{\frac{1}{2}}Y_{ml}(\theta,\phi)u_{ml}(r,t), \quad (4.1)$$

where

$$u_{ml}(r,t)=\underset{\omega\to\infty}{\text{l.i.m.}}\int_0^\omega \exp(-ik^2t/2\mu)\phi_{ml}(k)\psi_l(r,k)dk. \quad (4.2)$$

The asymptotic behavior of $\psi_l(r,k)$ [see below Eq. (2.7)] now motivates the consideration of the function $\tilde{u}_t(r,\theta,\phi)$ defined by

$$r(\sin\theta)^{\frac{1}{2}}\tilde{u}_t(r,\theta,\phi)=\underset{L\to\infty}{\text{l.i.m.}}\sum_L(\sin\theta)^{\frac{1}{2}}Y_{ml}(\theta,\phi)\tilde{u}_{ml}(r,t), \quad (4.3)$$

where

$$\tilde{u}_{ml}(r,t)=\underset{\omega\to\infty}{\text{l.i.m.}}\int_0^\omega \exp(-ik^2t/2\mu)\phi_{ml}(k)\chi_l(r,k)dk, \quad (4.4)$$

and in Eq. (4.4), $\chi_l(r,k)=(2/\pi)^{\frac{1}{2}}\sin(kr-l\pi/2+\delta_l(k))$. It is easy to show using the theory of Fourier transforms in $L^2(-\infty,\infty)$ that $\tilde{u}_{ml}(r,t)$ belongs to $L^2(0,\infty)$ for all t and that

$$\int_0^\infty |\tilde{u}_{ml}(r,t)|^2dr\leqslant 2\int_0^\infty |\phi_{ml}(k)|^2dk. \quad (4.5)$$

As the first main step in the derivation of Eq. (1.1), it will now be shown that

$$\lim_{|t|\to\infty}\|u_t-\tilde{u}_t\|=0. \quad (4.6)$$

By Eq. (2.3)

$$\|u_t-\tilde{u}_t\|^2=\sum_{l=0}^\infty\sum_{m=-l}^{l}\int_0^\infty |u_{ml}(r,t)-\tilde{u}_{ml}(r,t)|^2dr. \quad (4.7)$$

Minkowski's inequality applies to the integrals of Eq. (4.7). Therefore, by using Eq. (4.5) and the corresponding equation for $\int_0^\infty|u_{ml}(r,t)|^2dr$, which follows from Eq. (2.6), it is seen that the convergence of the series on the right-hand side of Eq. (4.7) is uniform with respect to t for $-\infty<t<\infty$. Therefore, if

$$\lim_{|t|\to\infty}\int_0^\infty |u_{ml}(r,t)-\tilde{u}_{ml}(r,t)|^2dr=0 \quad (4.8)$$

for all (l,m), Eq. (4.6) is valid.

The rest of the discussion requires $k>0$. For this reason, functions $u_{mlN}(r,t)$ and $\tilde{u}_{mlN}(r,t)$ are defined by restricting the k integration in Eqs. (4.2) and (4.4) to the interval $[N^{-1},N]$, $(1<N<\infty)$. It is not hard to prove (see p. 55 of I) that

$$\int_0^\infty |u_{ml}(r,t)-\tilde{u}_{ml}(r,t)|^2dr\to 0 \quad\text{as}\quad |t|\to\infty$$

if

$$\lim_{|t|\to\infty}\int_0^\infty |u_{mlN}(r,t)-\tilde{u}_{mlN}(r,t)|^2dr=0 \quad (4.9)$$

for all N. Now

$$u_{mlN}(r,t)-\tilde{u}_{mlN}(r,t)=\int_{1/N}^N \exp(-ik^2t/2\mu)\phi_{ml}(k)\times[\psi_l(r,k)-\chi_l(r,k)]dk. \quad (4.10)$$

Also, for all r and N, $\phi_{ml}(k)(\psi_l(r,k)-\chi_l(r,k))$ is summable on $[1/N,N]$. Hence, the Riemann-Lebesgue lemma shows that

$$\lim_{|t|\to\infty}[u_{mlN}(r,t)-\tilde{u}_{mlN}(r,t)]=0 \quad (4.11)$$

for all $0\leqslant r<\infty$. Consequently, if in Eq. (4.9) the limit can be carried under the integral sign, the proof that $\|u_t-\tilde{u}_t\|\to 0$ will be accomplished. Consider first

$$\int_0^R |u_{mlN}(r,t)-\tilde{u}_{mlN}(r,t)|^2dr.$$

For $0\leqslant r\leqslant R$ and $1/N\leqslant k\leqslant N$, $\psi_l(r,k)-\chi_l(r,k)$ is bounded. Hence, by Eq. (4.10) $|u_{mlN}(r,t)-\tilde{u}_{mlN}(r,t|$ $\leqslant K$ for all t and consequently, for all $1<N<\infty$ and all $0<R<\infty$

$$\lim_{|t|\to\infty}\int_0^R |u_{mlN}(r,t)-\tilde{u}_{mlN}(r,t)|^2dr =\int_0^R \lim_{|t|\to\infty}|u_{mlN}(r,t)-\tilde{u}_{mlN}(r,t)|^2dr=0. \quad (4.12)$$

It is therefore sufficient to show that

$$\lim_{R\to\infty}\int_R^\infty |u_{mlN}(r,t)-\tilde{u}_{mlN}(r,t)|^2dr=0, \quad (4.13)$$

uniformly with respect to t for $-\infty<t<\infty$.

