

LECTURES ON SCATTERING THEORY

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Lecture notes prepared by Andrew Hassell, based on lectures given by the author at the Australian National University in October and November, 2001.

The first two lectures are devoted to describing the basic concepts of scattering theory in a very compressed way. A detailed presentation of the abstract part can be found in [33] and numerous applications in [30] and [36]. The last two lectures are based on the recent research of the author.

1. INTRODUCTION TO SCATTERING THEORY. TRACE CLASS METHOD

1. Let us, first, indicate the place of scattering theory amongst other mathematical theories. This is very simple: it is a subset of perturbation theory. The ideology of perturbation theory is as follows. Let H_0 and $H = H_0 + V$ be self-adjoint operators on a Hilbert space \mathcal{H} , and let V be, in some sense, small compared to H_0 . Then it is expected that the spectral properties of H are close to those of H_0 . Typically, H_0 is simpler than H , and in many cases we know its spectral family $E_0(\cdot)$ explicitly. The task of perturbation theory is to deduce information about the spectral properties of $H = H_0 + V$ from those of H_0 . We shall always consider the case of self-adjoint operators on a Hilbert space \mathcal{H} .

The spectrum of a self-adjoint operator has two components: discrete (i.e., eigenvalues) and continuous. Hence, perturbation theory has two parts: perturbation theory for the discrete spectrum, and for the continuous spectrum. Eigenvalues of H_0 can generically be shifted under arbitrary small perturbations, but the formulas for these shifts are basically the same as in the finite dimensional case, $\dim \mathcal{H} < \infty$, which is linear algebra. On the contrary, the continuous spectrum is much more stable.

Example. Let

$$H_0 = -\Delta, \quad H = -\Delta + v(x), \quad v(x) = \overline{v(x)}, \quad v \in L^\infty(\mathbb{R}), \quad (1.1)$$

be self-adjoint operators on the Hilbert space $\mathcal{H} = \mathcal{L}^2(\mathbb{R})$. Denote by Φ the Fourier transform. Then

$$H_0 = \Phi^* |\xi|^2 \Phi, \quad (1.2)$$

so that the spectrum of H_0 is the same as that of the multiplication operator $|\xi|^2$. Moreover, we know all functions of the operator H_0 and, in particular, its spectral family explicitly. In the case considered V is multiplication by the function v . Thus, each of the operators H_0 and V is very simple. However, it is not quite so simple to understand their sum, the Schrödinger operator $H = H_0 + V$. Nevertheless, it is easy to deduce from the Weyl theorem that, if $v(x) \rightarrow 0$ as $|x| \rightarrow \infty$, then

the essential spectrum of H is the same as that of H_0 and hence it coincides with $[0, \infty)$.

Scattering theory requires classification of the spectrum in terms of the theory of measure. Each measure may be decomposed into three parts: an absolutely continuous part, a singular continuous part, and a pure point part. The same classification is valid for the spectral measure $E(\cdot)$ of a self-adjoint operator H . Thus, there is a decomposition of the Hilbert space $\mathcal{H} = \mathcal{H}^{\perp\perp} \oplus \mathcal{H}^{sc} \oplus \mathcal{H}^{pp}$ into the orthogonal sum of invariant subspaces of the operator H ; the operator restricted to $\mathcal{H}^{\perp\perp}$, \mathcal{H}^{sc} or \mathcal{H}^{pp} shall be denoted H^{ac} , H^{sc} or H^{pp} , respectively. The pure point part corresponds to eigenvalues. The singular continuous part is typically absent. Actually, a part of scattering theory is devoted to proving this for various operators of interest, but in these lectures we study only the absolutely continuous part H^{ac} of H . The same objects for the operator H_0 will be labelled by the index '0'. We denote P_0 the orthogonal projection onto the absolutely continuous subspace $\mathcal{H}_0^{\perp\perp}$ of H_0 .

The starting point of scattering theory is that the absolutely continuous part of self-adjoint operator is stable under fairly general perturbations. However assumptions on perturbations are much more restrictive than those required for stability of the essential spectrum. So scattering theory can be defined as perturbation theory for the absolutely continuous spectrum. Of course, it is too much to expect that $H^{ac} = H_0^{ac}$. However, we can hope for a unitary equivalence:

$$H^{ac} = UH_0^{ac}U^*, \quad U : \mathcal{H}_0^{\perp\perp} \rightarrow \mathcal{H}^{\perp\perp} \text{ onto.}$$

The first task of scattering theory is to show this unitary equivalence. We now ask: how does one find such a unitary equivalence U ? This is related (although the relationship is not at all obvious) to the second task of scattering theory, namely, the large time behaviour of solutions

$$u(t) = e^{-iHt}f.$$

of the time-dependent equation

$$i\frac{\partial u}{\partial t} = Hu, \quad u(0) = f \in \mathcal{H}.$$

If f is an eigenvector, $Hf = \lambda f$, then $u(t) = e^{-i\lambda t}f$, so the time behaviour is evident. By contrast, if $f \in \mathcal{H}^{\perp\perp}$, one cannot, in general, calculate $u(t)$ explicitly, but scattering theory allows us to find its asymptotics as $t \rightarrow \pm\infty$. In the perturbation theory setting, it is natural to understand the asymptotics of u in terms of solutions of the unperturbed equation, $iu_t = H_0u$. It turns out that, under rather general assumptions, for all $f \in \mathcal{H}^{\perp\perp}$, there are $f_0^\pm \in \mathcal{H}_0^{\perp\perp}$ such that

$$u(t) \sim u_0^\pm(t), \quad t \rightarrow \pm\infty, \quad \text{where } u_0^\pm(t) = e^{-iH_0t}f_0^\pm,$$

or, to put it differently,

$$\lim_{t \rightarrow \pm\infty} \|e^{-iHt}f - e^{-iH_0t}f_0^\pm\| = 0. \quad (1.3)$$

Hence f_0^\pm and f are related by the equality

$$f = \lim_{t \rightarrow \pm\infty} e^{iHt}e^{-iH_0t}f_0^\pm,$$

which justifies the following fundamental definition given by C. Møller [23] and made precise by K. Friedrichs [8].

DEFINITION 1.1. *The limit*

$$W_{\pm} = W_{\pm}(H, H_0) = s\text{-}\lim_{t \rightarrow \pm\infty} e^{iHt} e^{-iH_0 t} P_0,$$

if it exists, is called the wave operator.

It follows that $f = W_{\pm} f_0^{\pm}$. The wave operator has the properties

- (i) W_{\pm} is isometric on $\mathcal{H}_r^{\updownarrow}$.
- (ii) $W_{\pm} H_0 = H W_{\pm}$ (the *intertwining property*).

In particular, $\mathcal{H}_r^{\updownarrow}$ is unitarily equivalent, via W_{\pm} , to the restriction $H|_{\text{ran } W_{\pm}}$ of H on the range $\text{ran } W_{\pm}$ of the wave operator W_{\pm} and hence $\text{ran } W_{\pm} \subset \mathcal{H}^{\updownarrow}$.

DEFINITION 1.2. *If $\text{ran } W_{\pm} = \mathcal{H}^{\updownarrow}$, then W_{\pm} is said to be complete.*

It is a simple result that $W_{\pm}(H, H_0)$ is complete if and only if the ‘inverse’ wave operator $W_{\pm}(H_0, H)$ exists. Thus, if W_{\pm} exists and is complete (at least for one of the signs), H_0^{ac} and H^{ac} are unitarily equivalent. It should be emphasized that scattering theory is interested only in the canonical unitary equivalence provided by the wave operators.

Another important object of scattering theory

$$\mathbf{S} = W_{+}^{*} W_{-} \tag{1.4}$$

is called the scattering operator. It commutes with H_0 , $\mathbf{S} H_0 = H_0 \mathbf{S}$, which follows directly from property (ii) of the wave operators. Moreover, it is unitary on $\mathcal{H}_r^{\updownarrow}$ if both W_{\pm} are complete. In the spectral representation of the operator H_0 , the operator \mathbf{S} acts as multiplication by the operator-valued function $S(\lambda)$ known as the scattering matrix (see the next lecture, for more details).

An important generalization of Definition 1.1 is due to Kato [19].

DEFINITION 1.3. *Let J be a bounded operator. Then the modified wave operator $W_{\pm}(H, H_0, J)$ is defined by*

$$W_{\pm}(H, H_0, J) = s\text{-}\lim_{t \rightarrow \pm\infty} e^{iHt} J e^{-iH_0 t} P_0, \tag{1.5}$$

when this limit exists.

Modified wave operators still enjoy the intertwining property

$$W_{\pm}(H, H_0, J) H_0 = H W_{\pm}(H, H_0, J),$$

but of course their isometricity on $\mathcal{H}_r^{\updownarrow}$ can be lost.

2. We have seen that the wave operators give non-trivial spectral information about H . Thus, it is an important problem to find conditions guaranteeing the existence of wave operators. There are two quite different methods: the trace class method, and the smooth method (see the next lecture). The trace class method is the principal method of abstract scattering theory. For applications to differential operators, both methods are important.

