From: QUANTUM MECHANICS IN MATHEMATICS, CHEMISTRY, AND PHYSICS
Edited by Karl E. Gustafson, and William P. Reinhardt
(Plenum Publishing Corporation, 1981)

TOTAL CROSS SECTIONS IN NON-RELATIVISTIC SCATTERING THEORY

Volker Enss

Institut für Mathematik
Ruhr-Universität
D-4630 Bochum 1, F.R. Germany

and

Barry Simon

Departments of Mathematics and Physics
Princeton University
Princeton, N.J. 08544, U.S.A.

ABSTRACT

Using time-dependent geometric methods we obtain simple explicit upper bounds for total cross sections σ_{tot} in potential- and multiparticle-scattering. σ_{tot} is finite if the potential decays a bit faster than r^{-2} (in three dimensions) or if weaker direction dependent decay requirements hold. For potentials with support in a ball of radius R bounds are given which depend on R but not on the potential.

We obtain upper bounds on σ_{tot} for large coupling constant λ, the power of λ depending on the falloff of the potential. For spherically symmetric potentials the variable phase method gives also a lower bound growing with the same power of λ.

In the multiparticle case for charged particles interacting with Coulomb forces the effective potential between two neutral clusters decays sufficiently fast to imply finite total cross sections for atom-atom scattering.

We reexamine the definitions of classical and quantum cross sections to discuss some puzzling discrepancies.

1. OUTLINE

The total scattering cross section in quantum mechanics is a simple measure for the strength of a potential when it influences a homogeneous beam of particles with given energy and direction of flight. It can be easily measured in experiments, therefore various approximation schemes have been developed for its calculation. On the other hand relatively little attention has been paid to a mathematically rigorous treatment, probably because it is a rather special quantity derived from basic objects like the scattering amplitude or the scattering operator S. Moreover various assumptions and estimates were motivated by technical rather than physical reasons. In contrast to the conventional time independent approach Amrein and Pearson [1] used time dependent methods to obtain new results. In Amrein, Pearson,and Sinha [2] this was extended to prove finiteness of the total cross section in the multiparticle case if all pairs of particles which lie in different clusters interact with short range forces.

In our approach we add geometric considerations to the previous ones. The main bounds are derived by following the localization of wave packets as they evolve in time. This method is both mathematically simple and physically transparent. Nevertheless it allows to recover or improve most results with simpler proofs. We need not average over directions but we keep the direction of the incident beam fixed. The main defect of the geometric method so far is that we have to average over a small energy range; our bounds blow up in the sharp-energy limit. Consequently we get poor bounds for the low energy behavior or (connected by scaling) for obstacle scattering with the radius going to zero.

In Section 3 we determine the decay requirements for infinitely extended potentials which guarantee finite total cross sections both for the isotropic and anisotropic cases. They are close to optimal. We obtain explicit bounds which have the correct small coupling and high energy behavior. The Kupsch-Sandhas trick is used in the next section to give a bound independent of the potential if the latter has its support inside a ball of radius R. The bound has the correct large R behavior.

One of our main new results combines the two bounds to establish a connection between the decay of the potential at infinity and the rate of increase of the total cross section in the strong coupling limit (Section 5). The variable phase method gives lower bounds with the same rate of increase for spherically symmetric potentials.

The main advantage of time dependent (and geometric) methods is that two cluster scattering is almost as easy to handle as two particle (= potential-) scattering. One has to use a proper effective potential between the clusters which may decay faster than the pair potentials due to cancellations. For a system of charged particles interacting via Coulomb pair potentials the effective potential between neutral clusters (atoms) decays fast enough to give a finite total cross section for atom-atom scattering (including rearrangement collisions and breakup into charged clusters). This new result is derived in Section 7.

In quantum mechanics textbooks usually the classical total cross section is defined first and then the quantum total cross section is derived by analogy. Therefore it is puzzling that both quantities differ considerably even if the quantum corrections should be small. E. g. the quantum cross section is twice as big as the classical one for scattering from big hard spheres ("shadow scattering"), even when $\hbar \to 0$.

In Section 2 we examine the limits involved in the derivation of the quantum total cross section and show that it is basically a pure wave- (and not particle-) concept. This suggests our definition of the quantum total cross section (2.5), which agrees with the traditional one for suitable potentials. (Or one might use (2.5) as an equivalent expression for σ_{tot} which is convenient for estimates.) This point of view explains naturally the discrepancies; we discuss some aspects of the classical limit in Section 6.

For detailed references to earlier and related work see [1,2, 8, 11]. We restrict ourselves here to three dimensions, the results for general dimension as well as various refinements and extensions can be found in [8].

One of us (V.E.) would like to thank the Institute for Advanced Study, Princeton, for its hospitality and support under the Albert Einstein visiting professorship endowed by the Federal Republic of Germany and for a travel grant provided by Deutsche Forschungsgemeinschaft. Another of us (B.S.) acknowledges partial support by the National Science Foundation under Grant No. MCS 78-01885.

2. THE DEFINITION OF CLASSICAL AND QUANTUM TOTAL CROSS SECTIONS

When scattering experiments are performed with microscopic particles like atoms, electrons, nuclei, then (in contrast to billard balls) it is practically impossible to observe the time evolution of individual projectiles. We have to restrict ourselves to very few observables which can be measured well enough,

e. g. the direction of flight of the particle when it has passed the target. This direction is asymptotically constant, thus there is enough space and time available to measure it with arbitrary precision. In classical physics where the possibility to prepare particles with a given trajectory is not restricted by basic principles, the scattering angle depends strongly on the impact parameter. If the latter cannot be controlled the next best thing is to use a homogeneous beam of incoming particles and to observe the distribution of the outgoing particles over the scattering angles. This is the *classical differential cross section*. Let the incoming beam consist of particles flying in the direction $\hat{e}$ with momentum p and a given density (= number of particles per unit area orthogonal to $\hat{e}$); then one defines:

$$\sigma_{\text{class}}(p,\hat{e};d\Omega) = \frac{\text{number of particles deflected into } d\Omega}{\text{density of particles}}$$

where $d\Omega$ does not contain $\hat{e}$. Integrating over the outgoing directions yields the *classical total cross section*:

$$\sigma_{\text{tot,class}}(p,\hat{e}) = \int_{S^2} \sigma(p,\hat{e};d\Omega)$$

$$= \frac{\text{number of deflected particles}}{\text{density of particles}}$$

(If one thinks of an experiment running forever one should understand the numerators and denominators per given time interval.) Note that the idealization of a beam of finite density which is homogeneous in the plane perpendicular to the beam direction $\hat{e}$, necessarily involves infinitely many particles for two reasons. First one would need infinitely many particles per unit area, but this is compensated by the denominator in the definition of the cross section. The second infinity is more delicate which comes from the infinite extension of the beam. If the target has finite size (potential of compact support) then only the particles which hit the target can be deflected, the infinitely many particles which miss the target go on into the forward direction $\hat{e}$ and won't be counted. (The infinite extension of the beam allows to specify the beam independent of the size and localization of the target.) Excluding *one single* direction from the observation we have singled out the finitely many particles of interest (for finite density) out of the infinitely many incoming. This prevents us from measuring the total cross section exactly if the incoming beam cannot be prepared with all particles having the same direction. The (idealized) concept of the total cross section requires for its definition that there are beams of incoming particles with a sharp direction. On the other hand it is irrelevant whether beams with sharp energy (or modulus of the momentum p) are available or not. We will use this freedom below.

