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The Flux-Across-Surfaces Theorem and Zero-Energy Resonances[1]

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In this contribution we shall first introduce the Flux Across Surfaces (FAS) theorem, placing it in the general context of the Quantum Scattering Theory. Then we shall review briefly the theory of resonances in non-relativistic Quantum Mechanics and outline a proof of the FAS theorem for non-relativistic potential scattering, which covers also the case in which there is a zero energy resonance.

KEY WORDS: Quantum scattering theory; Schroedinger equation; probability density current; quantum resonances.

1. SETTING UP THE PROBLEM

The "flux across surfaces" theorem is of fundamental importance in the formulation of scattering theory in Quantum Mechanics. It gives a relation between what is observed in a scattering experiment and the basic object that is discussed in every textbook in Quantum Mechanics, i.e., the scattering amplitude. In abstract scattering theory, for scattering of a particle by a time independent potential, the scattering cross-section is essentially defined to be the probability $P(\Sigma, \psi_0)$ that the particle is detected by an apparatus with active surface Σ placed very far away from the region of interaction when the particle (or rather the beam of particles) is prepared at time $t = 0$ in a state ψ_0.

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Essentially, one argues that this probability is related to the corresponding asymptotic outgoing state ψ_{out} by the relation

$$P(\Sigma, \psi_0) = \int_{C_\Sigma} |\hat{\psi}_{\text{out}}(k)|^2 \, dk \tag{1.1}$$

where C_Σ is the cone generated by Σ with vertex in a point P which belongs to the region of interaction (the precise choice of the point is irrelevant if the active surface is sufficiently far away) and $\hat{\psi}$ is the Fourier transform of ψ (so that k is the momentum of the outgoing particle in suitable units).

From (1.1) the textbook relationship between the differential cross section and the scattering amplitude can be deduced, with the help of a statistical assumption on the beam of incoming particles. We refer to the book of ref. 1, Chap. 7, or to ref. 11.

The problem of deducing (1.1) from more basic principles had a first answer through Dollard's theorem;[10] this theorem states that, assuming existence and asymptotic completeness of the wave operator

$$W_+ = \text{s}-\lim_{t \to +\infty} e^{iHt} e^{-iH_0 t}$$

(where $H = H_0 + V$, V is the potential, and H_0 the free hamiltonian), one has

$$\lim_{t \to \infty} \int_{C_\Sigma} |\psi_t(x)|^2 \, dx = \int_{C_\Sigma} |\hat{\psi}_{\text{out}}(k)|^2 \, dk.$$

In order that this answer be satisfying, one must assume that $P(\Sigma, \psi_0)$ can be identified with the probability that the particle is detected in the cone C_Σ in the distant future.

However the experimental set up by which one measures the cross section is more closely related to the probability that the particle is detected by the active surface Σ at *any time* in the time interval during which the detector is active.

The physics of the scattering experiments is better described through a collection of distant detectors, surrounding the region in which the interaction takes place, firing at a random time; the experimenter records the distribution of the location in which the firing has taken place.

A natural mathematical object connected with this physical description is the quantum mechanical flux. It is defined by introducing the probability density current $j^{\psi_t} \equiv \mathrm{Im}(\psi_t^* \nabla \psi_t)$, which satisfies the continuity equation

$$\frac{\partial \rho_t}{\partial t} + \nabla j^{\psi_t} = 0, \qquad \rho_t \equiv |\psi_t|^2$$

whenever ψ_t satisfies the Schrödinger equation. It is natural to think that the probability that the particle crosses in the interval of time $(t, t+dt)$ the element dS on the surface of Σ be given by

$$(j^{\psi_t} \cdot n)\, dS\, dt \tag{1.2}$$

where n is the normal versor to Σ (oriented outwards with respect to the region in which the interaction takes place).

There are two difficulties in this interpretation. First, the current at fixed time is a distribution which is not, in general, integrable over a surface (a manifold of codimension one). This can be cured by requiring some Sobolev regularity to the inintial datum, e.g., $\psi_0 \in H^2(\mathbb{R}^3)$, compare ref. 2, Section 2.

More serious can be the fact that the flux at the time t and at the point $x \in \Sigma$ may be not outgoing; therefore the quantity in (1.2) may be negative, and not interpretable as a probability. On physical ground one expects that, if the detectors are placed "sufficiently far" from the scattering region, the flux be outgoing, but by the invariance under time translation of the entire theory one cannot expect this to be true uniformly in the initial data. Notice that this holds even for the case of a free particle.

The relevance of this point of view was recognized by Combes *et al.*[6] in 1975 and led them to formulate the "flux across surfaces conjecture," i.e., the statement that this physical intuition is correct if one lets the detectors be placed at an infinite distance and if some "reasonable" conditions are placed on the potential and on the initial state. Under these conditions (we return on this point later on) the conjecture was formulated in the following way: the following identification holds true

$$\begin{aligned}\sigma_{\mathrm{flux}}(\Sigma, \psi_0) &\equiv \lim_{R\to\infty} \lim_{T_2\to\infty} \int_{T_1}^{T_2} dt \int_{\Sigma_R} (j^{\psi_t} \cdot n)\, dS \\ &= \int_{C_\Sigma} |\mathscr{F}(W_+^{-1}\psi_0)(k)|\, dk\end{aligned} \tag{1.3}$$

where $\mathscr{F}$ is Fourier transform, Σ_R is the intersection of the cone C_Σ with the surface of the sphere of radius R and n is the normal to Σ oriented outwards (with respect to the cone). Notice that $\sigma_{\mathrm{flux}}(\Sigma, \psi_0)$ as defined by (1.3) is independent of T_1.

Remark. The conjecture says more. The following identity also holds

$$\sigma_{\text{flux}}(\Sigma, \psi_0) \equiv \lim_{R\to\infty} \lim_{T_2\to\infty} \int_{T_1}^{T_2} dt \int_{\Sigma_R} (j^{\psi_t} \cdot n)\, dS$$

$$= \lim_{R\to\infty} \lim_{T_2\to\infty} \int_{T_1}^{T_2} dt \int_{\Sigma_R} |(j^{\psi_t} \cdot n)|\, dS, \tag{1.4}$$

i.e., the flux is asymptotically outgoing.