The fundamental theorem for the trace class method is the Kato-Rosenblum theorem [15, 31, 16]. Recall that a compact operator T on \mathcal{H} is in the class \mathfrak{S}_p , $p > 0$, if

$$\|T\|_p^p = \sum (\lambda_j(T^*T))^{p/2} < \infty.$$

In particular, \mathfrak{S}_1 is called the trace class and \mathfrak{S}_2 is called the Hilbert-Schmidt class.

THEOREM 1.4. *If the difference $V = H - H_0$ belongs to the trace class, then the wave operators $W_{\pm}(H, H_0)$ exist.*

This is a beautiful theorem. It has a number of advantages, including:

(i) Since the conditions are symmetric with respect to the operators H_0 and H , the wave operators $W_{\pm}(H_0, H)$ also exist and hence $W_{\pm}(H, H_0)$ are complete.

(ii) The formulation is simple, but all proofs of it are rather complicated.

(iii) It relates very different sorts of mathematical objects: operator ideals, and scattering theory.

(iv) It is effective, since it is usually easy to determine whether V is trace class.

(v) It is sharp, in the sense that if H_0 and $p > 1$ are given, there is a $V \in \mathfrak{S}_p$ such that the spectrum of $H_0 + V$ is purely point.

However, Theorem 1.4 has a disadvantage: it is useless in applications to differential operators. Indeed, for example, for the pair (1.1) V is a multiplication operator which cannot be even compact (unless identically zero), and therefore Theorem 1.4 does not work. Nevertheless, it is still useful if one is only interested in the unitary equivalence of H^{ac} and $H_0 = H_0^{ac}$. In fact, it is sufficient to show that the operators $(H + c)^{-1}$ and $(H_0 + c)^{-1}$ are unitarily equivalent for some $c > 0$ or, according to Theorem 1.4, that their difference is trace class.

Actually, this condition is sufficient for the existence (and completeness) of the wave operators. More generally, the following result is true.

THEOREM 1.5. *Suppose that*

$$(H - z)^{-n} - (H_0 - z)^{-n} \in \mathfrak{S}_1$$

for some $n = 1, 2, \dots$ and all z with $\text{Im } z \neq 0$. Then the wave operators $W_{\pm}(H, H_0)$ exist and are complete.

Theorem 1.5 was proved in [3] for $n = 1$ and in [17] for arbitrary n . For semi-bounded operators, Theorem 1.5 follows from the Invariance Principle, due to Birman [1].

THEOREM 1.6. *Suppose that $\varphi(H) - \varphi(H_0) \in \mathfrak{S}_1$ for a real function φ such that its derivative φ' is absolutely continuous and $\varphi'(\lambda) > 0$. Then the wave operators $W_{\pm}(H, H_0)$ exist and*

$$W_{\pm}(H, H_0) = W_{\pm}(\varphi(H), \varphi(H_0)).$$

The operators $W_{\pm}(H, H_0)$ should be replaced here by $W_{\mp}(H, H_0)$ if φ' is negative.

3. A typical result of trace class theory in applications to differential operators is the following

THEOREM 1.7. *Let $H_0 = -\Delta + v_0(x)$ and $H = -\Delta + v_0(x) + v(x)$ on $L^2(\mathbb{R})$. Assume that $v_0 = \bar{v}_0$ is bounded and $v = \bar{v}$ satisfies*

$$|v(x)| \leq C \langle x \rangle^{-\rho}, \quad \langle x \rangle = (1 + |x|^2)^{1/2}, \quad (1.6)$$

for some $\rho > d$. Then the wave operators $W_{\pm}(H, H_0)$ exist and are complete.

For simplicity we shall give the *proof* only for $d = 1, 2$ or 3 . We proceed from Theorem 1.5 for $n = 1$. Choose $c > 0$ large enough so that $H_0 + c$ and $H + c$ are invertible. Then

$$(H + c)^{-1} - (H_0 + c)^{-1} = -(H + c)^{-1}V(H_0 + c)^{-1}.$$

Denote temporarily $H_{00} = -\Delta$. Since the operators

$$(H + c)^{-1}(H_{00} + c) = \text{Id} - (H + c)^{-1}(V_0 + V)$$

and, similarly, $(H_{00} + c)(H_0 + c)^{-1}$ are bounded, it suffices to check that

$$(H_{00} + c)^{-1}V(H_{00} + c)^{-1} = \left((H_{00} + c)^{-1}|V|^{1/2} \right) \text{sgn } v \left(|V|^{1/2}(H_{00} + c)^{-1} \right) \in \mathfrak{S}_1. \quad (1.7)$$

Note that $\Phi(H_{00} + c)^{-1}|V|^{1/2}$ is an integral operator with kernel

$$(2\pi)^{-d/2} e^{-ix \cdot \xi} (|\xi|^2 + c)^{-1} |v(x)|^{1/2},$$

which is evidently in $L^2(\mathbb{R}^{\neq})$. Thus, the operators $(H_{00} + c)^{-1}|V|^{1/2}$ and its adjoint $|V|^{1/2}(H_{00} + c)^{-1}$ are Hilbert-Schmidt and hence (1.7) holds.

Using Theorem 1.5 for $n > d/2 - 1$, it is easy (see [4], for details) to extend this result to an arbitrary d . On the contrary, the condition $\rho > d$ in (1.6) cannot be improved in the trace-class framework.

4. Theorem 1.4 admits the following generalization (see [26]) to the wave operators (1.5).

THEOREM 1.8. *Suppose that $V = HJ - JH_0 \in \mathfrak{S}_1$. Then the wave operators $W_{\pm}(H, H_0; J)$ exist.*

This result due to Pearson allows to simplify considerably the original proof of Theorem 1.4 and of its different generalizations. Although still rather sophisticated, the proof of Theorem 1.8 relies only on the following elementary lemma of Rosenblum.

LEMMA 1.9. *For a self-adjoint operator H , consider the set $\mathfrak{R} \subset \mathcal{H}^{ac}$ of elements f such that*

$$r_H^2(f) := \text{ess-sup } d(E(\lambda)f, f)/d\lambda < \infty.$$

If G is a Hilbert-Schmidt operator, then for any $f \in \mathfrak{R}$

$$\int_{-\infty}^{\infty} \|G \exp(-iHt)f\|^2 dt \leq 2\pi r_H^2(f) \|G\|_2^2.$$

Moreover, the set \mathfrak{R} is dense in \mathcal{H}^{ac} .

The wave operators were defined in terms of exponentials, e^{-itH} . There is also a ‘stationary’ approach, in which the exponentials are replaced by the resolvents $R(z) = (H - z)^{-1}$, $z = \lambda \pm i\varepsilon$, and the limit $t \rightarrow \pm\infty$ is replaced by the limit $\varepsilon \rightarrow 0$. In the trace class framework a consistent stationary approach was developed in the paper [2]. From analytical point of view it relies on the following result on boundary values of resolvents which is interesting in its own sake.

PROPOSITION 1.10. *Let H be a self-adjoint operator and let G_1, G_2 be arbitrary Hilbert-Schmidt operators. Then the operator-function $G_1 R(\lambda + i\varepsilon) G_2$ has limits as $\varepsilon \rightarrow 0$ (and $G_1 R(z) G_2$ has angular boundary values as $z \rightarrow \lambda \pm i0$) in the Hilbert-Schmidt class for almost all $\lambda \in \mathbb{R}$. Moreover, the operator-function $G_1 E(\lambda) G_2$ is differentiable in the trace norm for almost all $\lambda \in \mathbb{R}$.*

In particular, Proposition 1.10 allows one to obtain a stationary proof of the Pearson theorem (see the book [33]).

2. SMOOTH METHOD. SHORT RANGE SCATTERING THEORY

1. The smooth method relies on a certain regularity of the perturbation in the spectral representation of the operator H_0 . There are different ways to understand regularity. For example, in the Friedrichs-Faddeev model [7] H_0 acts as multiplication by independent variable in the space $\mathcal{H} = L_2(\Lambda; \mathfrak{H})$ where Λ is an interval and \mathfrak{H} is an auxiliary Hilbert space. The perturbation V is an integral operator with sufficiently smooth kernel.

Another possibility is to use the concept of H -smoothness introduced by T. Kato in [18].

DEFINITION 2.1. *Let G be an H -bounded operator; that is, suppose that $G(H+i)^{-1}$ is bounded. Then we say that G is H -smooth if there is a $C < \infty$ such that*

$$\int_{-\infty}^{\infty} \|Ge^{-iHt}f\|^2 dt \leq C^2 \|f\|^2 \quad (2.1)$$

for all $f \in \mathcal{H}$ or, equivalently,

$$\sup_{\text{Im } z \neq 0} \|G(R(z) - R(\bar{z}))G^*\| \leq 2\pi C^2. \quad (2.2)$$

In applications the assumption of H -smoothness of an operator G imposes too stringent conditions on the operator H . In particular, the operator H is necessarily absolutely continuous if kernel of G is trivial. This excludes eigenvalues and other singular points in the spectrum of H , for example, the bottom of the continuous spectrum for the Schrödinger operator with decaying potential or edges of bands if the spectrum has the band structure. However it is often suffices to verify H -smoothness of the operators $GE(X_n)$ where the union of intervals X_n exhausts \mathbb{R} up to a set of the Lebesgue measure zero. In this case we say that G is locally H -smooth.