Quantum mechanical scattering states for potentials vanishing at infinity are known to behave asymptotically like classical wave packets. Therefore it is reasonable to extend the notion of cross sections to quantum mechanics. However, a further limit is involved because there are no states with a sharp direction in the quantum mechanical state space. Let the z-axis be in the beam direction $\hat{e}$, then a sharp direction would mean that $p_x = p_y = 0$. By the uncertainty principle this implies infinite extension of the states in the x-y-directions. Thus the infinite extension of the state perpendicular to $\hat{e}$, which might look unnecessary in the classical case, is forced upon us in quantum scattering. We will have to handle wave functions which are constant in the plane perpendicular to $\hat{e}$, therefore the quantum cross section behaves like a quantity characteristic for classical waves rather than classical particles for any $\hbar > 0$. A classical particle approximation would require a wave packet well concentrated compared to a length typical for the potential. Thus it is no longer mysterious that in the classical limit ($\hbar \to 0$) the quantum cross section need not converge to the classical one (e. g. shadow scattering off hard spheres).

Another peculiarity of the classical cross section is its discontinuity under small changes of the potential. Consider e. g.

$$V_b(x,y,z) = (a+bx)\ \chi_{[-r,r]}(z)\ \chi_{[-R,R]}(x)\ \chi_{[-R,R]}(y)$$

for some parameters a,b,r,R where $r \ll R$. If the beam direction is along the z-axis (near the z-axis) for $b = 0$ the total cross section is zero (tiny) but for any $b \neq 0$ is jumps to $4R^2$ ($\approx 4R^2$). If one could easily count the particles which have been influenced by V(e. g. time delay for $a > 0$) the discontinuity of $\sigma_{\text{tot,class}}$ at $b = 0$ would disappear and it would always have the size of the geometric cross section $4R^2$. For such a potential with $b = 0$ the quasiclassical limit $\hbar \to 0$ of the quantum cross section does not converge at all!

Following the above considerations about the quantum cross section as a wave limit we use for its definition "plane wave packets" which are chosen to describe waves with a sharp direction of propagation $\hat{e}$ parallel to the z-axis, but they are normalized wave packets in the longitudinal direction, thus being as close as possible to a Hilbert space vector. For a given direction $\hat{e}$ the plane wave space $\mathcal{h}_{\hat{e}}$ is isomorphic to (and henceforth identified with) $L^2(\mathbb{R}, dz)$. The configuration space wave function is

$$g(x,y,z) = g(z) \text{ with } \int |g(z)|^2\, dz = 1. \tag{2.1}$$

In momentum space we denote by $\tilde{g}(k)$ the one-dimensional Fourier-transform

$$\tilde{g}(k) = (2\pi)^{-1/2} \int dz\, e^{-ikz} g(z), \tag{2.2}$$

corresponding to the three-dimensional Fourier transform

$$\hat{g}(\vec{k}) = \tilde{g}(k_z)(2\pi)\,\delta(k_x)\,\delta(k_y). \tag{2.3}$$

Since a beam should hit the target from one side only we assume:

$$\operatorname{supp} \tilde{g}(k) \subset (0,\infty), \tag{2.4}$$

which implies in (2.3) $k_z = |\vec{k}| =: k$.

The scattering operator S is the unitary operator which maps incoming states to the scattered outgoing waves, it is close to one on states which are weakly scattered. $(S-1)g$ corresponds to the scattered part of the wave g. The probability to detect a scattered particle is then $\|(S-1)g\|^2$ where the norm is that of the Hilbert space $\mathcal{H} = L^2(\mathbb{R}^3)$. Thus we *define* as the quantum mechanical *total cross section*

$$\int_0^\infty \sigma_{tot}(k,\hat{e})\, |\tilde{g}(k)|^2\, dk = \|(S-1)g\|^2, \tag{2.5}$$

where $g \in h_{\hat{e}}$ with (2.4). We will show below that for a class of potentials with suitable decay properties S-1 extends naturally from an operator on $\mathcal{H}$ to a bounded map from $h_{\hat{e}}$ into $\mathcal{H}$, then the definition makes sense. We average over the energy of the incident beam but keep the direction fixed. (See also the similar construction in [14].) Certainly we have to verify that our definition agrees with the conventional one given below.

Within the time independent theory of scattering for potentials with sufficiently fast decay the solutions of the Lippman Schwinger equation have the asymptotic form

$$\phi(\vec{k},\vec{x}) \sim \exp(i\vec{k}\cdot\vec{x}) + f(k;\hat{x}\leftarrow\hat{k})\,\frac{\exp(i\,k|x|)}{|x|} \quad ,$$

$f(k;\hat{x}\leftarrow\hat{k})$ is the continuous on shell scattering amplitude. Equivalently the kernel of S-1 in momentum space is

$$(S-1)(\vec{k}',\vec{k}) = \frac{i}{2\pi m}\,\delta(k'^2/2m - k^2/2m)\, f(k;\hat{k}'\leftarrow\hat{k})$$

where $\hat{k} = \vec{k}/k$, $k = |\vec{k}|$, etc. Then

$$\sigma_{tot}(k,\hat{e}) = \int d\Omega'\, |f(k;\hat{\omega}'\leftarrow\hat{e})|^2. \tag{2.6}$$

The physical motivation for this choice as given in most textbooks on quantum mechanics uses the "obvious" fact that $\exp(i\,\vec{k}\cdot\vec{x})$ describes an incoming homogeneous beam of particles with momentum k, direction $\hat{k}$ and density one (or $(2\pi)^{3/2}$) particle per unit area, similarly for the outgoing spherical wave.

More careful authors give the following time dependent justification. Let $\phi^{in}(\vec{k})$ be the (square integrable) wave function of a single incoming particle with momentum support well concentrated around a mean value $\vec{q}$. The corresponding outgoing state has a momentum space wave function

$$\phi^{out}(\vec{k}') = (S\,\phi^{in})(\vec{k}') = \int d^3k\,\delta(\vec{k}-\vec{k}')\,\phi^{in}(\vec{k}) +$$
$$+ \frac{i}{2\pi m}\int d^3k\,\delta(k'^2/2m-k^2/2m)\, f(k;\hat{k}'\leftarrow\hat{k})\,\phi^{in}(\vec{k}). \tag{2.7}$$

The "scattering into cones" papers [6, 9] show that the asymptotic direction of flight is $\hat{k}$ for the incoming and $\hat{k}'$ for the outgoing state. The first summand in (2.7) is then identified as "not deflected" and for continuous (or not too singular) f's the second term gives the deflected part. Although this splitting is natural it cannot be justified by observations for directions lying in the support of $\phi^{in}(\vec{k})$. Under this assumption the probability $w(\phi^{in})$ that a particle with incoming wave function ϕ^{in} will be deflected, is

$$w(\phi^{in}) = \int d^3k'\,\Big|\frac{i}{2\pi m}\int d^3k\,\delta(k'^2/2m-k^2/2m)\, f(k;\hat{k}'\leftarrow\hat{k})\,\phi^{in}(\vec{k})\Big|^2 =$$
$$= \|(S-1)\phi^{in}\|^2 .$$

