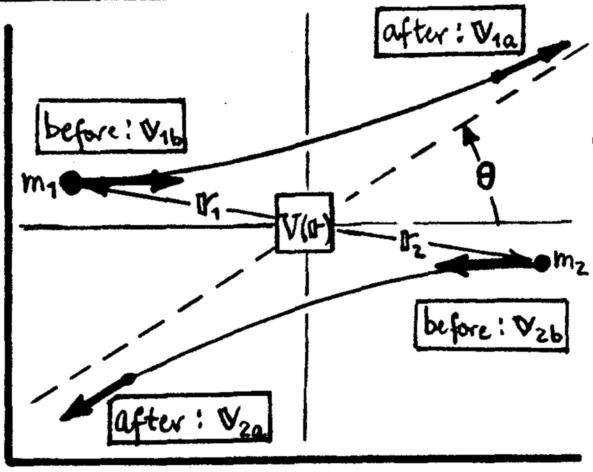
General description of a scattering event.

Ref. Davydov, ¶ 106-108; Sakurai, Secs. 7.1-7.3

QM Theory of Elastic Scattering



1) A "scattering" (QM or classical) refers to the change in trajectory of particles m_1 & m_2 during a "collision", as pictured at right. Initially m_1 & m_2 are at very large separation, are therefore free (for all practical purposes), and are moving at velocities $\mathbf{v}_{1b}$ & $\mathbf{v}_{2b}$. In time, the relative separation $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$ becomes small enough so that m_1 & m_2 interact via some potential $V(\mathbf{r})$. Here they can exchange momentum and thus alter each other's trajectories. After a long time, m_1 & m_2 are again far enough apart so that $V(\mathbf{r}) \to 0$ and the particles can again be considered free. But now they are moving at different velocities $\mathbf{v}_{1a}$ & $\mathbf{v}_{2a}$; they have been "scattered" through the $\measuredangle\, \theta$.

The problem is: given $\mathbf{v}_{1b}$ & $\mathbf{v}_{2b}$, and $V(\mathbf{r})$, find $\mathbf{v}_{1a}$ & $\mathbf{v}_{2a}$, and θ.

REMARKS on scattering problem.

1. The scattering is called "elastic" if the internal states of m_1 & m_2 do not change during the collision; only the kinetic character of the trajectories changes. m_1 & m_2 are treated like billiard balls, and this simplifies the QM problem considerably... m_1 & m_2 act like free particles before & after the collision, and can therefore be described by free particle wavefcns: $\phi(\mathbf{r}) \sim e^{i\mathbf{k}\cdot\mathbf{r}}$, $\mathbf{k} = \frac{m\mathbf{v}}{\hbar}$.

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2. m_1 & m_2 are "free" @ $t = -\infty$ (when $|\mathbf{r}_1 - \mathbf{r}_2|$ is "large") and again @ $t = +\infty$... meanwhile they undergo a transient coupling by $V(\mathbf{r})$, when $|\mathbf{r}|$ is "small". So the problem for just two particles has an intrinsic time dependence. We can eliminate time from the problem, however, by thinking of a continuous stream of identical particles m_1 entering from the left and colliding with a stream of m_2's from the right. Then the problem is steady-state, and we can use the time-independent Schrödinger Eqtn ($\forall\, t = \mp\infty$ freedom replaced by freedom @ $r \to \infty$).

REMARKS (cont'd)

3. Free particles (as $|\mathbf{r}| = |\mathbf{r}_1 - \mathbf{r}_2| \to \infty$) have wave fcns: $\phi(\mathbf{r}) = Ce^{i\mathbf{k}\cdot\mathbf{r}}$, where C is a norm cnst, and -- if the particle mass is m and its (kinetic) energy is E -- the wave # k satisfies: $k^2 = 2mE/\hbar^2$. The space-dependent ϕ's obey the free particle Schrodinger Eqtn, namely: $(\nabla^2 + k^2)\phi = 0$. Now, if in some region of space this free particle encounters some potential $V(\mathbf{r})$, then $\phi(\mathbf{r}) \to \psi(\mathbf{r})$, where ψ obeys the full Schrodinger Eqtn

$$\boxed{(\nabla^2 + k^2)\psi(\mathbf{r}) = \left[\frac{2m}{\hbar^2}V(\mathbf{r})\right]\psi(\mathbf{r})}. \tag{1}$$

In any region where $V(\mathbf{r}) \to 0$ (e.g. @ $|\mathbf{r}| \to \infty$), we will have $\psi \to$ some free particle $\tilde{\phi}$, but presumably with a different momentum $\mathbf{k} \to \tilde{\mathbf{k}} \neq \mathbf{k}$.

