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SCATTERING THEORY

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Lecture Notes on Scattering Theory*

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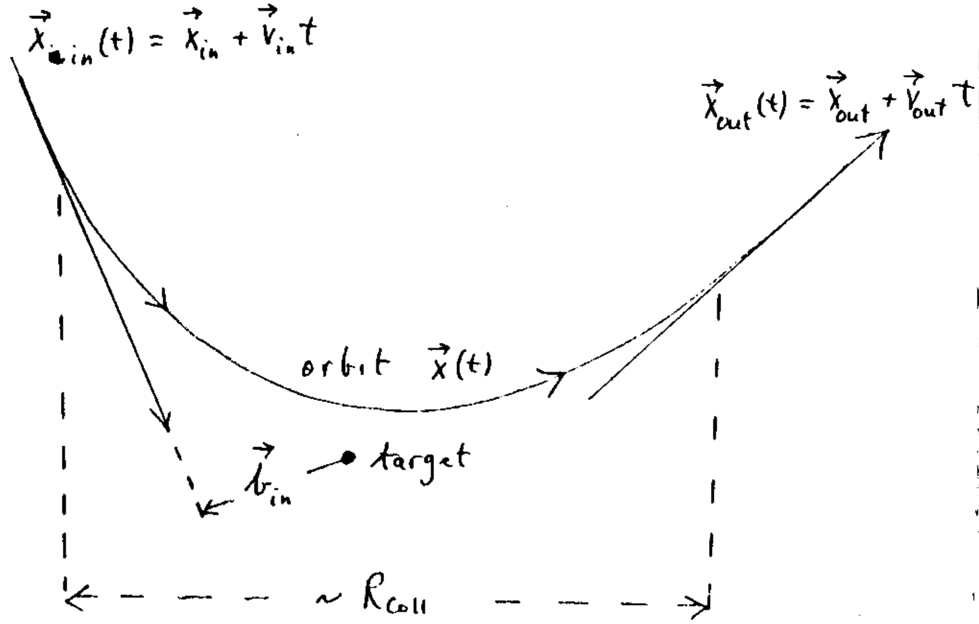
POTENTIAL SCATTERING

Consider a particle of mass μ incident on a real local potential $W(\vec{x})$. Classically, the



particle enters and exits the collision along in- and out-asymptotes, $\vec{x}_{in}(t)$ and $\vec{x}_{out}(t)$, respectively. (See J.R. Taylor, Scattering Theory, Wiley, New York, 1972.) These asymptotes are specified by the parameters $(\vec{x}_{in}, \vec{v}_{in})$ and $(\vec{x}_{out}, \vec{v}_{out})$. For reasonable potentials there is a one-one correspondence between the in- and out-asymptotes.

The orbit $\vec{x}(t)$ differs appreciably from a straight line only inside the interaction region, whose linear size is of order R_{coll}. Since our target has no structure, the collision is elastic ($|\vec{v}_{in}| = |\vec{v}_{out}| \equiv v$) and the classical collision duration is $t_{coll} \sim R_{coll}/v$. (If the potential has a Coulomb tail, the in- and out-asymptotes should be replaced by hyperbolic trajectories, and R_{coll} refers to the short-range part of the interaction, which is responsible for the deviation from pure Coulombic ~~p~~ motion.) Typical collision durations are less than 10^{-10} sec., often much smaller; for a 50 eV electron incident on a neutral atom, we have (e.g. R_{coll} ~ 100 a.u.) $t_{coll} \sim 10^{-15}$ sec.

In the usual scattering experiment we have a collimated beam of particles incident on a small volume containing many targets. The impact parameter, $\vec{b}_{in}$, that is, the component of $\vec{x}_{in}(t)$ perpendicular to $\vec{v}_{in}$, takes on random values, giving rise to a range of out-asymptotes.

In quantum mechanics we cannot simultaneously specify both $\vec{x}_{in}$ and $\vec{v}_{in}$ precisely. Rather, we represent the incoming particle by a localized wavepacket $|\Phi_{in}(t)\rangle$ which is peaked in both coordinate and momentum space, subject to the uncertainty principle $\Delta x \Delta p \sim \hbar$. The wavepacket moves with a group speed $\vec{v}_{in}$, and it spreads in space as it evolves forward in time. If Δx is the initial linear dimension of the wavepacket, the momentum distribution has a linear width $\delta p \sim \hbar/\Delta x$, and after a time t the wavepacket spreads ... $(\hbar/m\Delta x)t$, which is ~~[illegible]~~

negligible compared to the initial size Δx provided that $t \ll \mu(\Delta x)^2/\hbar$. This condition is normally satisfied for $t = t_{coll}$ so that wavepacket spreading can be neglected throughout the scattering process.

