On the role of the flux in scattering theory

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This paper is dedicated to the 60th birthday of Sergio Albeverio.

ABSTRACT. The often ignored quantum probability flux is fundamental for a genuine understanding of scattering theory as, in particular, expressed in the flux-across-surfaces theorem. This work splits into two parts. First we show how the flux enters into scattering theory and we give an elementary proof of the free flux-across-surfaces theorem. At least heuristically, the free theorem together with completeness of the wave operators implies the full flux-across-surfaces theorem. Therefore, in the second part, we discuss the proof of asymptotic completeness in potential scattering—the main focus of mathematical scattering theory so far. Of course this is well known, however, we found that the presentations of the proof (we looked at) showed no awareness of the crucial physical ingredient, namely the current positivity condition, a condition on the quantum flux. We wish to present here our understanding of the issues involved and we wish to emphasize that the arguments are all straightforward and natural: The proof uses Riemann-Lebesgue, compactness of operators and the current positivity condition.

1. Introduction

In Born's interpretation of the wave function Ψ_t at time t of a single particle of mass m, $\rho_t(x) := |\Psi_t(x)|^2$ is the probability density for finding the particle at x at that time. The consistency of this interpretation is ensured by the continuity equation

$$\frac{\partial \rho_t}{\partial t} + \nabla \cdot j^{\Psi_t} = 0 \tag{1.1}$$

where $j^{\Psi_t} = \mathrm{Im}\Psi_t^* \nabla \Psi_t$ is the quantum flux ($\hbar = m = 1$). Equation (1.1) holds whenever Ψ_t satisfies Schrödinger's equation.

The quantum flux is usually not considered to be of any operational significance. It is not related to any standard quantum mechanical measurement in the way, for example, that the density ρ, as the spectral measure of the position operator, gives the statistics for a position measurement. Nonetheless, it is hard to resist the suggestion that the quantum flux integrated over a surface gives the probability that the particle crosses that surface, i.e., that

$$j^{\Psi_t} \cdot dS dt \tag{1.2}$$

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is the probability that a particle crosses the surface element dS in the time dt. However, things are a little bit more complicated since $j^{\Psi_t} \cdot dSdt$ may be negative somewhere, in which case it cannot be a probability. A more careful analysis of the flux in Bohmian mechanics—that is quantum mechanics with particles having positions and hence trajectories—shows that $j^{\psi_t} \cdot dSdt$ is really the expected number of signed crossings through the (oriented) surface dS in the time dt. Thus $j^{\psi_t} \cdot dSdt$ coincides with the crossing *probability* whenever the particle crosses dS at most once and in the direction of the surface normal. In the following we will discuss potential scattering, a regime where this condition is expected to hold far away from the scattering center since the particle moves there essentially freely and radially.[1]

The next section will be concerned with a physically reasonable definition of the so-called scattering cross section for a quantum particle based on the quantum probability flux. The connection to abstract scattering theory is provided by the flux-across-surfaces theorem. We will give an elementary proof of the free flux-across-surfaces theorem, from which–at least heuristically–the full theorem follows, whenever the relevant wave functions are asymptotically moving according to the free dynamics, i.e. whenever the wave operators are asymptotically complete.

In Section 3 we will review the ingredients for answering the question, when wave functions move asymptotically freely. Of course this is all well known (see e.g. [**P**]), however, we like to focus on the crucial physical ingredient, namely the current positivity condition, a condition on the quantum flux.

2. The scattering cross section and the flux-across-surfaces theorem

The basic object that connects abstract scattering theory with experiment is the scattering cross section, that is, the probability that a detector covering the solid angle Σ, a subset of the unit sphere, would fire during a scattering experiment.

In mathematical physics this is generally defined to be

$$\sigma_{\text{cone}}(\Sigma) := \lim_{t\to\infty} \int_{C_\Sigma} |\psi_t(x)|^2 d^3x \,, \tag{2.1}$$

i.e., the asymptotic probability of finding the particle in the cone C_Σ spanned by Σ. Now Dollard's scattering-into-cones theorem [**Do**] connects this probability with the probability of finding its asymptotic momentum k in that cone:

$$\lim_{t\to\infty} \int_{C_\Sigma} |\psi_t(x)|^2 d^3x = \int_{C_\Sigma} \left| \widehat{W_+^{-1}\psi_0}(k) \right| d^3k \,. \tag{2.2}$$

Here $W_+ := \mathrm{s} - \lim_{t\to\infty} e^{iHt} e^{-iH_0t}$ is the wave operator, $H = H_0 + V$, with $H_0 = -\frac{1}{2}\Delta$, V a scattering potential and $\widehat{\ }$ denotes Fourier transformation.

So far the mathematics. But back to physics. $\sigma_{\text{cone}}(\Sigma)$ is the probability that at some large fixed time, when the position of the particle is measured, the particle is found in the cone C_Σ. But does one actually measure in a scattering experiment in what cone the particle happens to be found at some large but fixed time? Is it not rather the case that one of a collection of distant detectors surrounding the scattering center fires at some random time, a time that is not chosen by the experimenter? And isn't that random time simply the time at which, roughly speaking, the particle crosses the detector surface subtended by the cone?

This suggests that the relevant quantity for the scattering experiment should be the quantum flux. If the detectors are sufficiently distant from the scattering

[1] For a discussion of the near field scattering regime see [**DDGZ2**].

center the flux will typically be outgoing and (1.2) will be indeed the crossing probability. We obtain as the probability that the particle has crossed some distant surface during some time interval the integral of (1.2) over that time interval and that surface. The integrated flux thus provides us with a physical definition of the cross section:

$$\sigma_{\text{flux}}(\Sigma) := \lim_{R\to\infty} \int_0^\infty dt \int_{R\Sigma} j^{\psi_t} \cdot dS \,, \tag{2.3}$$

where $R\Sigma$ is the intersection of the cone C_Σ with the sphere of radius R. As before, one would like to connect this with the usual formulas and hence we need the counterpart of the scattering-into-cones theorem—the flux-across-surfaces theorem—which provides us with a formula for σ_{flux}:

$$\lim_{R\to\infty} \int_0^\infty dt \int_{R\Sigma} j^{\psi_t} \cdot dS = \int_{C_\Sigma} \left|\widehat{W_+^{-1}\psi_0}(k)\right|^2 d^3k \,. \tag{2.4}$$

The fundamental importance of the flux-across-surfaces theorem was first recognized by Combes, Newton and Shtokhamer [**CNS**]. It was proved only recently in [**AZ**] and [**TDM**] for short range potentials and in [**AP**] also for smooth long range potentials.