4. Now we claim Eq. (1) is just the eqtn we want to solve for the scattering problem. First -- with the idea of a steady stream of m's "colliding" with $V(\mathbf{r})$, we can get away with just the space-dependent analysis, replacing initial & final conditions of the particles being "free" at $t = \mp\infty$ with boundary conditions of $\psi \to \phi$(free) as $r \to \infty$. Second [per QM 507 Prob. # 17], when the interaction V is a fcn only of the relative position $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$, we can transform the two-body problem: m_1 @ $\mathbf{r}_1$ interacting with m_2 @ $\mathbf{r}_2$ by $V(\mathbf{r}_1 - \mathbf{r}_2)$, to an equivalent one-body problem: $m = \frac{m_1 m_2}{m_1 + m_2}$ interacting with $V(\mathbf{r})$, by means of the center-of-mass transformation.

So we proceed to solve Eq. (1) for the scattering problem, keeping in mind that k^2 is always (+)ve and unquantized, and $\psi \to \phi$(free) as $r \to \infty$.

The easiest way to think that $\psi \to \phi$(free) as $r \to \infty$ is to imagine that $V(\mathbf{r})$ is non-vanishing only in a limited region of space: $r \lesssim d$.

Solution for steady-state scattering ψ.

2) Eq. (1) is an inhomogeneous Helmholtz Equation for ψ(scattering), i.e.

$$\rightarrow (\nabla^2 + k^2)\psi(\mathbf{r}) = f(\mathbf{r}), \quad f(\mathbf{r}) = \frac{2m}{\hbar^2} V(\mathbf{r})\psi(\mathbf{r}). \qquad (2)$$

By results of probm #15, Lippmann-Schwinger version of Eq (2) above is:

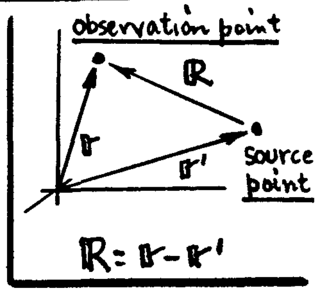
$$\psi(\mathbf{r}) = \phi(\mathbf{r}) + \frac{2m}{\hbar^2}\int d^3x'\, G(\mathbf{r},\mathbf{r}')V(\mathbf{r}')\psi(\mathbf{r}'),$$

w/ $[\nabla^2 + k^2]\, G(\mathbf{r},\mathbf{r}') = \delta(\mathbf{r}-\mathbf{r}')$, & $\phi(\mathbf{r})$ = free-particle plane wave.

So, we go directly to Eq. (5) next page.

... that

$$\rightarrow \boxed{(\nabla^2 + k^2)\, G(\mathbf{r},\mathbf{r}') = \delta(\mathbf{r}-\mathbf{r}')} \leftarrow \text{Dirac delta} \qquad (3)$$



Then, by the usual arguments★, a particular integral for (2) is:

$$\rightarrow \psi_P(\mathbf{r}) = \int_\infty d^3x'\, G(\mathbf{r},\mathbf{r}')\, f(\mathbf{r}'). \qquad (4)$$

The integral is over all space. Put in $f(\mathbf{r}')$ from Eq. (2), and add the homo-

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★ Multiply through Eq. (2) on the left by G, Eq. (3) on the left by ψ, and subtract to get:

$$\rightarrow \underbrace{G\nabla^2\psi - \psi\nabla^2 G}_{\nabla\cdot(G\nabla\psi - \psi\nabla G),\ \text{by Green's identity.}} = G f(\mathbf{r}) - \psi(\mathbf{r})\,\delta(\mathbf{r}-\mathbf{r}'),$$