While the fundamental importance of the identity (1.3) was recognized by Combes, Newton, and Stockhamer in 1975, the corresponding theorem was proved only recently, first for the free case (physically not interesting but mathematically not triviall) by Daumer *et al.*[7] and then, under various assumptions, by several Authors, with different techniques. For example, in ref. 23, the authors make use of the time-independent formulation of scattering theory and perform a thorough analysis of the properties of the (generalized) eigenfunctions of the Hamiltonian and of the corresponding Lippmann–Schwinger equation. In refs. 2 and 3, the authors use strategies taken from Geometrical Scattering Theory and theorems about time asymptotics of the evolution of the wave function, a method originated by Enss, see, e.g., ref. 21, based on the geometrical insight that, roughly speaking, wave functions orthogonal to the bound states and with support moving away from the scattering region, after a sufficiently long time will not feel the potential any more, and will thus move freely.

Remark. Other proofs have been inspired by the interpretation of Quantum Mechanics through Bohmian Mechanics, which gives an intuitive pictures of the flux in terms of crossings of the given surface by the path of the Bohmian particles.[7, 8] Or by the equivalence, as far as position measurements are concerned, between Quantum Mechanics and the Stochastic Mechanics first described by Nelson[18] and then developed, especially for scattering processes, by Carlen,[5] who gives a detailed study of the asymptotic behaviour pathwise. The proof through Stochastic Mechanics given by Posilicano and Ugolini[22] is particularly interesting as an alternative proof. Both these proofs, through Bohmian and Stochastic Mechanics, give actually more information, namely pathwise behaviour, and may shed some light on the problem of describing the correlation in the detection of several particles. A conjecture for the N-body problem was also given in a tentative way in ref. 6, and a more refined study of this problem is going to appear in ref. 14.

All these proofs are given under different assumptions, both on the potential and on the state of the system at time zero (or the asymptotic state at $t=+\infty$). All share the assumption that there is no zero energy resonances (the proofs that contain assumptions on the asymptotic outgoing state require that its energy spectrum is bounded away from zero, and it will be clear later on that such kind of states cannot "feel" a zero energy resonance).

It is common lore in physics that a quantum resonance is a sort of quasi-bound state. In this spirit, a convenient definition of zero-energy resonance is the following.

Definition 1.1. We say that $H=-\Delta+V$ has a *zero-energy resonance* (with respect to H_0) if there exist a distributional solution ψ_{res} of the Schrödinger equation $(-\Delta+V)\,\psi_{\mathrm{res}}=0$ such that $\langle x\rangle^{-\gamma}\,\psi_{\mathrm{res}}\in L^2(\mathbb{R}^3)$ for any $\gamma>1/2$ but *not* for $\gamma=0$. Here $\langle x\rangle=(1+|x|^2)^{1/2}$ as usual.

In other words, ψ_{res} fails to be an eigenstate since it does not decrease fast enough at infinity. It is shown in ref. 9 that the previous definition is equivalent, for a large class of potentials, to the more sophisticated and new fashioned ones.

It is relevant to notice that if there is a zero energy resonance then the resolvent $(H-k^2)^{-1}$, regarded in an appropriate sense (see Section 3), has a polar singularity in $k=0$. By computing the Laplace transform of the resolvent, one gets interesting information about the time evolution: in particular, when a zero energy resonance is present the decay of the wave-function for large times is slower than usual. More precisely, Jensen and Kato proved that for any $\psi\in\mathscr{H}_{\mathrm{ac}}(H)$ one has for $t\to\infty$ that

$$e^{iHt}\psi=(i\pi t)^{-1/2}\,\langle\psi,\psi_{\mathrm{res}}\rangle\,\psi_{\mathrm{res}}+(4i\pi)^{-1/2}\,t^{-3/2}B_1\psi+o(t^{-3/2}) \tag{1.5}$$

where the first term is present only if H has a zero energy resonance, B_1 is a suitable operator and the remainder term is small in a sense to be made precise, see ref. 17.

As far as the flux-across-surfaces problem is concerned, it is clear from (1.5) that the resonant case has some specific features. Indeed the assumption of absence of a zero energy resonance, or the absence in the initial state of energy spectrum near the lower end of the continuum part (the scattering regime concerns anyway the orthogonal complement of the bound states) is not without reason. Since the dynamics of the asymptotic states is free, the lower part of the energy spectrum is made of asymptotic states of very low momentum; therefore this states move away from the interaction region "very slowly" and the limit in (1.3) may not be achieved or, if achieved, may be different.

Given the order of the limits which are taken in (1.2) (first $T_2 \to \infty$ and then $R \to \infty$) one expects that this would not happen. But in any case this problem suggests that the case of a zero energy resonance should have a special treatment.

Notice that the map $\psi_0 \mapsto \sigma_{\text{flux}}(\Sigma, \psi_0)$ is not continuous in the Hilbert space topology, and therefore density theorems do not apply. Moreover, in presence of zero-energy resonances the the usual mapping properties of the (inverse of) the wave operators (to the extent that the outgoing state inherits the smoothness properties of the state at time zero) fail to hold.[24]

In order to get an insight into this problem, in ref. 20 Panati and Teta treat the case of a point interaction in $\mathbb{R}^3$. This model allows to find a very explicit expression for the resolvent and the evolution unitary group, as well as explicit conditions for the presence of a zero-energy resonance. Therefore the validity of (1.2) can be verified in a very explicit form; Panati and Teta found that in this special example of interaction, the flux across surface theorem holds even in presence of a zero energy resonance and without limitations on the support in energy of the initial state (some smoothness assumptions on the initial state are required for technical reasons).

The result is independent from the number of points where the point interactions are placed. On the other hand, it has been shown in ref. 15 that a large class of potentials can be approximated arbitrarily well by point interactions placed in a finite but very large number of points, properly distributed in space.