In this work, however, we will prove only the so called "free flux-across-surfaces theorem": Let $\psi_t := e^{-iH_0t}\psi_0$, then

$$\lim_{R\to\infty} \int_0^\infty dt \int_{R\Sigma} j^{\psi_t} \cdot dS = \int_{C_\Sigma} \left|\widehat{\psi_0}(k)\right|^2 d^3k \,. \tag{2.5}$$

The free theorem should be physically sufficient for wave functions that move asymptotically freely (cf. Section 3). This is because at finite times the flux through a distant surface should be essentially zero and at large times we have

$$\psi_t := e^{-iHt}\psi_0 \approx e^{-iH_0t} W_+^{-1}\psi_0 \,. \tag{2.6}$$

Thus the full time evolution becomes close to the free time evolution of $W_+^{-1}\psi_0$, albeit in L^2 only. But if one assumes that they also become close in the sense of the flux they generate, the full theorem follows from the free one.

The free flux-across-surfaces theorem was first proved in [**D**]. However, since it is of fundamental importance to scattering theory, it is worthwhile to present a simplified and elementary proof (see [**T**]) that could be part of a text book or lecture on scattering theory.

Let $\psi_0 \in \mathcal{S}(\mathbb{R}^n)$, the set of Schwartz functions, and $\psi_t := e^{-iH_0t}\psi_0$. We will show that for all $T \in \mathbb{R}$ and any measurable subset $\Sigma \subset S^{n-1}$ of the unit sphere

$$\lim_{R\to\infty} \int_T^\infty dt \int_{R\Sigma} j^{\psi_t} \cdot dS = \lim_{R\to\infty} \int_T^\infty dt \int_{R\Sigma} \left|j^{\psi_t} \cdot dS\right| = \int_{C_\Sigma} \left|\widehat{\psi_0}(k)\right|^2 d^3k \,. \tag{2.7}$$

In particular, the first equality shows that the flux is essentially outgoing at large distances and thus the left hand side provides the probabilities of interest. Secondly, we see that there is indeed no contribution to the flux at finite times and therefore the above heuristic argument seems valid.

Lets turn to the proof now. First note that it is sufficient to proof (2.7) for some fixed $T \geq 1$, since the domain $\mathcal{S}$ as well as the value of $|\widehat{\psi_0}(k)|$ is invariant under the free time evolution.

We proceed as in [**DDGZ1**] and write for $t \geq 1$

$$
\begin{aligned}
(2.8) \qquad \psi_t(x) &= \left(e^{-iH_0t}\psi_0\right)(x) = \int \frac{e^{i\frac{|x-y|^2}{2t}}}{(2\pi i t)^{\frac{n}{2}}}\psi_0(y)\,d^ny \\
&= \frac{e^{i\frac{x^2}{2t}}}{(it)^{\frac{n}{2}}}\widehat{\psi}_0\left(\frac{x}{t}\right) + \frac{e^{i\frac{x^2}{2t}}}{(2\pi i t)^{\frac{n}{2}}}\int e^{-i\frac{x\cdot y}{t}}\left(e^{i\frac{y^2}{2t}}-1\right)\psi_0(y)\,d^ny \\
&=: \alpha(x,t)+\beta(x,t)\,.
\end{aligned}
$$

The flux is now

$$
(2.9) \qquad j^{\psi_t}(x) = \mathrm{Im}(\psi_t^*(x)\nabla\psi_t(x)) = \frac{x}{t}t^{-n}\left|\widehat{\psi}_0\left(\frac{x}{t}\right)\right|^2 + N(x,t)\,,
$$

with

$$
\begin{aligned}
(2.10) \qquad N(x,t) &:= \mathrm{Im}\Big(t^{-n-1}\widehat{\psi}_0^*\left(\frac{x}{t}\right)\nabla\widehat{\psi}_0\left(\frac{x}{t}\right) + \beta^*(x,t)\nabla\alpha(x,t) \\
&\qquad +\alpha^*(x,t)\nabla\beta(x,t)+\beta^*(x,t)\nabla\beta(x,t)\Big)\,.
\end{aligned}
$$

We show as in [**DDGZ1**] that the first part of the flux in (2.9) gives rise to the right hand side of (2.7):

$$
\begin{aligned}
&\lim_{R\to\infty}\int_T^\infty dt\int_{R\Sigma} t^{-n-1}\left|\widehat{\psi}_0\left(\frac{x}{t}\right)\right|^2 x\cdot dS \\
&\quad= \lim_{R\to\infty}\int_T^\infty dt\int_{R\Sigma} t^{-n-1}\left|\widehat{\psi}_0\left(\frac{R\omega}{t}\right)\right|^2 R^n\,d\Omega \\
&\quad= \lim_{R\to\infty}\int_0^{R/T} d|k||k|^{n-1}\int_{R\Sigma}|\widehat{\psi}_0(k)|^2\,d\Omega = \int_{C_\Sigma}|\widehat{\psi}_0(k)|^2\,d^nk\,,
\end{aligned}
$$

where $dS = R^{n-1}d\Omega$, $d\Omega$ being Lebesgue-measure on the unit sphere S^{n-1} of $\mathbb{R}^n$. For the first equality we introduced spherical coordinates $x = R\omega$. For the second one we substituted $k := \frac{x}{t} = \frac{R\omega}{t}$, which, in particular, means that $d|k| = -Rt^{-2}dt$. Since $x\cdot dS = |x\cdot dS|$, all equalities in (2.7) hold, if we can show that

$$
(2.11) \qquad \lim_{R\to\infty}\int_T^\infty dt\int_{S_R}|N(x,t)\cdot dS| = 0\,.
$$