To represent a homogeneous beam one translates the incoming state by a vector $\vec{a}$ in the plane orthogonal to the mean direction $\vec{q}$, $\phi^{in}_{\vec{a}}(\vec{k}) = e^{-i\,\vec{a}\cdot\vec{k}}\phi^{in}(\vec{k})$, and one sums up the contributions for different $\vec{a}$'s. $\int d^2a$ represents a homogeneous beam with particle density one per unit area. The resulting number of deflected particles is then

$$\int d^2a\; w(\phi^{in}_{\vec{a}}) = \sigma_{tot}(\phi^{in}) \tag{2.8}$$
$$= \int d^3k\,(\hat{k}\cdot\hat{q})^{-1} \int d\Omega'\,|f(k;\hat{\omega}'\leftarrow\hat{k})|^2\,|\phi^{in}(\vec{k})|^2 .$$

In the limit $|\phi^{in}(\vec{k})|^2 \to \delta(\vec{k}-\vec{q})$ expression (2.6) for $\sigma_{tot}(q,\hat{q})$ is recovered and $|\phi^{in}(\vec{k})|^2 \to \delta(k_\perp)|\tilde{g}(k)|^2$ yields $\int dk\,\sigma_{tot}(k;\hat{e})|\tilde{g}(k)|^2$, the left hand side of (2.5). Note that the summation over $\vec{a}$'s is incoherent, we have added probabilities and not states, because we are interested only in interactions between the target and single particles, interference between particles in the beam has to be eliminated.

Let us now calculate the cross section according to our definition.

$$\|(S-1)g\|^2 = \int d^3k' \left| \frac{i}{2\pi m} \int d^3k \, \delta(k'^2/2m - k^2/2m) \right.$$

$$\left. f(k;\hat{k}'\leftarrow\hat{k})\,(2\pi)\,\delta(k_\perp)\,\tilde{g}(k) \right|^2$$

$$= \int dk \int d\Omega' \, |f(k;\hat{\omega}'\leftarrow\hat{e})|^2 \, |\tilde{g}(k)|^2 .$$

Thus our definition coincides with the conventional one if the scattering amplitude is continuous (or not too singular).

At first glance it seems strange that the incoherent superposition in (2.8) yields the same result as the coherent superposition of wave packets with strong correlations which forms the plane wave-packets. The following heuristic argument easily explains the phenomenon. Since $(S-1)g \in L^2(\mathbb{R}^3)$ the action of S-1 "localizes", it essentially annihilates the parts of the state which lie beyond some radius r. Let $R \gg r$ and use in the incoherent case (2.8) the normalized wave function

$$g(z)\;(2R)^{-1}\;\chi_{[-R,R]}(x)\;\chi_{[-R,R]}(y)$$

whose (3-dimensional) Fourier transform $\phi^{in}(\vec{k})$ obeys $|\phi^{in}(\vec{k})|^2 \to |\tilde{g}(k)|^2\,\delta(k_\perp)$ as $R \to \infty$ ($\tilde{g}$ is the 1-dim. Fourier transform). Then

$$w(\phi^{in}_{\vec{a}}) = \|(S-1)\phi^{in}_{\vec{a}}\|^2 \approx \begin{cases} (2R)^{-2}\,\|(S-1)g\|^2 & \text{for } |a_{1,2}| \le R \\ 0 & \text{otherwise} \end{cases}$$

and

$$\int d^2a \; w(\phi^{in}_{\vec{a}}) \approx \int_{-R}^{R} da_1 \int_{-R}^{R} da_2 \, \|(S-1)\phi^{in}_{\vec{a}}\|^2 \approx \|(S-1)g\|^2 .$$

The sharp direction - limit forces us to use states which are eventually constant in an area much larger than the localization region of S-1. Up to negligible boundary terms all contributions become parallel and the properly normalized coherent and incoherent superpositions do not differ.

In Section 6 we will return to the comparison of the wave picture and particle picture when we discuss the classical

limit. There we will explain why it is natural, although it looks unnatural, that the quantum cross section of a hard sphere is twice the corresponding one for classical particles ("shadow scattering"). In the same section we will explain why classical cross sections are generally infinite for potentials with unbounded support although the quantum cross sections may be finite.

3. THE BASIC ESTIMATE FOR σ_{tot}

We assume in this section that the potential $V(\vec{x})$ is a perturbation of the kinetic energy $H_o = -\frac{1}{2}\Delta$ with H_o-bound smaller than 1 (we have set $\hbar=1$ and the particle mass m=1, therefore momenta and velocities coincide). If the potential is of short range (we will impose stronger decay requirements shortly) then the isometric wave operators

$$\Omega^{\mp} = s - \lim_{t\to\pm\infty} e^{i\,Ht}\, e^{-i\,H_o t}$$

exist and are complete, the S-operator

$$S = (\Omega^-)^*\,\Omega^+$$

is unitary and on states in the domain of H_o the following "interaction picture" representation holds:

$$S-1 = (\Omega^-)^*\,[\Omega^+ - \Omega^-]$$

$$= (\Omega^-)^* \int_{-\infty}^{\infty} dt \; e^{i\,Ht}\,(iV)\,e^{-i\,H_o t} . \qquad (3.1)$$

Cook's estimate gives

$$\|(S-1)\phi\| \le \int_{-\infty}^{\infty} dt \, \|V\, e^{-i\,H_o t}\phi\| . \qquad (3.2)$$

Let $\phi_R \in \mathcal{H} = L^2(\mathbb{R}^3)$ be an approximating sequence of states which tends to the plane wave packet g as $R \to \infty$. For a suitable class of potentials we will show that

$$\lim_{R\to\infty}\; \sup_{R'>R} \int_{-\infty}^{\infty} dt \, \|V\, e^{-i\,H_o t}(\phi_{R'} - \phi_R)\| = 0 \qquad (3.3)$$

which implies by (3.2) convergence in $\mathcal{H}$ of $\lim_{R\to\infty} (S-1)\phi_R =: (S-1)g$ and the finite bound

$$\|(S-1)g\| \le \int_{-\infty}^{\infty} dt \, \|V\, e^{-i\,H_o t} g\| . \qquad (3.4)$$

It is convenient to use product functions

$$\phi_R(\vec{r}) = g(z)\ f_R(x,y) \tag{3.5}$$

because the free time evolution factorizes:

$$(e^{-i\,H_o t}\,\phi_R)(\vec{r}) = (e^{-i\,h_o t}\,g)(z)\ f_R(t;x,y)\ ,$$

where

$$h_o = -\frac{1}{2}\,d^2/dz^2,\quad f_R(t;x,y) = [\exp\{-\frac{i}{2}(\frac{d^2}{dx^2}+\frac{d^2}{dy^2})t\}f_R](x,y)\ .$$

In particular the plane wave packet space $h_{\hat{e}}$ is left invariant:

$$e^{-i\,H_o t}\,h_{\hat{e}} = e^{-i\,h_o t}\,h_{\hat{e}} = h_{\hat{e}}\,.$$

For Gaussian $f_R(x,y) = \exp[-(x^2+y^2)/R^2]$ it is well known that

$$|f_R(t;x,y)| \le 1 \qquad \forall\ t,x,y\ ,$$

and for any L,T,ε there is an R_o such that for $R > R_o$

$$||f_R(t;x,y)|^2 - 1| < \varepsilon \text{ if } x^2+y^2 < L^2, |t| < T\ . \tag{3.6}$$

Then for the convergence (3.3) it is necessary and sufficient to show the finiteness of the bound

$$\int_{-\infty}^{\infty} dt \| V\,e^{-i\,H_o t}\,g\|$$

$$= \int_{-\infty}^{\infty} dt\{\int dz \int dx\,dy |V(x,y,z)|^2\,|[e^{-i\,h_o t}\,g](z)|^2\}^{1/2} \tag{3.7}$$

$$\ge \int_{-\infty}^{\infty} dt\{\int d^3r\,|V(\vec{r})|^2\,|[e^{-i\,H_o t}\,gf_R](\vec{r})|^2\}^{1/2}\,. \tag{3.8}$$

The contribution to this integral is arbitrary small if for some L,T we have $|t| > T$ or $x^2+y^2 > L^2$ whereas inside this region the wave functions of $e^{-i\,H_o t}(\phi_{R'} - \phi_R)$ are small for $R' > R$ big enough. Any cutoff f_R which fulfills (3.6) gives the same result.