This suggests that the theorem is true in presence of a zero energy resonance also in potential scattering, under suitable assumption on the potential. And that the proof could be given adapting, with suitable modifications, the proof for point interactions. The difficulty lies in the fact that explicit estimates are no longer available, and one has to find the proper weaker estimates that hold in potential scattering and are still sufficient to complete the proof.

The paper of ref. 9, the contents of which are briefly reported in this note, provides such estimates, building on results of Jensen and Kato[17] on the analysis of resonances at the bottom of the continuous energy spectrum.

2. SETTING UP THE MATHEMATICAL PROBLEM

We shall discuss non-relativistic quantum mechanical scattering from a time-independent potential $V(x)$, $x \in \mathbb{R}^3$. We shall denote by H_0 the free hamiltonian that we shall take to be (in suitable units) $H_0 = -\Delta$. We shall assume that the potential V is such that the hamiltonian H, defined as $H=H_0+V$, is essentially self-adjoint on the domain of H_0, that it has neither positive eigenvalues nor singular continuous spectrum and that the absolutely continuous part of the spectrum is the interval $[0,+\infty)$.

These assumptions are in particular satisfied if V belongs to the class $(I)_n$ for $n\geqslant 2$. By that we mean that V belongs to $L^2(\mathbb{R}^3)$, is locally Hölder continuous except for a finite number of points, and that there exist $R_0>0$, $C_0>0$ and $\epsilon>0$ such that $|V(x)|\leqslant C_0\,|x|^{-\epsilon-n}$ for $|x|\geqslant R_0$. Moreover, under this assumption the wave operators $W_{\pm}=s-\lim_{t\to\pm\infty} e^{iHt}e^{-iH_0t}$ exists and are complete, i.e., the operator $S\equiv W_+^*W_-$ is unitary.

With the notation

$$U_t\equiv e^{-iHt},\qquad U_t^0\equiv e^{-iH_0t},\qquad \psi_t\equiv U_t\psi_0,\qquad \psi_0\in\sigma_{\mathrm{ac}}(H),$$

one has the existence of an element $\psi_{\mathrm{out}}(\psi_0)$ of the Hilbert space $L^2(\mathbb{R}^3)$ such that

$$\lim_{t\to\infty}\|\psi_t-U_t^0\psi_{\mathrm{out}}\|=0.$$

At this point, the proof of the Flux Across Surfaces (FAS) theorem has been given along two different lines. The first one relies on the time-independent theory of scattering, as developed by Kato and Ikebe and others, which is based on a detailed study of the generalized eigenfunctions corresponding to the continuous part of the spectrum of H.

The second one relies on the time-dependent approach initiated by Enss and that has became to be known as "geometrical scattering theory;" this approach is based on detailed estimates on the propagation properties in space of U_t as compared to U_t^0. This second method has the great advantage of soliciting physical intuition, and therefore is more apt for a visual description of the process that takes place. The role of the estimates which are needed to carry out the proofs is therefore more transparent, and the conditions on the potential are more clearly justified. And it may be more easily extended to the case of the N-body problem, because it leads to a more intrinsic separation among the channels and to a better use of the channel hamiltonian.

On the other hand, the geometric method relies more on the fact that at very large times the "true" motion becomes very close (in a suitable sense) to the free one, and therefore it leads naturally to assumptions on the outgoing states. We consider this a drawback, since the experimenter has at his disposal the preparation of the state at "time zero" but is unable to intervene on the state at a time remote in the future.

Remark. We consider the limit $t \to +\infty$ as a mathematical device to obtain formulas that are manageable, since the preparation of the experiment and its unfolding take place at finite times. Of course, this is justified if the convergence to the limit in (1.3) is sufficiently fast, and this requires in both methods delicate estimates. On the opposite, we will not consider the limit $t \to -\infty$, and this is the reason why we shall discuss only properties of the wave operator and not of the S-matrix.

Both methods rely on the fact that the theorem is valid for the free case ($V=0$) and the proof for the free case relies on stationary phase techniques. The two approaches differ substantially in obtaining the estimates necessary to prove the same result for the interacting case.

In proving the FAS theorem in the case of a zero energy resonance we shall follow the procedures of stationary scattering theory, for which the deep analysis by Jensen and Kato of the low energy behaviour of the generalized eigenfunctions is available.

We first sketch the proof of the FAS theorem in the case $V=0$ by using very explicitly the properties of the free propagation kernel.

Proposition 2.1. Let $V=0$. If the initial state is represented by a function in the Schwartz space $\mathscr{S}(\mathbb{R}^3)$ the FAS relation (1.3) holds true.

We follow the proof appearing in ref. 13.

Proof. For the free propagation one has

$$\begin{aligned}
\psi_t(x) &= \int_{\mathbb{R}^3} dy\, e^{i\frac{(x-y)^2}{2t}} (2\pi i t)^{-\frac{3}{2}} \psi_0(y) \\
&= e^{i\frac{x^2}{2t}} (it)^{-\frac{3}{2}} \hat{\psi}_0\left(\frac{x}{t}\right) + e^{i\frac{x^2}{2t}} (2\pi i t)^{-\frac{3}{2}} \int_{\mathbb{R}^3} e^{-i\frac{(x\cdot y)}{t}} \left(e^{i\frac{y^2}{2t}} - 1\right) \psi_0(y)\, dy \\
&\equiv \alpha(x,t) + \beta(x,t).
\end{aligned} \tag{2.1}$$

In (2.1) we have separated a term (α) which we expect to have the leading role (for free motion, asymptotically the momentum should be ratio of distance to time, in suitable units) and a term (β) with vanishing contribution for $t \to \infty$.

This type of splitting will play a major role also in the interacting case.

