

# Threshold Singularities of the $S$ -Matrix and Convergence of Haag-Ruelle Approximations

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**Abstract.** We establish a one-to-one correspondence between the continuity properties of the  $S$ -matrix at the 2-particle threshold and the rate of convergence of the Haag-Ruelle approximations  $\Psi(t)$  for asymptotic 2-particle states  $\Psi$  with smooth wavefunctions. It turns out that the norm distance  $\|\Psi - \Psi(t)\|$  approaches 0 like  $t^{-5/4}$  if the  $S$ -matrix has the normal threshold singularities and like  $t^{-3/4}$  in the exceptional case where the threshold has “absorbed” a bound state. These connections are valid both in relativistic quantum field theory and in non-relativistic models with short range interaction.

## I. Introduction

In [1] we investigated within the framework of quantum field theory the rate of convergence of the Haag-Ruelle-approximations  $\Psi(t)$  at large times  $t$  for arbitrary collision states  $\Psi$  with finite energy. In particular for states  $\Psi$  with smooth asymptotic wave functions we proved that the norm distance  $\|\Psi - \Psi(t)\|$  approaches 0 almost like  $t^{-3/4}$ . It is well known that this estimate can considerably be improved if  $\Psi$  corresponds to an asymptotic particle configuration where no two particles have the same velocity [2, 3]. Consequently, only those parts of  $\Psi$  which correspond to a configuration of particles with asymptotically coinciding velocities can cause a slow decrease of  $\|\Psi - \Psi(t)\|$ . Therefore one expects that the rate of convergence of  $\|\Psi - \Psi(t)\|$  is intimately connected with the threshold singularities of the  $S$ -matrix.

It is the aim of the present paper to study this connection in more detail. To this end we isolate, for large  $t$ , the leading contribution to  $\Psi - \Psi(t)$  and give an estimate of the remainder (Chapter II). For reasons of simplicity we shall restrict our attention to asymptotic 2-particle states. The expression thus obtained has a very simple structure and can be used to establish the desired connection (Chapters III and IV). It turns out that  $\|\Psi - \Psi(t)\|$  decreases asymptotically like  $t^{-5/4}$  if the

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$S$ -matrix has the usual singularity at the 2-particle threshold [4, 5]. Guided by experience with non-relativistic scattering theory, one can also imagine models in which the threshold has “absorbed” a bound state. In this exceptional case the  $S$ -matrix is more singular and the norm distance  $\|\Psi - \Psi(t)\|$  behaves asymptotically like  $t^{-3/4}$ . This coincides with the estimates derived from the basic principles and therefore we do not believe that the results given in [1] can be improved without further specification of the dynamics.

Another by-product of our investigations which might be interesting in its own right is that the elastic 2-particle scattering amplitude  $T(s, t)$  restricted to the forward direction  $t = 0$  can be defined as a locally square integrable function of  $s$  (except at the threshold). For the proof of this statement we apply a very direct method which does not make use of any sophisticated arguments (Chapter IV).

Finally we look at non-relativistic theories with short range inter-particle forces and discuss a simple model. As expected the results are completely analogous to the relativistic case (Chapter V).

Our assumptions and notation are the same as in [1]: we are dealing with a local, relativistic quantum theory of a chargeless massive particle with spin 0. It is an important feature of such models that the collision states can be created from the vacuum vector  $\Omega$  with the aid of a set  $\mathcal{P}$  of almost local, bounded 1-particle creation operators [1]. Let  $\Psi_f^{\text{out}}$  for example be an outgoing 2-particle state with a wavefunction  $f$  which has compact support in momentum space. Then one can find a suitable operator  $A \in \mathcal{P}$  to construct the Haag-Ruelle approximations of  $\Psi_f^{\text{out}}$

$$\Psi_f(t) = \int d^3x d^3y f(t|\mathbf{x}, \mathbf{y}) A(t, \mathbf{x}) A(t, \mathbf{y}) \Omega. \quad (1)$$

Here  $f(t|\mathbf{x}, \mathbf{y})$  denotes the configuration space wavefunction at time  $t$

$$f(t|\mathbf{x}, \mathbf{y}) = (2\pi)^{-3} \cdot \int d^3p d^3q e^{-it(\omega_p + \omega_q) + i(\mathbf{x}p + \mathbf{y}q)} \cdot \tilde{f}(\mathbf{p}, \mathbf{q}) \quad (2)$$

and  $\omega_p = (|\mathbf{p}|^2 + \mu^2)^{1/2}$ ,  $\mu$  being the mass of the particle. The approximations  $\Psi_f(t)$  converge strongly towards  $\Psi_f^{\text{out}}$  in the limit  $t \rightarrow \infty$  and an analogous statement holds for the incoming states.

## II. Asymptotic Expansion of Haag-Ruelle Approximations

It will be convenient in the following to assume that the wave function  $f$  of  $\Psi_f^{\text{out}}$  is arbitrarily often differentiable in momentum space. Yet in spite of this simplification the calculation of the leading contribution to  $\Psi_f^{\text{out}} - \Psi_f(t)$  for large  $t$  is still pretty technical and not very amusing. For this reason let us first of all sketch the idea of the proof and then go into details.

We start with the time derivative  $\partial_t \Psi_f(t)$  of the Haag-Ruelle approximation  $\Psi_f(t)$  defined in Eq. (1). It is well known that  $\partial_t \Psi_f(t)$  can be expressed as follows:

$$\partial_t \Psi_f(t) = \int d^3x d^3y f(t|\mathbf{x}, \mathbf{y}) j(t, \mathbf{x}) A(t, \mathbf{y}) \Omega \tag{3}$$

where  $j = (2\pi)^{-2} \cdot \int d^4p i \cdot (p_0 - \omega_p) \tilde{A}(p)$  is an almost local, bounded<sup>1</sup> operator which annihilates the vacuum. Since the norm of the commutator  $[j(t, \mathbf{x}), A(t, \mathbf{y})]$  decreases rapidly if  $|\mathbf{x} - \mathbf{y}|$  becomes large, only those regions of  $\mathbb{R}^6$  which are not too far separated from the plane  $\mathbf{x} = \mathbf{y}$  can contribute to the integral in Eq. (3). Accordingly, one decomposes the function  $f(t|\mathbf{x}, \mathbf{y})$  into two parts

$$f(t|\mathbf{x}, \mathbf{y}) = f\left(t\left|\frac{\mathbf{x} + \mathbf{y}}{2}, \frac{\mathbf{x} + \mathbf{y}}{2}\right.\right) + \left\{ f(t|\mathbf{x}, \mathbf{y}) - f\left(t\left|\frac{\mathbf{x} + \mathbf{y}}{2}, \frac{\mathbf{x} + \mathbf{y}}{2}\right.\right) \right\}$$

and the expression in the curly brackets can be neglected in the limit of large times. The main contribution  $f\left(t\left|\frac{\mathbf{x} + \mathbf{y}}{2}, \frac{\mathbf{x} + \mathbf{y}}{2}\right.\right)$  behaves asymptotically like a solution  $\hat{f}$  of the Klein-Gordon-equation with mass  $2\mu$  which is multiplied by  $t^{-3/2}$ . Therefore one splits  $f\left(t\left|\frac{\mathbf{x} + \mathbf{y}}{2}, \frac{\mathbf{x} + \mathbf{y}}{2}\right.\right)$  into  $t^{-3/2} \cdot \hat{f}\left(t\left|\frac{\mathbf{x} + \mathbf{y}}{2}\right.\right)$  and a part which can likewise be neglected. The expression thus obtained is the leading contribution to  $\partial_t \Psi_f(t)$  and since  $\Psi_f^{\text{out}} - \Psi_f(t) = \int_t^\infty d\tau \partial_\tau \Psi_f(\tau)$  this yields after a careful estimation of the remainder:

**Theorem 2.1.** *Let  $\tilde{f}$  be an element of  $\mathcal{S}(\mathbb{R}^6)$  with compact support. Then*

$$\Psi_f^{\text{out}} - \Psi_f(t) = \int_t^\infty d\tau \tau^{-3/2} \varrho_f(\tau) \Omega + O(t^{-3/2}) \quad \text{for } t > 0^2. \tag{4}$$

Here we have introduced the operator  $\varrho_f(\tau) = \int d^3z \hat{f}(\tau, \mathbf{z}) \varrho(\tau, \mathbf{z})$  where  $\varrho = \int d^3z' [j(\mathbf{z}'), A(-\mathbf{z}')] is an almost local creation operator and$

$$\hat{f}(\tau|\mathbf{z}) = (2\pi i)^{-3/2} \cdot \int d^3k e^{-i\tau\hat{\omega}_k + i\mathbf{z}\mathbf{k}} \cdot \frac{\hat{\omega}_k^{5/2}}{2\mu} \tilde{f}\left(\frac{\mathbf{k}}{2}, \frac{\mathbf{k}}{2}\right)$$

$$\text{with } \hat{\omega}_k = (|\mathbf{k}|^2 + 4\mu^2)^{1/2}.$$

<sup>1</sup> This is so since the Fourier-transform  $\tilde{A}(p)$  of  $A(x)$  has compact support. We may even assume that the support of  $\tilde{A}(p)$  is contained in the forward cone.