[14] The elements, u, constitute what has been referred to as the continuum subspace of H in earlier sections.

One sufficient condition is readily obtained from the asymptotic formula

$$\psi_l(r,k)-x_l(r,k)=0\left[\int_r^\infty V(y)dy\right]+0(1/r),\quad (4.14)$$

for $k>0$ and $r\to\infty$. [Equation (4.14) is readily deduced from Eq. (4.16).] Suppose $\int_r^\infty |V(y)|dy$ belongs to $L^2(R,\infty)$ for sufficiently large R. Then the Schwarz inequality applied to Eq. (4.10) shows that for all t and sufficiently large r,

$$|u_{mlN}(r,t)-\tilde{u}_{mlN}(r,t)|^2\leqslant g(r),\quad (4.15)$$

where $g(r)$ belongs to $L(R,\infty)$. Thus the condition expressed by Eq. (4.13) is satisfied. Consequently, Eq. (4.6) is valid.

The above condition on $V(r)$ can be replaced by the condition, $V(r)=0(r^{-1-\epsilon})$ as $r\to\infty$, for some $\epsilon>0$. This proved as follows. For $k>N^{-1}$ and $r>R(N,\epsilon)$, $\psi_l(r,k)$ satisfies the integral equation,

$$\psi_l(r,k)=x_l(r,k)-1/k\int_r^\infty \sin k(r-s)\times q(s)\psi_l(s,k)ds,\quad (4.16)$$

where $q(s)=l(l+1)/s^2+2\mu V(s)$. It follows from the iteration of Eq. (4.16) that as $r\to\infty$,

$$\psi_l(r,k)=x_{nl}(r,k)+0(r^{-(n+1)\epsilon}),\quad (4.17)$$

where $x_{nl}(r,k)$ is the function obtained by iterating Eq. (4.16) n times. Given ϵ, n can be chosen so that $n\epsilon>1$. This suffices to make $\psi_l(r,k)-x_{nl}(r,k)$ belong to $L^2(R,\infty)$ so that the argument below Eq. (4.13) can be applied to $\psi_l(r,k)-x_{nl}(r,k)$. Furthermore,

$$x_{nl}(r,k)-x_l(r,k)=\int_r^\infty dr_1G_k(r,r_1)x_l(r_1)+\cdots+\int_r^\infty dr_1\int_{r_1}^\infty dr_2\cdots\int_{r_{n-1}}^\infty dr_nG_k(r,r_1)G_k(r_1,r_2)\cdots\times G_k(r_{n-1},r_n)x_l(r_n),\quad (4.18)$$

where $G_k(x,y)=-k^{-1}q(y)\sin k(x-y)$.

With reference to Eq. (4.10), now consider

$$\xi(r,t)\equiv\int_{1/N}^N \exp(-ik^2t/2\mu)\phi_{ml}(k)\times[x_{nl}(r,k)-x_l(r,k)]dk.\quad (4.19)$$

For all r and t, Eq. (4.18) can be substituted into Eq. (4.19) and the k integral carried out first in each of the terms of the resulting sum. Moreover, the products

$$k^{-p}\sin k(r-r_1)\cdots\sin k(r_{p-1}-r_p)\sin(kr_p-l\pi/2+\delta_l(k))$$

can be decomposed into a sum of 2^p terms of the form $\sin(kZ-l\pi/2+\delta_l(k))$, or $\cos(kZ-l\pi/2+\delta_l(k))$ where Z is of the form $2r_i-2r_j+-+\cdots\pm r$.[15] In the definition of Z, r_i, r_j, etc., are selected from $r_1, r_2, r_3, \cdots, r_p$, and each distinct combination of 0, 1, 2, $\cdots$, p of them appears exactly once. Let

$$g_p(Z,t)=\int_{1/N}^N \exp(-ik^2t/2\mu)\phi_{ml}(k)k^{-p}\times\sin[kZ-l\pi/2+\delta_l(k)]dk.\quad (4.20)$$

By the theory of Fourier transforms

$$\int_0^\infty dZ|g_p(Z,t)|^2\leqslant\pi\int_{1/N}^N k^{-2p}|\phi_{ml}(k)|^2dk.\quad (4.21)$$

If $h_p(Z,t)$ is defined by Eq. (4.20) with $\cos(kZ-l\pi/2+\delta_l(k))$ in place of $\sin(kZ-l\pi/2+\delta_l(k))$, Eq. (4.21) applies with $h_p(Z,t)$ in place of $g_p(Z,t)$. With the k integrations done, $\xi(r,t)$ is given in part by a sum of terms of the form

$$\int_r^\infty dr_1q(r_1)\int_{r_1}^\infty dr_2q(r_2)\cdots\int_{r_{i-1}}^\infty dr_iq(r_i)g_p(Z,t)\times\int_{r_i}^\infty dr_{i+1}q(r_{i+1})\cdots\int_{r_{p-1}}^\infty dr_pq(r_p),\quad (4.22)$$

where Z contains r_i but none of the r_l for $l>i$. In addition, there are analogous terms with $h_p(Z,t)$ in place of $g_p(Z,t)$. Finally, there are terms with $g_p(r,t)$ and $h_p(r,t)$ which factor out of the integrals over the r_i. By applying the Schwarz inequality and Eq. (4.21) to the integrals containing $g_p(Z,t)$ and $h_p(Z,t)$, and by noting that as $r\to\infty$ $q(r)=0(r^{-1-\epsilon})$, it is readily verified that for all t as $r\to\infty$,