Integrate through this eqtn by $\int_V d^3x$ (volume V enclosed by surface S). Use Gauss' Theorem to convert the divergence on the LHS to a surface integral. Then...

$$\rightarrow \oint_S d\mathbf{S}\cdot[G\nabla\psi - \psi\nabla G] = \int_V d^3x\, G f(\mathbf{r}) - \psi(\mathbf{r}'); \ \delta\text{-fcn has projected out } \psi(\mathbf{r}').$$

Now interchange labelling $\mathbf{r}$ & $\mathbf{r}'$, noting that $G(\mathbf{r}',\mathbf{r}) = G(\mathbf{r},\mathbf{r}')$ is symmetric. So...

$$\rightarrow \psi(\mathbf{r}) = \int_V d^3x'\, G(\mathbf{r},\mathbf{r}')\, f(\mathbf{r}') + \oint_S d\mathbf{S}\cdot[\psi\nabla G - G\nabla\psi].$$

Surface term vanishes as $S\rightarrow\infty$. So: $\psi(\mathbf{r}) = \int_\infty d^3x'\, G(\mathbf{r},\mathbf{r}')\, f(\mathbf{r}')$, is an ∞-domain soln.

An Integral Equation for ψ(scattering). Remarks.

generous (plane-wave) solution $\phi(\mathbf{r})$ mentioned above. Then the solution to Eq. (1) [i.e. $(\nabla^2+k^2)\psi=(2m/\hbar^2)V\psi$] for the scattering wavefcn ψ is...

$$\boxed{\psi(\mathbf{r})=\phi(\mathbf{r})+\frac{2m}{\hbar^2}\int_\infty d^3x'\,G(\mathbf{r},\mathbf{r}')V(\mathbf{r}')\psi(\mathbf{r}')} \tag{5}$$

REMARKS on Eq. (5).

1. Eq. (5) is not really a "solution" for the unknown $\psi(\mathbf{r})$, because ψ appears on both sides of the equation. What we have done is to convert Schrödinger's differential equation for ψ to an <u>integral equation</u> for ψ... technically, Eq. (5) is a "Fredholm Equation of the second kind."[¶] The advantage of this is that we can easily do an <u>iteration</u> on Eq. (5)... it starts by approximating $\psi(\mathbf{r})\simeq\phi(\mathbf{r})$ in the RHS integral. Etc. See Eqs. (33)-(38) below.

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2. The free-particle plane-wave $\phi(\mathbf{r})$ which appears in (5) usually has some norm constant C attached, i.e. <u>$\phi(\mathbf{r})=C\exp(i\mathbf{k}\cdot\mathbf{r})$</u>, with $\mathbf{p}=\hbar\mathbf{k}$ representing the particle momentum. C can be chosen so that the particle flux density[†], viz.

$$\left[\begin{aligned}&\mathbf{J}=\frac{\hbar}{2im}(\phi^*\nabla\phi-\phi\nabla\phi^*),\ \text{w/}\ \phi(\mathbf{r})=Ce^{i\mathbf{k}\cdot\mathbf{r}}\\ &\Rightarrow\ \mathbf{J}=\frac{\hbar}{2im}|C|^2\cdot 2i\mathbf{k}=|C|^2\frac{\hbar\mathbf{k}}{m}=|C|^2\mathbf{v},\end{aligned}\right. \tag{6}$$

<u>Choose $C=1$.</u>

is "simple". The choice $C=1$ is appealing here... then $\mathbf{J}=\mathbf{v}$ is proportional to the incoming (or outgoing) free particle current. So we choose $C=1$.

Actually, the choice of C is not critical. When, later, we form the differential scattering cross-section [see Eq. (14) below], we can <u>normalize</u> the scattered particle intensity to unit incident particle intensity... then $|C|^2$ just gets divided out of the problem.