At this point we proceed differently from [**DDGZ1**]. We will show that there is a $c<\infty$ such that for every $0<\epsilon<1$

$$
(2.12) \qquad \sup_{x\in S_R}|N(x,t)| \leq ct^{-1-\epsilon}R^{-n+\epsilon}\,.
$$

Then (2.11) follows directly from this estimate:

$$
\begin{aligned}
(2.13) \qquad \lim_{R\to\infty}\int_T^\infty dt\int_{S_R}|N(x,t)\cdot dS| &\leq c\lim_{R\to\infty}R^{-1+\epsilon}\int_T^\infty t^{-1-\epsilon}\,dt \\
&= \frac{c}{\epsilon T^\epsilon}\lim_{R\to\infty}R^{-1+\epsilon} = 0\,.
\end{aligned}
$$

Thus it remains to show (2.12), which follows from inserting the following estimates for appropriate q into (2.10). Let $\|f\|_R := \sup_{x\in S_R}|f(x)|$ and $q\geq 0$, then there is a $c_q < \infty$, such that

$$\left\|\widehat{\psi}_0(\cdot/t)\right\|_R \le c_q\left(\frac{t}{R}\right)^q , \qquad \left\| |\nabla\widehat{\psi}_0(\cdot/t)| \right\|_R \le c_q\left(\frac{t}{R}\right)^q \tag{2.14}$$

$$\|\alpha(\cdot,t)\|_R \le c_q t^{-\frac{n}{2}}\left(\frac{t}{R}\right)^q , \qquad \| |\nabla\alpha(\cdot,t)| \|_R \le c_q t^{-\frac{n}{2}}\left(\frac{t}{R}\right)^q \tag{2.15}$$

$$\|\beta(\cdot,t)\|_R \le c_q t^{-\frac{n}{2}-1}\left(\frac{t}{R}\right)^q , \qquad \| |\nabla\beta(\cdot,t)| \|_R \le c_q t^{-\frac{n}{2}-1}\left(\frac{t}{R}\right)^q . \tag{2.16}$$

The estimates (2.14) and (2.15) follow from the assumption that $\psi_0 \in \mathcal{S}$, i.e., ψ_0, $\widehat{\psi}_0$ and their derivatives decay faster than any inverse polynomial.

We will prove (2.16) first for $q \in \mathbb{N}_0$ by using

$$e^{-i\frac{x\cdot y}{t}} = i^q\left(\frac{t}{|x|}\right)^q\left(\frac{x}{|x|}\cdot\nabla_y\right)^q e^{-i\frac{x\cdot y}{t}}$$

and doing q times integration by parts:

$$\begin{aligned}
|\beta(x,t)| &= (2\pi t)^{-\frac{n}{2}}\left|\int\left(\frac{t}{|x|}\right)^q\left[\left(\frac{x}{|x|}\cdot\nabla_y\right)^q e^{-i\frac{x\cdot y}{t}}\right]\left(e^{i\frac{y^2}{2t}}-1\right)\psi_0(y)\,d^ny\right| \\
&\le (2\pi t)^{-\frac{n}{2}}\left(\frac{t}{|x|}\right)^q\int\left|\left(\frac{x}{|x|}\cdot\nabla_y\right)^q\left(e^{i\frac{y^2}{2t}}-1\right)\psi_0(y)\right| d^ny\,.
\end{aligned}$$

To conclude the bound in (2.16) on $\|\beta\|_R$ for $q \in \mathbb{N}_0$ we are left to show that the integral decays like t^{-1}, which follows from a simple calculation:

$$\begin{aligned}
&\left\|\left(\frac{x}{|x|}\cdot\nabla_y\right)^q\left(e^{i\frac{y^2}{2t}}-1\right)\psi_0(y)\right\|_{L^1} = \\
&= \left\|\sum_{j=1}^{q}\begin{pmatrix} q \\ j\end{pmatrix}\left[\left(\frac{x}{|x|}\cdot\nabla_y\right)^j e^{i\frac{y^2}{2t}}\right]\left[\left(\frac{x}{|x|}\cdot\nabla_y\right)^{q-j}\psi_0(y)\right]\right. \\
&\quad + \left.\left(e^{i\frac{y^2}{2t}}-1\right)\left(\frac{x}{|x|}\cdot\nabla_y\right)^q\psi_0(y)\right\|_{L^1} \\
&\le \widetilde{c}_q\sum_{\substack{\mu:1\le|\mu|\le q\\ \nu:|\nu|=q-|\mu|}} t^{-|\mu|}\|y^\mu\partial_y^\nu\psi_0(y)\|_{L^1} + \frac{\widetilde{c}_q}{t}\sum_{\nu:1\le|\nu|\le q}\|y^2\partial_y^\nu\psi_0(y)\|_{L^1}\,.
\end{aligned}$$

Herein μ and ν denote multi-indices and we used that

$$\left|\left(e^{i\frac{y^2}{2t}}-1\right)\right| \le \frac{y^2}{2t}\,.$$

The case $q \in \mathbb{R}_0^+$ follows from interpolation: For $t/R \le 1$ resp. $t/R > 1$, $(t/R)^q$ is bounded by $(t/R)^n$ where n is the smallest integer larger than q resp. the largest integer smaller than q.

Since also $y\psi_0(y) \in \mathcal{S}$, the second estimate in (2.16) can be computed in the same way, doing, however, one more integration by parts. Thus (2.7) is proved.

