On the Flux-Across-Surfaces Theorem

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1 Abstract

The quantum probability flux of a particle integrated over time and a distant surface gives the probability for the particle crossing that surface at some time. We prove the free flux-across-surfaces theorem, which was conjectured by Combes, Newton and Shtokhamer [1], and which relates the integrated quantum flux to the usual quantum mechanical formula for the cross section. The integrated quantum flux is equal to the probability of outward crossings of surfaces by Bohmian trajectories in the scattering regime.

2 Introduction

Time-dependent scattering theory is concerned with the long-time behavior of wave packets ψ_t. Dollard's scattering-into-cones theorem [2, 3] asserts that, assuming, say, asymptotic completeness, the probability of finding a particle with a wave function $\psi \in \mathcal{H}_{ac}(H)$, the absolutely continuous subspace for the Hamiltonian H, in the far future in a given cone $C \subset \mathbb{R}^3$ (with vertex at the origin) equals the probability that the quantum mechanical momentum of $\Omega_-^\dagger \psi$ lies in the same cone,

$$\lim_{t\to\infty} \int_C d^3x |\psi_t(\mathbf{x})|^2 = \int_C d^3v |\widehat{\Omega_-^\dagger \psi}(\mathbf{v})|^2, \tag{1}$$

where $\Omega_- := \text{s-}\lim_{t\to\infty} e^{iHt}e^{-iH_0t}$ is the wave operator, $H = H_0 + V$ with the free Hamiltonian $H_0 = -\Delta/2$ (we choose units such that $\hbar = m = 1$) and the interaction potential V. $\hat{}$ denotes the Fourier transform. The scattering-into-cones theorem is regarded as fundamental, from which the expression for the differential cross section $\frac{d\sigma}{d\Omega} = |f(\theta, \phi)|^2$ from the time-independent theory is to be derived from the r.h.s. of (1) (e.g. [4], p. 356, [5]).

Combes, Newton and Shtokhamer [1] observed however that what is relevant for scattering theory is a formula for the probability that the particle crosses some distant surface at some time during the scattering process, since the detectors click at some *random* time, which is *not* chosen by the experimenter. Heuristically, this probability should be given by integrating the quantum mechanical probability flux over the relevant time interval and this surface. (The flux is often used that way in textbooks.) Combes, Newton and Shtokhamer hence conjectured the "flux-across-surfaces theorem"

$$\lim_{R\to\infty}\int_0^\infty dt\int_{C\cap\partial B_R}\mathbf{j}^{\psi_t}\cdot\mathbf{n}d\sigma=\int_C d^3v|\widehat{\Omega_-^\dagger\psi}(\mathbf{v})|^2, \tag{2}$$

where B_R is the ball with radius R and outward normal $\mathbf{n}$. To our knowledge there exists no proof of this theorem. A simpler statement, also not previously proven, is the "free flux-across-surfaces theorem," for freely evolving ψ_t,

$$\lim_{R\to\infty}\int_0^\infty dt\int_{C\cap\partial B_R}\mathbf{j}^{\psi_t}\cdot\mathbf{n}d\sigma=\int_C d^3v|\hat{\psi}(\mathbf{v})|^2 \tag{3}$$

which in a sense is physically good enough, because the scattered wave packet will move almost freely after the scattering has essentially been completed (see also [1]). We shall prove the "free flux-across-surfaces theorem" in this paper, commenting at the end on the general flux-across-surfaces theorem.

We want first to give the heuristic argument for (3). The flux should contribute to the integral in (3) only for large times, because the packet has to travel a long time before it reaches the distant sphere ∂B_R, so that we may use the long-time asymptotics of the free evolution. Writing

$$\psi_t(\mathbf{x})=(e^{-iH_0t}\psi)(\mathbf{x})=\int d^3y\frac{e^{i\frac{|\mathbf{x}-\mathbf{y}|^2}{2t}}}{(2\pi it)^{3/2}}\psi(\mathbf{y}) \tag{4}$$

and expanding the exponent of the propagator, we obtain

$$\psi_t(\mathbf{x})=\frac{e^{i\frac{x^2}{2t}}}{(it)^{3/2}}\hat{\psi}(\frac{\mathbf{x}}{t})+\frac{e^{i\frac{x^2}{2t}}}{(it)^{3/2}}\int\frac{d^3y}{(2\pi)^{3/2}}e^{-i\frac{\mathbf{x}\cdot\mathbf{y}}{t}}(e^{i\frac{y^2}{2t}}-1)\psi(\mathbf{y}) \tag{5}$$

so that for large times (the second term should be negligible since $|(e^{i\frac{y^2}{2t}}-1)|\to 0$ as $t\to\infty$)

$$\psi_t(\mathbf{x})\approx(it)^{-3/2}e^{i\frac{x^2}{2t}}\hat{\psi}(\frac{\mathbf{x}}{t}). \tag{6}$$

The importance of this asymptotics for scattering theory has long been recognized, see e.g. [7] and [2].

Consider now a cone C. Substituting $\mathbf{v}:=\frac{\mathbf{x}}{t}$ one readily obtains the scattering-into-cones theorem

$$\lim_{t\to\infty}\int_C d^3x|\psi_t(\mathbf{x})|^2=\int_C d^3v|\hat{\psi}(\mathbf{v})|^2. \tag{7}$$

But the l.h.s. of (7) should be unaffected if C is replaced by the truncated cone $C_R = C \cap B_R^c$, $B_R^c := \mathbb{R}^3 \backslash B_R$, for any $R > 0$. Thus writing $\int_{C_R} d^3x |\psi_t(\mathbf{x})|^2 = \int_0^t dt' \int_{C_R} d^3x \frac{\partial}{\partial t'} |\psi_{t'}(\mathbf{x})|^2 + \int_{C_R} d^3x |\psi_0(\mathbf{x})|^2$ and using the quantum flux equation $\frac{\partial}{\partial t}|\psi_t|^2 + \nabla \cdot \mathbf{j}^{\psi_t} = 0$ together with Gauss' theorem and taking $R \to \infty$ provides a heuristic argument for the free flux-across-surfaces theorem. Unfortunately, because of the difficulty in controlling the relevant approximations, this argument cannot be readily turned into a rigorous proof (see also [1]).