By the definition of $j(x)$ one has

$$j^{\psi_t}(x) = \frac{x}{t} t^{-3} \left| \hat{\psi}_0\left(\frac{x}{t}\right)\right|^2 + R_1(x,t) + R_2(x,t), \tag{2.2}$$

where R_1, R_2, explicitly given below, will give a negligible contribution to the flux in the scattering limit. The explicit form of R_1, R_2 is

$$R_1(x,t) = \mathrm{Im}\left(t^{-4}\hat{\psi}_0^*\left(\frac{x}{t}\right)\nabla\hat{\psi}_0\left(\frac{x}{t}\right)\right), \qquad R_2 = \mathrm{Im}(\beta^*\,\nabla\alpha + \alpha^*\,\nabla\beta + \beta^*\,\nabla\beta).$$

We first verify that the first term in (2.2) gives the correct result. Indeed one computes

$$\begin{aligned}
&\lim_{R\to\infty}\int_T^\infty dt\int_{\Sigma_R} t^{-4}\left|\hat{\psi}_0\left(\frac{x}{t}\right)\right|^2 (x\cdot n)\,d\sigma \\
&\quad= \lim_{R\to\infty}\int_T^\infty dt\int_{\Sigma_R} t^{-4}\left|\hat{\psi}_0\left(\frac{R\omega}{t}\right)\right|^2 R^3\,dR \\
&\quad= \lim_{R\to\infty}\int_0^{\frac{R}{T}} |k|^2\,d|k|\int_{\Sigma_R} |\hat{\psi}_0(k)|^2\,d\Omega \\
&\quad= \int_{C_\Sigma} |\hat{\psi}_0(k)|^2\,dk.
\end{aligned} \tag{2.3}$$

Here we have performed the change of variable $x = R\omega$, where $|\omega| = 1$, and we have set $R^2\omega\cdot n\,d\sigma = d\Omega$. Notice that the change of variables $k = \frac{x}{t} = \frac{R\omega}{t}$ means, in particular, $d|k| = -Rt^2\,dt$.

The remaining terms R_1 and R_2 can be estimated as follows: there exists a positive constants C_1, C_2 and a number $0 < \epsilon < 1$, such that for R and t large enough the following holds:

$$\sup_{x\in S_R} |R_i(x,t)| \leqslant C_i t^{-1-\epsilon} R^{-3+\epsilon} \qquad (i = 1, 2), \tag{2.4}$$

where $S_R \equiv \{x\in\mathbb{R}^3 : |x| = R\}$. This implies that the corresponding contribution to the flux is integrable in t uniformly in R and goes to zero in the limit $R\to\infty$.

The estimate in (2.4) can be obtained by integration by parts over the variable y, using a stationary phase argument and the identity, valid for any positive $q\in\mathbb{N}$,

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

and recalling that

$$|(e^{i\frac{y^2}{2t}}-1)|\leqslant\frac{y^2}{2t}.$$

The FAS relation (1.3) is thus proved for $\psi_0\in\mathscr{S}(\mathbb{R}^3)$. ∎

Remark. The estimates given above depend crucially on the non-relativistic dispersion dispersion law $H_0(k)=\frac{k^2}{2}$. In the relativistic case the analogous of the FAS theorem still holds, but the proof is substantially more complicated, see ref. 12 for the case of the Dirac equation.

3. A SKETCH OF THE PROOF

In this section we shall sketch a proof of the FAS theorem which includes the case of a resonance at zero energy. A more detailed version of this proof will be published elsewhere.[9]

The main tool in our analysis is the fact that the operator H can be "diagonalized," for the potentials we are considering, by means of the solutions $\Phi(x,k)$ of the Lippmann–Schwinger (LS) equation,

$$\Phi(x,k)=e^{ik\cdot x}-\int_{\mathbb{R}^3}\frac{e^{-i\,|k|\,|x-y|}}{4\pi\,|x-y|}V(y)\,\Phi(y,k)\,dy,\qquad \lim_{|x|\to\infty}\,(\Phi(x,k)-e^{ik\cdot x})=0. \tag{3.1}$$

It is well-known, after ref. 16, that this equation has a unique solution such that $\eta_k(x)\equiv\Phi(x,k)-e^{i(k\cdot x)}$ is a continuous function vanishing at infinity. In other words, the function $\eta_k(x)$ is the unique solution in the space of continuous functions vanishing at infinity of the equation

$$(1+G_{|k|}V)\,\eta_k=g_k,\qquad g_k(x)\equiv-\frac{1}{4\pi}\int_{\mathbb{R}^3}\frac{e^{-i\,|k|\,|x-y|}}{|x-y|}V(y)\,e^{ik\cdot y}\,dy, \tag{3.2}$$

where G_κ is the right inverse of $-\Delta-\kappa^2$ in $\mathscr{S}'(\mathbb{R}^3)$, given by convolution with $G_\kappa(x)=e^{i\kappa\,|x|}/|x|$. For the classical results on the LS equation one can see ref. 23 and references therein.

For our purposes it is more convenient to regard (3.1) as an equation in the weighted Sobolev space $H^{m,s}$, defined by

$$H^{m,s}(\mathbb{R}^3)\equiv\{u\in\mathscr{S}'(\mathbb{R}^3):\|(1+|x|^2)^{s/2}\,(1-\Delta)^{m/2}\,u\|_{L^2}<+\infty\}.$$

In this spaces equation (3.1) has still a unique solution (for suitable values of m,s), and the two solutions can be identified. The main advantage of the latter formulation is that the the map $\kappa \mapsto (-\Delta+\kappa^2)^{-1}$, $\kappa \in \mathbb{C}_+$, regarded as a map with values in the space of operators between weighted Sobolev spaces, can be continued as a continuous map to the closed upper half plane.[17] This will lead to a general definition of zero-energy resonance and resonance function.

