TOTAL CROSS SECTIONS IN NON-RELATIVISTIC SCATTERING THEORY

Volker Enss
Institut für Mathematik
Ruhr-Universität
D-44780 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 $\sigma_{\text{tot}}$ in potential- and multiparticle-scattering. $\sigma_{\text{tot}}$ 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 $\sigma_{\text{tot}}$ for large coupling constant $\lambda$, the power of $\lambda$ 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 $\lambda$.

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 the propagation of a 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 rather special to investigate in 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 multiscattering 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 one. 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 is that we have to average over a small energy range; our bounds blow up in the high-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 2 we determine the decay requirements for infinite 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 Kupash-Sandeas 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.

2. THE DEFINITION OF CLASSICAL AND QUANTUM TOTAL CROSS SECTIONS

The main advantage of time dependent (and geometric) methods is that two cluster scattering is almost as easy to handle as two particle (or 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 potential 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. (For one might use (2.5) as an equivalent expression for 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].

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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 $\theta$, then a sharp direction would mean that $P_z = P_\theta = 0$. 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 $\theta$, 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 $\theta$, 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.

$$V_B(x,y,z) = (a + b(x)) \gamma_{(-R,x)}(z) \gamma_{(-R,y)}(x) \gamma_{(-R,z)}(y)$$

for some parameters $a,b,R,x$. 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 $b \neq 0$ it jumps to $4\pi^2 a \hbar^2 R^2$. 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 $4\pi^2 R^2$. For such a potential with $b = 0$ the quasi-classical 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 $\theta$ parallel to the $x$-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 $\theta$ the plane wave space $H$ is isomorphic to (and henceforth identified with) $L^2(\mathbb{R},dx)$. The configuration space wave function is

$$g(x,y,z) = g(z) \text{ with } \int |g(z)|^2 \, dx = 1.$$  \hfill (2.1)
In momentum space we denote by \( \tilde{g}(k) \) the one-dimensional Fourier-transform
\[
\tilde{g}(k) = \frac{(2\pi)^{-1/2}}{i \sin k z} \tilde{g}(z),
\]
corresponding to the three-dimensional Fourier transform
\[
\tilde{g}(k) = \frac{1}{(2\pi)^3} \int \tilde{g}(\mathbf{r}) \, \delta(k - \mathbf{k}) \, d\mathbf{k}.
\]
Since a beam should hit the target from one side only we assume:
\[
\supp \tilde{g}(k) \subset \{ |\mathbf{k}| = |\mathbf{k}| \}.
\]
which implies in (2.3) \( |\mathbf{k}| = |\mathbf{k}| \).

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 \( I(S - 1)g \), where the norm is that of the Hilbert space \( \mathcal{H}^2(\mathbb{R}^2) \). Thus we define the quantum mechanical total cross section
\[
\sigma_{\text{tot}}(k, \mathbf{k}) = \int |\tilde{g}(k')|^2 \, dk = I(S - 1)g^2,
\]
where \( g \in \mathcal{H}^2(k) \) 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 \( \mathcal{H}^2(k) \) to a bounded map from \( \mathcal{H}^2(k) \) into \( \mathcal{H}^2(k) \), 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 Lippmann Swinger equation have the asymptotic form
\[
\phi^{\infty}(k, \mathbf{x}) = f(k, \mathbf{x}) \exp[i \mathbf{k} \cdot \mathbf{x}] + \frac{\exp[i \mathbf{k} \cdot \mathbf{x}]}{|\mathbf{k}|} |f(k, \mathbf{x})|,
\]
\( f(k, \mathbf{x}) \) is the continuous on shell scattering amplitude. Equivalently the kernel of \( S - 1 \) in momentum space is
\[
(S - 1)(k', k) = \frac{1}{2\pi m} \int \delta(k' - 2m \mathbf{k} - k) f(k, \mathbf{x}) \, d\mathbf{x},
\]
where \( k = |\mathbf{k}|, k = |\mathbf{k}| \), etc. Then
\[
\sigma_{\text{tot}}(k, \mathbf{k}) = \int |f(k, \mathbf{x})|^2 \, d\mathbf{x} = \sigma_{\text{tot}}(k, \mathbf{x})^2.
\]

The physical motivation for this choice as given in most textbooks on quantum mechanics uses the "obvious" fact that \( \exp(i k \cdot x) \) describes an incoming homogeneous beam of particles with momentum \( k \), direction \( \mathbf{k} \) and density \( \rho \) per unit area, similarly for the outgoing spherical wave.