[next page]

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† For the Schrödinger Eq.: $\frac{\partial\rho}{\partial t}+\nabla\cdot\mathbf{J}=0$, w/ $\rho=\psi^*\psi$ and $\mathbf{J}=\frac{\hbar}{2im}(\psi^*\nabla\psi-\psi\nabla\psi^*)$.

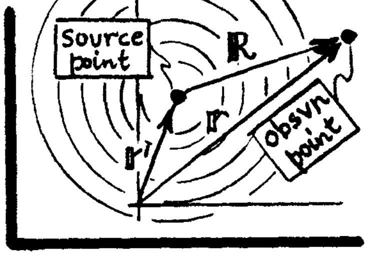
¶ Mathews & Walker "Math. Methods of ϕ" (Benjamin, 2nd ed., 1970), Chap. 11.

Green's Fcn for Scattering. Approxn for "before" and "after".

REMARKS on Eq(5) [cont'd]

3. To make Eq. (5) "work", we need to know the Green's fcn $G(\mathbf{r},\mathbf{r}')$, i.e. the solution to Eq. (3): $(\nabla^2+k^2)G(\mathbf{r},\mathbf{r}')=\delta(\mathbf{r}-\mathbf{r}')$. By standard methods*

$$\left[\!\left[\; G(\mathbf{r},\mathbf{r}') = -\frac{1}{4\pi R}e^{+ikR}, \quad \text{w/}\ \underline{\underline{R=|\mathbf{r}-\mathbf{r}'|}}. \right.\right. \qquad (7)$$



$G(R) \propto \frac{1}{R}e^{ikR}$ represents a spherical wave moving outward from the source point at $\mathbf{r}'$. The scattering wavefcn ψ of Eq (5) is:

$$\boxed{\psi(\mathbf{r}) = \phi(\mathbf{r}) - \frac{m}{2\pi\hbar^2}\int_\infty d^3x'\left(\frac{e^{ikR}}{R}\right)V(\mathbf{r}')\psi(\mathbf{r}')} \quad \begin{array}{l}\text{Davydov Eq. (106.8).}\\ m = \text{reduced mass,}\\ R=|\mathbf{r}-\mathbf{r}'|.\end{array} \qquad (8)$$

We will now use this ψ to solve our scattering problem.

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3) The integrand of the $\int_\infty d^3x'$ integral in (8) is appreciable only over values of $|\mathbf{r}'|$ where $V(\mathbf{r}')$ is non-zero. If we assume this region is small compared to the observation distance $r=|\mathbf{r}|$ (this is certainly true -- by definition -- before and after the collision), then we can use the approximation...

$$\rightarrow R = |\mathbf{r}-\mathbf{r}'| = \left[r^2 - 2\mathbf{r}\cdot\mathbf{r}' + \cancel{r'^2}^{\,0}\right]^{1/2} \simeq r - \hat{r}\cdot\mathbf{r}', \quad \text{w/}\ \hat{r}=\mathbf{r}/r. \qquad (9)$$

This neglects corrections of relative order $\left[\frac{\text{scattering}}{\text{region size}} \Big/ \frac{\text{observation}}{\text{distance}}\right]^2$. We can now