It is part of a common lore in scattering theory to think of a resonance as a complex pole of the resolvent for $\operatorname{Im}\kappa < 0$ (on the "unphysical sheet"). An analytic continuation of the resolvent below the entire real axis in κ is only possible for exponentially decreasing potentials; for a large class of potentials (e.g., dilation-analytic) the analytic extension is possible in a sector with vertex in the bottom of the continuous spectrum. In such cases, one can define non-zero resonances as poles of the continuation of the resolvent. But this is not possible for resonances at the bottom of the continuous spectrum. Without entering in too fine details (see refs. 9 and 17) we recall that for a general class of potentials the following holds:

Denote by $\mathscr{M}$ the kernel of $(1+G_0V)$ in $H^{1,-1/2-\epsilon}$ for $\epsilon>0$. (This space is independent on the choice of ε, provided ε is not too large.) The zero eigenspace of the operator $-\Delta+V$ in $L^2(\mathbb{R}^3)$ (bound states with zero energy) is a subspace of $\mathscr{M}$ and its complement in $\mathscr{M}$ is at most one-dimensional.

When this complement is not empty, its elements are called zero-energy resonance functions and the system is said to have a *zero-energy resonance*. Moreover $\phi \in \mathscr{M}$ belongs to $L^2(\mathbb{R}^3)$ iff $\langle V, \phi\rangle = 0$. If zero is not an eigenvalue of H, we can fix uniquely a canonical resonance function ψ_{res} by imposing the normalization condition $\langle V, \psi_{\text{res}}\rangle = (4\pi)^{-1/2}$. If zero is an eigenvalue of H, an additional condition is required in order to fix uniquely a canonical resonance function, see ref. 17.

In scattering theory one is interested in solving the Lippmann–Schwinger equation. This amounts to inverting the operator $1+G_\kappa V$ for κ on the real axis. According to ref. 17 this can be done continuously for $\kappa \in \mathbb{R}\setminus\{0\}$, with the following asymptotic expansion for $\kappa \to 0$, valid if the potential satisfies suitable assumptions.

Lemma 3.1. If there is a zero energy resonance with canonical resonance function ψ_{res} one has the following asymptotic expansion for $\kappa \to 0$, $\kappa \in \mathbb{R}_+$:

$$(1+G_\kappa V)^{-1} = \kappa^{-2}P_0V - i\kappa^{-1}(\langle\,\cdot\,, V\psi_{\text{res}}\rangle\,\psi_{\text{res}} - P_0VG_3VP_0V) + C_0 + \kappa C_1 + \mathscr{O}(\kappa^2) \tag{3.3}$$

where C_1, C_2 are suitable operators, P_0 is the projection operator in $L^2(\mathbb{R}^3)$ on the zero eigenspace of H and G_3 is the convolution operator with kernel $24\pi G_3(x, y) = |x-y|^2$. The remainder is small in the sense of the norm of operators between suitable weighted Sobolev spaces.

Remark. It should be remarked that (3.3) is an asymptotic expansion on the positve real axis, and the presence of the factors κ^{-1} and κ^{-2} do not correspond to poles of an analytic function but rather only to "polar-like" singularities on the real axis.

By exploiting (3.3) an asymptotic expansion for the Lippman–Schwinger eigenfunctions can be obtained. Indeed, denoting by $\{\psi_j\}_{j=1,\dots,m}$ any orthonormal basis for the null space of $-\Delta+V$ in $L^2(\mathbb{R}^3)$ (if zero is not an eigenvalue for H the corresponding terms should be omitted), one gets

$$\begin{aligned}\eta_k &= (1+G_{|k|}V)^{-1}\, g_k \\ &= \frac{1}{|k|^2}\sum_{j=1}^{m} \langle g_k, V\psi_j\rangle\, \psi_j - \frac{i}{|k|}(\langle g_k, V\psi_{\mathrm{res}}\rangle\, \psi_{\mathrm{res}} - P_0VG_3VP_0Vg_k) + \mathcal{O}(1)\end{aligned} \tag{3.4}$$

valid as $|k| \to 0$. The second-order polar singularity appearing in () is only apparent, since the corresponding "residue" is

$$\langle g_0, V\psi_j\rangle = \langle G_0V\, 1, V\psi_j\rangle = \langle V\, 1, G_0V\psi_j\rangle = -\langle V\, 1, \psi_j\rangle = 0,$$

where we used the fact that any function $\phi \in \mathcal{M}$ belongs to $L^2(\mathbb{R}^3)$ iff $\langle V, \phi\rangle = 0$. The previous observation is the key ingredient to prove the following lemma (see ref. 9 for a more precise statement).

Lemma 3.2. Let η_k be defined as $\eta_k = \Phi(x, k) - e^{i(k\cdot x)}$ where $\Phi(x, k)$ is the unique solution of the Lippmann–Schwinger equation such that η_k is continuous and vanishes at infinity. Under suitable assumptions on V, there exist complex numbers $\{r_j\}_{j=1,\dots,m}$ such that

$$\eta_k = r_0\, |k|^{-1}\, \psi_{\mathrm{res}} + \sum_{j=1}^{m} r_j\, |k|^{-1}\, \psi_j + \rho(\cdot, k) \tag{3.5}$$

where $r_0 = i\langle V, \psi_{\mathrm{res}}\rangle$ and the map $k \mapsto \rho(\cdot, k)$ from $\mathbb{R}^3\setminus\{0\}$ to $H^{1,-s}$ (with s large enough) has a bounded asymptotic expansion as $|k| \to 0$. If zero is not an eigenvalue of H, then the corresponding terms should be omitted.

The previous lemma provides us relevant information about the behaviour of the generalized eigenfunctions of H in the neighborhood of

$k=0$. We shall use it in the estimates by which we extend the proof of the theorem FAS to the potentials for which a zero-energy resonance is present.

Notice that Lemma 3.5 provides also relevant information about the asymptotic outgoing state ψ_{out}. Indeed, focusing for simplicity on the case in which zero is a resonance but not an eigenvalue for H, one has

$$\begin{aligned}\hat{\psi}_{\mathrm{out}}(k) &= \int_{\mathbb{R}^3} \Phi(x,k)^* \, \psi_0(x)(2\pi)^{-3/2}\, dx \\ &= \hat{\psi}_0(k) + \frac{r}{|k|} + \int_{\mathbb{R}^3} \rho(x,k)^* \, \psi_0(x)(2\pi)^{-3/2}\, dx, \end{aligned} \tag{3.6}$$

where $r = -i(2\pi)^{-3/2} \langle V, \psi_{\mathrm{res}} \rangle^* \langle \psi_{\mathrm{res}}, \psi_0 \rangle$. The expansion (3.6) shows the typical singular behaviour of the asymptotic outgoing state, as compared with the state at time zero, when the hamiltonian has a zero energy resonance.