<sup>2</sup> The symbol  $O(t^{-\alpha})$  denotes a strongly continuous vector-valued function for  $t > 0$  which decreases in norm like  $t^{-\alpha}$ .

As indicated above, to verify this theorem we need several estimates of wavefunctions in configuration-space which will be given in the sequel. Since the proofs are a straightforward application of methods already used in [1] we keep them brief.

**Lemma 2.2.** *Let  $\tilde{f}$  be an element of  $\mathcal{S}(\mathbb{R}^6)$  satisfying  $\tilde{f}(\mathbf{p}, \mathbf{p}) = 0$  for all  $\mathbf{p}$ . Then*

$$\int d^3x d^3y (1 + |\mathbf{x} - \mathbf{y}|)^{-2N} \cdot |f(t|\mathbf{x}, \mathbf{y})|^2 \leq c \cdot |t|^{-5} \quad \text{if } N \geq 3.$$

*Proof.* Using similar arguments to those in the proof of Lemma 3 of [1] one realizes that all configuration space wavefunctions  $f(t|\mathbf{x}, \mathbf{y})$  which behave in momentum space like  $\tilde{f}(\mathbf{p}, \mathbf{q}) = (\mathbf{p} - \mathbf{q})_i \cdot \tilde{g}(\mathbf{p}, \mathbf{q})$ ,  $\tilde{g} \in \mathcal{S}(\mathbb{R}^6)$  can be represented by

$$f(t|\mathbf{x}, \mathbf{y}) = t^{-1} \cdot \sum_{k=1}^3 (x-y)_k h_k(t|\mathbf{x}, \mathbf{y}) + t^{-1} \cdot h(t|\mathbf{x}, \mathbf{y}), \quad t \neq 0$$

where  $\tilde{h}_k$  and  $\tilde{h}$  are again from  $\mathcal{S}(\mathbb{R}^6)$ . Thus one gets

$$\int d^3x d^3y (1 + |\mathbf{x} - \mathbf{y}|)^{-2N} \cdot |f(t|\mathbf{x}, \mathbf{y})|^2 \leq \frac{16}{t^2} \cdot \int d^3x d^3y (1 + |\mathbf{x} - \mathbf{y}|)^{-2N} \cdot \left( \sum_{k=1}^3 |h_k(t|\mathbf{x}, \mathbf{y})|^2 + |h(t|\mathbf{x}, \mathbf{y})|^2 \right).$$

It follows from the work of Araki [6] and Ruelle [7] on solutions of the Klein-Gordon-equation that the integral on the right hand side of this inequality decreases like  $|t|^{-3}$  if  $N \geq 3$  and this proves the lemma for the special class of wavefunctions given above.

If  $\tilde{f}$  is any function satisfying the assumptions of the lemma then one can decompose it as follows:

$$\tilde{f}(\mathbf{p}, \mathbf{q}) = \sum_{1 \leq i+j+k \leq n} (\mathbf{p} - \mathbf{q})_1^i (\mathbf{p} - \mathbf{q})_2^j (\mathbf{p} - \mathbf{q})_3^k \tilde{g}_{ijk}(\mathbf{p}, \mathbf{q}) + \tilde{g}_n(\mathbf{p}, \mathbf{q}), \quad n \in \mathbb{N}.$$

$\tilde{g}_{ijk}, \tilde{g}_n$  are elements of  $\mathcal{S}(\mathbb{R}^6)$  and for  $\tilde{g}_n$  we have in addition the inequality  $(1 + |\mathbf{p} + \mathbf{q}|)^m \cdot |\tilde{g}_n(\mathbf{p}, \mathbf{q})| \leq c_{mn} \cdot |\mathbf{p} - \mathbf{q}|^n$ ,  $m \in \mathbb{N}$ . The first term of this decomposition is a sum of functions which all belong to the class just considered and therefore the lemma can be applied. To get an estimate of the remainder one splits  $\tilde{g}_n$  into ( $r \geq 1$ )

$$\tilde{g}_n(\mathbf{p}, \mathbf{q}) = \hat{h}(r[\mathbf{p} - \mathbf{q}]) \cdot \tilde{g}_n(\mathbf{p}, \mathbf{q}) + (1 - \hat{h}(r[\mathbf{p} - \mathbf{q}])) \cdot \tilde{g}_n(\mathbf{p}, \mathbf{q})$$

where  $\hat{h} \in \mathcal{C}^\infty(\mathbb{R}^3)$ ,  $\hat{h}(\mathbf{k}) = 0$  for  $|\mathbf{k}| \leq 1$  and  $\hat{h}(\mathbf{k}) = 1$  for  $|\mathbf{k}| \geq 2$ . Because of the support properties of  $(1 - \hat{h})$  the  $L^2(\mathbb{R}^6)$ -norm of  $(1 - \hat{h}(r[\mathbf{p} - \mathbf{q}])) \cdot \tilde{g}_n(\mathbf{p}, \mathbf{q})$  has the bound  $c \cdot r^{-n-3/2}$ . The non-overlapping part  $\hat{h}(r[\mathbf{p} - \mathbf{q}]) \cdot \tilde{g}_n(\mathbf{p}, \mathbf{q})$  can be estimated with the aid of Lemma 3 of [1] giving altogether

$$\int d^3x d^3y (1 + |\mathbf{x} - \mathbf{y}|)^{-2N} \cdot |g_n(t|\mathbf{x}, \mathbf{y})|^2 \leq c \cdot r^{-2n-3} + c_N \cdot r^{4N} \cdot t^{-2N}.$$

If one minimizes the right hand side of this inequality with respect to  $\tau$  it becomes evident that the integral decreases faster than  $|t|^{-5}$  for  $N \geq 3$  and large  $n$ .

This technique of decomposing the wavefunction  $\tilde{f}$  into a non-overlapping part  $\tilde{f}_r$  and a remainder  $\tilde{\Delta}f_r$ , also plays a key role in the proofs of the following two propositions. Since the non-overlapping part  $\tilde{f}_r$  can always be estimated with methods similar to those used in [1] we shall restrict ourselves to indicating why the contributions due to the remainder  $\tilde{\Delta}f_r$  decrease fast enough if  $r$  becomes large.

**Lemma 2.3.** *Let  $\tilde{f}$  be an element of  $\mathcal{S}(\mathbb{R}^6)$ . Then for sufficiently large  $N$*

$$\int d^3x d^3y (1 + |\mathbf{x} - \mathbf{y}|)^{-2N} \cdot \left| f(t|\mathbf{x}, \mathbf{y}) - f\left(t \left| \frac{\mathbf{x} + \mathbf{y}}{2}, \frac{\mathbf{x} + \mathbf{y}}{2} \right. \right) \right|^2 \leq c \cdot |t|^{-5}.$$

*Proof.* If  $\tilde{f}$  were antisymmetric the result would follow from the preceding lemma. Hence we may suppose  $\tilde{f}$  is symmetric. (Actually only this case is of interest to us anyway.) Taking this into consideration we get for  $\left\{ f(t|\mathbf{x}, \mathbf{y}) - f\left(t \left| \frac{\mathbf{x} + \mathbf{y}}{2}, \frac{\mathbf{x} + \mathbf{y}}{2} \right. \right) \right\}$  the representation

$$(2\pi)^{-3} \int d^3p d^3q e^{-it(\omega_p + \omega_q) + \frac{i}{2}(\mathbf{x} + \mathbf{y}) \cdot (\mathbf{p} + \mathbf{q})} \cdot \tilde{f}(\mathbf{p}, \mathbf{q}) (\cos \frac{1}{2}(\mathbf{x} - \mathbf{y}) \cdot (\mathbf{p} - \mathbf{q}) - 1).$$

Since  $(\cos \frac{1}{2}(\mathbf{x} - \mathbf{y}) \cdot (\mathbf{p} - \mathbf{q}) - 1)$  has a double zero at  $\mathbf{p} = \mathbf{q}$  and the derivatives with respect to  $\mathbf{p}$  and  $\mathbf{q}$  are bounded by polynomials in  $|\mathbf{x} - \mathbf{y}|$  one can conclude that the contribution of  $\tilde{\Delta}f_r$  to the integral under investigation decreases like  $r^{-10}$ . Consequently ( $N \geq 4$ )

$$\begin{aligned} \int d^3x d^3y (1 + |\mathbf{x} - \mathbf{y}|)^{-2N} \cdot \left| f(t|\mathbf{x}, \mathbf{y}) - f\left(t \left| \frac{\mathbf{x} + \mathbf{y}}{2}, \frac{\mathbf{x} + \mathbf{y}}{2} \right. \right) \right|^2 \\ \leq c \cdot r^{-10} + c_N \cdot r^{4(N-2)} \cdot t^{-2(N-2)} \end{aligned}$$

which shows that this expression decreases faster than  $|t|^{-5 + 15/N}$  and therefore “almost” like  $|t|^{-5}$  if  $N$  is large. For the proof that the integral decreases exactly like  $|t|^{-5}$  for some finite  $N$  a more refined decomposition of the integrand is necessary. (Compare the proof of Lemma 2.2.) Yet we omit the details.