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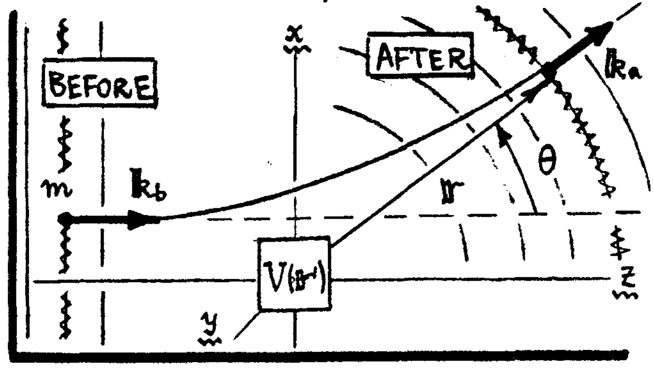
* See Jackson "Classical Electrodynamics" (Wiley, 2nd ed., 1975), Sec. 6.6. For: $(\nabla^2+k^2)G(\mathbf{r},\mathbf{r}')=\delta(\mathbf{r}-\mathbf{r}')$, on an ∞ domain, G depends only on the relative cd. $\mathbf{R}=\mathbf{r}-\mathbf{r}'$, and -- since there is no preferred direction in space -- in fact G should be spherically symmetric and depend only on $R=|\mathbf{R}|$. Then, w/o $\measuredangle$ dependence, in spherical cds: $\frac{1}{R}\frac{d^2}{dR^2}(RG)+k^2G=\delta(R)$. Everywhere but at $R=0$, G satisfies: $(RG)''+k^2(RG)=0$, so: $RG(R)=Ae^{\pm ikR}$, w/ A = cnst. Now, as $R\to 0$, have $G(R)\to A/R$, and since $\nabla^2(1/R) = -4\pi\delta(R)$, choose $A=-1/4\pi$. So: $G(R) = -(1/4\pi R)e^{\pm ikR}$, is solution to: $(\nabla^2+k^2)G=\delta(\mathbf{R})$, as used in (7). The $\frac{1}{R}e^{\pm ikR}$ are interpreted as spherical outgoing (+) or incoming (−) waves.

Asymptotic form of Ψ (scattering). Scattering Amplitude A.

use (9) in (8) to get a simplified Ψ in the asymptotic regions $r\to\infty$...

$$\Psi(\mathbf{r}) = \phi(\mathbf{r}) - \frac{m}{2\pi\hbar^2}\left(\frac{e^{ikr}}{r}\right)\int_\infty d^3x'\, e^{-ik\hat{r}\cdot\mathbf{r}'}\, V(\mathbf{r}')\Psi(\mathbf{r}'),\quad r \gg |\mathbf{r}'|_{MAX}. \qquad (10)$$



Now for some labelling. We suppose the incoming particle stream has momentum $\hbar\mathbf{k}_b$ and (in the free particle limit before the collision) is represented by the plane wave $\phi_b(\mathbf{r}) = e^{i\mathbf{k}_b\cdot\mathbf{r}}$; we put $\phi = \phi_b$ in Eq. (10). Now, as the scattering proceeds, Ψ evolves from ϕ_b (for $\infty \leftarrow r$ before the collision) to $\phi_b - (\int_\infty d^3x'$ correction) after the collision (when $r\to\infty$). The final momentum is $\hbar\mathbf{k}_a$, and for the phase factor in (10): $k\hat{r} = \mathbf{k}_a$ (this follows the $\mathbf{k}$ of the final state). The scattered wave can thus be written

$$\left[\begin{array}{l} \Psi(\mathbf{r}) = \phi_b(\mathbf{r}) + A(\mathbf{k}_b\to\mathbf{k}_a)\,\dfrac{e^{ikr}}{r},\ \text{after scattering;} \\[2ex] \text{w/ } A(\mathbf{k}_b\to\mathbf{k}_a) = -\dfrac{m}{2\pi\hbar^2}\displaystyle\int_\infty d^3x'\, e^{-i\mathbf{k}_a\cdot\mathbf{r}'}\, V(\mathbf{r}')\Psi(\mathbf{r}'). \end{array}\right] \qquad (11)$$

The scattering has the effect of generating spherical waves $\frac{1}{r}e^{ikr}$ which emanate from the scattering center $V(\mathbf{r}')$. The strength of these waves is governed by the coefficient A; A is known as the "scattering amplitude." A, which may be a fcn of the azimuthal $\measuredangle\varphi$ (in the xy plane above) as well as the colatitude (scattering) $\measuredangle\theta$, completely describes the collision.