$$\xi(r,t)=g_p(r,t)0(r^{-\epsilon})+h_p(r,t)0(r^{-\epsilon})+0(r^{-\frac{1}{2}(1+\epsilon)}),\quad (4.23)$$

for all fixed l, m, and N. In Eq. (4.10), $(\psi_l(r,k)-x_l(r,k))$ is now written as $(\psi_l(r,k)-x_{nl}(r,k))+(x_{nl}(r,k)-x_l(r,k))$. It then follows from Eq. (4.17) (with $n\epsilon>1$) and Eq. (4.19) that as $r\to\infty$,

$$u_{mlN}(r,t)-\tilde{u}_{mlN}(r,t)=\xi(r,t)+0(r^{-1-\epsilon})\quad (4.24)$$

Finally, Eqs. (4.24), (4.23), and (4.21) show that as $R\to\infty$,

$$\int_R^\infty |u_{mlN}(r,t)-\tilde{u}_{mlN}(r,t)|^2=0(R^{-\epsilon})\quad (4.25)$$

for all ϵ, l, m, N, and t. Therefore, Eq. (4.13) is satisfied and the validity of Eq. (4.6) is established.

The last step in the discussion is the proof that as $t\to\pm\infty$, $\tilde{u}(r,t)$ approaches its outgoing and incoming parts, respectively. Let $\phi_{ml}(k)$ be the function in Eq.

[15] If p is even, sine functions are obtained; if p is odd, cosine functions occur. If the number of factors r_i, r_j is even, r enters with a plus sign.

(4.2) and by definition let

$$r(\sin\theta)^{\frac{1}{2}}u_t^{\pm}(r,\theta,\phi) = \underset{L\to\infty}{\text{l.i.m.}} \sum_L (\sin\theta)^{\frac{1}{2}} Y_{ml}(\theta,\phi) u_{ml}^{\pm}(r,t), \quad (4.26)$$

where

$$u_{ml}^{\pm}(r,t) = \underset{\omega\to\infty}{\text{l.i.m.}} \int_0^{\omega} \exp(-ik^2t/2\mu)\phi_{ml}(k) \times (2\pi)^{-\frac{1}{2}} \exp[\pm i(kr-(l+1)\pi/2+\delta_l(k))]dk. \quad (4.27)$$

The $u_{ml}^{\pm}(r,t)$ belong to $L^2(0,\infty)$ for all t and their norms satisfy Eq. (4.5) without the factor of two. Moreover, by comparing Eqs. (4.3) and (4.4) with Eqs. (4.26) and (4.27) it is seen that

$$\tilde{u}_t = u_t^+ + u_t^-. \quad (4.28)$$

It will be shown at the end of this section that

$$\lim_{t\to\mp\infty} \|u_t^{\pm}\| = 0 \quad (4.29)$$

Therefore, by Eqs. (4.28), (4.6), and the definition of u_t above Eq. (4.1), if $Fu = \{\phi_{ml}(k),0\}$,

$$\lim_{t\to\pm\infty} \|[\exp(-iHt)]u - u_t^{\pm}\| = 0, \quad (4.30)$$

where $u_t^{\pm}$ are defined by Eqs. (4.26) and (4.27).

The desired asymptotic limits follow directly from Eq. (4.30). Let g belong to L^2 and let $F_0 g = \{\chi_{ml}(k)\}$. Equation (4.30) applies to g in the form in which H is replaced by H_0 and the $u^{\pm}{}_t$ are replaced by functions $g_t^{\pm}$, which are defined by replacing $\phi_{ml}(k)$ by $\chi_{ml}(k)$ and setting $\delta_l(k)$ equal to zero in Eqs. (4.26) and (4.27). Now let $g_{\pm} = F^{-1}\{\chi_{ml}(k)\exp(\pm i\delta_l(k)),0\}$. The application of Eqs. (4.30), (4.26), and (4.27) to each of these functions shows that

$$\lim_{t\to\mp\infty} \|e^{-iHt}g_{\pm} - e^{-iH_0t}g\| = 0. \quad (4.31)$$

Thus Eq. (1.1) is established.

The phase shift formulas for the wave operators can be given concisely in terms of F and F_0. In order to do this, the element $\{\theta_{ml}(k)\} = F_0 u$ is identified with the element $\{\theta_{ml}(k),0\}$ of the Hilbert space Γ consisting of all $\{\phi_{ml}(k),\alpha_{mln}\}$ such that the right-hand side of Eq. (2.9) is finite. With this convention, F and F^{-1} establish a one to one correspondence between L^2, and Γ while F_0 and F_0^{-1} establish a one to one correspondence between L^2 and the continuum subspace of Γ. The formulas for $\Omega_{\pm}$ are now very simple. By the definition of $\Omega_{\pm}$ below Eq. (1.1) and the definition of $g_{\pm}$ below Eq. (4.30),

$$\Omega_{\pm} = F^{-1}\exp(\pm i\delta_l(k))F_0. \quad (4.32)$$

By using (4.32) and the norm-preserving properties of F and F_0, it is easy to show that

$$\Omega_{\pm}^* = F_0^{-1}[\exp(\mp i\delta_l)]\tilde{P}_c F, \quad (4.33)$$

where $\tilde{P}_c$ is the projection operator for the continuum subspace of Γ, $(\tilde{P}_c\{\phi_{ml}(k),\alpha_{mln}\} = \{\phi_{ml}(k),0\})$. Equations (1.2) follow directly from Eqs. (4.32) and (4.33). Finally, from Eqs. (1.3), (4.32) and (4.33) it is seen that

$$S = F_0^{-1}[\exp(2i\delta_l(k))]F_0. \quad (4.34)$$

The relation of the Hilbert space operator, S, to the R matrix of the plane wave formulation of scattering theory will be taken up in the next section. This section will be concluded with an outline of the proof of Eq. (4.29), the complete details of which are given in Chapter IV of I.