In order to get an idea how the function  $f(t|\mathbf{z}, \mathbf{z})$  behaves asymptotically one can apply the method of stationary phase. The leading contribution turns out to be

$$\hat{\tilde{f}}(t|\mathbf{z}) = (2\pi)^{-3} \cdot \int d^3p d^3q e^{-it(\hat{\omega}_{\mathbf{p}+\mathbf{q}} + (\mathbf{p} - \mathbf{q}) \cdot S_{\mathbf{p}+\mathbf{q}}(\mathbf{p} - \mathbf{q}) + i\mathbf{z} \cdot (\mathbf{p} + \mathbf{q}))} \cdot \tilde{f}(\mathbf{p}, \mathbf{q}) \quad (5)$$

where  $S_{\mathbf{k}}$  is the  $3 \times 3$  matrix  $(S_{\mathbf{k}})_{ij} = \frac{1}{2\hat{\omega}_{\mathbf{k}}} \left( \delta_{ij} - \frac{k_i k_j}{\hat{\omega}_{\mathbf{k}}^2} \right)$  and

$$\hat{\omega}_{\mathbf{k}} = (|\mathbf{k}|^2 + 4\mu^2)^{1/2}.$$

For the difference between  $f(t|z, z)$  and  $\widehat{f}(t|z)$  we have the estimate:

**Lemma 2.4.** *Let  $\tilde{f}$  be an element of  $\mathcal{S}(\mathbb{R}^6)$ . Then*

$$\int d^3 z |f(t|z, z) - \widehat{f}(t|z)|^2 \leq c \cdot |t|^{-5}.$$

*Proof.* As in the preceding lemma we content ourselves with showing that this expression decreases “almost” like  $|t|^{-5}$ . To this end we represent the difference between  $f(t|z, z)$  and  $\widehat{f}(t|z)$  as follows:

$$f(t|z, z) - \widehat{f}(t|z) = (2\pi)^{-3} \cdot \int d^3 p d^3 q e^{iz(p+q)} \cdot \tilde{f}(\mathbf{p}, \mathbf{q}) \cdot \mathfrak{D}_t(\mathbf{p}, \mathbf{q})$$

where

$$\mathfrak{D}_t(\mathbf{p}, \mathbf{q}) = e^{-it(\omega_p + \omega_q)} - e^{-it(\widehat{\omega}_{p+q} + (\mathbf{p}-\mathbf{q}) \cdot S_{p+q}(\mathbf{p}-\mathbf{q}))}.$$

A straightforward calculation shows that

$$|\mathfrak{D}_t(\mathbf{p}, \mathbf{q})| \leq |t| \cdot |\mathbf{p} - \mathbf{q}|^4 \tilde{g}(\mathbf{p}, \mathbf{q})$$

where  $\tilde{g}(\mathbf{p}, \mathbf{q})$  is a continuous function which is polynomially bounded. Because of the fourfold zero of  $\mathfrak{D}_t(\mathbf{p}, \mathbf{q})$  at  $\mathbf{p} = \mathbf{q}$  the contribution due to  $\Delta \tilde{f}$ , can be estimated by  $c \cdot r^{-14} \cdot t^2$  giving altogether

$$\int d^3 z |f(t|z, z) - \widehat{f}(t|z)|^2 \leq c \cdot r^{-14} \cdot t^2 + c_N \cdot r^{2N} \cdot t^{-2N}$$

for arbitrary  $N \in \mathbb{N}$ . From this inequality the statement of the lemma follows at once.

For the proof of the theorem yet another inequality is needed. Using the fact that the operators  $A$  and  $j$  in Eq. (3) are almost local and  $j\Omega = j^*\Omega = 0$  one can show that

$$\begin{aligned} \|\partial_t \Psi_f(t)\|^2 &= \|\int d^3 x d^3 y f(t|\mathbf{x}, \mathbf{y}) j(t, \mathbf{x}) A(t, \mathbf{y}) \Omega\|^2 \\ &\leq c_N \cdot \int d^3 x d^3 y (1 + |\mathbf{x} - \mathbf{y}|)^{-2N} \cdot |f(t|\mathbf{x}, \mathbf{y})|^2 \end{aligned} \tag{6}$$

for all  $N \in \mathbb{N}$  with constants  $c_N$  not depending on  $f$  and  $t$  [1].

Now we are equipped with the tools needed to complete the argument. To begin with we replace the unspecified function  $\tilde{f}(\mathbf{p}, \mathbf{q})$  in  $\partial_t \Psi_f(t)$  by a more special wave function which coincides with  $\tilde{f}(\mathbf{p}, \mathbf{q})$  on the plane  $\mathbf{p} = \mathbf{q}$ ; the difference between the corresponding states is  $O(t^{-5/2})$  because of Lemma 2.2 and Relation (6). We take as the new wave-function

$$e^{-(\mathbf{p}-\mathbf{q}) \cdot S_{p+q}(\mathbf{p}-\mathbf{q})} \cdot \tilde{f}\left(\frac{\mathbf{p} + \mathbf{q}}{2}, \frac{\mathbf{p} + \mathbf{q}}{2}\right)$$

where  $S_{p+q}$  is the  $3 \times 3$  matrix introduced above. Since  $S_{p+q} \geq \frac{2\mu^2}{\widehat{\omega}_{p+q}^3} \cdot \mathbb{1}$  and  $\tilde{f} \in \mathcal{S}(\mathbb{R}^6)$  has compact support it is obvious that this function (which we shall again denote by  $\tilde{f}$ ) is an element of  $\mathcal{S}(\mathbb{R}^6)$ .

Then we proceed as was sketched in the first part of this chapter: we replace the function  $f(t|\mathbf{x}, \mathbf{y})$  in  $\partial_t \Psi_f(t)$  by  $f\left(t \left| \frac{\mathbf{x} + \mathbf{y}}{2}, \frac{\mathbf{x} + \mathbf{y}}{2} \right. \right)$ , the difference being  $O(t^{-5/2})$  because of Lemma 2.3 and Relation (6). Introducing  $\frac{1}{2}(\mathbf{x} + \mathbf{y})$  and  $\frac{1}{2}(\mathbf{x} - \mathbf{y})$  as new variables shows that the asymptotically leading contribution in  $\partial_t \Psi_f(t)$  has the form

$$8 \cdot \int d^3 z f(t|z, z) \varrho(t, z) \Omega$$

at which  $\varrho = \int d^3 z' [j(z'), A(-z')]$ . It is obvious that  $\varrho$  is again an almost local operator and  $\varrho^* \Omega = 0$ . Hence the norm of this state can be estimated as in deriving Relation (6):

$$\|\int d^3 z f(t|z, z) \varrho(t, z) \Omega\|^2 \leq c \cdot \int d^3 z |f(t|z, z)|^2$$

$c$  being a constant not depending on  $f$  and  $t$ . From this inequality and Lemma 2.4 it follows at once that  $f(t|z, z)$  may be replaced by  $\hat{f}(t|z)$  (see Relation (5)), the error being  $O(t^{-5/2})$ . Taking the special form of  $\hat{f}(\mathbf{p}, \mathbf{q})$  given above into consideration one gets after some trivial calculations

$$\hat{f}(t|z) = \frac{1}{8}(t-i)^{-3/2} (2\pi i)^{-3/2} \cdot \int d^3 k e^{-it\hat{\omega}_k + izk} \cdot \frac{\hat{\omega}_k^{5/2}}{2\mu} \hat{f}\left(\frac{\mathbf{k}}{2}, \frac{\mathbf{k}}{2}\right)$$

and this proves – using the notation of the theorem – that

$$\partial_t \Psi_f(t) = t^{-3/2} \cdot \varrho_f(t) \Omega + O(t^{-5/2}).$$

The required result then follows on integrating.

### III. An Equivalence-Theorem

The simple  $t$ -dependence of the leading contribution  $\int_t^\infty d\tau \tau^{-3/2} \varrho_f(\tau) \Omega$  will enable us to derive a useful relation between the rate of convergence of  $\Psi_f^{\text{out}} - \Psi_f(t)$  and certain continuity properties of the state  $\varrho_f \Omega \equiv \varrho_f(0) \Omega$  in momentum space. To begin with we note that

$$\varrho_f(t) \Omega = e^{it(H - \sqrt{\mathbf{P}^2 + 4\mu^2})} \cdot \varrho_f \Omega$$

where  $H$  is the Hamiltonian and  $\mathbf{P}$  the momentum operator. Our assumptions on the particle spectrum of the theory imply that the selfadjoint operator  $(H - \sqrt{\mathbf{P}^2 + 4\mu^2})$  has an isolated eigenvalue,  $-2\mu$ ,

and a continuous spectrum starting at  $-\mu$ . Obviously the eigenvalue  $-2\mu$  corresponds to the vacuum and the continuum between  $-\mu$  and 0 is exclusively due to 1-particle states. Taking into account the fact that  $\varrho_f \Omega$  is orthogonal to  $\Omega$  and all 1-particle states<sup>3</sup> we get therefore

$$\varrho_f(t) \Omega = \int_0^\infty e^{it\lambda} E(d\lambda) \varrho_f \Omega$$

where  $E(d\lambda)$  denotes the spectral measure of  $(H - \sqrt{\mathbf{P}^2 + 4\mu^2})$ . The integration of this equation yields after application of the Fubini-Tonelli theorem

$$\int_t^\infty d\tau \tau^{-3/2} \varrho_f(\tau) \Omega = t^{-1/2} \cdot \int_0^\infty \varphi(\lambda t) E(d\lambda) \varrho_f \Omega \quad \text{for } t > 0.$$

(Here we have introduced the function  $\varphi(u) = u^{1/2} \cdot \int_u^\infty dv v^{-3/2} e^{iv}$  which will be analysed to a certain extent in Appendix A.) The above relation together with Theorem 2.1 are the basis for the proof of the following proposition.