What is the quantum value for t_{coll}? For a typical nearly monoenergetic incident beam, Δp is sufficiently small that Δx is larger than R_{coll}. In this case one might think that ~~characteristic collision~~ t_{coll} ~~duration~~ is the time it takes the free particle wavepacket to pass a specific point in space. This latter time is $\sim \Delta x/v$, which we can rewrite as $\hbar/\Delta E$ where ΔE, the energy width of the free particle wavepacket, is $p\Delta p/\mu \sim \hbar(v/\Delta x)$ with $p = \mu v$. However, recall that the wavefunction ~~wavepacket~~ does not give information about

a single particle but rather about the statistical properties of an ensemble of particles. The effective quantum collision duration is, in fact, determined by the magnitude of the energy fluctuations which can occur during the collision. Fluctuations much larger than $E \equiv \frac{1}{2}\mu v^2$, the incident energy, are improbable; therefore $t_{coll} \sim \hbar/E$, the time over which energy fluctuations of order E may occur. Actually, the magnitude of the energy fluctuations is restricted not only by E but also by the difficulty of transferring a large amount of momentum to and from the particle. Momentum transfers much larger than $\sim \hbar/R_{coll}$ are improbable, and therefore energy fluctuations much larger than $(P/\mu)(\hbar/R_{cou})$ are improbable. If $E \gtrsim (P/\mu)(\hbar/R_{cou})$, that is, if $\mu v R_{cou}/\hbar \gtrsim 1$, the quantum time $\hbar/E$ is smaller than the classical time R_{cou}/v, and it is the latter time which characterizes the collision duration.

The out-asymptote is specified by a localized wavepacket $|\Phi_{out}(t)\rangle$.

We want to solve, in general, the time-dependent Schroedinger equation

$$i\hbar \frac{d}{dt} |\Psi(t)\rangle = H(t)|\Psi(t)\rangle \qquad (1)$$

subject to either the boundary condition

$$|\Psi(t)\rangle \to |\Phi_{in}(t)\rangle \quad \text{as } t \to -\infty \qquad (2a)$$

or

$$|\Psi(t)\rangle \longrightarrow |\Phi_{out}(t)\rangle \quad \text{as } t \to \infty . \qquad (2b)$$

(We allow the Hamiltonian $H(t)$ to be time-dependent.)

Since the Schroedinger equation is linear, we may write, for any t and t_0,

$$|\Psi(t)\rangle = U(t, t_0)\,|\Psi(t_0)\rangle \quad , \qquad (3)$$

where $U(t,t_0)$ is a linear operator, the <u>time-evolution operator</u>. Substituting (3) into (1) and noting that $|\Psi(t_0)\rangle$ is arbitrary, we have

$$i\hbar \frac{dU(t,t_0)}{dt} = H(t)\,U(t,t_0) \quad , \qquad (4a)$$

$$U(t,t) = 1 \quad . \qquad (4b)$$

~~If the Hamiltonian is time-indept, that is, if $H(t) \equiv H$, we have the formal solution~~

$$\cancel{U(t,t_0) = e^{-i(t-t_0)H/\hbar} \qquad (5)}$$

The formal solution of Eq. (4) is

$$\mathcal{U}(t,t_0) = \mathcal{T} \sum_n \frac{1}{n!} \left\{ -\frac{i}{\hbar} \int_{t_0}^{t} dt'\, H(t') \right\}^n$$

$$= \mathcal{T} \exp\left\{ -\frac{i}{\hbar} \int_{t_0}^{t} dt'\, H(t') \right\} , \qquad (5)$$

where the time-ordering operator $\mathcal{T}$ rearranges a product of n one-dimensional integrals $\int_{t_0}^{t} dt_j\, H(t_j)$, $j = 1, 2, \cdots, n$, as a single n-dimensional integral whose integrand $H(t_n) H(t_{n-1}) \cdots H(t_1)$ is ordered so that $t_n > t_{n-1} > \cdots > t_1$.

We can easily establish several useful properties of $\mathcal{U}(t,t_0)$. The group property

$$\mathcal{U}(t,t_0) = \mathcal{U}(t,t')\,\mathcal{U}(t',t_0) \qquad , (6)$$

follows from (3) upon noting that if $|\Psi(t')\rangle = \mathcal{U}(t',t_0)|\Psi(t_0)\rangle$ we have

$$|\Psi(t)\rangle = \mathcal{U}(t,t')\,|\Psi(t')\rangle$$

$$= \mathcal{U}(t,t')\,\mathcal{U}(t',t_0)\,|\Psi(t_0)\rangle .$$

Physically realizable states of the particle are represented by vectors which belong to the Hilbert space of vectors with finite norm. On this space the Hamiltonian $H(t)$ is Hermitian, $H(t)^\dagger = H(t)$. Taking the adjoint of Eq. (4a), and regarding $H(t)$ as Hermitian, we have

$$i\hbar \frac{d}{dt}\, \mathcal{U}(t,t_0)^\dagger = -\,\mathcal{U}(t,t_0)^\dagger H(t) . \qquad (7)$$

It follows from Eqs. (4a) and (7) that

$$i\hbar \frac{d}{dt} \left\{ \mathcal{U}(t,t_0)^\dagger\, \mathcal{U}(t,t_0) \right\} = 0 ,$$

so that $\mathcal{U}(t,t_0)^\dagger \mathcal{U}(t,t_0)$ is constant in time. Putting $t = t_0$, we see from Eq. (4b) that this constant is unity. Hence $\mathcal{U}(t,t_0)$ is isometric:

$$\mathcal{U}(t,t_0)^\dagger\, \mathcal{U}(t,t_0) = 1 . \qquad (8)$$

It follows that $U(t,t_0)$ preserves the norm of the state vector $|\Psi(t)\rangle$:

$$\langle\Psi(t)|\Psi(t)\rangle = \langle\Psi(t_0)|\, U(t,t_0)^\dagger U(t,t_0)\,|\Psi(t_0)\rangle$$
$$= \langle\Psi(t_0)|\Psi(t_0)\rangle .$$