By Eqs. (4.26) and (2.3), Eq. (4.29) will hold as $t\to\infty$ if

$$\lim_{t\to\infty} \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \int_0^{\infty} |u_{ml}^-(r,t)|^2 dr = 0. \quad (4.35)$$

The series in Eq. (4.35) converges uniformly with respect to t, so it remains to be shown that the integrals tend toward zero. This is done by approximating $\phi_{ml}(k)\exp(-i\delta_l(k))$ (Eq. (4.27)) in mean square by a step function zero near the origin and zero for large k. This reduces the problem to the consideration of integrals of the type

$$\int_0^{\infty} \left| \int_a^b dk \exp(-ik^2t/(2\mu) - ikr) \right|^2 dr, \quad (4.36)$$

where $0<a<b<\infty$. For sufficiently large t, and all r, it can be shown that

$$\left| \int_a^b dk \exp(-ik^2t/(2\mu) - ikr) \right|^2 < A(r^2+B)^{-1}, \quad (4.37)$$

where A and B are positive constants, Moreover, the integral over k tends toward zero by the Riemann-Lebesgue lemma. Thus the $\lim(t\to\infty)$ can be taken inside the integrals over r in Eq. (4.36) and the limit is zero. Therefore Eq. (4.29) is valid insofar as u_t^- is concerned. The proof for $t\to-\infty$ is obtained by an identical argument.

V. RELATION OF S TO THE R MATRIX OF THE PLANE WAVE THEORY AND TO THE SCATTERING CROSS SECTION

In this section, the probability $P(\Omega)$ for scattering into a given solid angle, Ω, is computed from the time dependent formalism. The conditions under which $P(\Omega)$ can be described in terms of the R matrix are then discussed. Finally, a mathematically nonrigorous, but physically convincing argument is given, which shows that for wave packets of the type used in conventional scattering experiments,

$$P(\Omega) = \sigma(\Omega)P(\mathbf{a}), \quad (5.1)$$

where $\sigma(\Omega)$ is the usual scattering cross section averaged over energy, and $P(\mathbf{a})$ is the two dimensional probability density for the incident particle to strike the point, **a**, where the scatterer is located in a plane perpendicular to the motion of the incident particle. This is the result which one would desire for it guarantees that when multiple scattering and interference effects can be neglected the average number of particles scattered into Ω for N incident particles is equal to $Nt\rho\sigma(\Omega)$, where t is the target thickness and ρ the number of scatterers per unit volume.

The formula for $P(\Omega)$ is obtained as follows. Let $V(\Omega;a,b)$ designate the region $(0\leqslant a\leqslant r\leqslant b\leqslant\infty, \theta_0\leqslant\theta\leqslant\theta_1, \phi_0\leqslant\phi\leqslant\phi_1)$. Let $u_t=\exp(-iHt)u$, where $Fu=\{\phi_{ml}(k),0\}$ as in Sec. IV and consider the probability

$$P_t(\Omega;a,b)=\int_{V(\Omega;a,b)}|u_t|^2d\mathbf{x} \quad (5.2)$$

that the scattered particle be in $V(\Omega;a,b)$ at time t. From Eqs. (4.26), (4.27) and (4.30) it is easy to see that

$$\lim_{t\to\pm\infty}\left(P_t(\Omega;a,b)-\int_{V(\Omega;a,b)}|u_t^{\pm}(r,\theta,\phi)|^2d\mathbf{x}\right)=0, \quad (5.3)$$

and that for all t

$$\int_{V(\Omega;a,b)}|u_t^{\pm}(r,\theta,\phi)|^2d\mathbf{x}=\lim_{L\to\infty}\sum_{l=0}^{L}\sum_{m=-l}^{l}\sum_{l'=0}^{L}\sum_{m'=-l'}^{l'}\times\int_{\Omega}Y_{ml}(\theta,\phi)\bar{Y}_{m'l'}(\theta,\phi)d\Omega\int_a^b u_{ml}^{\pm}(r,t)\bar{u}_{m'l'}^{\pm}(r,t)dr, \quad (5.4)$$

the convergence of the series being uniform with respect to t. From Eq. (4.27) and the theory of Fourier transforms

$$\int_{-\infty}^{\infty}u_{ml}^{\pm}(r,t)\bar{u}_{m'l'}^{\pm}(r,t)dr=\int_0^{\infty}\exp[\pm i(\delta_l(k)-\delta_{l'}(k)-(l-l')\pi/2)]\times\phi_{ml}(k)\bar{\phi}_{m'l'}(k)dk. \quad (5.5)$$

Furthermore, for any finite c

$$\int_{-\infty}^{c}u_{ml}^{+}(r,t)\bar{u}_{m'l'}^{+}(r,t)dr=\int_0^{\infty}u_{ml}^{+}(c-s,\,t)\bar{u}_{m'l'}^{+}(c-s,\,t)ds, \quad (5.6)$$

where, by Eq. (4.27),

$$u_{ml}^{+}(c-s,\,t)=\underset{\omega\to\infty}{\mathrm{l.i.m.}}\int_0^{\omega}\exp(-ik^2t/2\mu)\phi_{ml}(k)(2\pi)^{-\frac{1}{2}}\exp(ikc)\times\exp[i(-ks-(l+1)\pi/2+\delta_l(k))]dk. \quad (5.7)$$