More careful authors give the following time dependent justification. Let \( \phi^{\infty}(k) \) be the square integrable wave function of a single incoming particle with momentum support well concentrated around a mean value \( \mathbf{q} \). The corresponding outgoing state has a momentum space wave function
\[
\phi^{\infty}(k') = (S - 1) \phi^{\infty}(k) + \int \frac{d^2k}{2\pi m} \delta(k' - 2m \mathbf{k} - k) \phi^{\infty}(k) + \frac{i}{2\pi m} \int d^2k' \delta(k' - 2m \mathbf{k} - \mathbf{q}) f(k', \mathbf{x}) \phi^{\infty}(k') = (S - 1) \phi^{\infty}(k).
\]

The "scattering into cones" papers [6, 9] show that the asymptotic direction of flight is \( k' \) for the incoming and \( k' \) for the outgoing state. The first summand in (2.7) is thus 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 \( \phi^{\infty}(k) \). Under this assumption the probability \( w(\phi^{\infty}) \) that a particle with incoming wave function \( \phi^{\infty} \) will be deflected, is
\[
w(\phi^{\infty}) = \int d^2k \int \frac{d^2k'}{2\pi m} \delta(k' - 2m \mathbf{k} - \mathbf{q}) f(k', \mathbf{x}) |\phi^{\infty}(k')|^2 = I(S - 1) \phi^{\infty}.
\]

To represent a homogeneous beam one translates the incoming state by a vector \( \mathbf{\delta} \) in the plane orthogonal to the mean direction \( \mathbf{q} \),
\[
\phi^{\infty}_\mathbf{\delta}(k) = \exp[-i \mathbf{\delta} \cdot \mathbf{k}] \phi^{\infty}(k),
\]
and one sums up the contributions for different \( \mathbf{\delta} \)'s. \( d^2\mathbf{\delta} \) represents a homogeneous beam with particle density one per unit area. The resulting number of deflected particles is then
\[
\int d^2\mathbf{\delta} \, w(\phi^{\infty}_\mathbf{\delta}) = \sigma_{\text{tot}}(\mathbf{\delta})
\]
\[
= \int d^2\mathbf{k} \int \frac{d^2k'}{2\pi m} |f(k', \mathbf{\delta})|^2 |\phi^{\infty}(k')|^2.
\]
In the limit \( |\phi^{\infty}(k')|^2 = \delta(k' - k) \) expression (2.6) for \( \sigma_{\text{tot}}(\mathbf{\delta}, \mathbf{q}) \) is recovered and \( |\phi^{\infty}(k')|^2 = \delta(k') \) yields
\[
\int d^2\mathbf{k} \sigma_{\text{tot}}(\mathbf{k}) |\phi^{\infty}(k')|^2, \quad \text{the left hand side of (2.5). Note that the}
\]
summed over \( \mathbf{\delta} \)'s is incoherent, we have added probabilities and
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3. THE BASIC ESTIMATE FOR CONTINUATION OF THE KINETIC ENERGY

We assume in this section that the potential \( V(r) \) is a perturbation of the kinetic energy, \( H = \frac{\mathbf{p}^2}{2m} + V(r) \). We are interested in the existence of solutions of the Schrödinger equation with potential \( V(r) \) and velocity \( \mathbf{v} \). The solutions of the equation will be sought in the form of \( \psi(r,\mathbf{v}) = e^{-iHt} \psi_0(r) \), where \( \psi_0(r) \) is a solution of the free Schrödinger equation.

The equation of motion for \( \psi(r,\mathbf{v}) \) is given by

\[
\frac{\partial \psi}{\partial t} = i(H - V(r)) \psi.
\]

The potential \( V(r) \) is assumed to be smooth and bounded, and the wave function \( \psi \) is assumed to be in the domain of \( H \). The following interpolation picture representation holds:

\[
\psi(r,\mathbf{v}) = \int d^3p \, e^{i\mathbf{p}\cdot\mathbf{v}} \psi(p),
\]

where \( \psi(p) \) is the momentum representation of \( \psi \).