We have the following

THEOREM 2.2. *Let $H - H_0 = G^*G_0$, where G_0 is locally H_0 -smooth and G is locally H -smooth. Then the wave operators $W_{\pm}(H, H_0)$ exist and are complete.*

This is a very useful theorem, yet the proof is totally elementary. To make it even more simple, we forget about the word ‘locally’ and assume that G_0 is H_0 -smooth and G is H -smooth. We write

$$\lim_{t \rightarrow \pm\infty} (e^{iHt}e^{-tH_0t}f_0, f) = (f_0, f) + \lim_{t \rightarrow \pm\infty} i \int_0^t (G_0e^{-sH_0}f_0, Ge^{-iHs}f) ds.$$

Since the left and right hand sides of the last inner product are $L^2(\mathbb{R})$, the limit on the right hand side exists. This shows existence of the *weak* limit. To show the strong limit, we estimate using (2.1)

$$\begin{aligned} |(e^{iHt}e^{-tH_0t}f_0, f) - (e^{iHt'}e^{-tH_0t'}f_0, f)| &= \left| \int_{t'}^t (G_0e^{-sH_0}f_0, Ge^{-iHs}f) ds \right| \\ &\leq C \|f\| \left(\int_{t'}^t \|G_0e^{-sH_0}f_0\|^2 ds \right)^{1/2}. \end{aligned}$$

Taking the sup over f with $\|f\| = 1$, we obtain

$$\|e^{iHt}e^{-tH_0t}f_0 - e^{iHt'}e^{-tH_0t'}f_0\| \leq C \left(\int_{t'}^t \|G_0e^{-sH_0}f_0\|^2 ds \right)^{1/2}$$

which goes to zero as t', t tend to infinity.

Of course Theorem 2.2 is not effective since the verification of H_0 - and especially of H -smoothness may be a difficult problem. In the following assertion the hypothesis only concerns the free resolvent, $R_0(z) = (H_0 - z)^{-1}$.

THEOREM 2.3. *Suppose V can be written in the form $V = G^*\Omega G$, where Ω is a bounded operator and $GR_0(z)G^*$ is compact for $\text{Im } z \neq 0$, and is norm-continuous up to the real axis except possibly at a finite number of points λ_k , $k = 1, \dots, N$. Then $W_{\pm}(H, H_0)$ exist and are complete.*

We give only a brief sketch of its proof. Set

$$X_n = (-n, n) \setminus \bigcup_{k=1}^N (a_k - n^{-1}, a_k + n^{-1}).$$

Since $\|GR_0(\lambda \pm i\varepsilon)G^*\|$ is uniformly bounded for $\lambda \in X_n$, the operator $GE_0(X_n)$ is H_0 -smooth (cf. the definition (2.2)).

To show a similar result for the operator-function $GR(z)G^*$, we use the resolvent identity

$$R(z) = R_0(z) - R_0(z)VR(z), \quad (2.3)$$

whence

$$GR(z)G^* = \left(\text{Id} + GR_0(z)G^*\Omega \right)^{-1} GR_0(z)G^*, \quad \text{Im } z \neq 0. \quad (2.4)$$

It easily follows from self-adjointness of the operator H that the homogeneous equation

$$f + GR_0(z)G^*\Omega f = 0 \quad (2.5)$$

has only the trivial solution $f = 0$ for $\text{Im } z \neq 0$. Since the operator $GR_0(z)G^*$ is compact, this implies that the inverse operator in (2.4) exists. By virtue of equation (2.4), the operator-function $GR(z)G^*$ is continuous up to the real axis except the points λ_k and the set \mathcal{N} of λ such that the equation (2.5) has a non-trivial solution for $z = \lambda + i0$ or $z = \lambda - i0$. The set \mathcal{N} is obviously closed. Moreover, it has the Lebesgue measure zero by the analytical Fredholm alternative. This implies that the pair G, H also satisfies the conditions of Theorem 2.2. It remains to use this theorem.

2. Let us return to the Schrödinger operator $H = -\Delta + v$. Potentials v satisfying (1.6) with $\rho > 1$ are said to be *short range*. Below in this lecture we make this assumption. Let us apply Theorem 2.3 to the pair $H_0 = -\Delta, H$. Put $r = \rho/2$ and $G = \langle x \rangle^{-r}$. One can verify (cf. the proof of Theorem 1.7) that $GR_0(z)G^*$ is compact for $\text{Im } z \neq 0$ (and arbitrary $r > 0$). Next we consider the spectral family $E_0(\lambda)$ which according to (1.2) satisfies

$$d(E_0(\lambda)f, f)/d\lambda = \|\Gamma_0(\lambda)f\|^2, \quad (2.6)$$

where

$$(\Gamma_0(\lambda)f)(\omega) = 2^{-1/2}\lambda^{(d-2)/4}\hat{f}(\sqrt{\lambda}\omega) \quad (2.7)$$

and $\hat{f} = \Phi f$ is the Fourier transform of a function f from, say, the Schwartz class. Thus, up to a numerical factor, $\Gamma_0(\lambda)f$ is the restriction of \hat{f} to the sphere of radius

$\sqrt{\lambda}$. Remark further that if $f \in \langle x \rangle^{-r} L^2(\mathbb{R})$, then \hat{f} belongs to the Sobolev space $H^r(\mathbb{R})$. Since $r > 1/2$, it follows from the Sobolev trace theorem that the operator

$$\Gamma_0(\lambda) \langle x \rangle^{-r} : L^2(\mathbb{R}) \rightarrow \mathbb{L}^{\neq}(\mathbb{S}^{-\neq})$$

is bounded and depends (in the operator norm) Hölder continuously on $\lambda > 0$. Therefore according to (2.6) the operator-function $GE_0(\lambda)G$ is differentiable and its derivative is also Hölder continuous. Now we use the representation

$$(R_0(z)Gf, Gf) = \int_0^\infty (\lambda - z)^{-1} d(E_0(\lambda)Gf, Gf),$$

which, by the Privalov theorem, implies that the operator-function $GR_0(z)G$ is continuous in the closed complex plane cut along $[0, \infty)$ except, possibly, the point $z = 0$. Applying Theorem 2.3, we now obtain

THEOREM 2.4. *Let v be short range. Then the wave operators $W_\pm(H, H_0)$ for the pair (1.1) exist and are complete.*

Theorem 2.4 implies that for every $f \in \mathcal{H}^{-1}$, there is f_0^\pm such that relation (1.3) holds. Using the well-known expression for kernel of the integral operator e^{-itH_0} (in the x -representation), we find that

$$(e^{-itH}f)(x) \sim e^{i|x|^2/4t} (2it)^{-d/2} \hat{f}_0^\pm(x/2t). \quad (2.8)$$

Here ‘ \sim ’ means that the difference of the left and right hand sides tends to zero in $L^2(\mathbb{R}^d)$ as $t \rightarrow \pm\infty$. Thus, the solution ‘lives’ in the region $|x| \sim |t|$ of (x, t) space.

As a by-product of our considerations we obtain that the operator-function $GR(z)G$ is continuous up to real axis, except a closed set of measure zero. More detailed analysis shows that this set consists of eigenvalues of the operator H (and possibly the point zero), so that the singular continuous spectrum of H is empty. Finally, we note that, by the Kato theorem, the operator H does not have positive eigenvalues. This gives the following assertion known as the limiting absorption principle.

THEOREM 2.5. *Let v be short range and $r > 1/2$. Then the operator-function $\langle x \rangle^{-r} R(z) \langle x \rangle^{-r}$ is norm-continuous in the closed complex plane cut along $[0, \infty)$ except negative eigenvalues of the operator H and, possibly, the point $z = 0$.*

3. Let us compare Theorems 1.7 and 2.4. If $v_0 = 0$, then Theorem 2.4 is stronger because, in assumption (1.6), it requires that $\rho > 1$ whereas Theorem 1.7 requires that $\rho > d$. Theorem 2.4 can be extended to some other cases, for example to periodic and long-range v_0 . In the first case the spectral family $E_0(\cdot)$ can be constructed rather explicitly. In the second case the limiting absorption principle can be also verified (see the next lecture). However, contrary to Theorem 1.7, the method of proof of Theorem 2.4 gives nothing for arbitrary $v_0 \in L^\infty$. Therefore the following question naturally arises.

Problem. Let $H_0 = -\Delta + v_0(x)$ and $H = -\Delta + v_0(x) + v(x)$ where v satisfies estimate (1.6) for $\rho > 1$. Do the wave operators $W_\pm(H, H_0)$ exist for an arbitrary $v_0 \in L^\infty$?