Now, to within a factor $\exp[i(kc-(l+1)\pi+2\delta_l(k))]$, $u_{ml}^{+}(c-s,\,t)$ has the same form as $u_{ml}^{-}(s,t)$. Hence, it is easily seen from the arguments below Eq. (4.35) and the Schwarz inequality that, for all finite c,

$$\lim_{t\to\infty}\int_{-\infty}^{c}u_{ml}^{+}(r,t)\bar{u}_{m'l'}^{+}(r,t)dr=0. \quad (5.8)$$

The same kind of argument applies to $u_{ml}^{-}(r,t)$ for $t\to-\infty$. Therefore, by Eqs. (5.2), (5.3), (5.4), and (5.8), for all $0\leqslant a<\infty$,

$$\lim_{t\to\pm\infty}P_t(\Omega;a,\infty)=\lim_{L\to\infty}\sum_{l=0}^{L}\sum_{m=-l}^{l}\sum_{l'=0}^{L}\sum_{m'=-l'}^{l'}\int_{\Omega}Y_{ml}(\theta,\phi)\bar{Y}_{m'l'}(\theta,\phi)d\Omega\times\int_0^{\infty}\exp[\pm i(\delta_l(k)-\delta_{l'}(k)-(l-l')\pi/2)]\times\phi_{ml}(k)\bar{\phi}_{m'l'}(k)dk$$
$$=\lim_{L\to\infty}\int_0^{\infty}dk\int_{\Omega}d\Omega\left|\sum_{l=0}^{L}\sum_{m=-l}^{l}Y_{ml}(\theta,\phi)\phi_{ml}(k)\times\exp[\pm i(\delta_l-l\pi/2)]\right|^2. \quad (5.9)$$

For finite a and b the limit is zero. Thus, the scattered particle is asymptotically outside of any sphere of finite radius a.

The probability, $P(\Omega)$, for scattering into the solid angle Ω should clearly be defined by the relation

$$P(\Omega)=\lim_{t\to\infty}P_t(\Omega,a,\infty). \quad (5.10)$$

Equation (5.9) then provides a formula for $P(\Omega)$ in terms of the phase shifts and the properties of the incident wave packet. The formula can be rendered more concise in terms of the Fourier transforms of the incoming and outgoing wave packets. As was shown in Sec. IV, as $t\to\infty$, $u_t\to\exp(-iH_0t)u^{\pm}$, where $F_0u^{\pm}=\{\phi_{ml}(k)\exp(\pm i\delta_l(k))\}$. Furthermore, as is proved in Appendix A, the Fourier-Plancherel transforms $\hat{u}^{\pm}(k,\theta,\phi)$ of $u^{\pm}$ satisfy the relation

$$k(\sin\theta)^{\frac{1}{2}}\hat{u}^{\pm}(k,\theta,\phi)=\lim_{L\to\infty}\sum_{l=0}^{L}\sum_{m=-l}^{l}(\sin\theta)^{\frac{1}{2}}Y_{ml}(\theta,\phi)\times(-i)^l\phi_{ml}(k)\exp(\pm i\delta_l(k)). \quad (5.11)$$

Consequently, by Eqs. (5.10), (5.9), and (5.11)

$$P(\Omega)=\int_0^{\infty}\int_{\Omega}|\hat{u}^{+}(k,\theta,\phi)|^2k^2dkd\Omega. \quad (5.12)$$

The physical interpretation of Eq. (5.12) is straightforward. The probability that the particle be scattered into Ω is equal to the probability that the momentum vector of the outgoing packet lie in Ω. This well-known result, which has just been shown to be a rigorous consequence of the time-dependent formalism, is the basis for the physical interpretation of calculations in which $\hat{u}^+(k,\theta,\phi)$ is obtained from a time-independent formalism.

The connection of the Hilbert space formulas with the R matrix can now be readily deduced. Let $P_-(\Omega)$ designate the probability that the incident particle be scattered into Ω in the absence of the scatterer. [Use $\hat{u}^-(k,\theta,\phi)$ in place of $\hat{u}^+(k,\theta,\phi)$ in Eq. (5.12).] Let

$$P'(\Omega)=\int_0^\infty\int_\Omega|\hat{u}^+(k,\theta,\phi)-\hat{u}^-(k,\theta,\phi)|^2k^2dkd\Omega. \quad (5.13)$$

It is easy to prove that

$$|P'(\Omega)-P(\Omega)|\leqslant P_-(\Omega)+2(P_-(\Omega)P(\Omega))^{\frac{1}{2}}. \quad (5.14)$$