3. When do wave functions move freely to infinity?

Traditionally mathematical physics of scattering was mainly concerned with the problem of showing asymptotic completeness. The goal is to show that under reasonable conditions on the potential V all states orthogonal to all bound states of the Hamiltonian $H = H_0 + V$ move, in a sense to be specified below, asymptotically freely in time. This picture is partly sustained by the feeling that wave functions in $\mathcal{H}_{\rm pp}(H)^{\perp}$ should travel in time to spatial infinity, which as far as we understand was only recently brought into play by Enss in proving theorems about the time asymptotics of wave function evolution. Indeed, the great step towards proving the desired asymptotic behavior was to use the geometrical insight that, roughly speaking, wave functions with spatial support moving away from the spatial support of the scattering potential will not feel the potential anymore and will thus move freely. Since the scattering potential is usually a spatially located object, this insight is kind of very natural.

The sense in which the time evolution becomes free is best understood as follows. Consider a time sequence $t_n \to \infty$[2] and the time evolved wave function $\psi_n := e^{-iHt_n}\psi_0$, $\psi_0 \in \mathcal{H}_{\rm pp}(H)^{\perp}$.

As n gets large it should be the case that ψ_n is already far away from the scatterer potential, so that its time evolution is more or less the free one: For $t > 0$

$$e^{-iHt}\psi_n \approx e^{-iH_0t}\psi_n \,,$$

hence

$$\psi_n \approx e^{iHt}e^{-iH_0t}\psi_n$$

and this put in the strongest possible terms becomes

$$\psi_n \approx \lim_{t\to\infty} e^{iHt}e^{-iH_0t}\psi_n \,. \tag{3.1}$$

Hence, as a first step, the existence of the wave operator

$$W_+ := \mathrm{s}-\lim_{t\to\infty} e^{iHt}e^{-iH_0t} \tag{3.2}$$

as a strong limit must be ensured (W_- stands for $t \to -\infty$). Back to (3.1). That is naturally sharpened to

$$\lim_{n\to\infty} \|(W_+ - 1)\psi_n\| = 0 \,, \tag{3.3}$$

i.e. the ψ_n become eigenfunctions of the wave operator. From this what is called asymptotic completeness of the wave operators follows immediately: To see that we use some relations which follow from the existence of W_+.

Writing

$$e^{iH(t+s)}e^{-iH_0(t+s)} = e^{iHs}e^{iHt}e^{-iH_0t}e^{-iH_0s}$$

we obtain the so called intertwining property

$$e^{-iHs}W_+ = W_+e^{-iH_0s} \,, \tag{3.4}$$

from which one infers that the range $R(W_+)$ is invariant under the H-time evolution. Strong differentiation of (3.4) with respect to s yields

$$HW_+ = W_+H_0 \tag{3.5}$$

on $\mathcal{D}(H_0)$ and thus, since on $R(W_+)$

$$W_+^* = W_+^{-1} \,, \tag{3.6}$$

[2] We will write everything for positive times, but it is understood that everything holds with some notational adjustment also for negative times.

we have

$$W_+^{-1} H W_+ = H_0 \,. \tag{3.7}$$

From this last equality we infer that the restriction of H to $R(W_+)$ is unitarily equivalent to H_0. In particular, this implies the important a priori

$$R(W_+) \subset \mathcal{H}_{\rm ac}(H) \,. \tag{3.8}$$

Now, on the other hand, since $R(W_+)$ is closed and invariant under the H-time evolution, we have for all wave functions ψ_0 satisfying (3.3) that $\psi_0 \in R(W_+)$.

Consequently, *completeness* of the wave operators, that is $R(W_+) = \mathcal{H}_{\rm ac}(H)$, follows as soon as one can establish (3.3) for all $\psi_0 \in \mathcal{H}_{\rm ac}(H)$. If (3.3) holds indeed for all $\psi_0 \in \mathcal{H}_{\rm pp}^{\perp}(H) = \mathcal{H}_{\rm cont}(H)$, *asymptotic completeness* of the wave operator follows, i.e. $R(W_+) = \mathcal{H}_{\rm ac}(H) = \mathcal{H}_{\rm cont}(H)$ and thus, in particular, $\mathcal{H}_{\rm sc}(H) = \emptyset$.

When trying to establish (3.3), it is clearly natural to focus first on $\mathcal{H}_{\rm ac}(H)$, since the singular part seems more mystical. It turns out, however, that we shall only need to establish (3.3) for $\psi_0 \in \mathcal{H}_{\rm ac}(H)$, because we shall obtain as a corollary of the proof: Any sequence of vectors ϕ_n belonging to a bounded energy interval and going weakly to zero splits into two sequences of vectors $\phi_n = \phi_n^{\rm out} + \phi_n^{\rm in}$ with $\phi_n^{\rm out}$ satisfying (3.3) and $\phi_n^{\rm in}$ satisfying the corresponding statement for W_-.

That is heuristically clear, since any sequence going weakly to zero can do so by either having members showing increasing fluctuations and thus increasing energy, or, if that is constrained, by leaving any spatially finite region. So the splitting will be one in outgoing and incoming waves.

Now Davies observed that from the above mentioned corollary of the proof $\mathcal{H}_{\rm sc}(H) = \emptyset$ follows: By assuming otherwise there exists an orthonormal sequence of vectors spanning a bounded energy subspace of $\mathcal{H}_{\rm sc}(H)$, and any orthonormal sequence converges weakly to zero. But then, by splitting that sequence into the two approximate eigenfunction sequences of W_+ and W_- we obtain that they both must be in the absolutely continuous subspace of H and therefore also the original sequence must be such.

We gave this quick argument to really keep the focus on proving completeness.