We can derive a further property of the evolution operator by starting from $U(t,t_0)\,U(t_0,t) = 1$, which follows from the group property, and premultiplying this equation by $U(t,t_0)^\dagger$, using the isometric property to give

$$U(t_0,t) = U(t,t_0)^\dagger . \qquad (9)$$

We immediately obtain another differential equation for $U(t,t_0)$ by using this last property in Eq. (7), with t and t_0 interchanged; ~~it~~ we have

$$i\hbar \frac{d}{dt_0} U(t,t_0) = -\,U(t,t_0)\,H(t_0) . \qquad (10)$$

From Eq. (10) and its adjoint we see that

$$i\hbar \frac{d}{dt_0}\left\{ U(t,t_0)\,U(t,t_0)^\dagger \right\} = 0 .$$

It follows that

$$U(t,t_0)\,U(t,t_0)^\dagger = 1 , \qquad (11)$$

and hence $U(t,t_0)$ is not merely isometric, it is unitary.

Having derived two differential equations for the evolution operator, we now derive two integral equations. We start from the expression

$$\underbrace{\mathcal{J}(t,t_0) =}_{\wedge} -\frac{i}{\hbar}\int_{t_0}^{t} dt' \left\{ U(t,t')\,\mathcal{H}(t')\,U_{tr}(t',t_0) - \left[\mathcal{H}(t')\,U(t',t)\right]^\dagger U_{tr}(t',t_0) \right\}$$

where $\mathcal{H}(t) = H(t) - i\hbar(d/dt)$ and where $\mathcal{U}_{tr}(t, t_0)$ is a trial approximation to $\mathcal{U}(t,t_0)$ satisfying the correct boundary condition $\mathcal{U}_{tr}(t_0, t_0) = 1$. Using Eq. (9) and recalling that $H(t')$ is Hermitian (on the space $\mathcal{S}$ of physically realizable states), the terms in $H(t')$ cancel in the integrand of $\mathcal{I}(t,t_0)$, and the right-hand side of Eq. (12) reduces to

$$\mathcal{I}(t,t_0) = -\frac{i}{\hbar}\int_{t_0}^{t} dt' \left\{ -i\hbar\, \mathcal{U}(t,t') \frac{d}{dt'} \mathcal{U}_{tr}(t',t_0) - i\hbar \frac{d\mathcal{U}(t,t')}{dt'} \mathcal{U}_{tr}(t',t_0) \right\}$$

$$= -\int_{t_0}^{t} dt' \frac{d}{dt'} \left[\mathcal{U}(t,t') \mathcal{U}_{tr}(t',t_0) \right]$$

$$= -\mathcal{U}_{tr}(t,t_0) + \mathcal{U}(t,t_0) .$$

Using, instead, $\mathcal{H}(t')\mathcal{U}(t',t) = 0$ on the right-hand side of Eq. (12) we obtain

$$\mathcal{I}(t,t_0) = -\frac{i}{\hbar}\int_{t_0}^{t} dt' \, \mathcal{U}(t,t')\mathcal{H}(t')\mathcal{U}_{tr}(t',t_0) .$$

It follows that

$$\mathcal{U}(t,t_0) = \mathcal{U}_{tr}(t,t_0) - \frac{i}{\hbar}\int_{t_0}^{t} dt' \, \mathcal{U}(t,t')\mathcal{H}(t')\mathcal{U}_{tr}(t',t_0) . \quad (13)$$

Taking the adjoint of Eq. (13), using Eq. (9), and interchanging t and t_0 we obtain the alternative integral equation

$$\mathcal{U}(t,t_0) = \mathcal{U}_{tr}(t,t_0) - \frac{i}{\hbar}\int_{t_0}^{t} dt' \left[\mathcal{H}(t')\mathcal{U}_{tr}(t',t) \right]^{\dagger} \mathcal{U}(t',t_0) . \quad (14)$$

At asymptotically large times the particle is at an asymptotically large distance from the target and it is governed by the free-particle Hamiltonian $H_0(t) \equiv H(t) - W$ (where W is the ~~target~~ ~~potential~~ interaction of the particle with the target). If there is no radiation field we have $H_0(t) = H_0 \equiv \vec{P}^2/2\mu$, the kinetic energy operator. The motion of the free particle is governed by $\mathcal{U}_0(t,t')$ where

$$i\hbar \frac{d}{dt} U_0(t,t') = H_0(t)\, U_0(t,t') , \qquad (15)$$

with $U_0(t,t) = 1$. The in- and out-asymptotes are represented by

$$|\Phi_{in}(t)\rangle = U_0(t,0)|\Phi_{in}\rangle , \qquad (16a)$$

$$|\Phi_{out}(t)\rangle = U_0(t,0)\,|\Phi_{out}\rangle , \qquad (16b)$$

~~and the state vector~~ ~~and the vector which represents the~~

and the scattering state at time t is represented by

$$|\Psi(t)\rangle = \lim_{t_0 \to -\infty} U(t,t_0)|\Phi_{in}(t_0)\rangle \qquad (17a)$$