**Theorem 3.1.** *Under the hypotheses of Theorem 2.1 the following statements are equivalent provided that  $\frac{1}{2} < \alpha < \frac{3}{2}$ :*

- i)  $\Psi_f^{\text{out}} - \Psi_f(t) = O(t^{-\alpha})$  for  $t > 0$ .
- ii)  $\|\int_0^\lambda E(d\lambda') \varrho_f \Omega\|^2 \leq c \cdot \lambda^{2\alpha-1}$  for  $\lambda \geq 0$ .

*Proof.* i) Our previous results imply that the first relation is equivalent to

$$t^{-1/2} \cdot \int_0^\infty \varphi(\lambda t) E(d\lambda) \varrho_f \Omega = O(t^{-\alpha}) \tag{a}$$

and taking the norm of this equation yields for large  $t$

$$\int_0^\lambda |\varphi(\lambda' t)|^2 \cdot (\varrho_f \Omega, E(d\lambda') \varrho_f \Omega) \leq c' \cdot t^{-2\alpha+1}.$$

We shall show in the appendix that  $\varphi(u)$  is continuous for  $u > 0$  and  $\lim_{u \downarrow 0} \varphi(u) = 2$ . Hence there exists a  $\delta > 0$  such that  $|\varphi(u)| \geq 1$  for  $0 \leq u \leq \delta$ .

From this it follows at once (putting  $t = \delta/\lambda$ ) that

$$\int_0^\lambda (\varrho_f \Omega, E(d\lambda') \varrho_f \Omega) \leq c \cdot \lambda^{2\alpha-1}.$$

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<sup>3</sup> This follows from the fact that the 1-particle creation operator  $A$  — and therefore also  $j$  — allows only timelike momentum transfers.



ii) Let us now estimate the norm of the leading contribution  $t^{-1/2} \cdot \int_0^\infty \varphi(\lambda t) E(d\lambda) \varrho_f \Omega$  on the assumption that the second relation holds. To begin with one realizes after partial integration that

$$\begin{aligned} t^{-1} \cdot \int_0^\infty |\varphi(\lambda t)|^2 (\varrho_f \Omega, E(d\lambda) \varrho_f \Omega) \\ = - \int_0^\infty d\lambda 2 \operatorname{Re} \{ \bar{\varphi}(\lambda t) \varphi'(\lambda t) \} \cdot \int_0^\lambda (\varrho_f \Omega, E(d\lambda') \varrho_f \Omega). \end{aligned}$$

(The contributions of the boundaries vanish since  $E(d\lambda)$  is a continuous measure in the region in question and  $\lim_{u \rightarrow \infty} \varphi(u) = 0$ .) Therefore one gets

$$\left\| t^{-1/2} \cdot \int_0^\infty \varphi(\lambda t) E(d\lambda) \varrho_f \Omega \right\|^2 \leq c \cdot t^{-2\alpha} \cdot \int_0^\infty d\lambda |2 \operatorname{Re} \{ \bar{\varphi}(\lambda) \varphi'(\lambda) \}| \lambda^{2\alpha-1}$$

and the integral on the right hand side of this inequality exists with the above mentioned restrictions on  $\alpha$ . (We again refer to the appendix.) Hence the leading contribution satisfies relation (a) and consequently

$$\Psi_f^{\text{out}} - \Psi_f(t) = O(t^{-\alpha}).$$

This theorem will prove to be useful as the connecting link between the threshold properties of the  $S$ -matrix and the rate of convergence of  $\Psi_f^{\text{out}} - \Psi_f(t)$ . Apart from this point it is also worth mentioning that it establishes the Hölder-continuity of the measure  $E(d\lambda)$  on the states  $\varrho_f \Omega$  at  $\lambda = 0$  because  $\Psi_f^{\text{out}} - \Psi_f(t) = O(t^{-3/4+\varepsilon})$  for all  $\varepsilon > 0$  as is known from [1].

#### IV. Influence of the Threshold — Singularities

So far we have dealt with the vector  $\varrho \Omega^4$  which does not have a direct physical significance. It is therefore the aim of the present section to replace  $\varrho \Omega$  by a vector which is more easily amenable to a physical interpretation but which differs only slightly from  $\varrho \Omega$  near the 2-particle threshold.

For this reason let us consider the wavefunction of  $\varrho \Omega$  in the space of the outgoing 2-particle states. Proceeding formally it is easy to verify that

$$\text{out}(\mathbf{p}, \mathbf{q} | \varrho \Omega) = \frac{\pi^3}{2\omega_{\frac{\mathbf{p}+\mathbf{q}}{2}}} \cdot \text{out} \left( \mathbf{p}, \mathbf{q} \left| j \left| \frac{\mathbf{p}+\mathbf{q}}{2} \right. \right) \cdot \left( \frac{\mathbf{p}+\mathbf{q}}{2}, A \Omega \right).$$

Assuming for the moment that this expression is continuous in  $\mathbf{p}$  and  $\mathbf{q}$ , it follows at once that the wavefunction of  $\varrho \Omega$  coincides with the 2-particle

<sup>4</sup> Throughout this chapter the smearing of  $\varrho$  with  $\hat{f}$  is of no account and will be omitted. All results remain valid if one replaces  $\varrho \Omega$  by  $\varrho_{\hat{f}} \Omega$ .

forward scattering amplitude  $T(s, 0)^5$  at the threshold  $\mathbf{p} = \mathbf{q}$  apart from kinematical factors. We shall therefore proceed from  $\varrho\Omega$  to a vector with essentially  $T(s, 0)$  as wavefunction and it will then be possible to infer from the behaviour of  $\|\int_0^\lambda E(d\lambda') \varrho\Omega\|$  at  $\lambda=0$  the properties of  $T(s, 0)$  near the threshold  $s = 4\mu^2$  and vice versa.

Carrying through this program rigorously one meets a serious technical difficulty since the restriction of the functional  $T(s, t)$  to the hyperplane  $t=0$  is a priori not well defined. Yet one can get around this using the following trick: since the norm of the commutator  $[j(\mathbf{z}), A(-\mathbf{z})]$  decreases rapidly if  $|\mathbf{z}|$  becomes large it is obvious that the state

$$\varrho_k \Omega = \int d^3 z \cos \mathbf{z} \mathbf{k} \cdot [j(\mathbf{z}), A(-\mathbf{z})] \Omega$$

is strongly differentiable with respect to  $\mathbf{k}$ . This smoothness property of  $\varrho_k \Omega$  will enable us to define a vector which may be interpreted as the integral  $\int E^{\text{out}}(d^3 k) \varrho_k \Omega$ ,  $E^{\text{out}}(d^3 k)$  being the measure projecting onto the outgoing 2-particle states with relative momentum in  $d^3 k$ . An easy formal calculation yields for the wavefunction of this vector

$$\text{out}(\mathbf{p}, \mathbf{q} | \int E^{\text{out}}(d^3 k) \varrho_k \Omega) = \frac{\pi^2}{8\omega_{\mathbf{p}}\omega_{\mathbf{q}}} \cdot T(s, 0) \cdot (\mathbf{p}, A\Omega)(\mathbf{q}, A\Omega) \quad (7)$$

which is exactly the desired expression. Since the left hand side of this equation is an element of  $L^2(\mathbb{R}^6)$  we believe that the sensible way to proceed is to define the restriction of the 2-particle scattering amplitude  $T(s, t)$  to the forward direction  $t=0$  as a locally square integrable function via relation (7).

Let us now state the proposition which gives a precise meaning to  $\int E^{\text{out}}(d^3 k) \varrho_k \Omega$ . (The proof is given in Appendix B.)

**Lemma 4.1.** *Let  $\Phi(\underline{x})$ ,  $\underline{x} \in \mathbb{R}^n$  be a  $n$ -times continuously differentiable (in the strong topology) vector-valued function with compact support and  $E(d^n x)$  an absolutely continuous projection-valued measure. Let  $P_j$  be any uniformly bounded sequence of operators with finite rank such that*

<sup>5</sup> We define (in the sense of distributions)

$$\text{out}(\mathbf{p}, \mathbf{q} | \mathbb{1} - S | \mathbf{p}', \mathbf{q}')^{\text{out}} = \delta(\omega_{\mathbf{p}} + \omega_{\mathbf{q}} - \omega_{\mathbf{p}'} - \omega_{\mathbf{q}'}) \delta(\mathbf{p} + \mathbf{q} - \mathbf{p}' - \mathbf{q}') \cdot T(s, t)$$

where  $s = (\omega_{\mathbf{p}} + \omega_{\mathbf{q}})^2 - |\mathbf{p} + \mathbf{q}|^2$  and  $t = (\omega_{\mathbf{p}'} + \omega_{\mathbf{q}'})^2 - |\mathbf{p}' + \mathbf{q}'|^2$ . It follows then with the aid of the well known reduction technique [3] that

$$T(s, t) \cdot (\mathbf{p}', A\Omega)(\mathbf{q}', A\Omega) = 4\pi\omega_{\mathbf{q}'} \cdot \text{out}(\mathbf{p}, \mathbf{q} | j | \mathbf{p}') \cdot (\mathbf{p}', A\Omega)$$

if

$$\mathbf{p} + \mathbf{q} = \mathbf{p}' + \mathbf{q}' \quad \text{and} \quad \omega_{\mathbf{p}} + \omega_{\mathbf{q}} = \omega_{\mathbf{p}'} + \omega_{\mathbf{q}'}$$