The basic estimate for continuation of the kinetic energy is derived from the following inequality:

\[
|\psi(r)|^2 \leq C \left( 1 + \frac{1}{r} \right)^{-\delta} \int d^3p \, |\psi(p)|^2 e^{2\pi \delta |\mathbf{p}|}
\]

which implies by (3.2) convergence in \( \mathbf{R} \) of the corresponding sequence of states which exist and are complete, the operators \( \mathbf{p} \), \( \mathbf{v} \) and \( \mathbf{r} \) possess stronger decay requirements.

In the previous section we will explain why classical phase space sections may be finite and dependent on the target and single particles, interference between particles in the beam being not desired.
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where we have fixed the z-axis in the beam direction \( \hat{e} \), and the one-dimensional estimate

\[
\left| \frac{\sqrt{d}}{\mathcal{W}(z)} \int e^{-i \eta(t) \hat{e}} g(z) \mathcal{W}^2(z) |e^{-i \eta(t) \hat{e}} g(z)|^2 dt \right|^{1/2}
\]

will imply finite total cross sections.

Here we have taken multiplication by \( V(x) \) as a map from \( \mathcal{H}_0 \) into \( \mathcal{K} \) and we have used that

\[
\mathcal{W}_V g = L^2(\mathbb{R}) \rightarrow \mathcal{L}(\mathbb{R})
\]

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

Lemma.

Let \( \psi(z) \) have the (one-dimensional) Fourier transform \( \hat{\psi}(k) \in C^\infty_0(\mathbb{R}) \), supp \( \psi \subset (-\delta, \delta) \). Define

\[
\hat{\psi}(k) = \hat{\psi}(k-v)
\]

Then for \( v > \delta \) there are \( C \) independent of \( v \) such that

\[
\int_{\mathbb{R}} \left| \int e^{-i \eta(t) \hat{e}} g(z) \right|^2 \leq C \left( 1 + |vt| \right)^{-\eta}
\]

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

\[
\left| \int e^{-i \eta(t) \hat{e}} g(z) \right| \leq C \left( 1 + |z| \right)^{-\eta}
\]

Next observe that

\[
\left| e^{-i \eta(t) \hat{e}} \psi_j(k) \right| = \left| e^{i \frac{v^2}{2} + k^2} e^{-i \eta(t) \hat{e}} \psi_j(k) \right|
\]

and

\[
\left| e^{-i \eta(t) \hat{e}} \psi_j(z) \right| = \left| e^{-i \eta(t) \hat{e}} \psi_j(z-vt) \right|
\]

Thus for \( |z-vt|/|t| > \delta \)

\[
\left| e^{-i \eta(t) \hat{e}} \psi_j(z) \right| \leq C \left( 1 + |z-vt| \right)^{-\eta}
\]

For \( |z|/|t| > 2 \) this implies (3.13).
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\[ \begin{align*}
&< \frac{1}{v} \int d|v| \left( 2 \hbar |v| t \frac{1}{2} + 2 \hbar |v| t \right) \frac{C_2 (\hbar^2 |v|)^{-2}}{\sqrt{\frac{1}{v}}} \\
&\leq C \sqrt{v} \left( |h(0)| + \frac{1}{d\Re h(0)} \right) = C \sqrt{v} |v|^{-1} \\
&\leq C (v^{-1} |h(0)| + \frac{1}{d\Re h(0)}) = C \sqrt{v} |v|^{-1} 
\end{align*} \]

where the constant \( C \) depends on the shape of the wave function \( \psi \), and is independent of \( v \) and \( W \).

Let us take for a function with \( \sup_k \psi \in C_r \) and \( \sup_k \psi_y = \psi \) if \( |k-v| < 5/2 \); furthermore introduce a coupling constant \( \lambda \), then we can sum our results in the following

**Theorem.** For the pair \( R \), \( W = R + J \) and incident beam direction \( \gamma \), the total cross section is bounded by

\[ \sigma_{\text{tot}}(k,\gamma) \leq C(\gamma) (\lambda/\sqrt{v})^{2} / |k|^{2} \]

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 \( |v|^{-1} \). Assume that \( V \) is locally square integrable and continuous outside a ball of radius \( r \). Then \( |v|^{-1} \) is finite if

\[ \int \frac{dx}{|z|^{1/2}} \left( \frac{d|x|}{|z|^{1/2}} \right)^{1/2} < \infty \]