$$= \lim_{t_0 \to \infty} U(t,t_0)|\Phi_{out}(t_0)\rangle . \qquad (17b)$$

Introducing ~~the operators~~

$$U^{\pm}(t) = \lim_{t_0 \to \mp\infty} U(t,t_0)\,U_0(t_0,0) , \qquad (18)$$

... (16) and (17) that

$$|\Psi(t)\rangle = U^{+}(t)\,|\Phi_{in}\rangle \qquad (19a)$$

$$= U^{-}(t)\,|\Phi_{out}\rangle . \qquad (19b)$$

The operators $U^{\pm}(t)$ are isometric, but they may not be unitary, even though they are limits of ~~operators~~ an operator $U(t,t_0)U_0(t_0,0)$ which is unitary for finite t_0 (and t). If the $U^{\pm}(t)$ are unitary they possess inverses $U^{\pm}(t)^{\dagger}$ which are defined on the whole Hilbert space $\mathcal{H}$, ~~which~~ and this implies that the ranges $\mathcal{R}^{\pm}$ of the operators $U^{\pm}(t)$, that is, the spaces onto which ~~Hilbert space~~ $\mathcal{H}$ is mapped by the $U^{\pm}(t)$, are equal to the whole of $\mathcal{H}$. ~~Hilbert space.~~ However, the ranges $\mathcal{R}^{\pm}$ are just the space of scattering states, since any vector in $\mathfrak{S}$ represents a suitable asymptote which is transformed by $U^+(t)$ or $U^-(t)$ into a unique scattering state. Thus if $H(t)$ supports bound states — this is possible only if $H(t)$ is time-indept., as in radiationless scattering — these bound states are excluded from the ranges $\mathfrak{R}^\pm$; in this case the $U^\pm(t)$ are not unitary. However, when a radiation field is present $H(t)$ does not support bound states, and presumably the $U^\pm(t)$ are unitary.

Using the isometric property of $U^-(t)$, we have from Eqs. (19a) and (19b) that

$$|\Phi_{out}\rangle = S\,|\Phi_{in}\rangle \qquad (20)$$

where the scattering operator S, which maps any in-asymptote onto its corresponding

out-asymptote, is defined as

$$S = U^-(t)^\dagger\, U^+(t) \,, \qquad (21)$$

and is independent of t. The scattering operator is unitary. This follows because $U^+(t)$ is a norm-preserving map of $\mathfrak{S}$ onto $\mathfrak{R}^+$, and $U^-(t)^\dagger$ is a norm-preserving map of $\mathfrak{R}^-$ onto $\mathfrak{S}$, so that, since $\mathfrak{R}^+ = \mathfrak{R}^-$, S is a norm-preserving map of $\mathfrak{S}$ onto itself; this is the condition for S to be unitary.

We now derive a formal expression for the scattering state vector. Putting $\mathcal{U}_{tr}(t',t_0) = U_0(t',t_0)$ in Eq. (13), and using Eq. (15) to write

$$\mathcal{H}(t')\,U_0(t',t_0) = [H(t') - H_0(t')]\,U_0(t',t_0) = W\,U_0(t',t_0)\,,$$

we have

$$\mathcal{U}(t,t_0) = \mathcal{U}_0(t,t_0) - \frac{i}{\hbar}\int_{t_0}^{t} dt'\, \mathcal{U}(t,t')\, W\, \mathcal{U}_0(t',t_0) \quad . \qquad (22)$$

It follows from Eq. (17a), noting that

$$\mathcal{U}_0(t,t_0)|\Phi_{in}(t_0)\rangle = |\Phi_{in}(t)\rangle \; ,$$

that the scattering state vector is

$$|\Psi^+(t)\rangle = |\Phi_{in}(t)\rangle - \frac{i}{\hbar}\int_{-\infty}^{t} dt'\, \mathcal{U}(t,t')\, W\, |\Phi_{in}(t')\rangle \; , \qquad (23)$$

where we have attached the superscript "plus" to indicate that $|\Psi^+(t)\rangle$ is specified by the in-asymptote boundary condition. In principle, we can insert our formal solution for $\mathcal{U}(t,t')$, from Eq. (5), and evaluate the right-hand side of Eq. (23) to give $|\Psi^+(t)\rangle$. We can derive an integral equation for $|\Psi^+(t)\rangle$ by using

$$\mathcal{U}(t,t_0) = \mathcal{U}_0(t,t_0) - \frac{i}{\hbar}\int_{t_0}^{t} dt'\, \mathcal{U}_0(t,t')\, W\, \mathcal{U}(t',t_0) \; , \qquad (24)$$

which follows from Eq. (14), putting $\mathcal{U}_{tr}(t',t'') = \mathcal{U}_0(t',t'')$ and noting Eq. (9). Combining Eqs (17a) and (24) we obtain the integral equation

$$|\Psi^+(t)\rangle = |\Phi_{in}(t)\rangle - \frac{i}{\hbar}\int_{-\infty}^{t} dt'\, \mathcal{U}_0(t,t')\, W\, |\Psi^+(t')\rangle \; . \qquad (25)$$