This problem is of course related to unification of trace class and smooth approaches. The following theorem does this to some extent:

THEOREM 2.6. *Assume that V is of the form $V = G^*\Omega G$, where Ω is a bounded operator, $GR_0(z)G^* \in \mathfrak{S}_p$ for some $p < \infty$, and $GR_0(z)G^*$ has angular boundary values in \mathfrak{S}_p for almost every $\lambda \in \mathbb{R}$. Then $W_{\pm}(H, H_0)$ exist and are complete.*

Note that, given Proposition 1.10, Theorem 2.6 provides an independent proof of Theorem 1.4. On the other hand, it resembles Theorem 2.3 of the smooth approach. However it gives nothing for the solution of the problem formulated above. Most probably, the answer to the formulated question is negative, which can be considered as a strong evidence that a real unification of trace class and smooth approaches does not exist.

4. The stationary method is intimately related to eigenfunction expansions of the operators H_0 and H . Let us discuss this relation on the example of the Schrödinger operator H with a short range potential. For the operator $H_0 = -\Delta$, the construction of eigenfunctions is obvious. Actually, if $\psi_0(x, \omega, \lambda) = e^{i\sqrt{\lambda}\omega \cdot x}$, then $-\Delta\psi_0 = \lambda\psi_0$. This collection of eigenfunctions is ‘complete’, so eigenfunctions are parametrized by $\omega \in \mathbb{S}^{d-1}$ (for fixed $\lambda > 0$). By the intertwining property, the wave operators $W_{\pm}(H, H_0)$ diagonalize H and hence

$$HW_{\pm}\Phi^* = |\xi|^2W_{\pm}\Phi^*.$$

Thus, at least formally, eigenfunctions of H , that is, solutions of the equation

$$-\Delta\psi + v\psi = \lambda\psi, \quad (2.9)$$

can be constructed by one of the two equalities $\psi_+(\omega, \lambda) = W_+\psi_0(\omega, \lambda)$ or $\psi_-(\omega, \lambda) = W_-\psi_0(\omega, \lambda)$.

It turns out that this definition can be given a precise sense, and one can construct solutions of the Schrödinger equation with asymptotics $\psi_0(x, \omega, \lambda)$ at infinity.

THEOREM 2.7. *Assume (1.6) is valid for some $\rho > d$. For every $\lambda > 0$ and $\omega \in \mathbb{S}^{d-1}$ there is a solution ψ of (2.9) such that*

$$\psi(x, \omega, \lambda) = e^{i\sqrt{\lambda}\omega \cdot x} + a(\hat{x}, \omega, \lambda)|x|^{-(d-1)/2}e^{i\sqrt{\lambda}|x|} + o(|x|^{-(d-1)/2}), \quad \hat{x} = x/|x|, \quad (2.10)$$

where a is a continuous function on $\mathbb{S}^{d-1} \times \mathbb{S}^{d-1}$.

We interpret the $e^{i\sqrt{\lambda}\omega \cdot x}$ term as an incoming plane wave, the $|x|^{-(d-1)/2}e^{i\sqrt{\lambda}|x|}$ term as an outgoing spherical wave, and the coefficient $a(\hat{x}, \omega, \lambda)$ is called the *scattering amplitude* for the incident direction ω and the direction of observation \hat{x} . Note that a solution of the Schrödinger equation is determined uniquely by the condition that, asymptotically, it is a sum of a plane and the outgoing spherical waves.

Under assumption (1.6) where $\rho > (d+1)/2$, eigenfunctions of the operator H may be constructed by means of the following formula:

$$\psi(\omega, \lambda) = \psi_0(\omega, \lambda) - R(\lambda + i0)V\psi_0(\omega, \lambda), \quad (2.11)$$

or, equivalently, as solutions of the Lippman-Schwinger equation

$$\psi(\omega, \lambda) = \psi_0(\omega, \lambda) + R_0(\lambda + i0)V\psi(\omega, \lambda).$$

We note that, strictly speaking, the second term in the right hand side of (2.11) is defined by the equality

$$R(\lambda + i0)V\psi_0(\omega, \lambda) = R(\lambda + i0)\langle x \rangle^{-1/2-\epsilon}(V\langle x \rangle^{(d+1)/2+2\epsilon})(\langle x \rangle^{-d/2-\epsilon}\psi_0(\omega, \lambda)), \quad (2.12)$$

where $\epsilon > 0$ is sufficiently small. Here $\langle x \rangle^{-d/2-\epsilon}\psi_0(\lambda, \omega) \in L^2(\mathbb{R}^d)$ and the operator $V\langle x \rangle^{(d+1)/2+2\epsilon}$ is bounded. Therefore, by the limiting absorption principle (Theorem 2.5), the function (2.12) belongs to the space $\langle x \rangle^{1/2+\epsilon}L^2(\mathbb{R}^d)$ for any $\epsilon > 0$. The asymptotics (2.10) is still true for arbitrary $\rho > (d+1)/2$ if the remainder $e(x) = o(|x|^{-(d-1)/2})$ is understood in the following averaged sense:

$$e(x) = o_{av}(|x|^{-(d-1)/2}) \iff \lim_{R \rightarrow \infty} \frac{1}{R} \int_{|x| \leq R} |e(x)|^2 dx = 0.$$

In this case the scattering amplitude $a(\hat{x}, \omega, \lambda)$ belongs to the space $L^2(\mathbb{S}^{d-1})$ in the variable \hat{x} uniformly in $\omega \in \mathbb{S}^{d-1}$.

It is often convenient to write ψ in terms of the parameter $\xi = \sqrt{\lambda}\omega \in \mathbb{R}$, instead of (ω, λ) . Thus, we set

$$\psi_-(x, \xi) = \psi(x, \omega, \lambda), \quad \psi_+(x, \xi) = \overline{\psi_-(x, -\xi)}.$$

The Schwartz kernels of the wave operators are intimately related to eigenfunctions. In fact, if we define ‘distorted Fourier transforms’ Φ_{\pm} by

$$(\Phi_{\pm}f)(\xi) = (2\pi)^{-d/2} \int_{\mathbb{R}^d} \overline{\psi_{\pm}(x, \xi)} f(x) dx,$$

so that $\Phi_{\pm}H = |\xi|^2\Phi_{\pm}$, then we have

$$W_{\pm} = \Phi_{\pm}^* \Phi_0, \quad (2.13)$$

where $\Phi_0 = \Phi$ is the classical Fourier transform. Notice that the right hand side is defined purely in terms of time-independent quantities. This can be taken to be the *definition* of the wave operators in the stationary approach to scattering theory. Historically, it was the first approach to the study of wave operators suggested by Povzner in [27, 28] and developed further in [10]. Under optimal assumption $\rho > 1$ in (1.6) Theorem 2.4 was obtained in [21].

It follows from (2.13) that the scattering operator

$$\mathbf{S} = W_+^* W_- = \Phi_0^* \Phi_+ \Phi_-^* \Phi_0. \quad (2.14)$$

Let H_0 be realized (via the Fourier transform) as multiplication by λ in the space $L^2(\mathbb{R}^+; \mathbb{L}^{\neq}(\mathbb{S}^{-\mathbb{K}}))$. Since \mathbf{S} commutes with H_0 and is unitary, it acts in this representation as multiplication by the operator-function (scattering matrix) $S(\lambda) : L^2(\mathbb{S}^{d-1}) \rightarrow L^2(\mathbb{S}^{d-1})$ which is also unitary for all $\lambda > 0$. It can be deduced from (2.14) that

$$(S(\lambda)f)(\omega) = f(\omega) + \gamma c(\lambda) \int_{\mathbb{S}^{d-1}} a(\omega, \omega', \lambda) f(\omega') d\omega', \quad (2.15)$$

where a is the scattering amplitude defined by (2.10) and

$$\gamma = e^{\pi i(d-3)/4}, \quad c(\lambda) = i(2\pi)^{-(d-1)/2} \lambda^{(d-1)/4}.$$

If assumption (1.6) is satisfied for $\rho > 1$ only, then the scattering matrix satisfies the relation

$$S(\lambda) = \text{Id} - 2\pi i \Gamma_0(\lambda) \left(V - VR(\lambda + i0)V \right) \Gamma_0^*(\lambda), \quad (2.16)$$

which generalizes (2.15). Here $\Gamma_0(\lambda)$ is the operator (2.7). Since $\langle x \rangle^{-r} V \langle x \rangle^{-r}$ is a bounded operator for $r = \rho/2 > 1/2$, we see that (2.16) is correctly defined. It follows from formula (2.16) that the operator $S(\lambda) - \text{Id}$ is compact. Thus, the spectrum of $S(\lambda)$ (which lies on the unit circle by unitarity) is discrete, and may accumulate only at the point 1. Moreover, if

$$|\partial^\alpha v(x)| \leq C_\alpha \langle x \rangle^{-\rho-|\alpha|} \quad (2.17)$$

for all multi-indices α (and $\rho > 1$), then the kernel $k(\omega, \omega')$ of the operator $S(\lambda) - \text{Id}$ is smooth for $\omega \neq \omega'$ and $|k(\omega, \omega')| \leq C|\omega - \omega'|^{-d+\rho}$.