Showing the existence of the wave operators is standard—Reed Simon call it Cook's method—but it is nevertheless worthwhile to see how it is done, because from there on the way is pretty straightforward. Cook observed that

$$\begin{aligned} ||(W_+ - 1)\phi|| &= \lim_{t\to\infty} || \int_0^t ds \frac{d}{ds} e^{isH} e^{-isH_0}\phi|| \\ &= \lim_{t\to\infty} || \int_0^t ds e^{isH} V e^{-isH_0}\phi|| \le \int_0^\infty ds ||V e^{-isH_0}\phi||, \end{aligned} \tag{3.9}$$

where it is sufficient to have integrability on a dense set of vectors in L^2. The differentiation in the second equality needs that $e^{-isH_0}\phi \in \mathcal{D}(H)$, the domain of H, and we simply concentrate on V for which $\mathcal{D}(H) \subset \mathcal{D}(H_0)$ and to make it more simple, we assume V to be H_0-bounded with relative bound $v < 1$:

$$||V(H_0 + i)^{-1}|| \le v. \tag{3.10}$$

In view of (3.9) it is now heuristically very clear what must happen: The potential will fall off at spatial infinity to zero, while the H_0-time evolved wave function ϕ will leave any spatially bounded region. The integrand should thus go to zero, and we may hope that it does so in an integrable way whenever the potential decays sufficiently fast at spatial infinity. With a little experience on Fourier transforms, one may already foresee that the hope is well founded, having in mind the proof of Riemann Lebesgue, or what Reed Simon refer to as stationary phase method.

But before we come to that in more detail, let's consider (3.9) and (3.3) conjointly, with $\psi_n \in \mathcal{H}_{\rm ac}$ as we agreed to do. Believing as we do that ψ_n goes out to infinity already, the H_0-time evolution can only be of help, so interchanging unreflectedly integration with first taking the limit $n \to \infty$ we should get (3.3) without much ado. Even if we understate the problem of showing (3.3) as we certainly do, its good to keep the simple logic of the argument in mind. Because whatever one now attempts as next step to make the argument rigorous, one will be led to the same technicalities and eventually to the right track. We shall demonstrate that on the appearance of an important technical tool, the *compact* operators.

But let us first look at the existence problem (3.9), and let us try to work the problem a little further. Here's the idea. We formulate that $e^{-isH_0}\phi$ leaves any region very quickly which grows slower in time than what the particle will typically travel: If $\phi \in \mathcal{S}$ and

$$\operatorname{supp}\widehat{\phi} \in B_b \cap {B_a}^c, \tag{3.11}$$

balls of radii $0 < a < b$ around the origin (such ϕ form a dense set), then for any $l \in \mathbb{N}$ and with χ denoting the characteristic function

$$||\chi_{B_{\frac{1}{2}at}}(x)e^{-itH_0}\phi|| \le C(\phi,l)(\frac{1}{1+t})^l. \tag{3.12}$$

This comes from the usual Riemann–Lebesgue trick: In the case of one space dimension observe that

$$e^{i\omega S(k)} = \frac{1}{i\omega S'}\frac{d}{dk}e^{i\omega S(k)} \tag{3.13}$$

and write

$$\begin{aligned} \phi(x,t) = e^{-itH_0}\phi \quad &= \quad (2\pi)^{\frac{3}{2}}\int dk e^{ik\cdot x}e^{i\frac{k^2}{2}t}\widehat{\phi}(k) \\ &= (2\pi)^{\frac{3}{2}}\int dk e^{(1+x+t)\frac{ik\cdot x+i\frac{k^2}{2}t}{1+x+t}}\widehat{\phi}(k) \\ &= (2\pi)^{\frac{3}{2}}\int dk e^{i\omega\frac{k\cdot x+\frac{k^2}{2}t}{1+x+t}}\widehat{\phi}(k). \end{aligned} \tag{3.14}$$

Observing that, by our restrictions (3.11) and the indicator function in (3.12), S' is bounded away from zero, one uses repeatedly (3.13) and partial integration (as often as large as we want to have the exponent on $\frac{1}{\omega}$). That gives us an estimate on $\phi(x,t)$ which we insert into the l.h.s. of (3.12). The constant C in (3.12) contains the sup-norm of derivatives of $\widehat{\phi}$. The straight forward generalization of this trick to higher dimensions is known as Hörmander's theorem.

We shall now use (3.12) on (3.9) by inserting some 1's (which is of course standard procedure)

$$||V(H_0-i)^{-1}(\chi_{B_{\frac{1}{2}as}}(x)+\chi_{B^c_{\frac{1}{2}as}}(x))(H_0-i)e^{-isH_0}\phi||\,.$$

Using triangular inequality we obtain integrability of the first term in view of (3.12) and the fact that we can factor out $\|V(H_0-i)^{-1}\|$ according to (3.10) and that $H_0 - i$ commutes with e^{-isH_0} and leaves the support of $\widehat{\phi}$ invariant.

For the second term to be norm–integrable we require

$$\|V(H_0-i)^{-1}\chi_{B^c_{\frac{1}{2}as}}(x)\| \tag{3.15}$$

to be integrable, which is the so called Enss condition on V. It is a straightforward matter of calculation to convince oneself that (3.15) holds true for potentials falling off like $\mathrm{O}(\frac{1}{x^{1+\epsilon}})$.

It should be clear that the integrability (cf.(3.12)) of the first term is crucial, and that requires smoothness of the wave function, guaranteed by the energy bounds (3.11) which we may equivalently express as

$$\chi_{a<E<b}(H_0)\phi = \phi\,. \tag{3.16}$$

To make that manifest we restate what we showed in the following way:

$$\int_0^\infty dt\|\chi_{B_{\frac{1}{2}at}}(x)\chi_{a<E<b}(H_0)e^{-itH_0}\phi\| < C(\phi) < \infty \tag{3.17}$$

so that we also see the product

$$\chi_{B_{\frac{1}{2}at}}(x)\chi_{a<E<b}(H_0)$$

appear. The very same object will appear in the following.

Back to (3.3). Suppose we wish first to be sure that $\psi_n \in \mathcal{H}_{ac}$ behaves as we believe it does, i.e. that it goes out to infinity. What is the simplest way to put that? It leaves any spatially bounded region? May be, but unquestionably simpler is to consider first the projection of ψ_n on ψ_0, $\langle\psi_n,\psi_0\rangle$. That goes to zero by Riemann Lebesgue, since $\psi_0 \in \mathcal{H}_{ac}$. Actually, using the spectral representation associated with ψ_0 on its cyclic subspace, one can easily see that $\langle\psi_n,\phi\rangle \to 0$, i.e. that ψ_n converges weakly to zero, whenever $\psi_0 \in \mathcal{H}_{ac}$, and thus that $\|\,|\phi\rangle\langle\phi,\psi_n\rangle\| \to 0$.