Instead we may more directly compute the flux using (6), from which we find for $t \to \infty$

$$\mathbf{j}^{\psi_t}(\mathbf{x}) = \mathrm{Im}\psi_t^*(\mathbf{x})\nabla\psi_t(\mathbf{x}) \approx t^{-3}|\hat{\psi}(\frac{\mathbf{x}}{t})|^2 \frac{\mathbf{x}}{t}. \tag{8}$$

Noting that the flux is purely outgoing for large times, i.e. parallel to the outward normal $\mathbf{n}$ of ∂B_R, we then find upon substituting $\mathbf{v} := \frac{\mathbf{x}}{t}$ that

$$\begin{aligned} \int_0^\infty dt \int_{C\cap\partial B_R} \mathbf{j}^{\psi_t} \cdot \mathbf{n} d\sigma &\approx \int_0^\infty dt \int_{C\cap\partial B_R} t^{-3}|\hat{\psi}(\frac{\mathbf{x}}{t})|^2 \frac{\mathbf{x}}{t} \cdot \mathbf{n}(\mathbf{x}) d\sigma \\ &= \int_C d^3v |\hat{\psi}(\mathbf{v})|^2. \end{aligned} \tag{9}$$

This calculation can smoothly be turned into a rigorous proof, to which we now turn.

3 The Flux-Across-Surfaces Theorem

First we fix the following notation, illustrated also in the figure.

For $R > 0$ let $B_R := \{\mathbf{x} \in \mathbb{R}^3 : x \leq R\}$ and $\partial B_R = \{\mathbf{x} \in \mathbb{R}^3 : x = R\}$, with $x = |\mathbf{x}|$. Further let $\mathbf{n} : \partial B_R \to \mathbb{R}^3$, $\mathbf{n}(\mathbf{x}) := \frac{\mathbf{x}}{x}$ be the outward normal of the sphere ∂B_R. The cone spanned by the subset $\Sigma \subset S^2 := \{\mathbf{x} \in \mathbb{R}^3 : x = 1\}$ of the unit sphere is $C := \{\lambda\mathbf{x} \in \mathbb{R}^3 : \mathbf{x} \in \Sigma, \lambda \geq 0\}$ and its intersection with the sphere ∂B_R is $R\Sigma := C \cap \partial B_R = \{R\mathbf{x} \in \mathbb{R}^3 : \mathbf{x} \in \Sigma\}$. Another characterization of cones is provided by the unit vector $\mathbf{n}_C$, $\|\mathbf{n}_C\| = 1$ and the opening angle $\theta_C \in [0, \pi]$, namely $C := \{\mathbf{x} \in \mathbb{R}^3 : \mathbf{x} \cdot \mathbf{n}_C > x \cos\theta_C\}$. We chose polar coordinates $(r, \theta, \phi), r \geq 0, \theta \in [0, \pi], \phi \in [0, 2\pi)$ centered at the origin, $\mathbf{x}(r, \theta, \phi) = (r \sin\theta\cos\phi, r\sin\theta\sin\phi, r\cos\theta)$, with the z-direction $\mathbf{n}_C$. In these polar coordinates $B_R = \{(r, \theta, \phi) : r \leq R\}$, $\partial B_R = \{(r, \theta, \phi) : r = R\}$ and $C = \{(r, \theta, \phi) : \theta < \theta_C\}$. The intersection of the cone C with the sphere ∂B_R is now $C \cap \partial B_R = \{(r, \theta, \phi) : r = R, \theta < \theta_C\}$ with outward normal $\mathbf{n}(\theta, \phi) = R^{-1}\mathbf{x}(R, \theta, \phi)$. $d\Omega = \sin\theta d\theta d\phi$ denotes the solid angle.

Theorem 3.1 *Let $\psi \in \mathcal{S}(\mathbb{R}^3)$ and $\psi_t := e^{-iH_0 t}\psi$. Then for all $T \geq 0$ and any cone C*

$$\lim_{R\to\infty} \int_T^\infty dt \int_{C\cap\partial B_R} \mathbf{j}^{\psi_t}(\mathbf{x}) \cdot \mathbf{n} d\sigma = \lim_{R\to\infty} \int_T^\infty dt \int_{C\cap\partial B_R} |\mathbf{j}^{\psi_t}(\mathbf{x}) \cdot \mathbf{n}| d\sigma = \int_C d^3v |\hat{\psi}(\mathbf{v})|^2. \tag{10}$$

Remark 3.2 The condition $\psi \in \mathcal{S}(\mathrm{I\!R}^3)$, the Schwarz space, is introduced for the sake of simplicity. The proof may be performed with milder assumptions. Note, however, that $\mathcal{S}(\mathrm{I\!R}^3)$ is a time invariant domain under the free evolution.

Remark 3.3 The reason for formulating the theorem slightly stronger than (3), including information also about the modulus of $\mathbf{j}^{\psi_t} \cdot \mathbf{n}$, is that in Bohmian mechanics (see remark 3.11) the first (second) flux integral in (10) gives simply the expected value of the number of signed crossings (the total number of crossings) by the Bohmian trajectories of the surface. If they both agree it is an easy consequence that (10) equals the asymptotic probability that the particle crosses $C \cap \partial B_R$ at some time in $[0, \infty)$.

It will be convenient to introduce a notion of closeness of fluxes.