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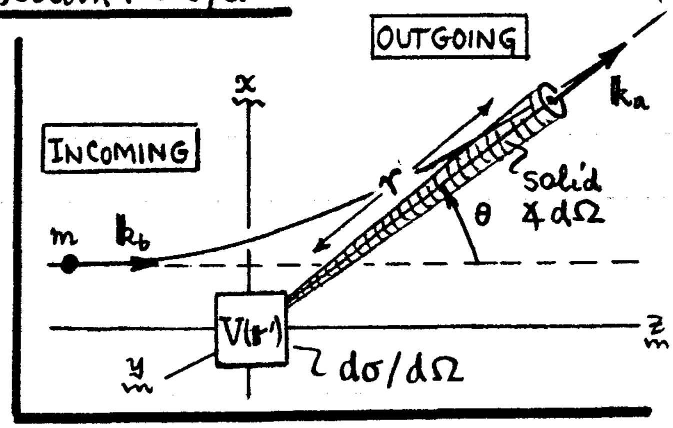
4) The scattering amplitude A of Eq. (11) can be related to the single most important measurable feature of the collision -- namely the differential scattering cross-section, which measures the relative number of particles

Definition of differential scattering cross-section: $d\sigma/d\Omega$.



scattered into a final solid ∢ $d\Omega$. Consider the scattered part of ψ in Eq. (11), viz.

$$\rightarrow \psi_{sc}(r) = \frac{A}{r} e^{ikr}. \qquad (12)$$

The radial current associated with this outgoing spherical wave (here $k = |\mathbf{k}_a|$) is:

$$\rightarrow J_r = \frac{\hbar}{2im}\left[\psi_{sc}^* \frac{\partial \psi_{sc}}{\partial r} - \psi_{sc}\frac{\partial \psi_{sc}^*}{\partial r}\right] = \frac{\hbar}{2im}|A|^2 \frac{1}{r^3}[2ikr] = \frac{|A|^2}{r^2}\frac{\hbar k}{m}. \qquad (13)$$

The # particles scattered into $d\Omega$ is $\propto J_r r^2 d\Omega = (\hbar|\mathbf{k}_a|/m)|A|^2$, while the # particles incident is $\propto |\mathbf{J}_b| = (\hbar|\mathbf{k}_b|/m)$, from Eq. (6). The ratio is:

$$d\sigma = \frac{\text{scattered into } d\Omega}{\text{incident}} = \frac{J_r r^2 d\Omega}{|\mathbf{J}_b|} = \frac{|\mathbf{k}_a|}{|\mathbf{k}_b|}|A(b\to a)|^2 d\Omega,$$

i.e., differential scattering cross-section $\Big\}$ $\boxed{\frac{d\sigma}{d\Omega} = \{|\mathbf{k}_a|/|\mathbf{k}_b|\}|A(b\to a)|^2}$. (14)

REMARKS on Eq. (14).

1. $d\sigma$ plays the role of an effective area offered by the potential $V(\mathbf{r}')$ to the incoming particle (b). If (b)'s trajectory intersects $d\sigma$, it gets scattered into $d\Omega$. If (b)'s trajectory falls outside $d\sigma$, nothing happens.

2. Whenever $d\sigma/d\Omega > 0$, there is a momentum change $\mathbf{k}_b$(before) $\rightarrow \mathbf{k}_a$(after) $\neq \mathbf{k}_b$, i.e. $\Delta\mathbf{k} = \mathbf{k}_b - \mathbf{k}_a \neq 0$. But if the collision is completely elastic, the energies $E(\text{before}) = \hbar^2 k_b^2/2m$ and $E(\text{after}) = \hbar^2 k_a^2/2m$ do not change. So $|\mathbf{k}_b| = |\mathbf{k}_a|$ for an elastic collision, and in (14): $d\sigma/d\Omega = |A(b\to a)|^2$.

3. The elastic scattering problem is thus reduced to evaluating the amplitude:

$$A(b\to a) = -\frac{m}{2\pi\hbar^2}\int_\infty d^3x'\, e^{i(\mathbf{k}_b - \mathbf{k}_a)\cdot \mathbf{r}'}\, V(\mathbf{r}')\underbrace{[\psi(\mathbf{r}')e^{-i\mathbf{k}_b\cdot\mathbf{r}'}]}_{\simeq 1}. \qquad (15)$$

in Eq. (11). As a first approxn, we can take $\psi(\mathbf{r}') \simeq \phi_b(\mathbf{r}')$; then the [ ] $\simeq 1$.