We could now conclude that ψ_n leaves any bounded region B_r if it were true that $\chi_{B_r}(x)$ were approximately a finite sum of such projectors or more generally a so called finite rank operator:

$$\text{is that true that } \chi_{B_r}(x) \approx \sum_{k=1}^{K} |\phi_k\rangle\langle\psi_k|\ ?\,,$$

because they map any weakly convergent sequence to a strongly convergent one.

But that is not true, as one quickly sees: It is natural to try a representation of $\chi_{B_r}(x)$ in terms of the discrete Fourier basis living on a cube containing B_r: But there is no energy cutoff at work, to make the representation approximately finite. But that can be put in by hand, since we can always restrict attention to a dense set of vectors. So instead of $\chi_{B_r}(x)$ consider $\chi_{B_r}(x)\chi_{a<E<b}(H)$ and to make life really simple, one convinces oneself first (easily by hand) of the fact that

$$\chi_{B_r}(x)\chi_{a<E<b}(H_0) \quad \text{is approximately finite rank}$$

and one should be satisfied with that because it turns out that more is not needed. Instead of $\chi_{a<E<b}(H_0)$ one may take by the way $f(H_0)$, with some smooth function f going to zero at infinity, and likewise some $g(x)$ and we shall use that replacement whenever we feel it appropriate.

At this point one should realize that we arrived at the classic example of a *compact* operator. Morally, any bounded operator living on bounded energy and spatial support wave functions is compact.

Note that, by the classical Bolzano Weierstrass theorem, a finite rank operator maps any bounded sequence to a sequence which has a convergent subsequence, and the latter property defines an compact operator. Furthermore all compact operators are operator–norm–limits of finite rank ones (not totally easy exercise). More importantly, all compact operators have the nice property that they map weakly convergent sequences to strongly convergent ones (a rather simple exercise). Finally products of bounded and compact operators are compact (very simple).

Having seen this we are immediately led to a good strategy of proof. Back to (3.3). We would now hope that $W_+ - 1$ can be shown to be compact, since the ψ_n go weakly to zero no matter what. Thinking of a time preserved and dense set of vectors given by $\psi = \chi_{a<E<b}(H)\psi$, it would suffice to have that

$$(W_+ - 1)\chi_{a<E<b}(H) \text{ is compact.} \tag{3.18}$$

In the attempt to show (3.18), one arrives via (3.9) at the task of showing

$$\int_0^\infty ds||Ve^{-isH_0}\chi_{a<E<b}(H)|| < \infty, \tag{3.19}$$

The idea is then to show that

$$\text{the operators} \quad Ve^{-isH_0}\chi_{a<E<b}(H) \quad \text{are compact,} \tag{3.20}$$

and that [3]

$$\text{the integral is operator–norm convergent.} \tag{3.22}$$

To see that (3.20) holds, suppose for the sake of a first quick rough argument that in $\psi_n = \chi_{a<E<b}(H)\psi_n$ we can substitute $\chi_{a<E<b}(H)$ by $\chi_{a<E<b}(H_0)$ (for n large enough). Then write for (3.20), like we did above:

$$V(H_0 - i)^{-1}(\chi_{B_R}(x) + \chi_{B_R^c}(x))(H_0 - i)e^{-isH_0}\chi_{a<E<b}(H_0)$$

and observe that

$$\|V(H_0 - i)^{-1}\chi_{B_R^c(x)}(H_0 - i)e^{-isH_0}\chi_{a<E<b}(H_0)\| \leq$$

$$\|V(H_0 - i)^{-1}\chi_{B_R^c(x)}\| \, \|(H_0 - i)e^{-isH_0}\chi_{a<E<b}(H_0)\| \to 0$$

as $R \to \infty$ by assumption (3.15), $\|(H_0 - i)e^{-isH_0}\chi_{a<E<b}(H_0)\|$ being finite. On the other hand

$$V(H_0 - i)^{-1}\chi_{B_R(x)}(H_0 - i)e^{-isH_0}\chi_{a<E<b}(H_0) = V(H_0 - i)^{-1}\chi_{B_R}(x)f(H_0)$$

is the product of a bounded (cf.(3.10)) and the compact operator, and thus compact. Hence no problem with that.

What we still must provide is the justification for replacing $\chi_{a<E<b}(H)\psi_n$ by $\chi_{a<E<b}(H_0)\psi_n$ (for n large enough) or, what amounts to the same task, replacing $f(H)$ by $f(H_0)$. The idea would be to show that $f(H) - f(H_0)$ is compact, which heuristically is clear since high energies are cut off by the compact support of f and large spatial distances are cut off by the decay of the potential, thus the difference lives on bounded energy and space wave functions. For the readers convenience

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[3] We emphasize that other natural ways to proceed, like looking at

$$\int_0^\infty ds\|Ve^{-isH_0}\chi_{a<E<b}(H)\psi_n\| < \infty \tag{3.21}$$

and trying to justify exchange of limit with integration (Lebesgue dominated convergence), lead eventually to the same presentation of the proof.