Definition 3.4 Two smooth functions $\mathbf{j}_1, \mathbf{j}_2 : \mathrm{I\!R}^3 \times \mathrm{I\!R} \to \mathrm{I\!R}^3$ are said to be "close in the sense of the asymptotic flux across surfaces," or $\mathbf{j}_1 \overset{FAS}{\sim} \mathbf{j}_2$, if for some $T > 0$

$$\lim_{R\to\infty} \int_T^\infty dt \int_{\partial B_R} |(\mathbf{j}_1 - \mathbf{j}_2) \cdot \mathbf{n}| d\sigma = 0. \tag{11}$$

Lemma 3.5 *Suppose that for* $\mathbf{j} : \mathrm{I\!R}^3 \times \mathrm{I\!R} \to \mathrm{I\!R}^3$ *and* $\mathbf{j}_0^\Phi(\mathbf{x}, t) := t^{-3} |\Phi(\frac{\mathbf{x}}{t})|^2 \frac{\mathbf{x}}{t}$ *with smooth* $\Phi \in L^2(\mathrm{I\!R}^3)$*, we have* $\mathbf{j} \overset{FAS}{\sim} \mathbf{j}_0^\Phi$*. Then for all cones* $C \subset \mathrm{I\!R}^3$ *and some* $T > 0$

$$\lim_{R\to\infty} \int_T^\infty dt \int_{C\cap\partial B_R} \mathbf{j}^{\psi_t}(\mathbf{x}) \cdot \mathbf{n}(\mathbf{x}) d\sigma = \lim_{R\to\infty} \int_T^\infty dt \int_{C\cap\partial B_R} |\mathbf{j}^{\psi_t}(\mathbf{x}) \cdot \mathbf{n}(\mathbf{x})| d\sigma = \int_C d^3v |\Phi(\mathbf{v})|^2. \tag{12}$$

Proof: By definition (3.4) it is sufficient to establish (12) for $\mathbf{j}^{\psi_t}$ replaced by $\mathbf{j}_0^\Phi$. Using spherical coordinates $\mathbf{x}(r, \theta, \phi) = (r \sin\theta \cos\phi, r \sin\theta \sin\phi, r \cos\theta)$ we compute

$$\begin{aligned}
\int_T^\infty dt \int_{C\cap\partial B_R} \mathbf{j}_0^\phi(\mathbf{x}) \cdot \mathbf{n}(\mathbf{x}) d\sigma &= \int_T^\infty dt \int_{C\cap\partial B_R} t^{-3} |\Phi(\frac{\mathbf{x}}{t})|^2 \frac{\mathbf{x}}{t} \cdot \mathbf{n}(\mathbf{x}) d\sigma \\
&= \int_T^\infty dt \int_\Sigma d\Omega R^2 t^{-3} |\hat{\phi}(\frac{\mathbf{x}(R, \theta, \phi)}{t})|^2 \frac{\mathbf{x}(R, \theta, \phi)}{t} \cdot \mathbf{n}(\theta, \phi).
\end{aligned}$$

Observing $\frac{\mathbf{x}(R,\theta,\psi)}{t} = \mathbf{x}(\frac{R}{t}, \theta, \psi)$ and substituting $v := \frac{R}{t}$ we obtain

$$\begin{aligned}
\lim_{R\to\infty} \int_T^\infty dt \int_{C\cap\partial B_R} \mathbf{j}_0^\Phi(\mathbf{x}) \cdot \mathbf{n}(\mathbf{x}) d\sigma &= \lim_{R\to\infty} \int_0^{R/T} dv v^2 \int_\Sigma d\Omega |\hat{\phi}(v, \theta, \psi)|^2 \\
&= \int_C d^3v |\Phi(\mathbf{v})|^2.
\end{aligned} \tag{13}$$

The observation that $\mathbf{x} \cdot \mathbf{n}(\mathbf{x}) = |\mathbf{x} \cdot \mathbf{n}(\mathbf{x})|$ finally shows that all equalities in (12) hold.

■

Lemma 3.6 *Let $\psi \in \mathcal{S}(\mathbb{R}^3), \psi_t := e^{-iH_0 t}\psi$ and $\mathbf{j}^{\psi_t} = \mathrm{Im}\psi_t^* \nabla \psi_t$. Then*

$$\mathbf{j}^{\psi_t}(\mathbf{x}, t) \overset{FAS}{\sim} \frac{\mathbf{x}}{t} t^{-3} |\hat{\psi}(\frac{\mathbf{x}}{t})|^2. \tag{14}$$

Proof: We verify the conditions in definition (3.4). For $t > 0$ we may write

$$\begin{aligned} \psi_t(\mathbf{x}) &= (e^{-iH_0 t}\psi)(\mathbf{x}) \\ &= \int d^3y \frac{e^{i\frac{|\mathbf{x}-\mathbf{y}|^2}{2t}}}{(2\pi i t)^{3/2}} \psi(\mathbf{y}) \\ &= \frac{e^{i\frac{x^2}{2t}}}{(it)^{3/2}} \hat{\psi}(\frac{\mathbf{x}}{t}) + \frac{e^{i\frac{x^2}{2t}}}{(it)^{3/2}} \int \frac{d^3y}{(2\pi)^{3/2}} e^{-i\frac{\mathbf{x}\cdot\mathbf{y}}{t}} (e^{i\frac{y^2}{2t}} - 1)\psi(\mathbf{y}). \end{aligned} \tag{15}$$

Since

$$|e^{i\frac{y^2}{2t}} - 1| \le 2 \tag{16}$$

for all $\mathbf{y} \in \mathbb{R}^3, t > 0$, we obtain that

$$f(\mathbf{v}, t) := \int \frac{d^3y}{(2\pi)^{3/2}} e^{-i\mathbf{v}\cdot\mathbf{y}} (e^{i\frac{y^2}{2t}} - 1)\psi(\mathbf{y}) \tag{17}$$

is well defined for all $\mathbf{v} \in \mathbb{R}^3$. Because $\psi \in \mathcal{S}(\mathbb{R}^3)$ we may interchange differentiation and integration to further obtain that f is differentiable on $\mathbb{R}^3 \times [T, \infty)$.