Therefore, if the incident beam is appropriately collimated, the scattering probability can be calculated accurately from $P'(\Omega)$ except near the forward direction. Now, by Eq. (5.11),

$$\begin{aligned}&k(\sin\theta)^{\frac{1}{2}}(\hat{u}^+(k,\theta,\phi)-\hat{u}^-(k,\theta,\phi))\\&=\underset{L\to\infty}{\text{l.i.m.}}\sum_{l=0}^{L}\sum_{m=-l}^{l}(\sin\theta)^{\frac{1}{2}}Y_{ml}(\theta,\phi)\\&\quad\times[\exp(2i\delta_l(k))-1](-i)^l\phi_{ml}(k)\exp(-i\delta_l(k))\\&=\underset{L\to\infty}{\text{l.i.m.}}\int_{4\pi}k(\sin\theta)^{\frac{1}{2}}R_L(\theta,\phi;\theta',\phi';k)\\&\qquad\times\hat{u}^-(k,\theta',\phi')d\Omega', \quad (5.15)\end{aligned}$$

where

$$\begin{aligned}&R_L(\theta,\phi;\theta',\phi';k)\\&=\sum_{l=0}^{L}\sum_{m=-l}^{l}Y_{ml}(\theta,\phi)\bar{Y}_{ml}(\theta',\phi')[\exp(2i\delta_l(k))-1],\\&=\sum_{l=0}^{L}(4\pi)^{-1}(2l+1)P_l(\cos\Theta)\\&\qquad\times[\exp(2i\delta_l(k))-1]. \quad (5.16)\end{aligned}$$

In obtaining Eq. (5.16), the addition theorem for spherical harmonics was used. The angle Θ is the angle between the vectors $\mathbf{k}'(k,\theta',\phi')$ and $\mathbf{k}(k,\theta,\phi)$. Aside from a multiplicative factor, $R_L(\theta,\phi;\theta',\phi';k)$ is just the sum of the first L terms of the series for the scattering amplitude which appears in the stationary-state formulation of scattering theory for monochromatic incident plane waves. Suppose that the series (5.16) converges to a function $R(\theta,\phi;\theta',\phi';k)$ in such a way that

$$\begin{aligned}&\lim_{L\to\infty}\int_{4\pi}k(\sin\theta)^{\frac{1}{2}}R_L(\theta,\phi;\theta',\phi';k)\hat{u}^-(k,\theta',\phi')d\Omega'\\&\quad=\int_{4\pi}k(\sin\theta)^{\frac{1}{2}}R(\theta,\phi;\theta',\phi';k)\hat{u}^-(k,\theta'\phi')d\Omega' \quad (5.17)\end{aligned}$$

for almost all (k,θ,ϕ). Then, the limit functions in Eqs. (5.15) and (5.17) are equal almost everywhere, and

$$\begin{aligned}&\hat{u}^+(k,\theta,\phi)-\hat{u}^-(k,\theta,\phi)\\&\qquad=\int_{4\pi}R(\theta,\phi;\theta',\phi';k)\hat{u}^-(k,\theta',\phi')d\Omega'. \quad (5.18)\end{aligned}$$

In this case, the scattering probability can be calculated from the incoming wave packet through Eqs. (5.18) and (5.13). The relation of $R(\theta,\phi;\theta',\phi';k)$ to the R matrix is the following. The R matrix, $R(\mathbf{k},\mathbf{k}')$, is defined by the formal relation[16]

$$\begin{aligned}&\hat{u}^+(k,\theta,\phi)-\hat{u}^-(k,\theta,\phi)\\&\quad=\iiint(-2\pi i)R(\mathbf{k},\mathbf{k}')\delta(E-E')\hat{u}^-(\mathbf{k}')d\mathbf{k}', \quad (5.19)\end{aligned}$$

where $E=k^2/2\mu$ and $\delta(E-E')$ is the Dirac delta function. Equation (5.19) means

$$\begin{aligned}&\hat{u}^+(k,\theta,\phi)-\hat{u}^-(k,\theta,\phi)\\&\qquad=-2\pi ik\mu\int_{4\pi}R(\mathbf{k},\mathbf{k}')\hat{u}^-(\mathbf{k}')d\Omega', \quad (5.20)\end{aligned}$$

where $|\mathbf{k}|=|\mathbf{k}'|$. By comparing Eqs. (5.20) and (5.18), it is seen that the R matrix is defined on the energy shell whenever the limit $R(\theta,\phi;\theta',\phi';k)$ of $R_L(\theta,\phi;\theta',\phi';k)$ exists and Eq. (5.17) is valid.

From the physical point of view, there is no point in discussing potentials for which Eq. (5.18) does not hold, because if the series in Eq. (5.16) does not converge fairly rapidly, the phase shift approach will be useless for computation anyway. It is possible, of course, to contemplate potentials for which the series (5.16) diverges for $\Theta=0$ since in practice the calculation of nonforward scattering using Eqs. (5.13) and (5.18) need not require integration over $\Theta=0$. The convergence of the series (5.16) and the validity of Eq. (5.17) can be tested by using the Born approximation for the phase shifts.[17] As is well known, it is sufficient for convergence for $\Theta\neq0$ that as $r\to\infty$ $V(r)=0(r^{-2-\epsilon})$, $\epsilon>0$.[18] The stronger condition $V(r)=0(r^{-3-\epsilon})$ is sufficient to guarantee absolute and uniform convergence for $0\leqslant\theta\leqslant\pi$.

The usual formula for $P'(\Omega)$ in terms of the differential scattering cross section is obtained by specializing $\hat{u}^-(k,\theta,\phi)$ so that it conforms to experimental conditions. This has been done by Ekstein,[16] Eisenbud,[19]

[16] See, for example, H. Eckstein, Phys. Rev. **101**, 880 (1956).
[17] D. S. Carter, Thesis, Princeton University, 1952 (unpublished).
[18] L. I. Schiff, *Quantum Mechanics* (McGraw-Hill Book Company, Inc., New York, 1949), 1st ed., p. 187, problem 5.
[19] L. Eisenbud, Thesis, Princeton University, 1948 (unpublished).

and Jauch.[20] An alternative formulation, based on the same physical arguments, is presented below.