For $\rho \in (1, (d+1)/2]$, construction of eigenfunctions, which behave asymptotically as plane waves, becomes a difficult problem. In particular, formula (2.11) makes no sense in this case. One can do something, but the construction of [32] is rather complicated and requires the condition (2.17). On the contrary, for arbitrary $\rho > 1$ we can construct solutions which formally correspond to averaging of $\psi(x, \omega, \lambda)$ over $\omega \in \mathbb{S}^{d-1}$. To illustrate this idea, let us first consider the free case $v = 0$. Then, for any $b \in C^\infty(\mathbb{S}^{d-1})$, the function

$$u(x) = \int_{\mathbb{S}^{d-1}} e^{i\sqrt{\lambda}\omega \cdot x} b(\omega) d\omega$$

satisfies $-\Delta u = \lambda u$ and, by the stationary phase arguments, it has asymptotics

$$u(x) = c(\lambda)^{-1} |x|^{-(d-1)/2} \left(\bar{\gamma} b(\hat{x}) e^{i\sqrt{\lambda}|x|} - \gamma b(-\hat{x}) e^{-i\sqrt{\lambda}|x|} \right) + o(|x|^{-(d-1)/2}).$$

In the general case one can also construct solutions of the Schrödinger equation (2.9) with the asymptotics of incoming and outgoing spherical waves.

THEOREM 2.8. *Assume (1.6) is valid for some $\rho > 1$. Let u be a solution of the Schrödinger equation (2.9) satisfying*

$$\int_{|x| \leq R} |u(x)|^2 dx \leq CR, \text{ for all } R \geq 1.$$

Then there are $b_\pm \in L^2(\mathbb{S}^{d-1})$ such that

$$u(x) = |x|^{-(d-1)/2} \left(\bar{\gamma} b_+(\hat{x}) e^{i\sqrt{\lambda}|x|} - \gamma b_-(-\hat{x}) e^{-i\sqrt{\lambda}|x|} \right) + o_{av}(|x|^{-(d-1)/2}). \quad (2.18)$$

Functions b_\pm are related by the scattering matrix: $b_+ = S(\lambda)b_-$. Conversely, for all $b_+ \in L^2(\mathbb{S}^{d-1})$ (or $b_- \in L^2(\mathbb{S}^{d-1})$), there is a unique function $b_- \in L^2(\mathbb{S}^{d-1})$ (or $b_+ \in L^2(\mathbb{S}^{d-1})$), and a unique solution u of (2.9) satisfying (2.18).

3. LONG RANGE SCATTERING THEORY

There are different and, to a large extent, independent methods in long range scattering (see [36]). Here we shall give a brief presentation of the approach of the paper [34] which relies on the theory of smooth perturbations.

1. The condition (1.6) with $\rho > 1$ is optimal even for the existence of wave operators for the pair $H_0 = -\Delta$, $H = -\Delta + v(x)$. For example, the wave operators do not exist if $v(x) = v_0 \langle x \rangle^{-1}$, $v_0 \neq 0$. Nevertheless the asymptotic behaviour of

the function $\exp(-iHt)f$ for large $|t|$ remains sufficiently close to the free evolution $\exp(-iH_0t)f_0$ if the condition (2.17) is satisfied for $|\alpha| \leq \alpha_0$ with α_0 big enough. Potentials obeying this condition for some $\rho \in (0, 1]$ are called long-range.

There are several possible descriptions of $\exp(-iHt)f$ as $t \rightarrow \pm\infty$. One of them is a modification of the free evolution which, in its turn, can be done either in momentum or in coordinate representations. Here we discuss the coordinate modification. Motivated by (2.8), we set

$$(U_0(t)f)(x) = \exp(i\Xi(x, t))(2it)^{-d/2} \hat{f}(x/(2t)), \quad (3.1)$$

where the choice of the phase function Ξ depends on v . Then the wave operators are defined by the equality

$$W_{\pm} = s\text{-}\lim_{t \rightarrow \pm\infty} e^{iHt}U_0(t). \quad (3.2)$$

To be more precise, these limits exist if the function $\Xi(x, t)$ is a (perhaps, approximate) solution of the eikonal equation

$$\partial\Xi/\partial t + |\nabla\Xi|^2 + v = 0.$$

For example, if $\rho > 1/2$, we can neglect here the nonlinear term $|\nabla\Xi|^2$ and set

$$\Xi(x, t) = (4t)^{-1}|x|^2 - t \int_0^1 v(sx)ds. \quad (3.3)$$

In the general case one obtains an approximate solution of the eikonal equation by the method of successive approximations. With the phase $\Xi(x, t)$ constructed in such a way, for an arbitrary $\hat{f} \in C_0^\infty(\mathbb{R}^d \setminus \{0\})$, the function $U_0(t)f$ is an approximate solution of the time-dependent Schrödinger equation in the sense that

$$\left| \int_1^{\pm\infty} \|(i\partial/\partial t - H)U_0(t)f\| dt \right| < \infty.$$

This condition implies that the vector-function $\partial e^{iHt}U_0(t)f/\partial t \in L^1(\mathbb{R})$ and hence the limit (3.2) exists. The modified wave operators have all the properties of usual wave operators. They are isometric, $W_{\pm}H_0 = HW_{\pm}$ and $\text{ran } W_{\pm} \subset \mathcal{H}^{\uparrow}$. As in the short-range case, the wave operator is said to be complete if $\text{ran } W_{\pm} = \mathcal{H}^{\uparrow}$. Only the completeness of W_{\pm} is a non-trivial mathematical problem. As we shall see below, it has a positive solution which implies that for every $f \in \mathcal{H}^{\uparrow}$, there is f_0^{\pm} such that (cf. (2.8))

$$(e^{-itH}f)(x) \sim e^{i\Xi(x, t)}(2it)^{-d/2} \hat{f}_0^{\pm}(x/2t). \quad (3.4)$$

Thus, in the short and long range cases, the large time asymptotics of solutions of the time-dependent Schrödinger equation differ only by the phase factor. In particular, in both cases they live in the region $|x| \sim |t|$ of (x, t) space.

2. For the proof of completeness of wave operators, we need some analytical results which we discuss now. Note first of all that the limiting absorption principle, Theorem 2.5, remains true if assumption (2.17) is satisfied for some $\rho > 0$ and $|\alpha| \leq 1$. However perturbative arguments of the previous lecture do not work for long range potentials. The simplest proof (see the original paper [24] or the book

[6]) of the limiting absorption principle relies in this case on the Mourre estimate:

$$iE(I)[H, A]E(I) \geq cE(I), \quad A = -i \sum_{j=1}^d (\partial_j x_j + x_j \partial_j), \quad c > 0, \quad (3.5)$$

where I is a sufficiently small interval about a given $\lambda > 0$. This is not too hard to prove for long-range two body potentials (but is much harder for multiparticle operators). To be more precise, the Mourre estimate implies that the operator-function $\langle x \rangle^{-r} R(z) \langle x \rangle^{-r}$ is norm-continuous up to positive half-axis, except a discrete set of eigenvalues of the operator H . In particular, the operator $\langle x \rangle^{-r}$ is locally H -smooth which is sufficient for scattering theory. Moreover, independent arguments (see, e.g., [30]) show that the Schrödinger operator H does not have positive eigenvalues.

Unfortunately, the operator $\langle x \rangle^{-1/2}$ is *not* (locally) H -smooth even in the case $v = 0$. However, there is a substitute:

THEOREM 3.1. *Let assumption (2.17) be satisfied for some $\rho > 0$ and $|\alpha| \leq 1$. Set*

$$(\nabla_j^\perp u)(x) = (\partial_j u)(x) - |x|^{-2} ((\nabla u)(x) \cdot x) x_j, \quad j = 1, \dots, d.$$

Then the operators $\langle x \rangle^{-1/2} \nabla_j^\perp E(\Lambda)$ are H -smooth for any compact $\Lambda \subset (0, \infty)$.

The *proof* is based on the equality

$$2|x|^{-1} \sum_{j=1}^d |\nabla_j^\perp u|^2 = ([H, \partial_r]u, u) + (v_1 u, u), \quad v_1(x) = O(|x|^{-1-\rho}),$$

which is obtained by direct calculation. Since $\langle x \rangle^{-(1+\rho)/2} E(\Lambda)$ is H -smooth, we only have to consider the term $[H, \partial_r]$. For this we note that

$$i \int_0^t ([H, \partial_r] e^{-isH} f, e^{-isH} f) ds = (\partial_r e^{-itH} f, e^{-itH} f) - (\partial_r f, f).$$

For $f \in \text{ran } E(\Lambda)$, the right hand side is bounded by $C(\Lambda) \|f\|^2$, so this shows H -smoothness of the operators $\langle x \rangle^{-1/2} \nabla_j^\perp E(\Lambda)$.

Note that the commutator method used for the proof of Theorem 3.1 goes back to Putnam [29] and Kato [20].