A considerable simplification results if $H(t) = H$ is time-indept. because we can perform the integration over t' in Eq. (5) to give

$$\mathcal{U}(t,t_0) = e^{-(i/\hbar)(t-t_0)H} \quad . \qquad (26)$$

We now assume that $H(t) = H$ is time-indept., until further notice, and we examine radiationless scattering in some detail. Let $|\vec{k}\rangle$ denote an eigenvector of the canonical momentum operator $\vec{P}$ with eigenvalue $\hbar\vec{k}$. We express $|\Phi_{in}\rangle$ in terms of its Fourier transform:

$$|\Phi_{in}\rangle = \int d^3k\, a_{in}(\vec{k})\, |\vec{k}\rangle \; . \qquad (27)$$

Noting that $\mathcal{U}_0(t,t_0)$ is given by Eq (26) with H replaced by $H_0 = \vec{P}^2/2\mu$, and using from Eqs. (16a) and (~~23~~ 27) that

$$|\Phi_{in}(t)\rangle = \int d^3k\, a_{in}(\vec{k})\, e^{-iE_k t/\hbar}\, |\vec{k}\rangle \quad . \qquad (28)$$

Using Eqs. (23), (26), and (28) we obtain

$$|\Psi^+(t)\rangle = \int d^3k\, a_{in}(\vec{k}) \Big\{ e^{-iE_k t/\hbar} |\vec{k}\rangle - \frac{i}{\hbar} \int_{-\infty}^{t} dt'\, e^{-iE_k t'/\hbar} \times e^{-(i/\hbar)(t-t')H}\, W|\vec{k}\rangle \Big\} \; . \qquad (29)$$

~~To perform the integration over t' we~~

We have interchanged the order of the integrals over $\vec{k}$ and t'. The integral over t' now does not formally converge because the integrand does not vanish at the lower limit $t \sim -\infty$. However, before interchanging the order of the integrals, we may insert a convergence factor $e^{\eta t'/\hbar}$ (into the integrand,) where η is positive but infinitesimal.

This amounts to replacing W by $We^{\eta t'/\hbar}$ in Eq. (23), so that W is unchanged for finite t' but is cut off for $t' \sim -\infty$. This has no physical consequence because $W|\Phi_{in}(t')\rangle$ vanishes anyway for $t' \sim -\infty$ since, in coordinate space, $|\Phi_{in}(t')\rangle$ represents a particle which for $t' \sim -\infty$ is asymptotically far from the target, ~~in a region~~ and W vanishes in this asymptotic region. With the convergence factor included, we may perform the integration over t' in Eq. (29) to give

$$|\Psi^+(t)\rangle = \int d^3k\, a_{in}(\vec{k})\, e^{-iE_k t/\hbar}\, |\Psi^+_k\rangle \; , \qquad (30)$$

where

$$|\Psi^+_k\rangle = |\vec{k}\rangle + G(E_k + i\eta) W|\vec{k}\rangle \; , \qquad (31)$$

and where $G(E)$ is the Green function, or resolvent, operator, defined as

$$G(E) = 1/(E-H) \; . \qquad (32)$$

Were we to choose $a_{in}(\vec{k}) = \delta^3(\vec{k}-\vec{K})$ we would obtain, from Eq. (30),

$$|\Psi^+(t)\rangle = e^{-iE_K t/\hbar}\,|\Psi^+_{\vec{K}}\rangle \, . \qquad (33)$$

Of course, this choice of $a_{in}(\vec{k})$ corresponds to a free particle whose momentum is precisely defined as $\hbar\vec{K}$, and consequently the particle is unlocalized in coordinate space so that $|\Phi_{in}\rangle$ cannot represent a particle localized on an asymptotic trajectory; indeed, $|\Phi_{in}\rangle$ has an infinite norm, and does not belong to the Hilbert space $\mathcal{H}$ of physically realizable states. Nor does $|\Psi^+_{\vec{K}}\rangle$, which also has infinite norm, belong to $\mathcal{H}$. However,

the fact that $\langle\Psi^+_{\vec{k}}|\Psi^+_{\vec{k}}\rangle = \infty$ suggests that we should interpret $|\Psi^+_{\vec{k}}\rangle$ as describing not one particle but infinitely many particles which do not interact with each other. Thus, while $|\Psi^+_{\vec{k}}\rangle$ does not represent the scattering of a single (localized) particle, it does represent the scattering of a uniform monoenergetic beam of noninteracting particles, each having a well-defined incident momentum $\hbar\vec{k}$.

Premultiplying Eq. (31) by $(E_k+i\eta-H)$ we obtain

$$(E_k+i\eta-H)|\Psi^+_k\rangle = i\eta|\vec{k}\rangle \, , \qquad (34)$$

so that in the limit $\eta\to 0$, $|\Psi^+_k\rangle$ is an eigenvector of H with eigenvalue E_k. The $|\Psi^+_k\rangle$ form the set of scattering state eigenvectors, which are orthogonal to the bound state eigenvectors, $|\Psi_b\rangle$. If we put $a_{in}(\vec{k}) = \delta^3(\vec{k}-\vec{K})$ in Eq. (25), using Eq. (37), we obtain

$$e^{-iE_k t/\hbar}|\Psi^+_{\vec{k}}\rangle = e^{-iE_k t/\hbar}|\vec{k}\rangle - \frac{i}{\hbar}\int_{t_0}^{t} dt'\, U_0(t,t')\, W e^{-iE_k t'/\hbar}|\Psi^+_{\vec{k}}\rangle. \quad (35)$$

Using Eq. (26), with H replaced by H_0, we can perform the integration over t' in Eq. (35) to yield the integral equation, usually referred to as the Lippmann-Schwinger equation,

$$|\Psi^+_{\vec{k}}\rangle = |\vec{k}\rangle + G_0(E_k + i\eta)W|\Psi^+_{\vec{k}}\rangle, \quad (36)$$

where $G_0(E) = 1/(E - H_0)$ is the free-particle resolvent.