In the bound (3.7) the potential enters only through the function

$$W(z) = \{\int dx\,dy\,|V(x,y,z)|^2\}^{1/2} \tag{3.9}$$

where we have fixed the z-axis in the beam direction $\hat{e}$, and the *one*-dimensional estimate

$$\|(S-1)g\| \le \int_{-\infty}^{\infty} \{\int dz\,W^2(z)|[e^{-i\,h_o t}\,g](z)|^2\}^{1/2}\,dt$$

$$= \int_{-\infty}^{\infty} dt\,\|W\,e^{-i\,h_o t}\,g\| < \infty \tag{3.10}$$

will imply finite total cross sections.

Here we have taken multiplication by $V(\vec{x})$ as a map from $h_{\hat{e}}$ into $\mathcal{H}$ and we have used that

$$\|V\,g\|_{L^2(\mathbb{R}^3)} = \|W\,g\|_{L^2(\mathbb{R})}\,. \tag{3.11}$$

We collect a few well known facts about wave packets in the following

<u>Lemma.</u>
Let $G(z)$ have the (one-dimensional) Fourier transform $\tilde{G}(k) \in C_o^\infty(\mathbb{R})$, supp $G \subset (-\delta,\delta)$. Define

$$\tilde{G}_v(k) := \tilde{G}(k-v)\,. \tag{3.12}$$

Then for $v > 2\delta$ there are C_m independent of v such that

$$\int_{|z| \le \frac{v}{2}t} dz\ |[e^{-i\,h_o t}\,G_v](z)|^2 \le C_m(1+|vt|)^{-m}\,. \tag{3.13}$$

<u>Proof.</u> Using the stationary phase method (see e.g. Theorem XI.14 in [12]) one easily shows that for $|z|/|t| > \delta$

$$|[e^{-i\,h_o t}\,G](z)| \le C'_m\,(1+|z|)^{-m}\,.$$

Next observe that

$$[e^{-i\,h_o t}\,G_v]^\sim(k) = e^{i\,t\,v^2/2}\,e^{i(k-v)vt}[e^{-i\,h_o t}\,G](k-v)\,,$$

and

$$|[e^{-i\,h_o t}\,G_v](z)| = |[e^{-i\,h_o t}\,G](z-vt)|\ .$$

Thus for $|z-vt|\,/\,|t| > \delta$

$$|[e^{-i\,h_o t}\,G_v](z)| \le C'_m(1+|z-vt|)^{-m}\,.$$

For $|z| \le v|t|/2$ this implies (3.13) . □

Remark. With some obvious modifications the Lemma and the results below hold for an extremely wide class of "free" Hamiltonians $H_o(\vec{p})$ with velocity operator $\vec{\nabla}_p H_o(\vec{p})$. Only the constant $C(\delta)$ in (3.18) will change.

Let $F(|z| \leq R)$ be the operator of multiplication with the characteristic function of the indicated region. The real function $\psi \in C_o^\infty(\mathbb{R})$ should obey $0 \leq \psi(q) \leq 1$ and $\psi(q) = 1$(resp. 0) for $|q| \leq \delta$(resp. $\geq 2\delta$). Denote by $\psi(K)$ multiplication of wave functions $\tilde{g}(k)$ with $\psi(k)$, then $\psi(K)$ is in z-space convolution with a smooth kernel of rapid decay.

A one-dimensional potential W is called a *short range potential* if

$$\| W\, \psi(K)\, F(|z| \geq R)\| =: h(R) \in L^1(\mathbb{R}_+, dR), \tag{3.14}$$

or equivalently

$$\| W\, F(|z| \geq R)\, \psi(K)\| \in L^1(\mathbb{R}_+, dR) .$$

Going back to the three dimensional potential V from which W was derived in (3.9) and using (3.11) for V as a map from $h_{\hat{e}}$ into $\mathcal{H}$ we require (depending on the direction $\hat{e}$):

$$\| V\, \psi(K) F(|z| \geq R)\|_{h_{\hat{e}},\mathcal{H}} =: h(R) \in L^1(\mathbb{R}_+, dR) \tag{3.15}$$

with the corresponding norm

$$\| V\|_{\hat{e}} = h(0) + \int_0^\infty h(R)\, dR . \tag{3.16}$$

We will discuss simple sufficient conditions for (3.15) below, first we will complete our estimate (3.10).

Observe that $\psi(K-v)$ depends on v in z-space only through phase factors which commute with F and W, thus $\| W\, \psi(K-v) F(|z| \geq R)\| = h(R)$ for all v. Let $\tilde{g}$ have support in $(v-\delta, v+\delta), v > 2\delta$, then $g = \psi(K-v) g$ and with the Lemma we obtain

$$\| (S-1) g\| \leq \int_{-\infty}^{\infty} dt\, \| W\, e^{-i h_o t} g\|$$

$$\leq \int_{-\infty}^{\infty} dt \| W\, \psi(K-v)\, F(|z| \geq v|t|/2)\, e^{-i h_o t} g\|$$

$$+ \int_{-\infty}^{\infty} dt \| W\, \psi(K-v)\, F(|z| \leq v|t|/2)\, e^{-i h_o t} g\| \leq$$

$$\leq \frac{1}{v} \int_{-\infty} d(vt)\, \{2\, h(v|t|/2) + 2h(0)\, C_2 (1+|vt|)^{-2}\}$$

$$\leq C\, v^{-1} \{h(0) + \int_0^\infty dR\, h(R)\} = C\, v^{-1} \| V\|_{\hat{e}} \tag{3.17}$$

where the constant C depends on the shape of the wave function $\tilde{g}$, but it is independent of v and W.

Let us take for g a function with supp $\tilde{g} \subset (v-\delta, v+\delta)$ and $\tilde{g}(k) = 1$ for $|k-v| < \delta/2$; furthermore we introduce a coupling constant λ, then we can sum up our results in the following

Theorem. For the pair H_o, $H = H_o + \lambda V$ and incident beam direction $\hat{e}$ the total cross section is bounded by

$$\int_{v-\delta/2}^{v+\delta/2} \sigma_{tot}\, (k, \hat{e})\, dk \leq C(\delta)\, (\lambda/v)^2\, \| V\|_{\hat{e}}^2 . \tag{3.18}$$

Note that the bound can be calculated explicitly and that it depends on the beam direction for non-isotropic forces. It is correct or close to optimal in its dependence on several properties as we will discuss now.