It is useful to introduce

$$\mathbf{g}(\mathbf{v}, t) := \nabla f(\mathbf{v}, t) = -i \int \frac{d^3y}{(2\pi)^{3/2}} e^{-i\mathbf{v}\cdot\mathbf{y}} (e^{i\frac{y^2}{2t}} - 1)\mathbf{y}\psi(\mathbf{y}). \tag{18}$$

Further we put

$$\alpha(\mathbf{x}, t) := \frac{e^{i\frac{x^2}{2t}}}{(it)^{3/2}} \hat{\psi}(\frac{\mathbf{x}}{t}) \tag{19}$$

and

$$\beta(\mathbf{x}, t) := \frac{e^{i\frac{x^2}{2t}}}{(it)^{3/2}} f(\frac{\mathbf{x}}{t}, t), \tag{20}$$

i.e. $\psi_t(\mathbf{x}) = \alpha(\mathbf{x}, t) + \beta(\mathbf{x}, t)$, and

$$\nabla\alpha(\mathbf{x}, t) = \frac{e^{i\frac{x^2}{2t}}}{(it)^{3/2}} \left(i\frac{\mathbf{x}}{t}\hat{\psi}(\frac{\mathbf{x}}{t}) + \frac{1}{t}(\nabla\hat{\psi})(\frac{\mathbf{x}}{t}) \right) \tag{21}$$

$$\nabla\beta(\mathbf{x}, t) = \frac{e^{i\frac{x^2}{2t}}}{(it)^{3/2}} \left(i\frac{\mathbf{x}}{t} f(\frac{\mathbf{x}}{t}, t) + \frac{1}{t}\mathbf{g}(\frac{\mathbf{x}}{t}, t) \right). \tag{22}$$

We may thus write

$$\begin{aligned} \mathbf{j}^{\psi_t}(\mathbf{x}) &= \mathrm{Im}(\psi_t^*(\mathbf{x})\nabla\psi_t(\mathbf{x})) \\ &= \mathrm{Im}(\alpha^*(\mathbf{x}, t)\nabla\alpha(\mathbf{x}, t) + \beta^*(\mathbf{x}, t)\nabla\alpha(\mathbf{x}, t) + \alpha^*(\mathbf{x}, t)\nabla\beta(\mathbf{x}, t) + \beta^*(\mathbf{x}, t)\nabla\beta(\mathbf{x}, t)) \\ &= \frac{\mathbf{x}}{t} t^{-3} |\hat{\psi}(\frac{\mathbf{x}}{t})|^2 + N(\mathbf{x}, t), \end{aligned} \tag{23}$$

with

$$N(\mathbf{x},t) := \mathrm{Im}\Big(t^{-4}\hat{\psi}^*(\frac{\mathbf{x}}{t})\nabla\hat{\psi}(\frac{\mathbf{x}}{t}) + \beta^*(\mathbf{x},t)\nabla\alpha(\mathbf{x},t) + \alpha^*(\mathbf{x},t)\nabla\beta(\mathbf{x},t) + \beta^*(\mathbf{x},t)\nabla\beta(\mathbf{x},t)\Big). \tag{24}$$

Thus to obtain (14) we need only show that (11) is satisfied for some $T > 0$ and $\mathbf{j}_1 - \mathbf{j}_2$ given by (24). We shall make use of the bounds

$$\sup_{\mathbf{v}\in\mathbb{R}^3, t>0} |f(\mathbf{v},t)| \leq 2(2\pi)^{-3/2}\|\psi\|_1 =: c_f, \tag{25}$$

$$\sup_{\mathbf{v}\in\mathbb{R}^3, t>0} |g(\mathbf{v},t)| \leq 2(2\pi)^{-3/2}\|y\psi(\mathbf{y})\|_1 =: c_g \tag{26}$$

($\|\cdot\|_1$ denotes the norm in L_1) and the fact that

$$\lim_{R\to\infty} f(\mathbf{v},\frac{R}{v}) = 0 \quad \forall \mathbf{v}\in\mathbb{R}^3. \tag{27}$$

(Note that $f(\mathbf{v},\frac{R}{v})$ is well defined even for $\mathbf{v} = 0$ by (17).) (25) and (26) hold since $|e^{\frac{iy^2}{2t}} - 1| \leq 2$ for all $\mathbf{v},\mathbf{y}\in\mathbb{R}^3, t > 0$. Since $\psi\in L_1(\mathbb{R}^3)$ and $\lim_{R\to\infty}|e^{i\frac{y^2 v}{2R}} - 1| = 0$ for all $\mathbf{v},\mathbf{y}\in\mathbb{R}^3$, (27) follows by dominated convergence.

We analyze the contribution of the expressions on the r.h.s. of (24) term by term. For the first term we obtain, using $|\mathrm{Im} z| \leq |z|$, the substitution $v = \frac{R}{t}$, and the Schwarz inequality

$$\begin{aligned}
|\mathrm{Im}\int_T^\infty dt \int_{\partial B_R} t^{-4}\hat{\psi}^*(\frac{\mathbf{x}}{t})\mathbf{n}\cdot\nabla\hat{\psi}(\frac{\mathbf{x}}{t})d\sigma| &\leq \int_T^\infty dt\int_\Sigma d\Omega R^2 t^{-4}|\hat{\psi}(\frac{\mathbf{x}}{t})||\nabla\hat{\psi}(\frac{\mathbf{x}}{t})| \\
&\leq \int_0^\infty dv v^2 \int_\Sigma d\Omega R^{-1}|\hat{\psi}(\mathbf{v})||\nabla\hat{\psi}(\mathbf{v})| \\
&\leq R^{-1}\|\hat{\psi}\|_2 \||\nabla\hat{\psi}|\|_2 \to 0
\end{aligned} \tag{28}$$

as $R\to\infty$, since $\hat{\psi}\in\mathcal{S}$.