Suppose that the scatterer is located at the point whose cartesian coordinates are $(a_1,a_2,0)$ in the reference frame in which the scattered beam is directed along the positive x_3 axis. If the change of location of the scatterer from the origin to $(a_1,a_2,0)$ is taken into account in the usual way, it follows from Eqs. (5.13) and (5.18) that

$$P'(\Omega)=\int_\Omega d\Omega\int_0^\infty dk\left|\int_{4\pi} R(\theta,\phi;\theta',\phi';k)\times\exp(i\mathbf{k}'\cdot\mathbf{a})\hat{u}^-(k,\theta',\phi')d\Omega'\right|^2. \quad (5.21)$$

Now, with a typical beam (beam diam ~ 1 cm, momentum $\sim 10^8$ cm^{-1}), $\hat{u}^-(k,\theta',\phi')$ goes to zero strongly outside a forward cone of apex angle $\sim 10^{-8}$ rad centered on the x_3 axis. Thus, in cases of physical interest $R(\theta,\phi;\theta',\phi';k)$ can certainly be replaced by $R(\theta,\phi;0,0;k)$. This leads to

$$P'(\Omega)\approx\int_\Omega d\Omega\int_0^\infty dk\sigma_k(\theta,\phi)\times\left|(2\pi)^{-1}\int_0^\pi\int_0^{2\pi}\exp(i\mathbf{k}'\cdot\mathbf{a})\hat{u}^-(k,\theta',\phi')\times k^2\sin\theta'd\theta'd\phi'\right|^2, \quad (5.22)$$

where

$$\sigma_k(\theta,\phi)=|k^{-1}\sum_{l=0}^\infty(2l+1)P_l(\cos\theta)\exp(i\delta_l(k))\sin\delta_l(k)|^2. \quad (5.23)$$

It will be recognized that $\sigma_k(\theta,\phi)$ is the differential cross section as usually defined. Equation (5.22) can be further transformed by noting that with $k\sim 10^8$ and $\theta'\sim 10^{-8}$, it will be a very good approximation to write[21]

$$(2\pi)^{-1}\int_0^\pi\int_0^{2\pi}\exp(i\mathbf{k}'\cdot\mathbf{a})\hat{u}^-(k,\theta',\phi')k^2\sin\theta'd\theta'd\phi'$$
$$\approx(2\pi)^{-1}\int_{-\infty}^\infty\int_{-\infty}^\infty\exp(i\mathbf{k}'\cdot\mathbf{a})\hat{u}^-(k_1,k_2,k)dk_1dk_2$$
$$\approx(2\pi)^{-\frac{1}{2}}\int_{-\infty}^\infty\exp(-ikx_3)u^-(a_1,a_2,x_3)dx_3. \quad (5.24)$$

Finally, with conventional collimation, it should be possible to describe the beam in terms of packets of the form

$$u^-(x_1,x_2,x_3)=g(x_1,x_2)e(x_3). \quad (5.25)$$

[20] See the first article of footnote 2. In this discussion the energy spread of the incoming packet is not considered.

[21] The final result in Eq. (5.24) is obtained from the theory of Fourier transforms and implies physically harmless mathematical restrictions on $u^-(x_1,x_2,x_3)$.

In this event, Eq. (5.22) becomes

$$P'(\Omega)\approx P(\mathbf{a})\int_\Omega d\Omega\int_0^\infty dk\sigma_k(\theta,\phi)|\hat{e}(k)|^2, \quad (5.26)$$

where $\hat{e}(k)$ is the Fourier transform of $e(x_3)[\hat{e}(k)=0$ for $k<0]$ and $P(\mathbf{a})=|g(a_1,a_2)|^2$. Since $u^-(x_1,x_2,x_3)$ is normalized, $\int_{-\infty}^\infty\int_{-\infty}^\infty P(\mathbf{a})da_1da_2=1$ and $\int_0^\infty|\hat{e}(k)|^2=1$. Equation (5.26), which because of Eq. (5.14) is practically equivalent to Eq. (5.1), is the final result. It shows how the cross section is to be averaged over the energy spectrum of the incoming beam, and shows explicity through $P(\mathbf{a})$ how the scattering decreases when the target is not in the center of the beam.

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APPENDIX A

In this appendix, the relation between the Fourier-Plancherel transform, $\hat{u}(k_1,k_2,k_3)$, of $u(x_1,x_2,x_3)$ and the transform, $\{\phi_{ml}(k)\}$, for $V=0$ is established. Let $u_n(r,\theta,\phi)$ be equal to $u(r,\theta,\phi)$ for $0\leqslant r\leqslant n$ and zero otherwise. Because of the norm-preserving properties of both transforms and because $u_n\to u$ in mean square, $\hat{u}_n\to\hat{u}$, and $\phi_{mln}(k)\to\phi_{ml}(k)$ in mean square. ($\{\phi_{mln}(k)\}\equiv F_0u_n$.) Since $\hat{u}_n$ and $\hat{u}$ belong to L^2, they possess expansions of the form given in Eqs. (2.1)–(2.3). Let $\gamma_{mln}(k)$ and $\gamma_{ml}(k)$ correspond, respectively, to the quantity called $\alpha_{ml}(r)$ in these equations. Clearly, $\gamma_{mln}(k)\to\gamma_{ml}(k)$ in mean square. Furthermore,