There are some simple sufficient conditions for $\| V\|_{\hat{e}} < \infty$. Assume that V is locally square integrable and continuous outside a ball of radius ρ. Then $\| V\|_{\hat{e}}$ is finite if

$$\int_\rho^\infty d\zeta \sup_{|z| > \zeta} \{\int dx \int dy\, V^2(x,y,z)\}^{1/2} < \infty . \tag{3.19}$$

If singularities may occur at arbitrary distances we use the fact that $\psi(K)$ maps $L^2(\mathbb{R})$ into $L^\infty(\mathbb{R})$ in z-space and the kernel decays rapidly. Therefore the decay of local L^2-norms is sufficient and we obtain

$$\| V\|_{\hat{e}} \leq \text{const} \int_0^\infty d\zeta \sup_{|z'| \geq \zeta} \int_{|z-z'| \leq 1} dz \quad \{\int dx \int dy\, V^2(x,y,z)\}^{1/2}. \tag{3.20}$$

We will get a finite total cross section if the potential is bounded at infinity by

$$|x|^{-(1/2)-\varepsilon} |y|^{-(1/2)-\varepsilon} |z|^{-1-\varepsilon}, \quad \varepsilon > 0 . \tag{3.21}$$

The total cross section is finite for all directions if the decay is like

$$|\vec{r}|^{-2} (\ln|\vec{r}|)^{-1-\varepsilon},\ \varepsilon > 0 . \tag{3.22}$$

Up to a square root of the logarithm (see [11]) this is optimal. Using the variable phase method of Calogero [4] and Babikov [3] one proves that the total cross section is infinite for some spherically symmetric potential with $|\vec{r}|^{-2} (\ln|\vec{r}|)^{-1/2}$ - decay (see the remark after Prop. 2.3 and Appendix 2 in [8]).

If the coupling constant λ is small or the energy high (i.e. (λ/v) small) then the Born approximation converges and it gives the same $(\lambda/v)^2$ - behavior as our bound (3.18).

Also in the strong coupling limit $\lambda \to \infty$ (v fixed) there is for any $\mu < 2$ a spherically symmetric potential with $\|V\|_{\hat{e}} < \infty$ such that the total cross section increases at least like $(\lambda)^{\mu}$. For potentials with faster decay, however, we will prove a slower increase in λ in Section 5.

The main drawback of our geometric method is that we do not get estimates for sharp energy: our bound $C(\delta)$ in (3.18) remains bounded but does not decrease like $O(\delta)$ as $\delta \to 0$. Related to this we get poor estimates on the low energy behavior. The reason for this limitation is our estimate

$$\left\| \int_{-\infty}^{\infty} dt\, e^{i Ht}\, V\, e^{-i H_0 t} g \right\| \tag{3.23}$$

$$\leq \int_{-\infty}^{\infty} dt\, \| V\, e^{-i H_0 t} g \| . \tag{3.24}$$

For a small momentum spread δ (and similarly for potentials with small support) the size of the wave packet g in z-space becomes large compared to the size of the region where V is strong; the main contribution to the integral (3.23) comes from a time interval $\sim \delta^{-1}$. In the continuous spectral subspace for H, away from zero-energy resonances, one expects a growth

$$\left\| \int_{-\delta^{-1}}^{\delta^{-1}} dt\, e^{+i Ht}\, V \right\| \sim \delta^{-1/2}$$

rather than the δ^{-1} of our estimate. The cancellations in (3.23) which are lost in (3.24) would be necessary to get good bounds for sharp energies (or small obstacles).

To sum up our strategy in this section was as follows:

according to our definition (2.5) of σ_{tot} we have to estimate $\|(S-1)g\|$ for plane wave packets g. It is bounded by

$$\int_{-\infty}^{\infty} dt\, \| V\, e^{-i H_0 t} g \| . \tag{3.25}$$

This expression is particularly convenient because it uses *freely* evolving wave packets and the potential V, but it does not use the full Hamiltonian H. The same properties are shared by the first order Born approximation which will give better approximations in the parameter range of its applicability. Our bound, however, is a universal upper bound.

The travelling plane wave packet $e^{-i H_0 t} g$ is mainly localized in a region where $z \approx v\,t$, $v \in \operatorname{supp} \tilde{g}$, the velocity(=momentum) support of g; the tails into the classically forbidden region decay rapidly. Thus one has to control that V as a map from suitable plane wave packets localized in $|z| \geq R$ into the Hilbert space is of short range (has a norm integrable in R). This is exactly what the $\|\cdot\|_{\hat{e}}$-norm controls (the factor $\psi(K)$ is simply a regularization which smoothes out local singularities; it does not affect the decay properties of the potential). At each time the effect of the potential on the plane wave packet is independent of the mean velocity v, but the time necessary for the wave packet to pass the potential behaves like v^{-1}. Thus the $(\lambda/v)^2 \|V\|_{\hat{e}}^2$ -bound is quite natural.

For potentials V with stronger singularities like the Rollnik class which are form bounded perturbations of H_0 one can use the intertwining property of the wave operators to get the estimate

$$\|(S-1)g\| \leq \int_{-\infty}^{\infty} dt \| \psi[(2H^{a.c.})^{1/2} - v]\ V\ \psi[(2H_0)^{1/2} - v]\, e^{-i H_0 t} g \|$$

for states with momentum support around v. Here we have used that $g = \psi(K-v)g = \psi[(2H_0)^{1/2} - v] g$ for these states.

If the interaction term

$$\psi[(2H^{a.c.})^{1/2} - v)]\ V\ \psi[(2H_0)^{1/2} - v]$$

is of short range as a map from plane wave packets into the Hilbert space *uniform* in v, then all the above results remain true. There is another way to handle even stronger local singularities with the Kupsch-Sandhas trick, explained in the next section. But then the high energy decay in (3.18) is lost.

4. POTENTIALS OF COMPACT SUPPORT

If the support of the potential V is contained in a ball of radius R then the classical total cross section can at most be πR^2 no matter what the potential is. We have just counted all particles entering the interaction region as potentially being deflected. Similarly in the quantum case we get a uniform bound (independent of the potential) by estimating the part of the plane wave packet which can possibly be influenced by the potential. The technical trick used for this estimate is due to Kupsch and Sandhas [10].

Let $j(|\vec{r}|) = 1$ (resp. 0) if $|\vec{r}| \leq 1$ (resp. ≥ 2) be a smooth cutoff function and define

$$j_R(|\vec{r}|) = j(|\vec{r}| / R). \tag{4.1}$$

For any $R < \infty$ and any $\Phi \in \mathcal{H}$ we have

$$\| j_R e^{-i H_o t} \Phi \| \to 0 \text{ as } |t| \to \infty , \tag{4.2}$$

and the same is true if Φ is replaced by a plane wave packet g (see the Lemma in Section 3). Therefore

$$\begin{aligned} \Omega &= \text{s-lim } e^{i Ht} e^{-i H_o t} \\ &= \text{s-lim } e^{i Ht} (1-j_R) e^{-i H_o t} \end{aligned} \tag{4.3}$$

and with the Cook argument

$$\begin{aligned} \Omega^+ - \Omega^- &= i \int_{-\infty}^{\infty} dt\, e^{i Ht} \{H(1-j_R) - (1-j_R) H_o\} e^{-i H_o t} \\ &= -i \int_{-\infty}^{\infty} dt\, e^{i Ht} [H_o, j_R] e^{-i H_o t} \\ &= i \int_{-\infty}^{\infty} dt\, e^{i Ht} \{\tfrac{1}{2} (\Delta j_R) + (\vec{\nabla} j_R) \cdot \vec{\nabla}\} e^{-i H_o t} . \end{aligned} \tag{4.4}$$

Here we have used that $V(1-j_R) = 0$ if V has support inside a ball of radius R, no matter how bad the singularities of V may be. If for the description of hard cores or other severe local singularities an identification operator is used to define the wave operators then the second line of (4.3) and (4.4) are still true for big enough R.