For the second term

$$\mathrm{Im}\,\beta^*\nabla\alpha = \mathrm{Im}\, t^{-3} f^*(\frac{\mathbf{x}}{t},t)\left(i\frac{\mathbf{x}}{t}\hat{\psi}(\frac{\mathbf{x}}{t}) + \frac{1}{t}(\nabla\hat{\psi})(\frac{\mathbf{x}}{t})\right) \tag{29}$$

we obtain, similarly using (25),

$$\begin{aligned}
|\mathrm{Im}\int_T^\infty dt\int_{\partial B_R}\beta^*\nabla\alpha\cdot\mathbf{n}d\sigma| &\leq \int_T^\infty dt\int_\Sigma d\Omega R^2 t^{-3}|f^*(\frac{\mathbf{x}}{t},t)|(|\frac{R}{t}\hat{\psi}(\frac{\mathbf{x}}{t})| + \frac{1}{t}|\nabla\hat{\psi}(\frac{\mathbf{x}}{t})|) \\
&\leq \int_0^\infty dv\int_\Sigma d\Omega v^2|f^*(\mathbf{v},\frac{R}{v})|(|\hat{\psi}(\mathbf{v})| + \frac{1}{R}|\nabla\hat{\psi}(\mathbf{v})|) \\
&\leq \int_0^\infty dv\int_\Sigma d\Omega v^2|f^*(\mathbf{v},\frac{R}{v})||\hat{\psi}(\mathbf{v})| + \frac{1}{R}c_f\||\nabla\hat{\psi}|\|_1.
\end{aligned}$$

The second term tends to zero as $R\to\infty$, and the first term also vanishes: using (25) and the fact that $\hat{\psi}\in L^1(\mathbb{R}^3)$ we see that the integrand is dominated by an integrable function uniformly in R, so that with (27) the integral vanishes for $R \to \infty$ by dominated convergence.

For

$$\mathrm{Im}\,\alpha^* \nabla \beta = \mathrm{Im}\, t^{-3} \hat{\psi}^*(\frac{\mathbf{x}}{t}) \left(i\frac{\mathbf{x}}{t} f(\frac{\mathbf{x}}{t}, t) + \frac{1}{t} g(\frac{\mathbf{x}}{t}, t) \right) \quad (30)$$

we may proceed in an analogous manner and obtain

$$\begin{aligned} |\mathrm{Im} \int_T^\infty dt \int_{\partial B_R} \alpha^* \nabla \beta \cdot \mathbf{n} d\sigma| &\leq \int_T^\infty dt \int_\Sigma d\Omega R^2 t^{-3} |\hat{\psi}^*(\frac{\mathbf{x}}{t})| (|\frac{R}{t} f(\frac{\mathbf{x}}{t}, t)| + \frac{1}{t} |\mathbf{g}(\frac{\mathbf{x}}{t}, t)|) \\ &\leq \int_0^\infty dv \int_\Sigma d\Omega v^2 |\hat{\psi}^*(\mathbf{v})| (|f(\mathbf{v}, \frac{R}{v})| + \frac{1}{R} |\mathbf{g}(\mathbf{v}, \frac{R}{v})|) \\ &\leq \int_0^\infty dv \int_\Sigma d\Omega v^2 |\hat{\psi}^*(\mathbf{v})| |f(\mathbf{v}, \frac{R}{v})| + c_g \frac{1}{R} \|\hat{\psi}\|_1 \\ &\to 0 \text{ as } \quad R \to \infty. \end{aligned} \quad (31)$$

It remains to show that for some $T > 0$

$$\lim_{R \to \infty} \int_T^\infty dt \int_{\partial B_R} |\beta^* \nabla \beta \cdot \mathbf{n}| d\sigma = 0. \quad (32)$$

Now,

$$\begin{aligned} \beta^* \nabla \beta &= i t^{-3} f^*(\frac{\mathbf{x}}{t}, t) \int \frac{d^3 y}{(2\pi)^{3/2}} e^{-i\frac{\mathbf{x}}{t}\cdot\mathbf{y}} (e^{i\frac{y^2}{2t}} - 1)(\frac{\mathbf{x}}{t} - \frac{\mathbf{y}}{t}) \psi(\mathbf{y}) & (33) \\ &= -i t^{-3} f^*(\frac{\mathbf{x}}{t}, t) \int \frac{d^3 y}{(2\pi)^{3/2}} e^{-i\frac{\mathbf{x}}{t}\cdot\mathbf{y}} (\frac{\mathbf{x}}{t} - \frac{\mathbf{y}}{t}) \psi(\mathbf{y}) \\ &+ i t^{-3} f^*(\frac{\mathbf{x}}{t}, t) \int \frac{d^3 y}{(2\pi)^{3/2}} e^{-i\frac{\mathbf{x}}{t}\cdot\mathbf{y}} e^{i\frac{y^2}{2t}} (\frac{\mathbf{x}}{t} - \frac{\mathbf{y}}{t}) \psi(\mathbf{y}) \\ &= t^{-3} f^*(\frac{\mathbf{x}}{t}, t) \int \frac{d^3 y}{(2\pi)^{3/2}} \left(\nabla_\mathbf{y} e^{-i\frac{\mathbf{x}}{t}\cdot\mathbf{y}} \right) \psi(\mathbf{y}) & (34) \\ &+ i t^{-4} f^*(\frac{\mathbf{x}}{t}, t) \nabla \hat{\psi}(\frac{\mathbf{x}}{t}) & (35) \\ &- t^{-3} f^*(\frac{\mathbf{x}}{t}, t) \int \frac{d^3 y}{(2\pi)^{3/2}} \nabla_\mathbf{y} \left(e^{-i\frac{\mathbf{x}}{t}\cdot\mathbf{y}} e^{i\frac{y^2}{2t}} \right) \psi(\mathbf{y}). & (36) \end{aligned}$$