Remark. Notice that the polar singularity of $\hat{\psi}_{\mathrm{out}}$ disappears whenever ψ_0 satisfies the "pseudo-orthogonality" condition $\langle \psi_{\mathrm{res}}, \psi_0 \rangle = 0$. An analogous condition appears in the case of a point interaction hamiltonian, see ref. 20.

The regularity of the generalized eigenfunctions away from the origin in k has been studied in much detail in ref. 23. They proved the following.

Lemma 3.3. Let $V \in (I)_n$, $n \geqslant 3$. Then:

(i) For every fixed $x \in \mathbb{R}^3$ the function $\Phi_\pm(x,\cdot)$ belongs to $C^{n-2}(\mathbb{R}^3 \setminus \{0\})$ and the partial derivatives $\partial_k^\alpha \Phi_\pm(x,k)$ for every multindex $\alpha \in \mathbb{N}^3$ with $|\alpha| \leqslant n-2$ are continuous with respect to $x \in \mathbb{R}^3$ and $k \in \mathbb{R}^3 \setminus \{0\}$.

(ii) for every compact set $K \subset \mathbb{R}^3$ containing the origin, and for every multindex α with $|\alpha| \leqslant n-2$ there are constants C_K, $C_{K,\alpha}$ such that

$$\sup_{k \in \mathbb{R}^3 \setminus K,\, x \in \mathbb{R}^3} |\Phi_\pm(x,k)| \leqslant C_K,$$

$$\sup_{k \in \mathbb{R}^3 \setminus K,\, x \in \mathbb{R}^3} |\partial_k^\alpha \Phi_\pm(x,k)| \leqslant C_{K,\alpha}(1+|x|)^{|\alpha|}.$$

We use now the information contained in Lemmas 3.2 and 3.3 to sketch the proof the FAS theorem for hamiltonian operators with a zero-energy resonance. The expansion of the solution $\psi_t(x)$ in terms of the solutions of the Lippman–Schwinger equation reads

$$\begin{aligned}\psi_t(x) &= (2\pi)^{-3/2} \int_{\mathbb{R}^3} e^{-ik^2 t} \Phi(x, k)\, \hat{\psi}_{\text{out}}(k)\, dk \\ &= (2\pi)^{-3/2} \left(\int_{\mathbb{R}^3} e^{-ik^2 t} e^{ik \cdot x} \hat{\psi}_{\text{out}}(k)\, dk + \int_{\mathbb{R}^3} e^{-ik^2 t} \eta(x, k)\, \hat{\psi}_{\text{out}}(k)\, dk \right) \\ &\equiv \alpha(x, t) + \beta(x, t), \end{aligned} \tag{3.7}$$

where we have used the relation $W_+ = \mathscr{F}^{-1} \mathscr{F}_+$ between the wave operator W_+, the Fourier transform $\mathscr{F}$ and the Friedrichs map $\mathscr{F}_+$ which diagonalizes the projection of the hamiltonian on the absolutely continuous part of its spectrum.

Since the current j can be written as

$$j \equiv \operatorname{Im}(\alpha^* \nabla\alpha + \alpha^* \nabla\beta + \beta^* \nabla\alpha + \beta^* \nabla\beta), \tag{3.8}$$

in view of the fact that the theorem FAS holds for the free case (which corresponds to $\beta = 0$), the proof of the theorem in the interacting case amounts to the proof that

$$\lim_{R \to \infty} \int_T^\infty \int_{\Sigma_R} |j_1(x, t) \cdot n|\, d\sigma = 0, \tag{3.9}$$

where $j_1 \equiv j - \operatorname{Im}(\alpha^* \nabla\alpha)$.

To prove (3.9) one can proceed essentially as in the free case, using integration by parts and stationary phase techniques, once has enough control of the smoothness and asymptotic behaviour in k of $\hat{\psi}_{\text{out}}(k)$ and of $\Phi(x, k)$.

Both are controlled by the properties of $\eta(x, k)$; the properties for k away from the origin are summarized in Lemma 3.3, while the asymptotic expansion for $k \to 0$ is described in Lemma 3.2.

We shall restrict attention from now on to the case in which there are no bound state at the bottom of the continuum spectrum. If one or more such bound states are present, the estimates follow similar patterns.

In estimating the integral of j_1 we shall separate the contribution in $\eta(x, k)$ and $\hat{\psi}_{\text{out}}(k)$ for small values of k from that at large values. This corresponds to extract the singular part of these terms, so that one has

$$\alpha(x, t) \equiv \alpha_{\text{reg}}(x, t) + \alpha_{\text{sing}}(x, t) \tag{3.10}$$

where

$$\alpha_{\mathrm{reg}}(x,t)=\int e^{i(k\cdot x)-ik^2t}\left(\hat{\psi}_{\mathrm{out}}(k)-\frac{r}{|k|}e^{-|k|^2}\right),$$

and

$$\alpha_{\mathrm{sing}}(x,t)=\int e^{i(k\cdot x)-ik^2t}\,\frac{r}{|k|}\,e^{-|k|^2}.$$