we repeat the usual argument: One argues that $(H-i)^{-1}-(H_0-i)^{-1}=(H-i)^{-1}V(H_0-i)^{-1}$ is compact by writing

$$(H-i)^{-1}V(H_0-i)^{-1}\chi_{B_R(x)}+(H-i)^{-1}V(H_0-i)^{-1}\chi_{B_R(x)^c}\,,$$

and noting that the adjoint of the first term is the product of the compact operator $\chi_{B_R(x)}(H_0-i)^{-1}$, $(H_0-i)^{-1}$ playing the role of the energy cut off, and the bounded $V(H-i)^{-1}=V(H_0-i)^{-1}(H_0-i)(H-i)^{-1}$, this being bounded by (3.10) and the fact that $(H_0-i)(H-i)^{-1}$ is bounded as an everywhere defined closed operator. The second operator goes in norm to zero by (3.15). Then that holds also for polynomials of $p((H-i)^{-1})-p((H_0-i)^{-1})$, where one relies on the Cauchy integral representation

$$((H-i)^{-1})^n=\int_{\text{small circle around i}}\frac{(H-z)^{-1}}{z-i}dz\,,$$

which on $((H-i)^{-1})^n-((H_0-i)^{-1})^n$ exists as norm limit of the compacts $(H-z)^{-1}-(H_0-z)^{-1}$, and thus these powers are compact. But then polynomials of $\frac{1}{x+i}$ and $\frac{1}{x-i}$ are dense in the continuous functions vanishing at infinity by the general Stone Weierstrass theorem.

Be that as it may, we should be clear that until now we encountered no real obstacle. Nothing really substantial had to be overcome. That will now come in the attempt to prove (3.22). To make it short: (3.22) is simply false. It couldn't be right, since one can always find a vector supported initially very far away from the scattering center and moving towards it under the H_0-time evolution, so that for any large time there is a wave function overlapping the potential. However, that cannot happen for the sequence ψ_n, since they move out, and this suggests that we should go back to (3.21) (cf. footnote 3). But we can't apply the Riemann–Lebesgue argument which led to (3.12) because we need uniformity, and we can't control the smoothness of the ψ_n in a uniform way.

We are now at the heart of the problem. If one spends some time on this one convinces oneself quickly that we need some further characterization of the special sequence ψ_n and it's clear, that we should not attempt to try to control smoothness in a uniform way. We should rather observe that until now we did not really try hard to formulate what it means that the ψ_n move out.

At this point the quantum flux comes into play. Knowing its meaning, it's easy to formulate a condition, which really says that the particle moves *out* to infinity:

The quantum flux j^{ψ_n} must point outward on any (spherical) surface surrounding the scatterer, i.e.

$$j^{\psi_n}\cdot dS\geq 0,\ dS\subset\partial B_R,\ \text{for all } R>0 \text{ for } n\to\infty. \tag{3.23}$$

We called this the current positivity condition [**DDGZ2**], and its directly based on the meaning of the flux. The trouble is that that condition is not easy to work with. Therefore we reshape it a bit: We think for simplicity in (3.23) already of spherical surfaces centered at zero. Let $x, |x|=R$ denote the vector to a point on the surface, then (3.23) holds, if

$$j^{\psi_n}\cdot x\geq 0 \text{ for all } R>0 \text{ for } n\to\infty\,,$$

and by a standard trick we get something useful: Since the support of the ψ_n should anyhow be concentrated further and further away and since "every part of the wave function should move outward", we integrate this over all space and get

$$\lim_{n\to\infty}\int dx j^{\psi_n}\cdot x \geq 0$$

which is now the quantum mechanical expectation of an operator (with $p = -i\nabla$):

$$\int dx\, j^{\psi_n}\cdot x = \langle\psi_n, \frac{1}{2}(p\cdot x + x\cdot p)\psi_n\rangle\,,$$

so that we replace (3.23) by using $D = p\cdot x + x\cdot p$ (we come now back to standard techniques, the operator D is referred to as Mourre–operator) with

$$\lim_{n\to\infty}\langle\psi_n, D\psi_n\rangle \geq 0\,.$$

Thus we are led to formulate that the ψ_n become asymptotically eigenfunctions of the projector P^+, projecting on the positive eigenspace of D, i.e. we finally arrive at

$$\lim_{n\to\infty}\|P^+\psi_n - \psi_n\| = 0\,. \tag{3.24}$$

In other words we must show that

$$\lim_{n\to\infty}\|P^-\psi_n\| = 0\,, \tag{3.25}$$

where $P^- + P^+ =$ Identity. It is a straightforward calculation to diagonalize D and one finds quickly that the spectral decomposition is $d\lambda|\lambda\rangle\langle\lambda|\otimes 1$ acting on $L^2(r^2dr)\otimes L^2(d\omega)$ (where we used the splitting into spherical coordinates $x = (r,\omega)$) with

$$P^+\phi(r,\omega) = \int_0^\infty d\lambda r^{\frac{i}{2}\lambda}r^{-\frac{3}{2}}\int u^2du u^{-\frac{i}{2}\lambda}u^{-\frac{3}{2}}\phi(u,\omega). \tag{3.26}$$

I shall not give more details on D, but only remark that one easily finds that D is unitarily equivalent to the one dimensional momentum operator, so that its spectral properties are clear.

We must go back to the problem at hand. Things really work out now. Suppose (3.25) were true. Then we need only show that

$$\|(W_+ - 1)f(H_0)P^+\psi_n\| \to 0,$$

and the question whether $(W_+ - 1)f(H_0)P^+$ is compact imposes itself. Morally, that ought to be true, because P^+ leaves only outgoing wave functions. Thus contributions can only come from wave functions supported around the scattering center, and $f(H_0)$ makes the energy bounded. Again we have bounded energy and spatial wave function being relevant only.