Treating (35) like (29) we see that (35) doesn't contribute. Partial integration of (34) + (36) yields

$$\begin{aligned} \mathbf{a}(\mathbf{x}, t) &:= t^{-3} f^*(\frac{\mathbf{x}}{t}, t) \int \frac{d^3 y}{(2\pi)^{3/2}} \left(e^{-i\frac{\mathbf{x}}{t}\cdot\mathbf{y}} e^{i\frac{y^2}{2t}} \nabla_\mathbf{y} \psi(\mathbf{y}) - e^{-i\frac{\mathbf{x}}{t}\cdot\mathbf{y}} \nabla_\mathbf{y} \psi(\mathbf{y}) \right) \\ &= t^{-3} f^*(\frac{\mathbf{x}}{t}, t) \int \frac{d^3 y}{(2\pi)^{3/2}} e^{-i\frac{\mathbf{x}}{t}\cdot\mathbf{y}} (e^{i\frac{y^2}{2t}} - 1) \nabla_\mathbf{y} \psi(\mathbf{y}) \\ &= -t^{-3} f^*(\frac{\mathbf{x}}{t}, t) \int \frac{d^3 y}{(2\pi)^{3/2}} \frac{t^2}{x^2} (\nabla_\mathbf{y}^2 e^{-i\frac{\mathbf{x}}{t}\cdot\mathbf{y}}) (e^{i\frac{y^2}{2t}} - 1) \nabla_\mathbf{y} \psi(\mathbf{y}) \\ &= -t^{-1} x^{-2} f^*(\frac{\mathbf{x}}{t}, t) \int \frac{d^3 y}{(2\pi)^{3/2}} e^{-i\frac{\mathbf{x}}{t}\cdot\mathbf{y}} \nabla_\mathbf{y}^2 \left((e^{i\frac{y^2}{2t}} - 1) \nabla_\mathbf{y} \psi(\mathbf{y}) \right), \end{aligned} \quad (37)$$

with two partial integrations in the last step.

Now

$$\begin{aligned}\nabla_{\mathbf{y}}(e^{i\frac{y^2}{2t}}-1) &= it^{-1}\mathbf{y}e^{i\frac{y^2}{2t}},\\ \nabla^2_{\mathbf{y}}(e^{i\frac{y^2}{2t}}-1) &= (-\frac{y^2}{t^2}+3it^{-1})e^{i\frac{y^2}{2t}}\end{aligned} \tag{38}$$

and

$$|e^{i\frac{y^2}{2t}}-1| \le \frac{y^2}{2t}, \tag{39}$$

so that for $t \ge T > 0$

$$|\nabla^2_{\mathbf{y}}((e^{i\frac{y^2}{2t}}-1)\nabla_{\mathbf{y}}\psi(\mathbf{y}))| \le |h(\mathbf{y})|t^{-1} \tag{40}$$

with some $h \in \mathcal{S}(\mathbb{R}^3)$ appropriately chosen. Hence,

$$|\int \frac{d^3y}{(2\pi)^{3/2}} e^{-i\frac{\mathbf{x}}{t}\cdot\mathbf{y}} \Big(\nabla^2_{\mathbf{y}}((e^{i\frac{y^2}{2t}}-1)\nabla_{\mathbf{y}}\psi(\mathbf{y}))\Big)| \le t^{-1}\int \frac{d^3y}{(2\pi)^{3/2}}|h(\mathbf{y})| =: ct^{-1}. \tag{41}$$

Thus we arrive at

$$|\mathbf{a}(\mathbf{x},t)| \le ct^{-2}x^{-2}|f(\frac{\mathbf{x}}{t},t)|, \tag{42}$$

and with $\mathbf{R}(\theta,\psi) := \mathbf{x}(R,\theta,\psi)$ we obtain

$$\int_T^\infty dt \int_{\partial B_R} |\mathbf{a}\cdot\mathbf{n}|d\sigma \quad \le \quad c\int_T^\infty dt t^{-2}\int_\Sigma d\Omega |f(\frac{\mathbf{R}}{t},t)|. \tag{43}$$

On the one hand (cf. (25))

$$\sup_{t\ge T, R>0} |f(\frac{\mathbf{R}}{t},t)| \le c_f, \tag{44}$$

and on the other hand with the Riemann-Lebesgue lemma

$$\lim_{R\to\infty} |f(\frac{\mathbf{R}}{t},t)| = 0 \ \forall\ t > 0. \tag{45}$$

Hence the r.h.s. of (43) tends to zero (dominated convergence) as $R \to \infty$ and we have thus finished the the proof of lemma (3.6). ■

Corollary 3.7 *For some $T > 0$, Theorem (3.1) holds .*

The analysis so far actually establishes the theorem for any $T > 0$. We now show that the restriction $T > 0$ can be removed.

Lemma 3.8 *For all $-\infty < T_1 < T_2 < \infty$*

$$\lim_{R\to\infty} \int_{T_1}^{T_2} dt \int_{\partial B_R} |\mathbf{j}^{\psi_t}(\mathbf{x})\cdot\mathbf{n}|d\sigma = 0. \tag{46}$$

Proof: First observe that

$$\int_{T_1}^{T_2} dt \int_{\partial B_R} |\mathbf{j}^{\psi_t}(\mathbf{x})\cdot \mathbf{n}| d\sigma \leq 4\pi \int_{T_1}^{T_2} dt R^2 \sup_{\mathbf{x}\in\partial B_R} |\psi_t(\mathbf{x})||\nabla\psi_t(\mathbf{x})|. \tag{47}$$