We have subtracted a term proportional to $e^{-|k|^2}$ in order to be able to do the (gaussian) integrations explicitly. Similarly, from the LS equation one has

$$\beta(x,t)=\int\frac{V(y)}{|x-y|}\,\Gamma(x,y;t)\,dy \tag{3.11}$$

where (omitting a factor $(2\pi)^{3/2}$)

$$\Gamma(x,y;t)=\Gamma_{\mathrm{sing},1}(x,y;t)+\Gamma_{\mathrm{sing},2}(x,y;t)+\Gamma_{\mathrm{reg}}(x,y;t) \tag{3.12}$$

with

$$\Gamma_{\mathrm{sing},2}(x,y;t)=r\,r_0\,\psi_{\mathrm{res}}(y)\int e^{-i(k^2t+|k|\,|x-y|)-2|k|^2}\,|k|^{-2}\,dk$$

$$\Gamma_{\mathrm{sing},1}(x,y;t)=r_0\,\psi_{\mathrm{res}}(y)\int e^{-i(k^2t+|k|\,|x-y|)-|k|^2}f_1(k)\,|k|^{-1}$$

$$\Gamma_{\mathrm{reg}}(x,y;t)=\int e^{-i(k^2t+|k|\,|x-y|)}f_1(k)(e^{ik\cdot y}+\rho(y,k))\,dk$$

where

$$f_1(k)\equiv\hat{\psi}_{\mathrm{out}}(k)-\frac{r}{|k|}\,e^{-|k|^2}, \tag{3.13}$$

so that on the singular part one can do the (gaussian) integration explicitly.

We shall make repeatedly make use of the following simple lemmas

Lemma 3.4. Let $\mathscr{L}$ be the linear space of functions on $\mathbb{R}^3$ defined by the following condition:

$$\mathscr{L}\equiv\{f\in\mathscr{S}'(\mathbb{R}^3):\hat{f}\in L^1,\,|y|\,\hat{f}(y)\in L^1,\,\nabla\hat{f}\in L^1\}.$$

Define $\phi_f(x,t) \equiv \int_{R^3} e^{ik\cdot x} e^{-ik^2 t} f(k)\, d^3k$. Then for every function $f \in \mathscr{L}$ and for every $0 \leqslant \mu \leqslant 1$ there is a constant $c_{f,\mu}$ such that the following inequality holds

$$|\phi_f(x,t)| \leqslant c_{f,\mu} t^{-3/2} \left(\frac{t}{|x|}\right)^{\mu}, \tag{3.14}$$

for $t \geqslant T_0 > 0$.

Notice that $\mathscr{L} \subset C_\infty(\mathbb{R}^3)$, as a consequence of the Riemann–Lebesgue lemma.

Proof. We prove (3.14) for $\mu = 0$ and for $\mu = 1$. The case $0 < \mu < 1$ follows from an interpolation argument. In the case $\mu = 0$, Eq. (3.14) is verified because

$$\phi_f(x,t) = (e^{-iH_0 t} \hat{f}\,)(x) = e^{i\frac{x^2}{2t}} (4\pi i t)^{-3/2} \int_{\mathbb{R}^3} e^{-i(\frac{x}{t}\cdot y)} e^{i\frac{y^2}{2t}} \hat{f}(y)\, dy,$$

so that

$$|\phi_f(x,t)| \leqslant C t^{-3/2} \, \|\hat{f}\|_{L^1}.$$

To prove (3.14) for $\mu = 1$ notice that one has, for $q, y \in \mathbb{R}^3$

$$e^{i(q\cdot y)} = (-i)\, |q|^{-1} \left(\frac{q}{|q|} \cdot \nabla_y\right) e^{i(q\cdot y)}$$

so that, by integration by parts and standard density arguments

$$\check{g}(q) = i\, |q|^{-1} \int_{\mathbb{R}^3} e^{i(q\cdot y)} \left(\frac{q}{|q|} \cdot \nabla_y\right) g(y)\, dy$$

whenever the right hand side is finite. This gives

$$\frac{|x|}{t} |\phi_f(x,t)| \leqslant \frac{C}{t^{3/2}} \sum_{r=1}^{3} \int_{R^3} |t^{-1} y_r e^{i\frac{y^2}{2t}} \hat{f}(y) + e^{i\frac{y^2}{2t}} \partial_r \hat{f}(y)|\, dy.$$

Since by assumption $y_r \hat{f}(y)$ and $\nabla \hat{f}$ belong to $L^1(\mathbb{R}^3)$ we have proved (3.14) also for $\mu = 1$. ∎

Lemma 3.5. Let $\tilde{f}(\kappa) \equiv \int_{S^2} f(\kappa\omega)\, d\omega$ the angular average of f. Let

$$\mathscr{L}_0 \equiv \left\{ f \in \mathscr{L} : |\tilde{f}(\kappa)| \leqslant C\langle\kappa\rangle^{-3-\varepsilon}, \left|\frac{d\tilde{f}}{d\kappa}(\kappa)\right| \leqslant C\langle\kappa\rangle^{-2-\varepsilon} \right\}.$$

If $f \in \mathscr{L}_0$ the following holds

$$\left| \int_0^\infty e^{-i(\kappa^2 t + \kappa\,|x|)} \tilde{f}(\kappa)\, d\kappa \right| \leqslant \frac{C'}{|x|+t}.$$

Proof. Define

$$\eta \equiv |x| + t, \qquad \xi(\kappa) \equiv \frac{\kappa^2 t + \kappa\,|x|}{|x|+t}.$$

One has, denoting with a prime the derivative with respect to κ

$$\xi' \leqslant \inf\{1, \kappa\}, \qquad \xi'' \leqslant 2.$$

Integrating by parts and noticing that asymptotically for large values of κ

$$\frac{1}{\xi'} \simeq \kappa^{-1}, \qquad \frac{\xi''}{(\xi')^2} \simeq \kappa^{-2}$$

one completes the proof. ∎

Remark. Lemma 3.4 says that for functions in $\mathscr{L}$ we can "exchange" some weaker decrease at $t \to \infty$ in order to have a better decrease for $R \to \infty$. Notice that a decrease in time as $t^{-3/2}$ is not necessary for integrability.

The previous lemmas are used to control the behaviour at large R of the integral of j_1 over time and over the sphere of radius R in $\mathbb{R}^3$ once one can prove that the regular part of the integrand belongs to the space $\mathscr{L}_0$.