From what we already did, we see that the problem boils down to showing that (starting from (3.19) putting in the usual 1's and observing also (3.15))

$$\int_0^\infty ds\|\chi_{B_{\frac{1}{2}as}}(x)e^{-isH_0}f(H_0)P^+\| < \infty. \tag{3.27}$$

But that follows now easily by the Riemann–Lebesgue trick (cf.(3.13)), showing good integrability of $(e^{-itH_0}f(H_0)P^+\phi)(x,t)$. For that observe, that with $\mathcal{F}$ denoting the operator of Fourier transformation

$$(e^{-itH_0}f(H_0)P^+\phi)(x,t) = (\mathcal{F}^{-1}e^{-it\frac{k^2}{2}}f(k^2/2)\mathcal{F}P^+\mathcal{F}^{-1}\mathcal{F}\phi)(x,t)\,,$$

and we need $\mathcal{F}P^+\mathcal{F}^{-1}$, which is easily found:

$$\mathcal{F}x\mathcal{F}^{-1} = -p\,,$$

and thus $\mathcal{F}D\mathcal{F}^{-1} = -D$ and thus $\mathcal{F}P^+\mathcal{F}^{-1} = P^-$. Hence, ignoring irrelevant constants,

$$\begin{aligned}(e^{-itH_0}f(H_0)P^+\phi)(x,t) &= \int dke^{-ik\cdot x-it\frac{k^2}{2}}f(k^2/2)P^-\widehat{\phi}(k)\\ &= \langle e^{ik\cdot x+it\frac{k^2}{2}}f(k^2/2),P^-\widehat{\phi}\rangle = \langle P^-e^{ik\cdot x+it\frac{k^2}{2}}f(k^2/2),\widehat{\phi}\rangle\\ &\leq \|P^-e^{ik\cdot x+it\frac{k^2}{2}}f(k^2/2)\|\,\|\phi\|\,. \end{aligned} \tag{3.28}$$

Next observe that by Plancherel for the λ-transform

$$\|P^-\Phi\|^2 = \int_{-\infty}^{0} d\lambda|\langle\lambda,\Phi\rangle|^2\,,$$

with $\Phi = e^{ik\cdot x+it\frac{k^2}{2}}f(k^2/2)$ and $\langle\lambda,\Phi\rangle$ its λ-transform. We need integrability in λ and then good integrability of the norm in t.

From (3.26) we see that, with θ denoting the angle between k and x:

$$\langle\lambda,\Phi\rangle(\lambda,\theta) = \int_0^\infty |k|^{\frac{1}{2}}e^{i(\frac{t}{2}k^2+ik\cdot x-\frac{\lambda}{2}ln|k|)}f(k^2/2)d|k|$$

and we need the asymptotics for large λ and t. To apply now the Riemann–Lebesgue argument, observe the important fact that only those $\lambda\leq 0$ are relevant (that's the work of P^-), so that the differential of the relevant phase (compare with (3.14))

$$\frac{d}{d|k|}S = \frac{t|k|+\frac{|\lambda|}{2|k|}+|x|cos\theta}{1+t+|\lambda|}$$

is bounded away from zero: For $\frac{|x|}{t}\in B_{\frac{a}{2}}$ and supp$f\subset B_a^c$

$$t|k|+\frac{|\lambda|}{2|k|}-|x| > at+\frac{|\lambda|}{2|k|}-\frac{at}{2} = \frac{at}{2}+\frac{|\lambda|}{2|k|}\,.$$

There is no problem applying the Riemann Lebesgue argument to get for any $n\in\mathbb{N}$

$$|\langle\lambda,\Phi\rangle| \leq (\frac{1}{1+t+|\lambda|})^n$$

and from that it's easy to finally get (3.27).

We are almost done. There is only (3.25) left to be established. That however goes with a nice trick: We established compactness of $(W_+-1)f(H_0)P^+$, so by the same token $(W_--1)f(H_0)P^-$ is compact, and so is the adjoint $P^-f(H_0)(W_-^*-1)$, and to the adjoint we are naturally led by the standard argument that it suffices to show

$$\|P^-f(H_0)\psi_n\|\to 0\,,$$

as we shall see now.

$$\|P^-f(H_0)\psi_n\| \leq \|P^-f(H_0)(W_-^*-1)\psi_n\| + \|P^-f(H_0)W_-^*\psi_n\|\,,$$

and while the first term goes to zero by compactness, we are left with showing that

$$\|P^-f(H_0)W_+^*\psi_n\| = \|P^-f(H_0)e^{-it_nH_0}W_-^*\psi\|\to 0\,,$$

where we used the intertwining property (3.4). But for that it suffices to show that for all ϕ

$$\|P^-f(H_0)e^{-it_nH_0}W_-^*\phi\| = 0\,,$$

which we can be done by showing that

$$\text{s} - \lim \|P^- f(H_0) e^{-it_n H_0}\| = 0\,,$$

which can be done on $\mathcal{S}$—the usual density argument. And that can then be done by the Riemann–Lebesgue argument which we just employed along the same lines (it's even a little simpler now). That is all.

Finally, let us go back to the issue of *asymptotic completeness*, i.e. we wish to establish that $\sigma_{\rm sc}(H) = \emptyset$.[4] We note that we only used that the sequence ϕ_n converges weakly to zero, except in the last step (establishing (3.25)), where we explicitly used that $\phi_n = e^{-iHt_n}\phi$. But that last step is not needed for what we wish to establish now. Suppose that the singular continuous spectrum $\sigma_{\rm sc}(H)$ is nonempty, then the subspace $\mathcal{H}_{\rm sc}$ is infinite dimensional and thus contains an orthonormal sequence of vectors ϕ_n with $f(H)\phi_n = \phi_n$, f compactly supported and $0 \notin \text{supp} f$. In

$$\phi_n = f(H)P^+\phi_n + f(H)P^-\phi_n$$

we can again replace $f(H)$ by $f(H_0)$ since $f(H) - f(H_0)$ is compact and the sequences $P^+\phi_n$ and $P^-\phi_n$ converge weakly to zero. Now we consider the sequences $\phi_n^+ = f(H_0)P^+\phi_n$ and $\phi_n^- = f(H_0)P^-\phi_n$ separately. Recalling that we established compactness of $(W_+ - 1)f(H_0)P^-$ and $(W_- - 1)f(H_0)P^+$ we conclude that ϕ_n^+ satisfies (3.3) and ϕ_n^- the corresponding statement for W_-. Thus both sequences belong to $\mathcal{H}_{\rm ac}$ and the same must be true for ϕ_n also, leading to a contradiction.

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[4] Note that the following argument also proves that nonzero eigenvalues of H are of finite multiplicity and can accumulate only at 0.

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