$s\text{-}\lim_{j \rightarrow \infty} P_j = \mathbb{1}$ . Then the integrals  $\int E(d^n x) P_j \Phi(\underline{x})$  are defined as Bochner-integrals [9] and the limit

$$s\text{-}\lim_{j \rightarrow \infty} \int E(d^n x) P_j \Phi(\underline{x}) = \int E(d^n x) \Phi(\underline{x})$$

exists independently of the special choice of the sequence  $P_j$ . Furthermore

$$\left\| \int E(d^n x) \Phi(\underline{x}) \right\| \leq V(\mathbb{G}) \cdot \sup_{\mathbf{x} \in \mathbb{R}^n} \left\| \frac{\partial}{\partial x_1} \cdots \frac{\partial}{\partial x_n} \Phi(\underline{x}) \right\|$$

where  $\mathbb{G} \subset \mathbb{R}^n$  denotes the support of  $\left\| \frac{\partial}{\partial x_1} \cdots \frac{\partial}{\partial x_n} \Phi(\underline{x}) \right\|$  and  $V(\mathbb{G})$  its volume.

Since  $E^{\text{out}}(d^3 k)$  is an absolutely continuous projection-valued measure and  $\varrho_{\mathbf{k}} \Omega$  an arbitrarily often differentiable vector-valued function one can conclude that the integral  $\int E^{\text{out}}(d^3 k) h(\mathbf{k}) \varrho_{\mathbf{k}} \Omega$  exists if  $h$  is a smooth function with compact support. Recalling that  $\varrho_{\mathbf{k}} \Omega$  is a state of finite energy we see that only a bounded region in  $\mathbf{k}$ -space can contribute to the above integral. Hence if  $h_R$  is a sequence of smooth functions with compact support and  $h_R(\mathbf{u}) = 1$  for  $|\mathbf{u}| \leq R$  then the integral  $\int E^{\text{out}}(d^3 k) h_R(\mathbf{k}) \varrho_{\mathbf{k}} \Omega$  is independent of  $R$  for sufficiently large  $R$ . This establishes the existence of

$$\int E^{\text{out}}(d^3 k) \varrho_{\mathbf{k}} \Omega = s\text{-}\lim_{R \rightarrow \infty} \int E^{\text{out}}(d^3 k) h_R(\mathbf{k}) \varrho_{\mathbf{k}} \Omega.$$

It remains to show that this vector differs only slightly from  $\varrho \Omega$  near the 2-particle threshold: let  $h$  be a smooth function,  $h(\mathbf{u}) = 1$  for  $|\mathbf{u}| \leq 1$  and  $h(\mathbf{u}) = 0$  for  $|\mathbf{u}| \geq 2$ . Then the preceding lemma guarantees that the integral  $\int E^{\text{out}}(d^3 k) h\left(\frac{\mathbf{k}}{\sqrt{\lambda}}\right) \varrho_{\mathbf{k}} \Omega$  exists for all  $\lambda > 0$ . Since the function  $\{\varrho_{\mathbf{k}} - \varrho\} \Omega$  has a double zero at  $\mathbf{k} = 0$  the second part of Lemma 4.1 implies that

$$\left\| \int E^{\text{out}}(d^3 k) h\left(\frac{\mathbf{k}}{\sqrt{\lambda}}\right) \{\varrho_{\mathbf{k}} - \varrho\} \Omega \right\| \leq c \cdot \lambda \quad \text{for } \lambda > 0 \tag{8}$$

and this proves that the difference between  $\varrho \Omega$  and  $\int E^{\text{out}}(d^3 k) \varrho_{\mathbf{k}} \Omega$  is small in the neighbourhood of the threshold.

We are now in a position to establish the desired connection between the continuity properties of  $\|\int_0^\lambda E(d\lambda') \varrho \Omega\|$  at  $\lambda = 0$  and  $T(s, 0)$  at  $s = 4\mu^2$ .

**Lemma 4.2.** *The following statements are equivalent for small  $\lambda > 0$  if  $\frac{1}{2} < \alpha < \frac{3}{2}$ :*

- i)  $\|\int_0^\lambda E(d\lambda') \varrho \Omega\|^2 \leq c \cdot \lambda^{2\alpha-1}$ .
- ii)  $\int_{4\mu^2}^{4\mu^2+\lambda} ds (s - 4\mu^2)^{1/2} |T(s, 0)|^2 \leq c' \cdot \lambda^{2\alpha-1}$ .

*Proof.* Since  $\varrho\Omega$  is a state of finite energy only the asymptotic 2-particle component of  $\varrho\Omega$  can contribute to the first integral if  $\lambda$  is small<sup>6</sup>. Now let  $E_{\max}$  be the maximum energy of  $\varrho\Omega$ . Then one can find two positive numbers  $\alpha$  and  $\beta$  depending only on  $E_{\max}$  such that for all  $\mathbf{p}$  and  $\mathbf{q}$  satisfying  $\omega_{\mathbf{p}} + \omega_{\mathbf{q}} \leq E_{\max}$

$$\alpha \cdot |\mathbf{p} - \mathbf{q}|^2 \leq \omega_{\mathbf{p}} + \omega_{\mathbf{q}} - (|\mathbf{p} + \mathbf{q}|^2 + 4\mu^2)^{1/2} \leq \beta \cdot |\mathbf{p} - \mathbf{q}|^2. \quad (b)$$

Realizing how  $E(d\lambda)$  acts on the asymptotic 2-particle space it follows from this inequality that for sufficiently small  $\lambda > 0$  the first relation of the lemma is equivalent to  $\left\| \int E^{\text{out}}(d^3k) h\left(\frac{\mathbf{k}}{\sqrt{\lambda}}\right) \varrho\Omega \right\|^2 \leq \hat{c} \cdot \lambda^{2\alpha-1}$  and therefore also to  $\left\| \int E^{\text{out}}(d^3k) h\left(\frac{\mathbf{k}}{\sqrt{\lambda}}\right) \varrho_{\mathbf{k}}\Omega \right\|^2 \leq \hat{c} \cdot \lambda^{2\alpha-1}$  because of inequality (8).

Now with the aid of Relation (7) one gets

$$\begin{aligned} & \left\| \int E^{\text{out}}(d^3k) h\left(\frac{\mathbf{k}}{\sqrt{\lambda}}\right) \varrho_{\mathbf{k}}\Omega \right\|^2 \\ &= \frac{\pi^4}{64} \cdot \int \frac{d^3p}{2\omega_{\mathbf{p}}} \frac{d^3q}{2\omega_{\mathbf{q}}} \left| h\left(\frac{\mathbf{p}-\mathbf{q}}{\sqrt{\lambda}}\right) T(s, 0) \frac{(\mathbf{p}, A\Omega)(\mathbf{q}, A\Omega)}{\omega_{\mathbf{p}}\omega_{\mathbf{q}}} \right|^2. \end{aligned}$$

Using Inequality (b) once more and changing variables one can conclude that the behaviour of this expression coincides for small  $\lambda > 0$  with that of

$$\int_{4\mu^2}^{4\mu^2 + \lambda} ds (s - 4\mu^2)^{1/2} |T(s, 0)|^2 \cdot h(s)$$

where  $h(s)$  is continuous for  $s > 4\mu^2$  and  $\lim_{s \downarrow 4\mu^2} h(s) > 0$ . From these facts the proposition follows immediately.

With this lemma and Theorem 2.1 now we have at our disposal the information connecting the rate of convergence of the Haag-Ruelle approximations with the properties of the  $S$ -matrix near the 2-particle threshold.

**Theorem 4.3.** *The following statements are equivalent if  $\frac{1}{2} < \alpha < \frac{3}{2}$ :*

- i)  $\Psi_f^{\text{out}} - \Psi_f(t) = O(t^{-\alpha}), t > 0$  for all  $\tilde{f} \in \mathcal{S}(\mathbb{R}^6)$  with compact support.
- ii)  $\int_{4\mu^2}^{4\mu^2 + \lambda} ds (s - 4\mu^2)^{1/2} |T(s, 0)|^2 \leq c \cdot \lambda^{2\alpha-1}$  for small  $\lambda > 0$ .

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<sup>6</sup> This is the only place throughout this paper where we really need the asymptotic completeness of the theory.

From this theorem and the fact that  $\Psi_f^{\text{out}} - \Psi_f(t) = O(t^{-3/4+\varepsilon})$ ,  $\varepsilon > 0$  in all theories which are compatible with our assumptions [1] we can furthermore conclude:

**Corollary 4.4.** *For small  $\lambda > 0$  and arbitrary  $\varepsilon > 0$  the estimate*

$$\int_{4\mu^2}^{4\mu^2+\lambda} ds (s - 4\mu^2)^{1/2} |T(s, 0)|^2 \leq c_\varepsilon \cdot \lambda^{1/2-\varepsilon}$$

holds.  $c_\varepsilon$  is a number which does not depend on  $\lambda$  but which may tend to  $\infty$  if  $\varepsilon \rightarrow 0$ .