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

\[ \int |z|^{-1/2} \sup_{|z|-\epsilon} \left( \frac{d|x|}{|z|^{1/2}} \right)^{1/2} \leq C |z|^{-1} \]

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

\[ |x|^{-1/2} \sqrt{\frac{1}{v}} \leq C |z|^{-1/2} \]

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

$$l^{-2} (\frac{\text{d}l}{\text{d}t})^{-1} e^{-\epsilon} \epsilon > 0.$$  

(3.22)

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

If the coupling constant $\lambda$ is small or the energy high (i.e., $(\lambda/v)$ 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 $\lambda = (\nu \text{ fixed})$ there is for any $u < 2$ a spherically symmetric potential with $\text{Im} \lambda < \epsilon$ such that the total cross section increases at least like $(\lambda)^u$. For potentials with faster decay, however, we will prove a slower increase in $\lambda$ 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

$$\| \text{d}t \psi(t) \|_{L^2} \psi(t) g \|_{L^2} \psi(t) g \| = \| \frac{\text{d}t}{\text{d}t} \psi(t) \|_{L^2} \psi(t) g \|_{L^2} \psi(t) g \| \leq \frac{\text{d}t}{\text{d}t} \psi(t) \|_{L^2} \psi(t) g \|_{L^2} \psi(t) g \|.$$  

(3.23)

(3.24)

For a small momentum spread $\delta$ (and similarly for potentials with small support) the size of the wave packet $g$ in $\mathbb{R}^3$ 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 $\delta^{-1}$

$$\| \text{d}t \psi(t) \|_{L^2} \psi(t) g \| \sim \delta^{-1/2} \delta^{-1}$$

rather than the $\delta^{-1}$ 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:

\[ \tag{3.25} \]

This expression is particularly convenient because it uses exactly 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 $e^{itH_0} g$ is mainly localized in a region where $\| \psi(t) \|_{L^2} \psi(t) g \|_{L^2} \psi(t) g \| \leq \| \psi(t) \|_{L^2} \psi(t) g \|_{L^2} \psi(t) g \|$. Thus the $(\lambda/v)^2$-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

$$\| \psi(t) \|_{L^2} \psi(t) g \|_{L^2} \psi(t) g \| \leq \| \psi(t) \|_{L^2} \psi(t) g \|_{L^2} \psi(t) g \|.$$  

for states with momentum support around $v$. Here we have used that $g = \psi(X) \psi(t) g = \psi(2\pi \mathbb{Z}) \psi(t) g$ for these states.

If the interaction term $\psi(2\pi \mathbb{Z}) \psi(t) g$ 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 Kupershmidt-Sanders 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 \( 
\pi R^2 \) 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 Kupach and Sandhas [10].

Let \( j_l (|z|) = 1 (\text{resp.} 0) \) if \( |z| \leq 1 \) (\text{resp.} \geq 2) be a smooth cutoff function and define

\[
j_R (|z|) = j_l (|z| / R).
\]  

(4.1)

For any \( R > = \) and any \( \theta \in \mathbb{K} \) we have

\[
1 j_R e^{-i H_0 t} \theta t \to 0 \text{ as } |t| \to \infty,
\]

(4.2)

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

\[
\Theta = s \lim \frac{e^{-i H_0 t}}{H_0} e^{-i H_0 t} = s \lim \frac{e^{-i H_0 t}}{H_0} (1 - i \frac{1}{R}) e^{-i H_0 t}
\]

(4.3)

and with the Cook argument

\[
\Theta e^{-i H_0 t} = \int dt \frac{e^{-i H_0 t}}{H_0} (H_0 (1 - i \frac{1}{R}) e^{-i H_0 t} =
\]

\[
- i \frac{1}{e^{i H_0 t}} H_0 (1 - i \frac{1}{R}) e^{-i H_0 t}
\]

(4.4)

Here we have used that \( V (1 - i \frac{1}{R}) = 0 \) 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 \( R \).

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 Merin and Pearson [11] gave a bound independent of \( \lambda \) for potentials of compact support and \( \lambda \) increasing as \( \lambda^2 \) otherwise. Martin [11] proved a \( \lambda^2 \) bound for spherically symmetric Rössler potentials. Actually the increase in the coupling constant \( \lambda \) will depend on the decay at infinity of the potential.