Rather than specify the scattering state vector by the in-asymptote boundary condition, we could specify it by the out-asymptote boundary condition. Thus, using Eq. (17b) with Eq. (22), we obtain instead of Eq. (23) the

equation

$$|\Psi^-(t)\rangle = |\Phi_{out}(t)\rangle + \frac{i}{\hbar}\int_t^{\infty} dt'\, U(t,t')W|\Phi_{out}(t')\rangle, \quad (37)$$

where the superscript "minus" reminds us that $|\Psi^-(t)\rangle$ is specified by the out-asymptote boundary condition. Instead of Eq. (25) we have

$$|\Psi^-(t)\rangle = |\Phi_{out}(t)\rangle + \frac{i}{\hbar}\int_t^{\infty} dt'\, U_0(t,t')\, W|\Psi^-(t')\rangle. \quad (38)$$

To perform the integration over t', when $H(t) = H$, we must insert a convergence factor $e^{-\eta t'/\hbar}$, and Eqs. (31) and (36) are replaced by

$$|\Psi^-_{\vec{k}}\rangle = |\vec{k}\rangle + G(E_k - i\eta)W|\vec{k}\rangle, \quad (39)$$

$$= |\vec{k}\rangle + G_0(E_k - i\eta)W|\Psi^-_{\vec{k}}\rangle. \quad (40)$$

$|\Psi^-_{\vec{k}}\rangle$ is also an eigenvector of H with eigenvalue E_k.

The bound state vectors $\{|\Phi_b\rangle\}$ together with the scattering state eigenvectors $\{|\Psi^+_{\vec k}\rangle\}$ or $\{|\Psi^-_{\vec k}\rangle\}$ form a complete set. The $\{|\Psi^\pm_{\vec k}\rangle\}$ are normalized as

$$\langle\Psi^\pm_{\vec k'}|\Psi^\pm_{\vec k}\rangle = \mathcal{N}_k\, \delta^3(\vec k' - \vec k). \qquad (41)$$

(The $\{|\vec k\rangle\}$ have a similar normalization.)

Let s denote the scale of the normalization, that is, s has the units of $\langle\Psi^\pm_{\vec k'}|\Psi^\pm_{\vec k}\rangle$ and is unity in these units. The normalization factor $\mathcal{N}_k$ has the dimensions of s/volume.

The number of particles in a beam described by $|\Psi^\pm_{\vec k}\rangle$ is $\langle\Psi^\pm_{\vec k}|\Psi^\pm_{\vec k}\rangle/s$, which is infinite. If $n(\vec k)\,d^3k$ is the number of states in the element d^3k, the completeness of the set of bound and scattering state eigenvectors can be expressed as

$$\frac{1}{s}\int d^3k\, n(\vec k)\,|\Psi^\pm_{\vec k}\rangle\langle\Psi^\pm_{\vec k}| + \sum_b |\Psi_b\rangle\langle\Psi_b| = 1, \qquad (42)$$

with $\langle\Psi_{b'}|\Psi_b\rangle = \delta_{b'b}$. Premultiplying Eq. (42) by $\langle\Psi^\pm_{\vec k'}|$, and postmultiplying by $|\Psi^\pm_{\vec k''}\rangle$, we obtain, using Eq. (41) and the orthogonality of the bound and scattering state eigenvectors,

$$\frac{1}{s}\, n(\vec k')\,\mathcal{N}_{k'}\langle\Psi^\pm_{\vec k'}|\Psi^\pm_{\vec k''}\rangle = \langle\Psi^\pm_{\vec k'}|\Psi^\pm_{\vec k''}\rangle.$$

Hence we have $n(\vec k) = s/\mathcal{N}_k$.

We are now ready to calculate the cross section for a beam of particles, that is incident along an asymptote represented by $|\Phi_{in}\rangle$, to scatter from the target and emerge along an asymptote represented by $|\Phi_{out}\rangle$. We assume that the out-asymptote is different from, and distinguishable from, the in-asymptote so that $\langle\Phi_{out}|\Phi_{in}\rangle = 0$. We start by imagining the beam to have a finite spatial extent and to consist of a large but finite number of localized particles, defined momentum close to $\hbar\vec{k}_i$. We look at scattering into an out-asymptote state in which the particles are ~~fairly~~ localized but have a fairly sharply defined momentum close to $\hbar\vec{k}_f$. Thus $|\Phi_{in}(t)\rangle$, $|\Phi_{out}(t)\rangle$, and $|\Psi^+(t)\rangle$ each have finite norm, equal to the normalization scale s multiplied by the number of particles in the beam. In the end we pass to the limit where the in- and out-asymptote momenta are precisely defined, (and the number of particles in the beam is infinite. We begin by calculating the number of particles which at time t are in the state represented by $|\Phi_{out}(t)\rangle$. This number is

$$N_{out}(t) = \left|\langle \Phi_{out}(t) | \Psi^+(t)\rangle\right|^2 / s^2 . \qquad (43)$$