We want to apply dominated convergence. With

$$\psi_t(\mathbf{x}) = (2\pi)^{-3/2}\int d^3k e^{i\mathbf{k}\cdot\mathbf{x}} e^{-i\frac{k^2 t}{2}}\hat{\psi}(\mathbf{k}), \tag{48}$$

and

$$\nabla\psi_t(\mathbf{x}) = i(2\pi)^{-3/2}\int d^3k e^{i\mathbf{k}\cdot\mathbf{x}} e^{-i\frac{k^2 t}{2}}\mathbf{k}\hat{\psi}(\mathbf{k}), \tag{49}$$

we have that

$$\sup_{\mathbf{x}\in\mathbb{R}^3, t\in\mathbb{R}} |\nabla\psi_t(\mathbf{x})| \leq (2\pi)^{-3/2}\|k\hat{\psi}(\mathbf{k})\|_1. \tag{50}$$

Since $\psi\in\mathcal{S}(\mathbb{R}^3)$ we may perform n partial integrations in (48) to obtain

$$\begin{aligned}\psi_t(\mathbf{x}) &= (2\pi)^{-3/2}x^{-n}\int d^3k\Big[(\frac{1}{i}\nabla_k)^n e^{i\mathbf{k}\cdot\mathbf{x}}\Big] e^{-i\frac{k^2 t}{2}}\hat{\psi}(\mathbf{k}) \\ &= (-1)^n(2\pi)^{-3/2}x^{-n}\int d^3k e^{i\mathbf{k}\cdot\mathbf{x}}\Big[(\frac{1}{i}\nabla_k)^n e^{-i\frac{k^2 t}{2}}\hat{\psi}(\mathbf{k})\Big].\end{aligned} \tag{51}$$

We estimate

$$|(\frac{1}{i}\nabla_k)^n e^{-i\frac{k^2 t}{2}}\hat{\psi}(\mathbf{k})| \leq |h(\mathbf{k})|(1+t^n) \tag{52}$$

for some $h\in\mathcal{S}(\mathbb{R}^3)$. For $n=2$ we thus have

$$\begin{aligned}R^2\sup_{\mathbf{x}\in\partial B_R}|\psi_t(\mathbf{x})||\nabla\psi_t(\mathbf{x})| &\leq (2\pi)^{-3/2}\|k\hat{\psi}(\mathbf{k})\|_1\int d^3k|(\frac{1}{i}\nabla_k)^2 e^{-i\frac{k^2 t}{2}}\hat{\psi}(\mathbf{k})| \\ &\leq c'(1+t^2)\in L^1(T_1,T_2).\end{aligned} \tag{53}$$

For $n=3$ and any fixed $t\in[T_1,T_2]$ we obtain

$$\begin{aligned}R^2\sup_{\mathbf{x}\in\partial B_R}|\psi_t(\mathbf{x})||\nabla\psi_t(\mathbf{x})| &\leq (2\pi)^{-3/2}R^{-1}\|k\hat{\psi}(\mathbf{k})\|_1\int d^3k|(\frac{1}{i}\nabla_k)^3 e^{-i\frac{k^2 t}{2}}\hat{\psi}(\mathbf{k})| \\ &\leq c''R^{-1}(1+t^3)\to 0\end{aligned} \tag{54}$$

for $R\to\infty$. Now we use dominated convergence in (47) and are done. ■

Theorem (3.1) now follows directly from Cor.(3.7) and Lemma (3.8).

Remark 3.9 The extension of our result to the free evolution of N particles is straightforward. The extension to the interacting case, i.e. a proof of (2) (even for one-particle scattering), is open. The theory of generalized eigenfunction expansions [8] can be used to control the space-time behavior of $\psi_t(\mathbf{x})$ and of the flux $\mathbf{j}^{\psi_t}$. We may expand

$\psi_t(\mathbf{x}) = (2\pi)^{-3/2}\int d^3k e^{-i\frac{k^2 t}{2}}\phi(\mathbf{x},\mathbf{k})\widehat{\Omega_-^\dagger\psi}(\mathbf{k})$, where $\phi(\mathbf{x},\mathbf{k})$ are solutions of the Lippmann-Schwinger equation

$$\phi(\mathbf{x},\mathbf{k}) = e^{i\mathbf{k}\cdot\mathbf{x}} - \frac{1}{2\pi}\int d^3y \frac{e^{-ik|\mathbf{x}-\mathbf{y}|}}{|\mathbf{x}-\mathbf{y}|}V(\mathbf{y})\phi(\mathbf{y},\mathbf{k}), \tag{55}$$

(with *incoming* spherical waves). The important connection between the wave operators, generalized eigenfunctions and the Fourier transform is expressed by $\widehat{\Omega_-^\dagger\psi}(\mathbf{k}) = (2\pi)^{-3/2}\int d^3x\phi^*(\mathbf{x},\mathbf{k})\psi(\mathbf{x})$. For a proof of (2), relying essentially on a stationary phase argument, we need additional smoothness properties of the eigenfunctions which, to our knowledge, have not yet been established. More precisely, we need to know that $\phi(\mathbf{x},\cdot) \in C^\infty(\mathbb{R}^3 \setminus \{0\})$ for all $\mathbf{x} \in \mathbb{R}^3$, $\phi(\cdot,\mathbf{k}) \in C^\infty(\mathbb{R}^3)$ for all $\mathbf{k} \in \mathbb{R}^3 \setminus \{0\}$, and $\sup_{\mathbf{x}\in\mathbb{R}^3,\mathbf{k}\in\mathbb{R}^3\setminus\{0\}}\phi(\mathbf{x},\mathbf{k}) < \infty$. The closest we could get was, with [8] and [4] Theorem XI.41 and XI.70, that for $V \in L^2(\mathbb{R}^3)$ locally Hölder continuous with the possible exception of finitely many singularities and $|V(\mathbf{x})| = O(x^{-2-h})$ for some $h > 0$, $\phi(\mathbf{x},\mathbf{k})$ is bounded and continuous for $\mathbf{x} \in \mathbb{R}^3$ and $\mathbf{k} \in D \subset \mathbb{R}^3 \setminus \{0\}$, where D is *compact*. It is well known that for $V \in C^\infty(\mathbb{R}^3)$ the solutions ϕ of the stationary Schrödinger equation obey $\phi \in C^\infty(\mathbb{R}^3)$ and thus the solutions $\phi(\cdot,\mathbf{k})$ of the Lippmann-Schwinger equation, which are special solutions of the stationary Schrödinger equation parametrized by $\mathbf{k}$, are in $C^\infty(\mathbb{R}^3)$ (see [6], Theorem IX.62). It remains to be shown that for any $\mathbf{x} \in \mathbb{R}^3$ both $\phi(\mathbf{x},\cdot) \in C^\infty(\mathbb{R}^3 \setminus \{0\})$ and $\sup_{\mathbf{x}\in\mathbb{R}^3,\mathbf{k}\in\mathbb{R}^3\setminus\{0\}}|\phi(\mathbf{x},\mathbf{k})| < \infty$. This should be true for potentials which are sufficiently smooth and have sufficiently strong decay at infinity [9].