Theorem. Let \( \lambda (t) \) obey for some \( \alpha > 2 \), \( x := |x| \geq R \) :

\[
|V (x)| \leq \text{const.} (1 + x)^{-\alpha},
\]

(5.1)

or

\[
|V (x)| \leq \text{const.} e^{-\lambda x}
\]

(5.2)

then for given direction \( \theta \) and Hamiltonian \( H_0 + \lambda \nu \)

\[
\int d \theta \text{ tot} (k, \theta; \lambda) \leq \text{const.} (\lambda / \nu)^{2/(\alpha - 1)}
\]

(5.3)

or

\[
k_0^2 (\lambda / \nu)
\]

(5.4)
where \( \nu > 2\delta \), \( (\lambda/\nu) > 2 \).

**Remark.** The power \( \nu \) in (5.3) is correct because there are spherically symmetric potentials decaying like (5.1) with a lower bound increasing like (5.3). For \( \nu > 3 \), trace class methods give similar results (see Appendix 2 and 3 in [9]).

**Proof.** Using \( \psi_0 \) (4.1) we get in (4.4) in addition to the commutator a tail term \( 3V(1-r)^{1/2} \). Combining the bounds (3.18) for the tail part and (4.5) for the inner part which is independent of \( \nu \) and \( \lambda \), we obtain

\[
\int_{r \leq \delta} \| \psi_0 (k, \cdot, \lambda) \|_2 \leq C \delta \| R^2 + (\lambda/\nu)^2 \|_2 (1-\lambda/r)^{1/2}.
\]

We minimize the bound by choosing \( R = (\lambda/\nu)^{1/(\nu-1)} \) in case (5.1) and \( R = (\lambda/\nu)^{1/(\nu-1)} \) in case (5.2).

6. THE CLASSICAL LIMIT

So far we have chosen our units such that Planck's constant \( h=1 \). We then insert it to study the classical limit \( \hbar \to 0 \) for the pair \( H = - (\hbar^2/2) \partial_x^2 + V \). The wave number is \( \nu \nu^{-1} \) for the physical momentum \( \nu \) (velocity). Scattering the mass this corresponds to scattering for the pair \( H = - (1/2) \partial_x^2 + H_0 + V \); thereby the S-operator and its kernel in \( k \)-space are not changed. With the physical momentum \( \nu \) fixed the wave vector \( k \) diverges as \( \hbar \to 0 \) and the coupling constant \( \lambda \) grows as \( \hbar^{-2} \). In terms of the quantities of the previous section we have \( \nu \nu^{-1} \) (\( \hbar = \text{const.} \) is the physical velocity), thus \( (\lambda/\nu) \nu^{-1} \) 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 \( e \).

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 \( \sigma_{\text{tot}} \) in the quasiclassical regime and moreover allows to give bounds on the constant in (4.5) for the large \( R \) behavior.

**NON-RELATIVISTIC SCATTERING THEORY**

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 \( e \). Let \( g \in C^\infty(\mathbb{R}) \) be smooth with \( g(0) = 1 \) (resp. \( 0 \) if \( |x| < \delta \) (resp. \( |x| > \delta \)). Define for \( R>0 \)

\[
f_{R,s}(x,y) = g((x-y)^2 - R - 2s)/s,
\]

this implies

\[
f_{R,s}(x,y) = \begin{cases} 1 & \text{for } x^2 + y^2 < (R+2s)^2 \\ 0 & \text{for } x^2 + y^2 > (R+3s)^2. \end{cases}
\]

Now split the plane wave packet \( g \) as

\[
g = g f_{R,s} + g(1-f_{R,s})
\]

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

\[
\| f_{R,s} \|_2^2 \leq |g(\nu-(R+3s))^2
\]

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

Now consider the normalized sequence of wave packets

\[
\mathfrak{Q}_n(k) = (\hbar) k^{1/2} \delta(\hat{k}-\mathfrak{q}_n(k-x/k))
\]

for \( \mathfrak{q}_n \in C^\infty(\mathbb{R}) \), \( v \) a given physical velocity. Then in the limit \( \hbar \to 0 \)

\[
|\mathfrak{q}_n(z)|^2 dz \to \delta(z) dz \text{ and the distribution of the physical momentum } p = \hbar k \text{ converges to } \delta(p-v) dp.
\]