As for the part that is singular for $|k| \to 0$, in view of the explicit polar form of the singularity, one has at disposal explicit estimates, which are obtained by straightforward gaussian integration. We recall them (C_μ is a suitable constant).

$$\left| \int e^{i(k\cdot x)\,t - ik^2 t - k^2}\, |k|^{-1}\, dk \right| \leqslant C_\mu\, |x|^{-1}\, t^{-1/2} \left(\frac{|x|}{\sqrt{t}} \right)^\mu, \qquad -1 \leqslant \mu \leqslant 1,$$

$$\left| \int e^{-ik^2 t + i\,|k|\,|x-y| - k^2}\, |k|^{-1}\, dk \right| \leqslant C_\mu t^{-1} \left(\frac{|x-y|}{\sqrt{t}} \right)^\mu, \qquad 0 \leqslant \mu \leqslant 2,$$

$$\left| \int e^{-ik^2 t + i\,|k|\,|x-y| - k^2}\, |k|^{-2}\, dk \right| \leqslant C_\mu t^{-1} \left(\frac{|x-y|}{\sqrt{t}} \right)^\mu, \qquad 0 \leqslant \mu \leqslant 1.$$

To prove the FAS Theorem, i.e., that (3.9) is satisfied, it remains to prove that the functions

$$f_1(k) \equiv \psi_{\text{out}}(k) - r\,\frac{e^{-|k|^2}}{|k|}, \quad f_2(k) \equiv k\psi_{\text{out}}(k), \quad f_3(k) \equiv |k|^{-1}\,(f_1(k) - f_1(0)), \tag{3.15}$$

belong to the space $\mathscr{L}_0$. If this is the case, one can use the previous estimates to prove (3.9). Indeed, the only term that cannot be controlled using the previous estimates is

$$\begin{aligned} j_{cr}(x,t) &\equiv \frac{x}{|x|}\,\mathrm{Im}\left[\left(\int \frac{V(y)}{|x-y|}\,\Gamma_{\text{sing},2}(x,y;t)\,dy\right)^{*}\left(\int \frac{V(y)}{|x-y|^2}\,\Gamma_{\text{sing},2}(x,y;t)\,dy\right)\right] \\ &= C\,\frac{x}{|x|}\int dy \int dy'\,\frac{V(y)\,V(y')\,\psi_{\text{res}}(y)\,\psi_{\text{res}}(y')}{|x-y|\,|x-y'|^2} \\ &\quad \times \mathrm{Im}[\phi_{cr}(x-y;t)^{*}\,\phi_{cr}(x-y';t)], \end{aligned}$$

where we have used the reality of ψ_{res} and we define ϕ_{cr} as

$$\phi_{cr}(x-y,t) \equiv \int e^{-i(k^2 t + |k|\,|x-y| - k^2)}\,|k|^{-2}\,dk.$$

One more gaussian integration leads to the following estimate

$$\phi_{cr}(x-y;t) = \frac{c_\mu}{\sqrt{t}}\,(e^{z^2})_{z = \frac{i\,|x-y|}{\sqrt{1+it}}} + r(x,t)$$

where

$$|r(x,t)| \leqslant \frac{C_\mu}{\sqrt{t}}\left(\frac{|x|}{t}\right)^{\mu}, \qquad -1 \leqslant \mu \leqslant 0.$$

The property of the second term is sufficient to prove the vanishing of its contribution for $R \to \infty$. As for the first term, one can use the bound, for $z = \frac{i\,|x-y|}{\sqrt{1+it}}$

$$|\mathrm{Im}(e^{z_1^2 + z_2^2})| \leqslant \frac{C}{t^{1/4}}\,(|x_1 - y_1|^2 + |x_2 - y_2|^2)^{1/4}.$$

From our assumptions on the potentials it follows that

$$\int dy \int dy' \, \frac{(|x-y|^2+|x-y'|^2)^{1/4}}{|x-y|^2\,|x-y'|} V(y)\,V(y')\,\psi_{\mathrm{res}}(y)\,\psi_{\mathrm{res}}(y') \leqslant \frac{C}{|x|^{5/2}} \tag{3.16}$$

and then that

$$|j_{cr}(x,t)| \leqslant \frac{C_{1,\mu}}{|x|^{5/2}\,t^{5/4}} + \frac{C_{2,\mu}}{|x|^3\,t}\left(\frac{|x|}{\sqrt{t}}\right)^{2\mu}, \qquad -1 \leqslant \mu \leqslant 0. \tag{3.17}$$

This is sufficient to prove that also the contribution of this last term to the integral of j_1 goes to zero when $R \to \infty$.

We are left with the task of finding conditions on the potential and on the initial state ψ_0 in order that the functions f_1, f_2, and f_3, defined in (3.15), belong to the space $\mathscr{L}_0$. This goal requires explicit information on the properties of wave operators when the system has a zero-energy resonance, a completely not trivial task, see ref. 24. Explicit conditions on V and ψ_0 have been found, for the case of a bounded potential, with completely different methods in ref. 19. As for unbounded potentials the problem is still open, and discussed in more detail in ref. 9. We can therefore state the FAS theorem in the following form.

Theorem 3.6. Assume $V \in (I)_n$ for $n \geqslant 15$, and that the hamiltonian $H = H_0 + V$ has a zero energy resonance or/and eigenvalue. Let $\psi_0 \in \mathscr{H}_{\mathrm{ac}}(\mathbb{R}^3) \cap \mathscr{S}(\mathbb{R}^3)$ be such that ψ_{out} corresponds to functions $f_i \in \mathscr{L}_0$, $i = 1,\ldots, 3$, see (3.15). Then the FAS relation (1.3) holds true, for any $T_1 \in \mathbb{R}$.

Remark. Under suitable assumptions on the potential one may deduce that the functions f_1, f_2, and f_3 (related to ψ_{out} by (3.15)) belong to $\mathscr{L}_0$ using convenient decay properties of ψ_0 and the properties of the solutions of the Lippmann–Schwinger equation.

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