3. Our proof of completeness relies on consideration of wave operators (1.5) with a specially chosen operator J . Let us look for J in the form of a pseudodifferential operator

$$(Jf)(x) = (2\pi)^{-d/2} \int_{\mathbb{R}^d} e^{ix \cdot \xi} p(x, \xi) \hat{f}(\xi) d\xi. \quad (3.6)$$

We shall work in the class of symbols $\mathcal{S}_{\rho, \delta}^m$ consisting of functions $p(x, \xi) \in C^\infty(\mathbb{R} \times \mathbb{R})$ satisfying the estimates

$$|\partial_x^\alpha \partial_\xi^\beta p(x, \xi)| \leq C_{\alpha, \beta} \langle x \rangle^{m - \rho|\alpha| + \delta|\beta|}$$

for all multi-indices α and β . In addition, we shall assume that p vanishes for $|\xi| \geq R$, for some R . The number m is called the *order* of the symbol, and of the corresponding pseudodifferential operator. Compared to the usual calculus, here the roles of x and ξ are interchanged: we require some decay estimates as $|x| \rightarrow \infty$, rather than as $|\xi| \rightarrow \infty$ in the usual situation. We shall assume that

$0 \leq \delta < 1/2 < \rho \leq 1$. The symbol $p(x, \xi)$ of the operator J belongs to the class $\mathcal{S}_{\rho, \delta}^0$. We recall that operators of order zero are bounded on $L^2(\mathbb{R}^d)$.

Since

$$de^{iHt} J e^{-iH_0 t} / dt = ie^{iHt} (HJ - JH_0) e^{-iH_0 t},$$

it is desirable to find such J that the *effective perturbation* $HJ - JH_0$ be short-range (a pseudodifferential operator of order $-1 - \varepsilon$ for $\varepsilon > 0$). This means that $\psi(x, \xi) = e^{ix \cdot \xi} p(x, \xi)$ is an approximate eigenfunction of the operator H , with eigenvalue $|\xi|^2$, for each ξ . Let us look for ψ in the form $\psi(x, \xi) = e^{i\phi(x, \xi)}$. Then

$$(-\Delta + v(x) - |\xi|^2)\psi = (|\nabla\phi|^2 + v(x) - |\xi|^2 - i\Delta\phi)\psi,$$

which leads to the eikonal equation

$$|\nabla\phi|^2 + v(x) = |\xi|^2.$$

Suppose that

$$\phi(x, \xi) = x \cdot \xi + \Phi(x, \xi), \quad (3.7)$$

where

$$\partial_x^\alpha \partial_\xi^\beta \Phi(x, \xi) = O(|x|^{1-\rho-|\alpha|}). \quad (3.8)$$

Then

$$|\nabla\phi|^2 + v(x) - |\xi|^2 = 2\xi \cdot \nabla\Phi + |\nabla\Phi|^2 + v(x) \quad (3.9)$$

and neglecting the nonlinear term we obtain the equation

$$2\xi \cdot \nabla_x \Phi + v(x) = 0. \quad (3.10)$$

We need its two solutions given by the equalities

$$\Phi_\pm(x, \xi) = \pm \frac{1}{2} \int_0^\infty (v(x \pm t\xi) - v(\pm t\xi)) dt. \quad (3.11)$$

Clearly, these functions Φ_\pm satisfy assumption (3.8) but only off a conic neighbourhood of $x = \mp\xi$.

Thus, two problems arise. The first is that, to obtain in (3.6) a symbol p_\pm from the class $\mathcal{S}_{\rho, \delta}^0$, we need to remove by a cut-off function $\zeta_\pm(x, \xi)$ a small conic neighbourhood of the set $\hat{x} = \mp\hat{\xi}$. Thus, we are obliged to consider the wave operators for two different operators J_\pm . This idea appeared in [11] and will be realized below. The second problem is that the term $|\nabla\Phi|^2$ neglected in (3.9) is ‘short range’ only for $\rho > 1/2$. Of course, it is easy to solve the eikonal equation by iterations, considering at each step a linear equation of type (3.10), and to obtain a ‘short range’ error for arbitrary $\rho > 0$. However, even after the cut-off by the function $\zeta_\pm(x, \xi)$, we obtain the symbol p_\pm from the class $\mathcal{S}_{\rho, 1-\rho}^0$, which is bad if $\rho \leq 1/2$. To overcome this difficulty, we need to take into account the oscillating nature of p_\pm (see [35]).

4. Below we suppose that $\rho > 1/2$. Let $\sigma_\pm \in C^\infty$ be such that $\sigma_\pm(\theta) = 1$ near ± 1 and $\sigma_\pm(\theta) = 0$ near ∓ 1 . We construct J_\pm by the formula (3.6) where

$$p_\pm(x, \xi) = e^{i\Phi_\pm(x, \xi)} \zeta_\pm(x, \xi) \quad (3.12)$$

and the cut-off function $\zeta_\pm(x, \xi)$ essentially coincides with $\sigma_\pm(\langle \hat{x}, \hat{\xi} \rangle)$. We deliberately ignore here some technical details which can be found in [34]. For example, strictly speaking, additional cut-offs of low and high energies by a function of $|\xi|^2$

and of a neighbourhood of $x = 0$ by a function of x should be added to $\zeta_{\pm}(x, \xi)$. Then the operators J_{\pm} so constructed are pseudodifferential operators of order 0 and type $(\rho, \delta = 1 - \rho)$.

Note that Theorem 2.2 extends automatically to the wave operators (1.5). Thus, we are looking for a factorization

$$HJ_{\pm} - J_{\pm}H_0 = G^*\Omega G,$$

where G is locally H_0 - and H -smooth and the operator Ω is bounded. Let us recall that the operator $\langle x \rangle^{-r}$ is H -smooth, for any $r > 1/2$. Since zeroth order pseudodifferential operators are bounded on $L^2(\mathbb{R}^d)$, a factorization as above would have been true if $HJ - JH_0$ were of order $-1 - \epsilon$ for some $\epsilon > 0$.

However, the pseudodifferential operator $HJ_{\pm} - J_{\pm}H_0$ has symbol decaying only as $|x|^{-1}$; this is from one derivative of $-\Delta$ hitting $e^{ix \cdot \xi}$ and one hitting ζ_{\pm} . Notice that the symbol of the ‘bad’ term equals

$$-2ie^{i\Phi_{\pm}(x, \xi)} \langle \xi, \nabla_x \sigma_{\pm}(\langle \hat{x}, \hat{\xi} \rangle) \rangle.$$

It only decays as $|x|^{-1}$ but is supported outside a conic neighbourhood of the set where $\hat{x} = \hat{\xi}$ or $\hat{x} = -\hat{\xi}$. Therefore,

$$HJ - JH_0 = \sum_{j=1}^d (\langle x \rangle^{-1/2} \nabla_j^{\perp})^* \Omega_j (\langle x \rangle^{-1/2} \nabla_j^{\perp}) + \langle x \rangle^{-r} \Omega_0 \langle x \rangle^{-r}, \quad r > 1/2,$$

where Ω_j , $j = 0, 1, \dots, d$, are order zero pseudodifferential operators. Using Theorem 3.1 for the first d terms, and the limiting absorption principle for the last one, we obtain

PROPOSITION 3.2. *The wave operators $W_{\pm}(H, H_0, J_{\tau})$ and $W_{\pm}(H_0, H, J_{\tau}^*)$ exist for $\tau = ‘+’$ and $\tau = ‘-’$.*

The next step is to verify

PROPOSITION 3.3. *The operators $W_{\pm}(H, H_0; J_{\pm})$ are isometric and $W_{\pm}(H, H_0; J_{\mp}) = 0$.*

Indeed, it suffices to check that

$$\text{s-} \lim_{t \rightarrow \pm\infty} (J_{\pm}^* J_{\pm} - I) e^{-iH_0 t} = 0 \quad (3.13)$$

and

$$\text{s-} \lim_{t \rightarrow \pm\infty} J_{\mp}^* J_{\mp} e^{-iH_0 t} = 0. \quad (3.14)$$

According to (3.12), up to a compact term, $J_{\mp}^* J_{\mp}$ equals the pseudodifferential operator Q_{\mp} with symbol $\zeta_{\mp}^2(x, \xi)$. If $t \rightarrow \pm\infty$, then the stationary point $\xi = x/(2t)$ of the integral

$$(Q_{\mp} e^{-iH_0 t} f)(x) = (2\pi)^{-d/2} \int_{\mathbb{R}^d} e^{i\langle \xi, x \rangle - i|\xi|^2 t} \zeta_{\mp}^2(x, \xi) \hat{f}(\xi) d\xi \quad (3.15)$$

does not belong to the support of the function $\zeta_{\mp}^2(x, \xi)$. Therefore supposing that $f \in \mathcal{S}(\mathbb{R}^d)$ and integrating by parts, we estimate integral (3.15) by $C_N(1 + |x| + |t|)^{-N}$ for an arbitrary N . This proves (3.14). To check (3.13), we apply the same arguments to the PDO with symbol $\zeta_{\pm}^2(x, \xi) - 1$.

Now it is easy to prove the asymptotic completeness.