Remark 3.10 The mathematical physics of scattering theory is mainly concerned with the existence and asymptotic completeness of wave operators $\Omega_\pm := \text{s-}\lim_{t\to\mp\infty} e^{iHt}e^{-iH_0t}$. The wave operators may be used to control the long-time behavior of wave packets $\psi_t := e^{-iHt}\psi$, in the sense of $\psi_t \overset{L^2}{\sim} e^{-iH_0t}\Omega_-^\dagger\psi$, i.e. the difference vanishes in L^2 as $t \to \infty$. Dollard's lemma implies that for $\phi_t := e^{-iH_0t}\phi$

$$\phi_t(\mathbf{x}) \overset{L^2}{\sim} e^{i\frac{x^2}{2t}}(it)^{-3/2}\hat{\phi}(\frac{\mathbf{x}}{t}). \tag{56}$$

Asymptotic completeness of the wave operators implies, among other things, that for any $\psi \in \mathcal{H}_{ac}(H)$ there is a $\phi \in L^2$ such that $\lim_{t\to\infty}\|e^{-iHt}\psi - e^{-iH_0t}\phi\|_2 = 0$, where $\phi = \Omega_-^\dagger\psi$ with Ω_- unitary on $\mathcal{H}_{ac}(H)$ (see, e.g., [4]). It then follows by the triangle inequality that for any $\psi \in \mathcal{H}_{ac}$

$$\psi_t(\mathbf{x}) \overset{L^2}{\sim} e^{i\frac{x^2}{2t}}(it)^{-3/2}\widehat{\Omega_-^\dagger\psi}(\frac{\mathbf{x}}{t}). \tag{57}$$

From this the general scattering-into-cones theorem (1) follows easily (see. e.g. [2]). This is however not sufficient to prove the physically relevant flux-across-surfaces theorem. The notion of closeness which should be used here is the closeness of fluxes in the sense of the asymptotic flux across surfaces introduced in definition (3.4), and not the closeness of wave functions in L^2.

Remark 3.11 In the context of Bohmian mechanics [10, 11, 12, 13, 14], a theory of point particles moving along trajectories defined by an ODE arising from the wave function, with velocity $\mathbf{j}^{\psi_t}/|\psi|^2$, a theory that can be shown to underly the quantum formalism (see. e.g. [15, 16]), it follows easily from Theorem (3.1) that

$$\lim_{R\to\infty} \mathbb{P}^{\psi}(\mathbf{x}_e^R \in R\Sigma) = \lim_{R\to\infty} \int_0^{\infty} dt \int_{R\Sigma} \mathbf{j}^{\psi_t} \cdot \mathbf{n} d\sigma \tag{58}$$

where $\mathbf{x}_e^R$ is the position at which the trajectory first crosses the sphere ∂B_R and $\mathbb{P}^{\psi}$ is the quantum equilibrium measure, given by the density $|\psi|^2$. This provides a natural definition of the cross section measure.

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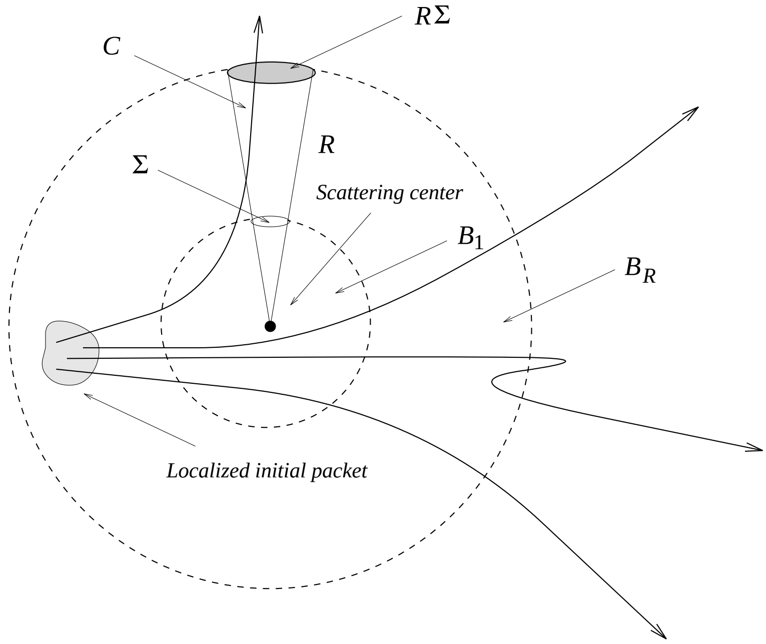

Figure 1: The initial wave packet evolves under the influence of the scatterer at the origin. In Bohmian mechanics (see remark 3.11) the flow lines of the corresponding flux represent the possible trajectories of the particle.