Inserting the "potential" $\{\frac{1}{2} \Delta j_R + (\vec{\nabla} j_R) \cdot \vec{\nabla}\}$ in the estimates of the preceding section, e.g. (3.19) with $\rho = 0$, one easily obtains

<u>Theorem.</u> Let $H = H_o + V$, V any potential with support contained in a ball of radius $R \geq R_o$, then for $v > 2\delta$

$$\int_{v-\delta}^{v+\delta} \sigma_{tot}(k,\hat{e})\, dk \leq \text{const. } R^2, \tag{4.5}$$

where the constant depends on δ and R_o but is independent of v,R and V.

Except for the value of the constant in (4.5) (see Section 6 for estimates) the bound is saturated for large R by hard cores giving $2\pi R^2$. The energy decay has disappeared because the gradient applied to g in (3.17) yields an increase proportional to v. The remarks following (3.24) showed why the small R behavior of our simple bound is not optimal. The correct behavior as $R \to 0$ should be a constant because there are point interactions with non trivial scattering, see [8] for a discussion.

5. STRONG COUPLING BEHAVIOR

For strong coupling, when the Born approximation does not converge, the traditional time independent method yields finiteness of the total cross section but no control on its size because a Fredholm alternative is used to solve the Lippman Schwinger equation. Recently Amrein and Pearson [1] gave a bound independent of λ for potentials of compact support and increasing as λ^2 otherwise. Martin [11] proved a λ^4-bound for spherically symmetric Rollnik potentials. Actually the increase in the coupling constant λ will depend on the decay at infinity of the potential.

<u>Theorem.</u> Let $V(\vec{r})$ obey for some $\alpha > 2$, $r := |\vec{r}| \geq R_o$:

$$|V(\vec{r})| \leq \text{const. } (1 + r)^{-\alpha} , \tag{5.1}$$

or

$$|V(\vec{r})| \leq \text{const. } e^{-\mu r} \tag{5.2}$$

then for given direction $\hat{e}$ and Hamiltonian $H_o + \lambda V$

$$\int_{v-\delta}^{v+\delta} \sigma_{tot}(k,\hat{e};\lambda)\, dk \leq D(\delta) \begin{cases} (\lambda/v)^{\gamma}, \gamma = 2/(\alpha-1) & (5.3) \\ \text{or} \\ \ln^2(\lambda/v) & (5.4) \end{cases}$$

where $v > 2\delta$, $(\lambda/v) > 2$.

Remark. The power γ in (5.3) is correct because there are spherically symmetric potentials decaying like (5.1) with a lower bound increasing like (5.3). For $\alpha > 3$ trace class methods give similar results (see Appendix 2 and 3 in [8]).

Proof. Using j_R (4.1) we get in (4.4) in addition to the commutator a tail term $\lambda V(1-j_R)$. Combining the bounds (3.18) for the tail part and (4.5) for the inner part which is independent of V and λ, we obtain

$$\int_{v-\delta}^{v+\delta} \sigma_{tot}(k,\hat{e};\lambda)dk \leq D(\delta)[R^2 + (\lambda/v)^2 \| V(1-j_R)\|_e^2] .$$

We minimize the bound by choosing $R = (\lambda/v)^{1/(\alpha-1)}$ in case (5.1) and $R = (\mu')^{-1} \ln(\lambda/v)$, $\mu' < \mu$ in case (5.2). □

6. THE CLASSICAL LIMIT

So far we have chosen our units such that Planck's constant $\hbar=1$. We reinsert it to study the classical limit $\hbar\to 0$ for the pair $H_o = -(\hbar^2/2)\Delta$, $H = H_o + V$. The wave number is $\vec{k}=\hbar^{-1}\vec{p}$ for the physical momentum $\vec{p}$(= velocity). Scaling the time this corresponds to scattering for the pair $H_o = -(1/2)\Delta$, $H = H_o + \hbar^{-2} V$; thereby the S-operator and its kernel in $\vec{k}$-space are not changed. With the physical momentum $\vec{p}$ fixed the wave vector k diverges as $\hbar^{-1}$ in the classical limit $\hbar\to 0$ and the coupling constant λ grows as $\hbar^{-2}$. In terms of the quantites of the previous section we have $v \sim \hbar^{-1}$ ($\hbar$ v = const is the physical velocity), thus $(\lambda/v) \sim \hbar^{-1}$ diverges and the classical limit is a strong coupling limit. We have seen that the total cross section then generally diverges unless the potential has compact support. Therefore infinitely extended potentials will in general have infinite classical total cross sections.

Fix now an obstacle or potential of compact support and let F be its area as seen from the fixed incident beam direction $\hat{e}$. The classical cross section can be determined with any beam which covers F, the particles passing outside F will miss the target and they do not contribute. Similarly in the quantum case the part of the plane wave packet which is at time t = 0 far-away from F will hardly be scattered by the potential. The main contribution to the total cross section comes from the part that covers F, the outside part does not contribute in the classical limit $\hbar\to 0$. This gives simple estimates of σ_{tot} in the quasiclassical regime and moreover allows to give bounds on the constant in (4.5) for the large R behavior.

For simplicity we treat obstacles inside a ball of radius R, the changes necessary to treat other shapes are obvious.

Similar to (3.5) we use a family of smooth cutoff functions in the plane perpendicular to $\hat{e}$. Let $\phi \in C^\infty(\mathbb{R})$ be monotone with $\phi[u] = 1$ (resp. 0) if $u \leq 0$ (resp. ≥ 1). Define for $R,s > 0$

$$f_{R,s}(x,y) := \phi[\{(x^2+y^2)^{1/2} - R - 2s\}/s], \qquad (6.1)$$

this implies

$$f_{R,s}(x,y) = \begin{cases} 1 & \text{for } x^2+y^2 \leq (R+2s)^2 \\ 0 & \text{for } x^2+y^2 \geq (R+3s)^2 . \end{cases} \qquad (6.2)$$

Now split the plane wave packet g as

$$g = g\, f_{R,s} + g(1-f_{R,s}) \qquad (6.3)$$

then the Hilbert space norm of the first summand is bounded by

$$\| g\, f_{R,s}\|^2 \leq \|g\|^2\, \pi(R+3s)^2 \qquad (6.4)$$

where the norm of g is in $L^2(\mathbb{R})$.

Now consider the normalized sequence of wave packets

$$\tilde{g}_\hbar(k) = (\hbar)^{1/4}\, \tilde{G}[\sqrt{\hbar}(k-v/\hbar)]$$

for $\tilde{G} \in C_o^\infty(\mathbb{R})$, v a given physical velocity. Then in the limit $\hbar\to 0$ $|g_\hbar(z)|^2$ dz converges to $\delta(z)$ dz and the distribution of the physical momentum $p = \hbar$ k converges to $\delta(p-v)dp$.

With the free time evolution generated by $h_o = -(\hbar^2/2)d^2/dz^2$ the estimate (3.13) of the Lemma in Section 3 can be changed to

$$\int_{|z|\leq vt/2} dz\ |[e^{-i h_o t} g_\hbar](z)|^2 \leq C_m \hbar^m (1+|vt|)^{-m}. \qquad (6.5)$$

As in Section 4 we use again the Kupsch-Sandhas trick for the estimate of

$$\|(S-1)g_\hbar\ (1-f_{R,s})\| \qquad (6.6)$$
$$\leq \int_{-\infty}^{\infty} dt\ \|\{(1/2)(\Delta j)+(\vec{\nabla} j)\cdot\vec{\nabla}\}\ e^{-i H_o t}\ g_\hbar(1-f_{R,s})\|$$

where we choose $j \in C_0^\infty$ with $j(\vec{r}) = 1(0)$ if $|\vec{r}| \leq R(\geq R+s)$ and $|\vec{\nabla} j|$, Δj are proportional to s^{-1}, s^{-2}. The support of the "bounded potential" in curly brackets in (6.6) is contained in a ball of radius R+s. With the estimate (6.5) the time integration in (6.6) has a contribution for $|t| \geq 2(R+s)/v$ which is bounded by const $\hbar^m (s^{-1}+s^{-2})$.