THEOREM 3.4. *Suppose that condition (2.17) is fulfilled for $\rho > 1/2$ and all α . Then the wave operators $W_{\pm}(H, H_0; J_{\pm})$ exist, are isometric and complete.*

Since $W_{\pm}(H_0, H; J_{\pm}^*) = W_{\pm}^*(H, H_0; J_{\mp})$, it follows from Proposition 3.3 that $W_{\pm}(H_0, H; J_{\mp}^*) = 0$. This implies that

$$\lim_{t \rightarrow \pm\infty} \|J_{\mp}^* e^{-iHt} f\| = 0, \quad f \in \mathcal{H}^{ac}. \quad (3.16)$$

Let us choose the functions σ_{\pm} in such a way that $\sigma_{+}^2(\theta) + \sigma_{-}^2(\theta) = 1$. Then

$$J_{+} J_{+}^* + J_{-} J_{-}^* = \text{Id} + K$$

for a compact operator K and hence

$$\|J_{+}^* e^{-iHt} f\|^2 + \|J_{-}^* e^{-iHt} f\|^2 = \|f\|^2 + o(1)$$

as $|t| \rightarrow \infty$. Now it follows from (3.16) that

$$\lim_{t \rightarrow \pm\infty} \|J_{\pm}^* e^{-iHt} f\| = \|f\|.$$

This is equivalent to isometricity of the wave operators

$$W_{\pm}(H_0, H; J_{\pm}^*) = W_{\pm}^*(H, H_0; J_{\pm}),$$

so that $W_{\pm}(H, H_0; J_{\pm})$ are complete.

We emphasize that Theorem 3.4 and, essentially, its proof remain valid for an arbitrary $\rho > 0$.

Now it is easy to justify the asymptotics (3.4). By existence and completeness of the wave operator $W_{\pm}(H, H_0, J_{\pm})$, we have

$$\lim_{t \rightarrow \pm\infty} \|e^{-itH} f - J_{\pm} e^{-itH_0} f_0^{\pm}\| = 0, \quad f_0^{\pm} = W_{\pm}(H_0, H, J_{\pm}^*) f.$$

The critical point $\xi(x, t)$ of the integral

$$(J_{\pm} e^{-itH_0} f_0^{\pm})(x) = (2\pi)^{-d/2} \int_{\mathbb{R}^d} e^{ix \cdot \xi} e^{i\Phi_{\pm}(x, \xi)} \zeta_{\pm}(x, \xi) e^{-it|\xi|^2} \hat{f}_0^{\pm}(\xi) d\xi \quad (3.17)$$

is defined by the equation

$$2t\xi(x, t) = x + \nabla_{\xi} \Phi_{\pm}(x, \xi(x, t)), \quad \pm t > 0,$$

so that $\xi(x, t) = x/(2t) + O(|t|^{-\rho})$. Applying stationary phase to the integral (3.17), we obtain formula (3.4) with function

$$\Xi(x, t) = |x|^2/(4t) + \Phi_{\pm}(x, x/(2t)),$$

which equals (3.3).

5. In the long range case the scattering operator \mathbf{S} is defined again by formula (1.4) where $W_{\pm} = W_{\pm}(H, H_0, J_{\pm})$. Thus, again \mathbf{S} is unitary and commutes with H_0 , so defines a family of scattering matrices $S(\lambda)$ which are unitary operators on $L^2(\mathbb{S}^{d-1})$ for $\lambda > 0$.

However the structure of the spectrum of the scattering matrix in the short and long range cases are completely different. Typically, in the long range case the spectrum of $S(\lambda)$ covers the unit circle. The nature of this spectrum is in general not known, except in the radially symmetric case (that is, when the potential v is a function only of $|x|$). In that case, the scattering matrix commutes with the Laplacian on \mathbb{S}^{d-1} , so it breaks up into the orthogonal sum of finite dimensional operators. Hence the spectrum is dense pure point in this case.

The kernel $s(\omega, \omega', \lambda)$ of $S(\lambda)$ is still smooth away from the diagonal, but near the diagonal it, typically, has the form (for $\rho < 1$)

$$s(\omega, \omega', \lambda) \sim c(\omega, \lambda) |\omega - \omega'|^{-(d-1)(1+\rho^{-1})/2} e^{i\theta(\omega, \omega', \lambda)}, \quad (3.18)$$

where $\theta(\omega, \omega', \lambda)$ is asymptotically homogeneous of order $1 - \rho^{-1}$ as $\omega - \omega' \rightarrow 0$.

In the long range case practically nothing is known about eigenfunctions, which behave asymptotically as plane waves. Moreover, as shows the explicit formula (see, e.g., [22]) for the Coulomb potential $v(x) = v_0|x|^{-1}$, in this case the separation of the asymptotics of eigenfunctions into the sum of plane and spherical waves loses, to a large extent, its sense. On the contrary, Theorem 2.8 extends [9] to arbitrary long range potentials.

4. THE SCATTERING MATRIX. HIGH ENERGY AND SMOOTHNESS ASYMPTOTICS

This section relies on the paper [37].

1. Let us begin with the short range case, (1.6) with $\rho > 1$. Then there is a stationary representation (2.16) of the scattering matrix. Using the Sobolev trace theorem and the dilation transformation $x \mapsto \lambda^{-1/2}x$, we can show (see [36], for details) that, for any $r > 1/2$, the operator (2.7) satisfies the estimate

$$\|\Gamma_0(\lambda)\langle x \rangle^{-r}\| \leq C(r)\lambda^{-1/4}.$$

Similarly, one can control the dependence on λ in the limiting absorption principle, which yields

$$\|\langle x \rangle^{-r}R(\lambda + i0)\langle x \rangle^{-r}\| \leq C(r)\lambda^{-1/2}.$$

The representation (2.16) allows us to study by a simple iterative procedure the behaviour of the scattering matrix $S(\lambda)$ in the two asymptotic regimes of interest, namely for high energies and in smoothness of its kernel. In fact these two regimes are closely related. Namely, we use the resolvent identity (2.3) and substitute its right hand side in place of the resolvent $R(\lambda + i0)$ in (2.16). This gives us a series known as the Born approximation:

$$S(\lambda) = \text{Id} - 2\pi i \sum_{n=0}^N (-1)^n \Gamma_0(\lambda) V \left(R_0(\lambda + i0) V \right)^n \Gamma_0^*(\lambda) + \sigma_N(\lambda).$$

The error term, $\sigma_N(\lambda)$ is $O(\lambda^{-(N-2)/2})$ in operator norm, and in addition gets smoother and smoother in the sense that $\sigma_N(\lambda) \in \mathfrak{S}_{\alpha_N(\mathfrak{N})}$, where $\alpha_N \rightarrow 0$ as $N \rightarrow \infty$.

However, the Born approximation has several drawbacks. First, it is actually quite complicated, involving multiple oscillating integrals of higher and higher dimensions as n increases. Second, it does not apply to long range potentials, or to magnetic, even short range, potentials. Here we discuss another, much simpler, form of approximation which applies to all these situations but requires assumptions of the type (2.17).

2. To give an idea of the approach, suppose first for simplicity that $v \in C_0^\infty(\mathbb{R})$ (though the argument can be applied to a wider class of potentials). Let the solution of the Schrödinger equation (2.9) be defined by formula (2.11). By (2.16), the integral kernel $k(\omega, \omega', \lambda)$ of the operator $S(\lambda) - \text{Id}$ may be written as

$$k(\omega, \omega', \lambda) = -i\pi(2\pi)^{-d}\lambda^{(d-2)/2} \int_{\mathbb{R}^d} e^{-i\sqrt{\lambda}x \cdot \omega} v(x) \psi(x, \omega', \lambda) dx. \quad (4.1)$$

Since this is an integral over a compact region, to analyze the asymptotics of $k(\omega, \omega', \lambda)$ as $\lambda \rightarrow \infty$, it suffices to construct the asymptotics of $\psi(x, \omega, \lambda)$ for bounded x as $\lambda \rightarrow \infty$.

This can be done by the following well known procedure [5]. Assuming for a moment only (2.17) for $\rho > 1$, one seeks $\psi(x, \omega, \lambda)$ in the form

$$\psi(x, \xi) = e^{ix \cdot \xi} b(x, \xi), \quad b(x, \xi) = \sum_{n=0}^N (2i|\xi|)^{-n} b_n(x, \hat{\xi}), \quad b_0 = 1, \quad \xi = \sqrt{\lambda} \omega. \quad (4.2)$$

Plugging (4.2) into the Schrödinger equation (2.9), and equating powers of $|\xi|$, we obtain equations

$$\hat{\xi} \cdot \nabla_x b_{n+1} = -\Delta b_n + v b_n. \quad (4.3)$$

The remainder term

$$r_N(x, \xi) = e^{-ix \cdot \xi} (-\Delta + v(x) - |\xi|^2) \psi(x, \xi)$$

is then given by

$$r_N(x, \xi) = (2i|\xi|)^{-N} (-\Delta b_N(x, \hat{\xi}) + v(x) b_N(x, \hat{\xi})).$$

Equations (4.3) can be explicitly solved:

$$b_{n+1}(x, \hat{\xi}) = \int_{-\infty}^0 \left(-\Delta b_n(x + t\hat{\xi}, \hat{\xi}) + v(x + t\hat{\xi}) b_n(x + t\hat{\xi}, \hat{\xi}) \right) dt.$$

It is easy to see that

$$\begin{aligned} |\partial_x^\alpha \partial_\xi^\beta b_n(x, \hat{\xi})| &\leq C_{\alpha, \beta} \langle x \rangle^{-(\rho-1)n - |\alpha|} |\xi|^{-|\beta|}, \\ |\partial_x^\alpha \partial_\xi^\beta r_N(x, \xi)| &\leq C_{\alpha, \beta} \langle x \rangle^{-1 - (\rho-1)(N+1) - |\alpha|} |\xi|^{-N - |\beta|}, \end{aligned} \quad (4.4)$$

except on arbitrary conic neighbourhoods of the bad direction $\hat{x} = \hat{\xi}$.