With the free time evolution generated by \( h_0 = -\partial_x^2/2 \) the estimate (3.13) of the Lemma in Section 3 can be changed to

\[
\| h_0 \mathfrak{q}_n \|_2^2 \leq C \hbar h_0 \| (1+i vt) \|^\nu,
\]

(6.5)

As in Section 4 we use again the Kupch-Sardas trick for the estimate of

\[
\mathfrak{a}_0^{(8-1)} \mathfrak{q}_n \mathfrak{a}_0^{(1-f_{R,s})} \mathfrak{a}_0
\]

(6.6)
where we choose $j \in \mathcal{O}$ with $j(z) = 1(z)$ if $|z| \leq R(\geq R+\delta)$ and

$$|j(z)|, \delta j$$

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 $R+\delta$. With the estimate (6.5) the time integration in (6.6) has a contribution for $|t| \geq 2(R+\delta)/v$ which is bounded by $\text{const} \, \mathcal{H}(s^{-1} + s^{-2})$.

It remains to estimate the tail of

$$e^{-i \mathcal{H}(s^{-1} + s^{-2})}$$

(6.7)

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

$$\lim_{\mathcal{H} \to 0} \sup_{|t| \leq 2R/v} \left| \int (1/2)(2j) \right| (\mathcal{H})^{-1} e^{-i \mathcal{H} \mathcal{H}(s^{-1} + s^{-2})} = 0.$$  

(6.8)

Thus the contribution to $g_{\text{tot}}$ from the outer part disappears

$$\lim_{\mathcal{H} \to 0} \int (s-i)^{-1} \phi \left(1 - f_{\mathcal{H}, R, s} \right) \right| = 0.$$  

(6.9)

With (6.4) and $f_{\text{tot}}(v; \mathcal{H} = 0) \leq 2v$ we obtain

$$\sigma_{\text{tot}}(v; \mathcal{H} = 0) = \lim_{\mathcal{H} \to 0} \int (s-i)^{-1} \phi \left(1 - f_{\mathcal{H}, R, s} \right) \right| \leq 4\pi R^2.$$  

(6.10)

In the classical limit the sharp energy quantum cross section is bounded by four times the geometric classical cross section of general shapes.

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

$$\sigma_{\text{tot}}(v; \mathcal{H}) \leq 2v \mathcal{H}/\mathcal{H}^4 + O(R^2).$$  

(6.11)

The remainder term can be estimated explicitly.

This bound (6.9) is saturated if $\mathcal{H} \to 0$ on $\mathcal{H} f$. This happens for potentials of the type

$$V(x,y,z) = x^2 + y^2 + \mathcal{H} \left( \mathcal{H} + 2 \right) v^2.$$  

(6.12)

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

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 $\mathcal{H} f$ and $S g f$ are approximately orthogonal and

$$\sigma_{\text{tot}}(k) = \int \mathcal{H} f \left(k, \mathcal{H} \right) \mathcal{H} f \left(k, \mathcal{H} \right) dk \approx 2\pi R^2 \mathcal{H}^2.$$  

(6.13)

For general shapes $X \setminus R^2$ is replaced by $2X$. 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 [7] 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 $2\mathcal{H}$ (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 $\rho$ 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 $\hbar (v/\rho)^{-1}$. The transition between the two regimes happens near a distance $D$ where the cone is as wide as the tube, i.e. $\mathcal{H} \rho^2 \mathcal{H}^2$. 

$$\sigma_{\text{tot}}(v; \mathcal{H}) \leq 2v \mathcal{H}/\mathcal{H}^4 + O(R^2).$$  

(6.11)
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 \( R < \rho \). Typically most particles which hit the target will be significantly deflected and are detected easily giving the classical geometric cross section \( \pi R^2 \). 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 gatters. Later it spreads into a cone with angles \( \tan \theta = \frac{R}{h(2\pi)^{-1}} \). For the main part of this wave to be detectable outside the cone of the incoming wave one has to choose \( \rho > R \). One can see these "shadow"-particles only if their cone region is wider than the tube of radius \( \rho \), i.e. beyond the minimal distance \( d \gg \rho \) from the target. To get an idea of the order of magnitude take a neutron of energy 100 e\( \text{V}, a \) target of radius \( 10^{-5} \) m and a beam ten times wider, then \( d \approx 2 \cdot 10^{-4} \) 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 \( \alpha \)) there is a subspace \( \mathcal{K}_\alpha \) of the state space \( \mathcal{K} \) consisting of product wave functions

\[
\psi = \psi_1 \psi_2 \]