It remains to estimate the tail of

$$e^{-i H_o t}(1-f_{R,s}(x,y)) \tag{6.7}$$

which propagates into the region $x^2+y^2 \leq (R+s)^2$ for the time interval $|t| \leq 2(R+s)/v \leq 4R/v$ (if $s \leq R$) independent of $\hbar$. Now we let s tend to zero slowly as $\hbar \to 0$, e.g. like a small power $\hbar^\varepsilon$, then the momentum distribution shrinks as $\hbar^{(1-\varepsilon)}$, we have to control propagation beyond a distance $\hbar^\varepsilon$ into the region where the "potential" of strength $\hbar^{-2\varepsilon}$ acts. The same kind of estimate as above yields

$$\lim_{\hbar\to 0} \sup_{|t| \leq 4R/v} \| \{(1/2)(\Delta j)+(\vec{\nabla} j)\cdot\vec{\nabla}\} \times e^{-i H_o t} g_\hbar (1-f_{R,s}) \| = 0. \tag{6.8}$$

Thus the contribution to σ_{tot} from the outer part disappears

$$\lim_{\hbar\to 0} \|(S-1) g_\hbar (1-f_{R,s})\| = 0.$$

With (6.4) and $\|S-1\| \leq 2$ we obtain

$$\sigma_{tot}(v;\hbar=0) := \lim_{\hbar\to 0} \|(S-1) g_\hbar f_{R,s}\|^2$$

$$\leq 4\pi R^2 .$$

In the classical limit the sharp energy quantum cross section is bounded by four times the geometric classical πR^2 (or 4F for general shapes).

By scaling one can see that the relevant quantity is the dimensionless $k R = p R/\hbar$ which has to be big. Thus $\hbar \to 0$ is equivalent to the high energy or large R limit for given physical $\hbar$. Using this (or an analogous estimate as above with s growing slightly slower than R) we can improve (4.5) in the Theorem of Section 4 ($\hbar$ fixed):

$$\int_{v-\delta}^{v+\delta} \sigma_{tot}(k,\hat{e})dk \leq 2\delta \, 4\pi R^2 + o(R^2). \tag{6.9}$$

The remainder term can be estimated explicitly.

This bound (6.9) is saturated if $S \approx -1$ on g f. This happens for potentials of the type

$$V(x,y,z) = a \, \chi_{[-r,r]}(z) \, \chi_{R^2}(x^2+y^2)$$

discussed in Section 2. For δ small and suitably adjusted parameters a and r depending on $v/\hbar$ the S operator can approximate any phase factor. In particular for $\hbar \to 0$ it oscillates between $S \approx -1$ and $S \approx 1$, therefore σ_{tot} does not converge as $\hbar \to 0$.

For typical potentials, however, the particles are deflected if they hit the target and only very few of them continue to fly approximately in the forward direction. Then g f and S g f are approximately orthogonal and

$$\int \sigma_{tot}(k) |\hat{g}(k)|^2 dk \approx 2\pi R^2 \|g\|^2. \tag{6.10}$$

For general shapes $2\pi R^2$ is replaced by 2 F. This is the well known "shadow scattering"-result which holds e.g. for hard spheres. A short time after the scattering g f and S g f are essentially localized in disjoint regions, thus for these particular beams simple amplitude measurements close to the target can be made. In Section 5 of [8] we propose a characterization of potentials which should be "typical" in the above sense.

To sum up this discussion we have seen that with our definition of the total cross section it is perfectly justified to use beams of finite width. For small but macroscopic targets (k R big enough depending on the admissible error) a beam is even wide enough if it just covers the target. Moreover for typical potentials simple measurements can be carried out near the target which should yield good approximate results.

On the other hand the conventional definition based on counters detecting deflected particles will always require a much wider beam. An extremely well collimated beam of finite width 2ρ (like a laser beam) will typically have the following shape. Up to a finite distance it looks like a plane wave restricted to a tube of radius ρ and asymptotically it looks like a spherical wave restricted to a cone. By the uncertainty principle the momentum- (=velocity-) spread perpendicular to the propagation direction is of the order $\hbar\rho^{-1}$ which should be small compared to the average velocity v. The opening angle of the asymptotic cone is then $\hbar(\rho v)^{-1}$. The transition between the two regimes happens near a distance D where the cone is as wide as the tube, i.e. $D \approx \rho^2 v/\hbar$.

A counter which should detect only deflected particles must be located outside the union of the tube and the cone where the incoming beam would propagate. Consider for example a target of radius $R \leq \rho$. Typically most particles which hit the target will be significantly deflected and are detected easily giving the classical geometric cross section πR^2. The subtle effects come from the "shadow", the particles missing behind the target; their wave function is the negative of the part of the plane wave packet restricted in the perpendicular direction to the radius R at time zero. Its tube region is contained in the bigger tube of the incoming beam and thus never matters. Later it spreads into a cone with angles $\tan\theta \leq \hbar(Rv)^{-1}$. For the main part of this wave to be detectable outside the cone of the incoming wave one has to choose $\rho \gg R$. One can see these "shadow"-particles only if their cone region is wider than the tube of radius ρ, i.e. beyond a minimal distance $d \gtrsim R\,\rho\,v/\hbar$ from the target. To get an idea of the order of magnitude take a neutron of energy 100 eV, a target of radius 10^{-5}m and a beam ten times wider, then $d \gtrsim 2 \cdot 10^{3}$m! Increasing the mass or energy of the projectile or the size of the target will only increase this distance. In the laboratory one will see nothing but the classical cross section for tiny but macroscopic targets if deflected particles are counted. (See also [13] where an approximate calculation for hard spheres is given.) Although both definitions of the total cross section agree asymptotically our definition has the advantage of giving a good approximate value from observations within a reasonable distance of the target.