From Eq. (25) we have, noting $\langle \Phi_{out}(t)|\Phi_{in}(t)\rangle = 0$,

$$\langle \Phi_{out}(t)|\Psi^+(t)\rangle = -\frac{i}{\hbar}\int_{-\infty}^{t} dt' \, \langle \Phi_{out}(t')| W e^{-\eta|t'|/\hbar} |\Psi^+(t')\rangle, \quad (4$$

where we have multiplied W by the convergence factor $e^{-\eta|t'|/\hbar}$ which, after our manipulations below, gaurantees convergence at the lower limit of the integral over t', and also at the upper limit when we let $t \to \infty$. From Eqs. (43) and (44) we have

$$\frac{dN_{out}(t)}{dt} = \frac{1}{s^2\hbar^2}\langle \Psi^+(t)| W e^{-\eta|t|/\hbar} |\Phi_{out}(t)\rangle \times \int_{-\infty}^{t} dt' \, \langle \Phi_{out}(t')| W e^{-\eta|t'|/\hbar} |\Psi^+(t')\rangle + \text{c.c.} \qquad (45)$$

where c.c. means "complex conjugate". We now put $a_{in}(\vec{k}) = \delta^3(\vec{k}-\vec{k}_i)$ and $a_{out}(\vec{k}) = \delta^3(\vec{k}-\vec{k}_f)$, so that $|\Phi_{out}(t)\rangle = \exp(-iE_{k_f}t/\hbar)|\vec{k}_f\rangle$ and $|\Psi^+(t)\rangle = \exp(-iE_{k_i}t/\hbar)|\Psi^+_{\vec{k}_i}\rangle$. We can readily perform the integration over t' in Eq. (45) to yield, for $t > 0$,

$$\frac{dN_{out}}{dt}(t) = \frac{2\eta}{\eta^2+(\Delta E)^2}\, e^{-\eta t/\hbar}\left\{2\cos(\Delta E t/\hbar) - e^{-\eta t/\hbar}\right\} \times \frac{1}{\hbar s^2}\left|T(\vec{k}_i \to \vec{k}_f)\right|^2 , \qquad (46)$$

where $\Delta E = E_{k_f} - E_{k_i}$ and where the scattering T-matrix is

$$T(\vec{k}_i \to \vec{k}_f) = \langle \vec{k}_f | W | \Psi^+_{\vec{k}_i} \rangle . \qquad (47)$$

The physical significance of the parameter η is that $\hbar/\eta$ is the characteristic time taken for the

beam to pass through the interaction region; the interaction $We^{-\eta|t|/\hbar}$ is nonnegligible only for times $|t| \lesssim \hbar/\eta$. Thus the collision is over after a time $t \sim \hbar/\eta$ and subsequently $dN_{out}(t)/dt$ vanishes exponentially because no further scattering can occur. In fact, $\hbar/\eta$ is the characteristic time for the wavepacket $|\Psi^+(t)\rangle$, which has a spatial extent greater than R_{coll}, to pass a given point in space. (Note that here $|\Psi^+(t)\rangle$ describes a beam of infinitely many particles, not a single particle, and $\hbar/\eta$ is the time taken for the beam, not an individual particle in the beam, to pass through the interaction region. The collision [illegible] single particle is, as discussed above, $\hbar/E_i$ or R_{cou}/v.) Thus the energy uncertainty ~~is~~ of the beam is of order η and we should consider scattering into ~~a~~ the group of states contained in a narrow energy interval (of width $\sim \eta$) centered at E_{k_f}. Since $d^3k = k^2 dk\, d\hat{k} = (\mu/\hbar^2)\, k\, dE_k\, d\hat{k}$, the density of states in the energy interval dE_k is

$$\rho'(\vec{k}) \equiv n(\vec{k})\, d^3k / dE_k$$

$$= (\mu s / \hbar^2 \mathcal{N}_k)\, k\, d\hat{k} \quad . \qquad (48)$$

To calculate the rate for scattering into this group of states we multiply the right-hand side of Eq. (46) by $\rho'(E_{k_f})\, dE_{k_f}$. Taking the limit $\eta \to 0$ and observing that in this limit

$$\frac{2\eta}{\eta^2 + (\Delta E)^2} = 2\pi\,\delta(\Delta E) \quad , \qquad (49)$$

we obtain ~~the~~ the time-independent rate for scattering into a group of states:

$$\frac{dN_{out}}{dt} = \frac{2\pi}{\hbar s^2}\, \rho'(\vec{k}_f)\, \left| T(\vec{k}_i \to \vec{k}_f) \right|^2 ; \qquad (50)$$