Roughly speaking this proposition says that  $T(s, 0)$  cannot be much more singular than  $(s - 4\mu^2)^{-1/2}$  at  $s = 4\mu^2$ . It is exactly this singularity which one expects if the threshold has “absorbed” a bound state. Since there is no reason to believe that the postulates of quantum field theory exclude the possibility of such models this justifies our conjecture – again using Theorem 4.3 – that the estimates for the rate of convergence of  $\Psi_f^{\text{out}} - \Psi_f(t)$  given in [1] cannot be improved without further specification of the dynamics. Apart from these exceptional models,  $T(s, 0)$  should be uniformly bounded in a suitable neighbourhood of the threshold  $s = 4\mu^2$  [4, 5]. In these normal cases one gets for small  $\lambda > 0$

$$\int_{4\mu^2}^{4\mu^2+\lambda} ds (s - 4\mu^2)^{1/2} |T(s, 0)|^2 \leq c \cdot \lambda^{3/2}$$

and this implies (via Theorem 4.3) that  $\Psi_f^{\text{out}} - \Psi_f(t) = O(t^{-5/4})$ ,  $t > 0$  for all asymptotic 2-particle states with wavefunctions  $\tilde{f} \in \mathcal{S}(\mathbb{R}^6)$  having compact support in momentum space.

## V. Comparison with Non-Relativistic Scattering Theory

The singularities of the  $S$ -matrix at the 2-particle threshold are due to asymptotic configurations of particles with small relative momentum and may be regarded as a non-relativistic effect. It is therefore not surprising that investigations within the framework of non-relativistic potential scattering theory yield exactly the same results as in quantum field theory. However, we still think it worth considering the non-relativistic case for two reasons: first the framework is simpler so the methods of proof become more transparent and secondly there is no lack of non-trivial models. Accordingly this chapter has two subsections. In the first one we give the analogues of Theorems 2.1, 3.1, and 4.3, and in the second one we consider a simple model: the scattering of a particle by a square – well potential.

a) *Some General Results*

Since in a non-relativistic 2-particle system the center of mass motion can be separated out it suffices for our purposes to consider a 1-particle system in an external potential. Therefore we assume that the Hamiltonian  $H$  has, on a suitable domain in configuration space, the form

$$H = -\Delta + V(\mathbf{x})$$

where  $\Delta$  is the Laplacian and  $V$  the potential. To exclude singular potentials with long range we require in addition

$$\int d^3x |(1 + |\mathbf{x}|^2) \cdot V(\mathbf{x})|^2 < \infty .$$

At present it is not known whether this condition ensures that the spectrum of the Hamiltonian has no unphysical pathologies. To exclude infinitely many bound states and a continuous singular part of the spectrum one needs more stringent assumptions [8]. Let us therefore explicitly assume that the Hamiltonian has the spectral decomposition

$$H = \sum_{k=1}^n \lambda_k E_k + \int_0^\infty \lambda E(d\lambda)$$

where  $E_k$  is the projection onto the subspace corresponding to the discrete eigenvalue  $\lambda_k$ . The projection valued measure  $E(d\lambda)$  is supposed to be absolutely continuous.

As in the relativistic case, the scattering states are usually constructed as strong limits of suitably chosen sequences: if  $\Psi^{\text{out}}$ , for example, denotes a vector which behaves at large times like the freely propagating state  $\Psi$ , then  $\Psi^{\text{out}} = \text{s-lim}_{t \rightarrow \infty} \Psi(t)$  where

$$\Psi(t) = e^{iHt} e^{-iH_0 t} \Psi .$$

( $H_0$  is the free Hamiltonian:  $H_0 = -\Delta$  in configuration space).

Having characterized the framework, we start our investigations as in Chapter II by isolating the asymptotically leading contribution to  $\Psi^{\text{out}} - \Psi(t)$ :

**Lemma 5.1.** *If  $\Psi$  is a state with a wavefunction  $\psi(\mathbf{x}) \in \mathcal{S}(\mathbb{R}^3)$  then*

$$\Psi^{\text{out}} - \Psi(t) = i^{-1/2} \tilde{\psi}(\mathbf{0}) \cdot \int_t^\infty d\tau \tau^{-3/2} e^{iH\tau} \hat{V} + O(t^{-3/2}) \quad \text{for } t > 0 .$$

$\hat{V}$  denotes the vector with the configuration space wave-function  $V(\mathbf{x})$ .

*Proof.* It suffices to consider the state  $\partial_t \Psi(t) = i \cdot e^{iHt} V e^{-iH_0 t} \Psi$ . Representing the vector  $V e^{-iH_0 t} \Psi$  in configuration space one gets

$$\begin{aligned} (V e^{-iH_0 t} \Psi)(\mathbf{x}) &= V(\mathbf{x}) (2\pi i t)^{-3/2} \cdot \int d^3 y e^{i \frac{|\mathbf{x}-\mathbf{y}|^2}{4t}} \cdot \psi(\mathbf{y}) \\ &= V(\mathbf{x}) (i t)^{-3/2} \cdot \tilde{\psi}(\mathbf{0}) + V(\mathbf{x}) (2\pi i t)^{-3/2} \cdot \int d^3 y \left( e^{i \frac{|\mathbf{x}-\mathbf{y}|^2}{4t}} - 1 \right) \cdot \psi(\mathbf{y}). \end{aligned}$$

The second term in the second line of this equation can be estimated as follows:

$$\begin{aligned} \left| \int d^3 y \left( e^{i \frac{|\mathbf{x}-\mathbf{y}|^2}{4t}} - 1 \right) \cdot \psi(\mathbf{y}) \right| &\leq (4|t|)^{-1} \cdot \int d^3 y |\mathbf{x} - \mathbf{y}|^2 |\psi(\mathbf{y})| \\ &\leq c' \cdot |t|^{-1} \cdot (1 + |\mathbf{x}|^2) \end{aligned}$$

$c'$  being independent of  $\mathbf{x}$  and  $t$ . Now it is easy to verify that

$$\| e^{iHt} (V e^{-iH_0 t} \Psi - (i t)^{-3/2} \cdot \tilde{\psi}(\mathbf{0}) \hat{V}) \|^2 \leq c \cdot |t|^{-5} \cdot \int d^3 x (1 + |\mathbf{x}|^2) V(\mathbf{x})^2$$

and integrating this inequality with respect to  $t$  yields the desired result.

It is not quite as simple to pass to momentum space in the non-relativistic case because  $H$  may have many bound states. However, these states do not contribute to the asymptotically leading part of  $\Psi^{\text{out}} - \Psi(t)$  as the next lemma shows.

**Lemma 5.2.** *Let  $\Psi$  be a state with a wavefunction  $\psi(\mathbf{x}) \in \mathcal{S}(\mathbb{R}^3)$ . Then*

$$\begin{aligned} \Psi^{\text{out}} - \Psi(t) &= i^{-1/2} \tilde{\psi}(\mathbf{0}) \cdot t^{-1/2} \cdot \int_0^\infty \varphi(\lambda t) E(d\lambda) \hat{V} + O(t^{-3/2}) \quad \text{for } t > 0, \\ (\varphi(u) &= u^{1/2} \cdot \int_u^\infty dv v^{-3/2} e^{iv} \text{ is the function introduced in Chapter III.}) \end{aligned}$$

*Proof.* We can restrict ourselves to showing that

$$\sum_{k=1}^n E_k \cdot \int_t^\infty d\tau \tau^{-3/2} e^{iH\tau} \hat{V} = O(t^{-3/2})$$

since if this is so only the continuous part of the spectrum of  $H$  contributes to the asymptotically leading term of  $\Psi^{\text{out}} - \Psi(t)$ . Then the statement follows from the arguments given in the first part of Chapter III. Now

$$E_k \cdot \int_t^\infty d\tau \tau^{-3/2} e^{iH\tau} \hat{V} = \left( \int_t^\infty d\tau \tau^{-3/2} e^{i\lambda_k \tau} \right) \cdot E_k \hat{V}$$

and this reduces the problem to a simple estimation of an integral. A straightforward calculation shows that the above expression is  $O(t^{-3/2})$  if  $\lambda_k \neq 0$ .

If  $\lambda_k = 0$  it turns out that  $E_k \hat{V} = 0$ : let  $\Psi_n, n \in \mathbb{N}$  be a sequence of vectors with configuration space wavefunctions  $\psi(n^{-1} \mathbf{x}), \psi \in \mathcal{S}(\mathbb{R}^3)$  and  $\psi(\mathbf{0}) = 1$ . Since  $V(\mathbf{x}) \in L^2(\mathbb{R}^3)$  it follows that  $s\text{-}\lim_{n \rightarrow \infty} V \Psi_n = \hat{V}$ . It is

also easy to verify that  $\|H_0 \Psi_n\|^2 = n^{-1} \cdot \int d^3 p |p|^4 |\hat{\psi}(p)|^2$  proving  $s\text{-}\lim_{n \rightarrow \infty} H_0 \Psi_n = 0$ . Hence if  $\Phi$  is an eigenvector of  $H$  with eigenvalue 0 then

$$(\Phi, \hat{V}) = \lim_{n \rightarrow \infty} (\Phi, V \Psi_n) = - \lim_{n \rightarrow \infty} (\Phi, H_0 \Psi_n) = 0$$

and this clearly shows that  $E_k \hat{V} = 0$ .