7. TWO CLUSTER SCATTERING

So far we have studied potential scattering. This is equivalent to two particle scattering if one can separate off the center of mass motion, i.e. if the potential depends only on the relative position of the particles. Similarly one can consider in the multiparticle case scattering of two bounded subsystems like atoms; the relative position and momentum of the centers of mass for the two subsystems corresponds to position and momentum in potential scattering. A "channel" is specified if both the decomposition of the particles into clusters and the bound states for each cluster are given. For each channel (labelled by the index α) there is a subspace $\mathcal{H}_\alpha$ of the state space $\mathcal{H}$ consisting of product wave functions

$$\phi \prod_i \eta_i \tag{7.1}$$

where ϕ is the square integrable function which describes the relative motion of the centers of mass of the clusters, and η_i are the cluster bound state wave functions. The cluster Hamiltonian $H(\alpha)$ which leaves $\mathcal{H}_\alpha$ invariant is obtained from the full Hamiltonian

H as $H(\alpha) = H - I_\alpha$, where I_α is the sum of all potentials which couple particles in different clusters. The channel wave operators are mappings from $\mathcal{H}_\alpha$ into $\mathcal{H}$ defined as

$$\Omega_\alpha^{\mp} = \lim_{t\to\pm\infty} e^{i\,Ht}\, e^{-i\,H(\alpha)t} \tag{7.2}$$

and the full wave operators

$$\Omega^{\mp} = \bigoplus_\alpha \Omega_\alpha^{\mp} \tag{7.3}$$

are isometric mappings into $\mathcal{H}$ from $\oplus\,\mathcal{H}_\alpha$ which is interpreted as space of outgoing or incoming configurations, respectively. The scattering operator

$$S = (\Omega^-)^* \,\Omega^+$$

maps incoming configurations into outgoing ones. (See Section XI.5 of [12] for details.) For the channel α and a given incoming state $\Psi_\alpha \in \mathcal{H}_\alpha$ one has

$$\|(S-1)\Psi_\alpha\| \leq \|(\Omega_\alpha^+ - \Omega_\alpha^-)\Psi_\alpha\| \tag{7.4}$$

$$\leq \int_{-\infty}^{\infty} dt\, \|I_\alpha\, e^{-iH(\alpha)t}\,\Psi_\alpha\| \tag{7.5}$$

similar to the two particle case. (7.4) is an equality if asymptotic completeness holds.

Fix now a *two* chuster channel α, then the incoming wave function in $\mathcal{H}_\alpha$ is of the form

$$\Psi_\alpha = \phi_\alpha\, \eta_1\, \eta_2 \tag{7.6}$$

and ϕ_α is a function of one variable, the relative coordinate of the two centers of mass. (As usual we have separated off the total center of mass motion.) The total cross section is now defined analogously. In addition to the clusters which are scattered elastically and deflected one also counts all excitations, breakup and rearrangement collisions. In our wave-limit approach we use incoming plane wave packets of the channel α described by

$$g_\alpha := g\, \eta_1\, \eta_2 \tag{7.7}$$

where η_i are the corresponding bound state wave functions (or one if the cluster consists of a single particle) and g is the familiar plane wave packet for the relative center of mass motion, obtained as a limit of square integrable functions as discussed in Section 3. We now define

$$\int_0^\infty \sigma_{tot}(k,\hat{e};\alpha)\,|\tilde{g}(k)|^2\,dk := \|(S-1)g_\alpha\|^2, \tag{7.8}$$

and we use (7.5) as a simple estimate.

$H(\alpha)$ acts trivially on η_1 and η_2 and reduces on g to $h_\alpha = -(1/2\,m_\alpha)\,d^2/dz^2$ where m_α is the reduced mass of the two clusters. Therefore

$$\|I_\alpha e^{-i\,H(\alpha)t} g_\alpha\| = \|V_\alpha e^{-i\,h_\alpha t} g\| \tag{7.9}$$

with the effective potential between the clusters

$$V_\alpha(\vec{r}) = [\int |I_\alpha(\vec{r},\zeta_1,\zeta_2)|^2\,|\eta_1(\zeta_1)|^2\,|\eta_2(\zeta_2)|^2\,d\zeta_1\,d\zeta_2]^{1/2} \tag{7.10}$$

Here $\vec{r}$ is the separation of centers of mass and ζ_i are the inner-cluster coordinates (of dimension 3(k-1) if k particles belong to the cluster). The analysis of Section 3 immediately applies and all we have to do in the multiparticle case is to control the decay of $V_\alpha(\vec{r})$ for a proof of finite total cross sections. On the other hand the analysis of Sections 4 - 6 cannot be used directly because effective potentials won't have compact support, and a growing coupling constant will change I_α and the bound state wave functions η_i simultaneously. This makes it difficult to control the strong coupling or classical limits.

Typical bound state wave functions (except at thresholds) have exponential decay [5]. If there are bound states with slow decay we will omit in the following the corresponding channels. If all pair potentials contributing to I_α

$$V_{ij}(\vec{r}_i - \vec{r}_j) = V_{ij}(\vec{r} + \vec{\zeta}_{1,i} - \vec{\zeta}_{2,j}) \tag{7.11}$$

decay faster than $|\vec{r}_i - \vec{r}_j|^{-2}$ as specified in (3.22), then the convolution in (7.10) preserves this property and the total cross section is finite. Of particular physical interest, however, is the case of long range pair potentials like the Coulomb force between charged particles which may nevertheless give rise to an

effective potential of short range. This is the case for atom-atom scattering. If both clusters are neutral then the contribution with slowest decay is the dipole-dipole potential which behaves as $|\vec{r}|^{-3}$.

Let i label the particles in one cluster and j label those in the other. Consider as a typical example pair potentials of the type

$$\begin{aligned} &e_i\,e_j|\vec{r}_i - \vec{r}_j|^{-1} + V_{ij}(\vec{r}_i - \vec{r}_j) \in L^2_{\ell oc} \\ &V_{ij}(\vec{u}) = O(|\vec{u}|^{-2-\varepsilon}) \text{ for } |\vec{u}| \geq R_o\,. \end{aligned} \tag{7.12}$$

If both clusters are neutral: $\Sigma e_i = \Sigma e_j = 0$, then $V_\alpha(\vec{r})$ satisfies (3.20). This proves the following

<u>Theorem.</u> Let N charged particles interact with pair potentials which fulfill (7.12). Let α be a channel with two neutral clusters whose bound state wave functions have rapid decay. Then

$$\int_{v-\delta}^{v+\delta} \sigma_{tot}(k,\hat{e};\alpha)\,dk \leq C(\delta)\;v^{-2}\|V_\alpha\|^2_{\hat{e}} \tag{7.13}$$

is finite and $C(\delta)$ is independent of the channel.

One expects that a similar result holds if one cluster is neutral and does not have a permanent dipole moment, but we cannot prove that ([7] and Section 6 of [8]).

REFERENCES

1. W.O. Amrein and D.B. Pearson, J. Phys. A <u>12</u>, 1469 (1979).
2. W.O. Amrein, D.B. Pearson, and K.B. Sinha, Nuovo Cimento <u>52A</u>, 115 (1979).
3. V.V. Babikov, Sov. Phys. Uspekhi <u>92</u>, 271 (1967).
4. F. Calogero, <u>The Variable Phase Approach to Scattering</u>, Academic Press, New York 1967.
5. P. Deift, W. Hunziker, B. Simon, and E. Vock, Commun. Math. Phys. <u>64</u>, 1 (1978).
6. J.D. Dollard, Commun. Math. Phys. <u>12</u>, 193 (1969).
7. V. Enss and B. Simon, Phys. Rev. Lett. <u>44</u>, 319 and 764 (1980).
8. V. Enss and B. Simon, Commun. Math. Phys., in press.
9. T.A. Green and O.E. Lanford, J. Math. Phys. <u>1</u>, 139 (1960).
10. J. Kupsch and W. Sandhas, Commun. Math. Phys. <u>2</u>, 147 (1966).
11. A. Martin, Commun. Math. Phys. <u>69</u>, 89 (1979) and <u>73</u>, 79 (1980).
12. M. Reed and B. Simon, <u>Methods of Modern Mathematical Physics, III Scattering Theory</u>, Academic Press, New York 1979.

13. R. Peierls, Surprises in Theoretical Physics, Princeton University Press, 1979.
14. T. Kato, Scattering Theory, in: Studies in Mathematics Vol 7, Studies in Applied Mathematics, A. H. Taub ed., The Mathematical Association of America, 1971; page 90-115.