(7.1)

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

\[
\mathbf{H}(\alpha) = H - \mathbf{I}_\alpha, \quad \text{where } I_\alpha \text{ is the sum of all potentials which couple particles in different clusters. The channel wave operators are mappings from } X_\alpha \text{ into } \mathcal{K} \text{ defined as}
\]

\[
\mathbf{G}_\alpha = \lim_{t \to \infty} e^{-iH(\alpha)t} = e^{-iH(\alpha)t} \quad \text{(7.2)}
\]

and the full wave operators

\[
\mathbf{G}^\dagger = \Psi_\alpha \mathbf{G}_\alpha \Psi_\alpha^\dagger \quad \text{(7.3)}
\]

are isometric mappings into \( \mathcal{K} \) from \( \Psi_\alpha \mathcal{K} \), which is interpreted as space of outgoing or incoming configurations, respectively. The scattering operator

\[
S = \mathbf{G}_\alpha \mathbf{G}_\alpha^\dagger
\]

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

\[
(\omega_{\alpha})^\dagger \Psi_\alpha \leq (\omega_{\alpha}^* - \mathbf{G}_\alpha^\dagger \Psi_\alpha \Psi_\alpha^\dagger \leq \frac{d\omega}{dt} \Psi_\alpha \Psi_\alpha^\dagger \leq \frac{d\omega}{dt} \Psi_\alpha \Psi_\alpha^\dagger \quad \text{(7.4)}
\]

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

Fix now a \( \omega_{\alpha} \) cluster channel \( \alpha \), then the incoming wave function in \( \mathcal{K}_\alpha \) is of the form

\[
\Psi_\alpha = \psi_1 \psi_2 \quad \text{(7.5)}
\]

and \( \psi_\alpha \) 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 \( \alpha \) described by

\[
\Psi_\alpha^\dagger = \mathbf{G}_\alpha \Psi_\alpha \Psi_\alpha^\dagger \quad \text{(7.6)}
\]
where $n_i$ 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

$$\int_0 \alpha \left| k \right|^2 dx = \alpha \left| k \right|^2,$$

(7.8)

and we use (7.5) as a simple estimate.

$H$ acts trivially on $\eta_1$ and $\eta_2$ and reduces on $g$ to $H = -(1/2 m_0) \frac{d^2}{dz^2}$ where $m_0$ is the reduced mass of the two clusters. Therefore

$$H_0 = \int_0 g_i \left( H \right) g_i = H g_i = H \eta_0 \eta_1 g_0 g_1$$

(7.9)

with the effective potential between the clusters

$$V_{12} = \int_0 g_i \left( \left( \eta_1, \eta_2 \right)^2 \right) \frac{d\eta_1}{d\omega_1} \frac{d\eta_2}{d\omega_2}$$

(7.10)

Here $\eta$ is the separation of centers of mass and $\zeta_i$ are the inner-cluster coordinates (of dimension 3 in 1, if $k$ particles belong to the cluster). The analysis of Section 3 immediately applies and all we have to do in the multparticle case is to control the decay of $V_{12}$ 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 $V_0$ and the bound state wave functions $\eta_i$ 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 $V_0$

$$V_{12} = V_{12} \left( \zeta_{1,2} \right)$$

(7.11)

decay faster than $1/\left| \zeta_{1,2} \right|^2$ 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 $1/\left| \zeta_{1,2} \right|^3$.

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

$$V_{1j} \left( \zeta_{1,2} \right) = \int_0 g_i \left( \zeta_{1,2} \right) \frac{d\eta_i}{d\omega_i}$$

(7.12)

If both clusters are neutral: $E_1 = E_2 = 0$, then $V_{1j}$ satisfies (3.20). This proves the following

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

$$\int_0 g_i \left( \zeta \right) \frac{d\eta_i}{d\omega_i} \leq 1/2 \int_0 \left| \zeta \right|^{-2}$$

(7.13)

is finite and $C(\zeta)$ 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 (7.1) and Section 6 of (8).

REFERENCES