$$\gamma_{mln}(k)=k\int_0^\pi\int_0^{2\pi}\bar{Y}_m(\theta,\phi)d\Omega(2\pi)^{-\frac{3}{2}}\times\int_0^n r'^2dr'\int_0^\pi\int_0^{2\pi}\exp(-i\mathbf{k}\cdot\mathbf{r}')u(r',\theta',\phi')d\Omega', \quad (A1)$$

where $\mathbf{k}$ is the radius vector to the point (k,θ,ϕ). In Eq. (A1), the order of integration can be reversed and the exponential can be expanded in terms of spherical harmonics and Bessel functions. In this way, there results

$$\gamma_{mln}(k)=(-i)^l\int_0^n\int_0^\pi\int_0^{2\pi}(kr)^{\frac{1}{2}}J_{l+\frac{1}{2}}(kr)\times\bar{Y}_{ml}(\theta,\phi)ru(r,\theta,\phi)drd\Omega$$
$$=(-i)^l\phi_{mln}(k). \quad (A2)$$

The last equality in Eq. (A2) follows from Eqs. (2.2) and (2.5) and the fact that for $V=0$ $\psi_l(r,k)$ is equal to $(kr)^{\frac{1}{2}}J_{l+\frac{1}{2}}(kr)$. It follows from Eq. (A2) and the convergence of $\gamma_{mln}(k)$ and $\phi_{mln}(k)$ that

$$\gamma_{ml}(k) = (-i)^l \phi_{ml}(k) \tag{A3}$$

almost everywhere. Furthermore, from the definition of $\gamma_{ml}(k)$ it is easy to see that for any finite K and $p>0$

$$\int_0^K \int_0^\pi \int_0^{2\pi} k^p |\hat{u}(k,\theta,\phi)|^2 k^2 dk d\Omega = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \int_0^K k^p |\phi_{ml}(k)|^2 dk. \tag{A4}$$

By taking $p=4$, it follows that $\|k^2\hat{u}\| < \infty$ if and only if Eq. (3.1) is satisfied. (Note that $V(r)=0$.) Furthermore, from Eq. (A3) and the bi-uniqueness of the transforms in question, it follows that when $\|k^2\hat{u}\| < \infty$, the function whose Fourier-Plancherel transform is $(k^2/2\mu)\hat{u}$ is identical with $F_0^{-1}\{(k^2/2\mu)\phi_{ml}(k)\}$. Hence, H_0, as defined by Eqs. (3.1) and (3.2), is equal to the operator multiplication by $k^2/2\mu$ in the space of Fourier-Plancherel transforms.

To see that the foregoing is true only with the boundary condition $\psi_0(x,k) = 0(x)$ for $x \to 0$, consider the radial part of the transform for $l=0$ without this condition.[22] For any function $u(r)$ belonging to $L^2(0,\infty)$

$$u(r) = \lim_{\omega\to\infty} \int_0^\omega \psi^\alpha(r,k)\phi^\alpha(k)dk, \tag{A5}$$

where

$$\phi^\alpha(k) = \lim_{\omega\to\infty} \int_0^\omega \psi^\alpha(x,k)u(x)dx. \tag{A6}$$

[22] E. C. Titchmarsh, *Eigenfunction Expansions Associated with Second Order Differential Equations* (Oxford University Press, London, England, 1946), p. 59.

The function $\psi^\alpha(r,k)$ is given by

$$\psi^\alpha(x,k) = \frac{2^{\frac{1}{2}}}{\pi^{\frac{1}{2}}} \left\{ \frac{\cos\alpha}{(\cos^2\alpha + k^2\sin^2\alpha)^{\frac{1}{2}}} \sin kx - \frac{k\sin\alpha}{(\cos^2\alpha + k^2\sin^2\alpha)^{\frac{1}{2}}} \cos kx \right\}. \tag{A7}$$

For $\alpha=0$, $\psi^\alpha(x,k)$ reduces to the function $\psi_0(x,k)$ which figures in Eqs. (2.4)–(2.6). Now consider the function $g(x_1,x_2,x_3) = \exp(-pr)$. It belongs to L^2 and it is readily verified that $\int\int\int |k^2\hat{g}(k_1,k_2,k_3)|^2 d\mathbf{k} < \infty$. Therefore, g belongs to the domain of the operator, multiplication by $k^2/2\mu$ in the space of Fourier-Plancherel transforms.

Let $x^\alpha(k)$ be the transform of g defined by Eqs. (2.1)–(2.6) for $V=0$ using the $\psi^\alpha(x,k)$. (Only the term with $l=0$ contributes.) In this case the function $u(r)$ in Eqs. (A5) and (A6) is $2\pi^{\frac{1}{2}}r\exp(-pr)$. Direct calculation now shows that as $k\to\infty$,

$$\begin{aligned} x^\alpha(k) &= (2\sqrt{2}/k^2)(1+0(k^{-2})); && \sin\alpha \neq 0, \\ &= 0(k^{-3}), && \sin\alpha = 0. \end{aligned} \tag{A8}$$

From Eq. (A8) it is clear that $k^2x^\alpha(k)$ belongs to $L^2(0,\infty)$ if and only if $\sin\alpha=0$. Therefore, $g(x_1,x_2,x_3)$ is in the domain of the operator, multiplication by $k^2/2\mu$ in the space of the transform defined by Eqs. (2.1)–(2.6) if and only if $\sin\alpha=0$. Thus, the domains of the operators, multiplication by $k^2/2\mu$ in the space of Fourier-Plancherel transforms, $\hat{u}$, and multiplication by $k^2/2\mu$ in the space of the transforms F_0u are identical if and only if $\sin\alpha=0$.