We require now that the wavefunction  $\psi \in \mathcal{S}(\mathbb{R}^3)$  of  $\Psi$  does not vanish at the threshold,  $\hat{\psi}(0) \neq 0$ . Under these premises the leading contribution of  $\Psi^{\text{out}} - \Psi(t)$  given in Lemma 5.2 is non-trivial and the following proposition holds:

**Lemma 5.3.** *The following statements are equivalent provided that  $\frac{1}{2} < \alpha < \frac{3}{2}$ :*

- i)  $\Psi^{\text{out}} - \Psi(t) = \mathbf{0}(t^{-\alpha})$  for  $t > 0$ .
- ii)  $\|\int_0^\lambda E(d\lambda') \hat{V}\|^2 \leq c \cdot \lambda^{2\alpha-1}$  for  $\lambda > 0$ .
- iii)  $\left\| \frac{1}{H + i\lambda} \hat{V} \right\|^2 \leq c' \cdot |\lambda|^{2\alpha-3}$  for  $\lambda \neq 0$ .

*Proof.* In order to establish the equivalence of i) and ii) one can take over the arguments given in Theorem 3.1. The equivalence of ii) and iii) becomes manifest after a simple calculation providing one recalls that  $E_k \hat{V} = 0$  if  $E_k$  is the projection onto the eigenvectors of  $H$  to the eigenvalue 0.

As in Chapter IV we shall now proceed from  $\hat{V}$  to a state with a wavefunction which is intimately connected with the scattering amplitude<sup>7</sup>. For this purpose we introduce the vector valued function  $\hat{V}_\lambda$ ,  $\lambda > 0$  which is represented in configuration space by  $\hat{V}_\lambda(\mathbf{x}) = V(\mathbf{x}) \cdot \frac{\sin \sqrt{\lambda} |\mathbf{x}|}{\sqrt{\lambda} |\mathbf{x}|}$ . (Note that  $\frac{\sin \sqrt{\lambda} |\mathbf{x}|}{\sqrt{\lambda} |\mathbf{x}|}$  is a rotationally invariant improper eigenstate of  $H_0$  corresponding to the eigenvalue  $\lambda$ .) Since  $(1 + |\mathbf{x}|^2) \cdot V(\mathbf{x}) \in L^2(\mathbb{R}^3)$  the function  $\hat{V}_\lambda$  is continuously differentiable in the strong topology and this guarantees (because of Lemma 4.1) that the vector

$$\int_0^\infty E(d\lambda') h\left(\frac{\lambda'}{\lambda}\right) \hat{V}_{\lambda'}, \quad \lambda > 0 \tag{9}$$

exists if  $h \in \mathcal{S}(\mathbb{R}^1)$ ,  $h(u) = 1$  for  $|u| \leq 1$  and  $h(u) = 0$  for  $|u| \geq 2$ . Making use of the fact that  $\|\partial_\lambda \{\hat{V}_\lambda - \hat{V}\}\| \leq c'$  and  $\|\hat{V}_\lambda - \hat{V}\| \leq c'' \cdot \lambda$  it follows

<sup>7</sup> The scattering amplitude  $T(|p|; \mathbf{n}, \mathbf{n}')$  is (in formal language) defined by  $\text{out}(\mathbf{p} | \mathbb{1} - S | \mathbf{p}')^{\text{out}} = 2\pi i \cdot \delta(|p|^2 - |p'|^2) T(|p|; \mathbf{n}, \mathbf{n}')$ ,  $\mathbf{n}, \mathbf{n}'$  being the unit vectors parallel to  $\mathbf{p}$  and  $\mathbf{p}'$  respectively. With this definition [8]

$$T(|p|; \mathbf{n}, \mathbf{n}') = \text{out}(\mathbf{p} | V | \mathbf{p}') \quad \text{for } |p| = |p'|.$$



furthermore that

$$\left\| \int_0^\infty E(d\lambda') h\left(\frac{\lambda'}{\lambda}\right) \{\hat{V}_{\lambda'} - \hat{V}\} \right\|^2 \leq c \cdot \lambda, \quad \lambda > 0 \tag{10}$$

which proves that  $\hat{V}$  coincides with the state given by (9) in a neighbourhood of the threshold.

For an interpretation of the vector (9) it is convenient to use the energy-angular momentum basis. We define

$$T\left(E; \begin{matrix} l & l' \\ m & m' \end{matrix}\right) = \pi \cdot |p| \int d\Omega \bar{Y}_{lm}(\mathbf{n}) \int d\Omega' Y_{l'm'}(\mathbf{n}') T(|p|; \mathbf{n}, \mathbf{n}'), \quad E = |p|^2$$

where  $Y_{lm}$  are the spherical harmonics corresponding to the angular momentum quantum numbers  $l, m$ . It follows at once from this definition that<sup>8</sup>

$$\text{out}\left(E; l, m \left| \int_0^\infty E(d\lambda') h\left(\frac{\lambda'}{\lambda}\right) \hat{V}_{\lambda'} \right.\right) = h\left(\frac{E}{\lambda}\right) E^{-1/4} \cdot T\left(E; \begin{matrix} l & 0 \\ m & 0 \end{matrix}\right)$$

and specializing to rotationally invariant potentials  $V$  one gets

$$\text{out}\left(E; l, m \left| \int_0^\infty E(d\lambda') h\left(\frac{\lambda'}{\lambda}\right) \hat{V}_{\lambda'} \right.\right) = \delta_{l0} \delta_{m0} h\left(\frac{E}{\lambda}\right) E^{-1/4} \cdot T\left(E; \begin{matrix} 0 & 0 \\ 0 & 0 \end{matrix}\right).$$

The final theorem is then an immediate consequence of these equations, Relation (10) and Lemma 5.3.

**Theorem 5.4.** *The following statements are equivalent for small  $\lambda > 0$  and  $\frac{1}{2} < \alpha < \frac{3}{2}$ :*

- i)  $\Psi^{\text{out}} - \Psi(t) = O(t^{-\alpha}), \quad t > 0$  for all  $\psi \in \mathcal{S}(\mathbb{R}^3)$ .
- ii)  $\left\| \int_0^\lambda E(d\lambda') \hat{V} \right\|^2 \leq c \cdot \lambda^{2\alpha-1}$ .
- iii)  $\int_0^\lambda dE E^{-1/2} \cdot \sum_{l,m} \left| T\left(E; \begin{matrix} l & 0 \\ m & 0 \end{matrix}\right) \right|^2 \leq c' \cdot \lambda^{2\alpha-1}$ .

If the potential  $V$  is rotationally invariant this expression can be simplified to

$$\int_0^\lambda dE E^{-1/2} \cdot \left| T\left(E; \begin{matrix} 0 & 0 \\ 0 & 0 \end{matrix}\right) \right|^2 \leq c' \cdot \lambda^{2\alpha-1}.$$

*b) A Simple Model*

For reasons of concreteness we finally consider the model of an attractive square-well potential with range  $a$  and strength  $V_0$ . (This

<sup>8</sup> The improper states  $|E; l, m\rangle^{\text{out}}$  are normalized by

$$\text{out}\langle E; l, m | E'; l', m'\rangle^{\text{out}} = \delta(E - E') \delta_{ll'} \delta_{mm'}.$$

potential and the corresponding Hamiltonian satisfy our assumptions.) It is our aim to determine both the rate of convergence of  $\Psi^{\text{out}} - \Psi(t)$  and the continuity properties of the S-matrix near the threshold. To this end we calculate the behaviour of  $\|\int_0^\lambda E(d\lambda') \hat{V}\|$  for small  $\lambda$  and then apply the preceding theorem.

It is obvious that only the  $l=0$  part of  $E(d\lambda')$  can contribute to the above integral since  $\hat{V}$  is spherically symmetric. Thus

$$\left\| \int_0^\lambda E(d\lambda') \hat{V} \right\|^2 = \int_0^\lambda dE |(\phi_E, \hat{V})|^2$$

where  $\phi_E$ ,  $E > 0$  are the regular solutions of the radial Schrödinger equation with angular momentum  $l=0$  which are normalized to an energy  $\delta$ -function. The differential equation for  $\phi_E$  reads

$$(H\phi_E)(r) = -\frac{1}{r^2} \frac{d}{dr} r^2 \frac{d}{dr} \phi_E(r) + V(r) \phi_E(r) = E\phi_E(r)$$

where  $V(r) = -V_0$  for  $r \leq a$  and  $V(r) = 0$  for  $r \geq a$ . It is trivial to calculate the regular solutions of this equation,

$$\begin{aligned} \phi_E(r) &= N_E \cdot (2\pi r)^{-1} \cdot \\ &\begin{cases} \sqrt{E} \cdot \sin \sqrt{E+V_0} r, & r < a \\ \sqrt{E+V_0} \cos \sqrt{E+V_0} a \cdot \sin \sqrt{E}(r-a) + \sqrt{E} \sin \sqrt{E+V_0} a \cdot \cos \sqrt{E}(r-a), & r \geq a \end{cases} \end{aligned}$$

and normalizing  $\phi_E$  to an energy  $\delta$ -function yields

$$|N_E| = E^{-1/4} \cdot (E \cdot \sin^2 \sqrt{E+V_0} a + (E+V_0) \cdot \cos^2 \sqrt{E+V_0} a)^{-1/2}.$$