The delta function ~~is~~ $\delta(\Delta E)$ ensures energy conservation, $|\vec{k}_f| = |\vec{k}_i|$. To calculate the differential cross section for scattering into the direction $\hat{k}_f$ we divide the rate by both $d\hat{k}_f$ and the flux of the incident beam. The wave function representing the incident beam is, in coordinate space,

$$\Phi_{in}(\vec{x}) \equiv \langle \vec{x} \,|\, \vec{k}_i \rangle = \mathcal{N}_{k_i}^{1/2}\, (2\pi)^{-3/2}\, e^{i \vec{k}_i \cdot \vec{x}} \quad . \; ($$

The flux is the magnitude of the current density

$$\vec{J}_i = \frac{1}{S} \mathrm{Re} \left\{ \Phi_{in}(\vec{x})^* \frac{\hbar}{i\mu} \nabla_{\vec{x}} \Phi_{in}(\vec{x}) \right\}$$

$$= \mathcal{N}_k (2\pi)^{-3/2} (\hbar \vec{k}_i / \mu S) . \quad (52)$$

It follows that the differential cross section is

$$\frac{d\sigma}{d\hat{k}_f}(\vec{k}_i \to \vec{k}_f) = |f(\vec{k}_i \to \vec{k}_f)|^2 , \quad (53)$$

where the scattering amplitude is

$$f(\vec{k}_i \to \vec{k}_f) = -(2\pi)^2 (\mu/\hbar^2 \mathcal{N}_k) T(\vec{k}_i \to \vec{k}_f); \quad (54)$$

the minus sign is merely conventional.

In general we cannot evaluate $T(\vec{k}_i \to \vec{k}_f)$ exactly since we do not know $|\Psi^+_{\vec{k}_i}\rangle$ exactly. However, as a first

approximation we can replace $|\Psi^+_{\vec{k}_i}\rangle$ by the state vector $|\vec{k}_i\rangle$ of the incoming free particles. This yields the "Born" approximation:

$$T(\vec{k}_i \to \vec{k}_f) \approx \langle \vec{k}_f | W | \vec{k}_i \rangle . \quad (55)$$

Successively better approximations can, if W is sufficiently weak, be generated through the Born expansion of the resolvent $G(E)$:

$$G(E) = G_0(E) \sum_{n=0}^{\infty} \{ W G_0(E) \}^n . \quad (56)$$

We can evaluate $G_0(E)$ in closed form. Let us choose the normalization factor $\mathcal{N}_k = 1$, so that $\langle \vec{k} | \vec{k}' \rangle = \delta^3(\vec{k} - \vec{k}')$ and

$$\int d^3k \, |\vec{k}\rangle\langle\vec{k}| = 1 . \quad (57)$$

we have

$$G_0(E) = G_0(E)\int d^3k\; |\vec{k}\rangle\langle\vec{k}|$$

$$= \int d^3k\; \frac{|\vec{k}\rangle\langle\vec{k}|}{E - \hbar^2k^2/2\mu}$$

since $G_0(E) = 1/(E - \vec{p}^{\,2}/2\mu)$. Hence

$$\langle\vec{x}|G_0(E)|\vec{x}\,'\rangle = (2\pi)^{-3}\int d^3k\; \frac{e^{i\vec{k}\cdot(\vec{x}-\vec{x}\,')}}{E - \hbar^2k^2/2\mu}$$

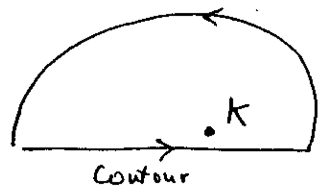
$$= (2\mu/\hbar^2)\,(2\pi)^{-3}\int_0^\infty k^2dk\int_{-1}^{1}d\mu\int_0^{2\pi}d\phi\;\frac{e^{ik\rho\mu}}{K^2-k^2}$$

where $\rho = |\vec{x}-\vec{x}\,'|$ and $E = \hbar^2K^2/2\mu$, with μ the cosine of the angle between $\vec{k}$ and $\vec{x}-\vec{x}\,'$. The integrand is indept. of ϕ, and so the integral over ϕ gives just a factor of 2π. Performing the integration over μ gives

$$\langle\vec{x}|G_0(E)|\vec{x}\,'\rangle = (2\mu/\hbar^2)\,\frac{(2\pi)^{-2}}{i\rho}\int_0^\infty k\,dk\,\frac{(e^{ik\rho}-e^{-ik\rho})}{K^2-k^2}$$

$$= (2\mu/\hbar^2)\,\frac{(2\pi)^{-2}}{i\rho}\int_{-\infty}^{\infty}\frac{k\,dk\,e^{ik\rho}}{K^2-k^2}\,, \qquad (58)$$

where we have used $\int_0^\infty dx\, f(-x) = \int_{-\infty}^0 dx\, f(x)$ in the last step. We now see that if K is real, the integrand is singular at $k = \pm K$. However, we are interested in values of E that have an infinitesimal imaginary part, $\pm i\eta$. We complete the contour of integration with a semicircle of infinite radius in the upper half of the complex k-plane. Suppose that $\mathrm{Im}(E) = \eta$. Then the integrand has a pole inside this contour at $k = K$, just above the real axis. Using Cauchy's thm we obtain



$$\langle\vec{x}|G_0(E+i\eta)|\vec{x}\,'\rangle = -\frac{\mu}{2\pi\hbar^2}\,\frac{e^{iK|\vec{x}-\vec{x}\,'|}}{|\vec{x}-\vec{x}\,'|}\,.$$

To be continued.