These results make it possible to evaluate the expansion coefficients of  $\hat{V}$  in the energy basis

$$|(\phi_E, \hat{V})| = 2V_0 \sqrt{E} |N_E| \cdot \left| \frac{\sin \sqrt{E+V_0} a - \sqrt{E+V_0} a \cdot \cos \sqrt{E+V_0} a}{E+V_0} \right|.$$

Inspecting this expression one realizes that the behaviour of  $|(\phi_E, \hat{V})|$  at  $E=0$  depends sensitively on the value of  $\sqrt{V_0} a$ . There are three significant cases to be distinguished:

i)  $\sqrt{V_0} a = (2n-1) \frac{\pi}{2}$ ,  $n \in \mathbb{N}$ : this implies  $|(\phi_E, \hat{V})| = E^{-1/4} h(E)^{10}$  and therefore  $\|\int_0^\lambda E(d\lambda') \hat{V}\|^2 = \lambda^{1/2} h(\lambda)$ . It follows then from Theorem 5.4

<sup>10</sup> Throughout this section  $h(u)$  denotes a function which is continuous for  $u > 0$  and  $\lim_{u \downarrow 0} h(u) > 0$ .

that the scattering amplitude  $T \begin{pmatrix} 0 & 0 \\ E & 0 \end{pmatrix}$  behaves like a non-vanishing constant at  $E=0$  and  $\Psi^{\text{out}} - \Psi(t) = O(t^{-3/4})$  for  $t > 0$ .

ii)  $\sqrt{V_0}a = \tan \sqrt{V_0}a$ : then  $|\langle \phi_E, \hat{V} \rangle| = E^{5/4}h(E)$ , hence  $\|\int_0^\lambda E(d\lambda') \hat{V}\|^2 = \lambda^{7/2}h(\lambda)$ . One can therefore conclude that (roughly speaking)  $\Psi^{\text{out}} - \Psi(t) = O(t^{-3/2})$  for  $t > 0$  and the scattering amplitude vanishes at least like  $E^{3/4}$  at  $E=0$ . (A better estimate cannot be obtained from the theorem because of the restrictions on  $\alpha$ .)

iii) All other possible values for  $\sqrt{V_0}a$ : in this case is  $|\langle \phi_E, \hat{V} \rangle| = E^{1/4}h(E)$  and thus  $\|\int_0^\lambda E(d\lambda') \hat{V}\|^2 = \lambda^{3/2}h(\lambda)$ . Consequently the scattering amplitude vanishes at  $E=0$  like  $E^{1/2}$  and  $\Psi^{\text{out}} - \Psi(t) = O(t^{-5/4})$  for  $t > 0$ .

Among all possible cases the last one occurs most frequently since  $V_0$  and  $a$  are not restricted by an additional condition. In this normal situation the scattering amplitude shows the famous  $E^{1/2}$  behaviour at the threshold and the approximations converge like  $\|\Psi^{\text{out}} - \Psi(t)\| \leq c \cdot t^{-5/4}$  for large  $t$ . In the exceptional Case i) a bound state is absorbed by the threshold and causes the slower  $t^{-3/4}$  decrease of  $\|\Psi^{\text{out}} - \Psi(t)\|$ . The remaining example is likewise something out of the ordinary: there the estimate  $\|\Psi^{\text{out}} - \Psi(t)\| \leq c \cdot t^{-3/2}$  holds for  $t > 0$  since the influence of the threshold can be neglected compared with the contributions of the bound states.

### Appendix A

In Chapter III we introduced the function  $\varphi(u) = u^{1/2} \cdot \int_u^\infty dv v^{-3/2} e^{iv}$ ,  $u > 0$ . We specify here some simple properties of  $\varphi(u)$  which were repeatedly used in our arguments:

- i)  $\varphi(u)$  is continuous for  $u > 0$  and  $\lim_{u \downarrow 0} \varphi(u) = 2$ .
- ii)  $|\varphi(u)| \leq 2 \cdot u^{-1}$  and  $|\varphi'(u)| \leq 2 \cdot (1 + u^{-1/2})$ .
- iii)  $|\text{Re}\{\bar{\varphi}(u) \varphi'(u)\}| \leq c \cdot u^{-3}$  for large  $u$ .

For the proof of these statements the following hints may suffice:

- i)  $\varphi(u) = u^{1/2} \cdot \int_u^\infty dv v^{-3/2} + u^{1/2} \cdot \int_u^\infty dv v^{-3/2}(e^{iv} - 1)$ . The first integral can be calculated explicitly and  $v^{-3/2}(e^{iv} - 1)$  is absolutely integrable.
- ii) It follows after partial integration that  $\varphi(u) = u^{1/2} \cdot (iu^{-3/2} e^{iu} - i\frac{3}{2} \int_u^\infty dv v^{-5/2} e^{iv})$  and therefore  $|\varphi(u)| \leq 2 \cdot u^{-1}$ . Similarly one can show

$$\begin{aligned} \varphi'(u) &= \frac{1}{2}u^{-1/2} \cdot \int_u^\infty dv v^{-3/2} e^{iv} - u^{-1} e^{iu} \\ &= \frac{1}{2}u^{-1/2} \cdot \int_u^\infty dv v^{-3/2}(e^{iv} - 1) - u^{-1}(e^{iu} - 1) \end{aligned}$$

hence  $|\varphi'(u)| \leq 2 \cdot (1 + u^{-1/2})$ .

iii) From the relations given in ii) one can conclude that  $\varphi(u) = iu^{-1}e^{iu} + O(u^{-2})$  and  $\varphi'(u) = -u^{-1}e^{iu} + O(u^{-2})$ . Therefore  $\operatorname{Re}\{\bar{\varphi}(u)\varphi'(u)\} = O(u^{-3})$ .

### Appendix B

We could not find a proof of Lemma 4.1 in the literature and therefore give it here:

$P_j$  is an operator of finite rank and can thus be expressed as a finite sum of operators of rank one:  $P_j\Phi = \sum_{m=1}^M c_m(\hat{\Psi}_m, \Phi) \cdot \Psi_m$ . It is therefore natural to define

$$\int E(d^n x) P_j \Phi(\underline{x}) = \sum_{m=1}^M c_m \int (\hat{\Psi}_m, \Phi(\underline{x})) \cdot E(d^n x) \Psi_m.$$

Since the functions  $(\hat{\Psi}_m, \Phi(\underline{x}))$  are continuously differentiable and have compact support the right hand side of this equation is well defined as a finite sum of Bochner integrals [9, Chapter III].

Now let  $\mathbb{X}$  be the Borel set  $\mathbb{X} = \{y: -\infty < y_1 \leq x_1 \cdots -\infty < y_n \leq x_n\}$  and  $\Theta_{\mathbb{X}}$  the associated characteristic function;  $E(\underline{x})$  stands for the projection  $E(\underline{x}) = \int \Theta_{\mathbb{X}}(\underline{x}') E(d^n x')$ . One gets immediately after partial integration

$$\begin{aligned} \int E(d^n x) P_j \Phi(\underline{x}) &= (-1)^n \sum_{m=1}^M c_m \cdot \int d^n x \left( \hat{\Psi}_m, \frac{\partial}{\partial x_1} \cdots \frac{\partial}{\partial x_n} \Phi(\underline{x}) \right) \cdot E(\underline{x}) \Psi_m \\ &= (-1)^n \int d^n x E(\underline{x}) P_j \frac{\partial}{\partial x_1} \cdots \frac{\partial}{\partial x_n} \Phi(\underline{x}) \end{aligned}$$

and consequently

$$\begin{aligned} &\| \int E(d^n x) P_j \Phi(\underline{x}) - \int E(d^n x) P_{j'} \Phi(\underline{x}) \| \\ &= \left\| \int d^n x E(\underline{x}) (P_j - P_{j'}) \frac{\partial}{\partial x_1} \cdots \frac{\partial}{\partial x_n} \Phi(\underline{x}) \right\| \\ &\leq V(\mathbb{G}) \cdot \sup_{x \in \mathbb{R}^n} \left\| (P_j - P_{j'}) \frac{\partial}{\partial x_1} \cdots \frac{\partial}{\partial x_n} \Phi(\underline{x}) \right\|. \end{aligned}$$

It is self evident that the set of vectors  $\frac{\partial}{\partial x_1} \cdots \frac{\partial}{\partial x_n} \Phi(\underline{x})$  is compact as continuous image of the compact set  $\mathbb{G}$ . Bearing in mind that the operators  $P_j$  are uniformly bounded and  $s\text{-}\lim_{j \rightarrow \infty} P_j = \mathbf{1}$  it follows that

$$\lim_{j, j' \rightarrow \infty} \sup_{\underline{x} \in \mathbb{R}^n} \left\| (P_j - P_{j'}) \frac{\partial}{\partial x_1} \cdots \frac{\partial}{\partial x_n} \Phi(\underline{x}) \right\| = 0.$$

This proves that the limit  $s\text{-}\lim_{j \rightarrow \infty} \int E(d^n x) P_j \Phi(x)$  exists. In the same way one establishes both the independence of this limit from the special choice of the sequence  $P_j$  and the estimate given for the norm of the limit vector.

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