If v is compactly supported, then the estimates in x are inessential, so it follows from (4.1) and (4.2) that

$$\begin{aligned} k(\omega, \omega', \lambda) &= -i\pi (2\pi)^{-d} \lambda^{(d-2)/2} \sum_{n=0}^N (2i\sqrt{\lambda})^{-n} \int_{\mathbb{R}^d} e^{i\sqrt{\lambda}x \cdot (\omega' - \omega)} v(x) b_n(x, \omega') dx \\ &\quad + O(\lambda^{(d-3)/2 - N/2}). \end{aligned}$$

Since N is arbitrary, this gives the asymptotic expansion of the scattering amplitude as $\lambda \rightarrow \infty$. We note that $k \in C^\infty(\mathbb{S}^{d-1} \times \mathbb{S}^{d-1})$ in the variables ω and ω' , so the smoothness asymptotics in the case $v \in C_0^\infty(\mathbb{R}^d)$ is trivial.

3. Finally, we give a universal formula which applies in both the long range and magnetic cases. We shall need two approximate solutions ψ_\pm of the Schrödinger equation

$$(i\nabla + a(x))^2 \psi_\pm + v(x) \psi_\pm = |\xi|^2 \psi_\pm.$$

We suppose that a vector (or magnetic) potential $a(x)$ as well as scalar potential $v(x)$ satisfy the condition (2.17) for some $\rho > 0$. Let us look for ψ_\pm in the form

$$\psi_\pm(x, \xi) = e^{i\phi_\pm(x, \xi)} b_\pm(x, \xi), \quad (4.5)$$

where $\phi = \phi_{\pm}$ is defined by formula (3.7) and $\Phi = \Phi_{\pm}$ satisfies (3.8). Plugging (4.5) into the Schrödinger equation, we obtain the eikonal equation for ϕ :

$$|\nabla_x \phi|^2 - 2a(x) \cdot \nabla_x \phi + v_0(x) = |\xi|^2, \quad v_0(x) = |a(x)|^2 + v(x). \quad (4.6)$$

If $\rho > 1$ and $a = 0$, then one can set $\Phi = 0$. In this case $\psi_{-}(x, \xi) = \psi(x, \xi)$ and $\psi_{+}(x, \xi) = \overline{\psi(x, -\xi)}$ where the function $\psi(x, \xi)$ was constructed in the previous subsection. However, even if a is short range (but does not vanish), then, for the study of the limit $\lambda \rightarrow \infty$, one cannot avoid the eikonal equation.

Once again, the equation (4.6) for function $\phi = \phi_{\pm}$ defined by formula (3.7) where $\Phi = \Phi_{\pm}$ can be solved by successive approximations:

$$\Phi(x, \xi) = \sum_{n=0}^{N_0} (2|\xi|)^{-n} \phi_n(x, \hat{\xi}).$$

Here

$$\begin{aligned} \hat{\xi} \cdot \nabla \phi_0 + \hat{\xi} \cdot a &= 0, \\ \hat{\xi} \cdot \nabla \phi_1 + |\nabla \phi_0|^2 - 2a \cdot \nabla \phi_0 + v_0 &= 0 \\ \hat{\xi} \cdot \nabla \phi_{n+1} + \sum_{m=0}^n \nabla \phi_m \cdot \nabla \phi_{n-m} - 2a \cdot \nabla \phi_n &= 0, \quad n \geq 1. \end{aligned}$$

So at every step we have an equation

$$\hat{\xi} \cdot \nabla_x \phi(x, \hat{\xi}) + f(x, \hat{\xi}) = 0,$$

with, possibly a long range function f . This equation can be solved by one of the two formulas (cf. (3.10), (3.11))

$$\phi_{\pm}(x, \xi) = \pm \int_0^{\infty} \left(f(x \pm t\hat{\xi}, \hat{\xi}) - f(\pm t\hat{\xi}, \hat{\xi}) \right) dt. \quad (4.7)$$

Using both signs '+' and '-', we obtain functions ϕ_{\pm} satisfying (4.6) up to a term $q_{\pm}(x, \xi)$ such that

$$|\partial_x^{\alpha} \partial_{\xi}^{\beta} q_{\pm}(x, \xi)| \leq C_{\alpha, \beta} \langle x \rangle^{-N_0 \rho - |\alpha|} |\xi|^{-N_0 - |\beta|}$$

for all (x, ξ) excluding an arbitrary conic neighbourhood of the direction $\hat{x} = \hat{\xi}$ for the minus sign, or $\hat{x} = -\hat{\xi}$ for the plus sign. One chooses and fixes N_0 such that $N_0 \rho > 1$.

Then for b_{\pm} one has the transport equation

$$-2i\xi \cdot \nabla b_{\pm} + 2i(a - \nabla \Phi_{\pm}) \cdot \nabla b_{\pm} - \Delta b_{\pm} + (-i\Delta \Phi_{\pm} + i \operatorname{div} a + q_{\pm}) b_{\pm} = 0. \quad (4.8)$$

As before, one looks for $b_{\pm} = b_{\pm}^{(N)}$ in the form (4.2) which gives standard equations

$$\hat{\xi} \cdot \nabla_x b_{n+1}^{(\pm)}(x, \hat{\xi}) = f_n^{(\pm)}(x, \hat{\xi}),$$

where $f_n^{(\pm)}$ are determined by functions $b_1^{(\pm)}, \dots, b_n^{(\pm)}$. All these equations are solved by formula (4.7) (but the term $f_n^{(\pm)}(\pm t\hat{\xi})$ can be dropped). Then the functions $b_n^{(\pm)}$ and the remainder $r_N^{(\pm)}$ in the transport equation satisfy estimates of the type (4.4) for some $\rho > 1$. As $N \rightarrow \infty$, we obtain a function (4.5) satisfying the Schrödinger equation with an arbitrary given accuracy both in the variables x and ξ .

Now we can give an approximate formula for the scattering amplitude. Remark that away from the diagonal, it is not hard to show that the kernel $s(\omega, \omega', \lambda)$ of the scattering matrix $S(\lambda)$ is smooth and $O(\lambda^{-\infty})$, so the main point is to understand the kernel when ω and ω' are close to some given point ω_0 . Let $\omega_0 \in \mathbb{S}^{d-1}$ be arbitrary, let Π_{ω_0} be the plane orthogonal to ω_0 and $x = z\omega_0 + y$, $y \in \Pi_{\omega_0}$. Set

$$s_0(\omega, \omega', \lambda) = \mp \pi i \lambda^{(d-2)/2} (2\pi)^{-d} \int_{\Pi_{\omega_0}} \left(\overline{\psi_+(y, \sqrt{\lambda}\omega)} \partial_z \psi_-(y, \sqrt{\lambda}\omega') - \overline{\partial_z \psi_+(y, \sqrt{\lambda}\omega)} \psi_-(y, \sqrt{\lambda}\omega') - 2i(a(y) \cdot \omega_0) \overline{\psi_+(y, \sqrt{\lambda}\omega)} \psi_-(y, \sqrt{\lambda}\omega') \right) dy. \quad (4.9)$$

Here $s_0 = s_0^{(N)}$ depends on N , since the construction above depends on a choice of N . On the contrary, it does not depend on N_0 which is fixed. Let $\Omega_{\pm} = \Omega_{\pm}(\omega_0, \delta) \subset \mathbb{S}^{d-1}$ be determined by the condition $\pm \omega \cdot \omega_0 > \delta > 0$ and $\Omega = \Omega_+ \cup \Omega_-$. Then we have

THEOREM 4.1. *For all integer p , there is an $N = N(p)$ such that*

$$\tilde{s}_0^{(N)}(\omega, \omega', \lambda) := s(\omega, \omega', \lambda) - s_0^{(N)}(\omega, \omega', \lambda) \in C^p(\Omega \times \Omega)$$

and

$$\|\tilde{s}_0^{(N)}(\cdot, \cdot, \lambda)\|_{C^p} \leq C\lambda^{-p}.$$

We make some brief comments on the proof of this theorem. Note that the representation formula (2.16) holds in the general short range case, when both electric and magnetic potentials are present. However it is useless for the proof of Theorem 4.1 even for purely electric short range potentials.

As in the previous lecture, one considers instead modified wave operators $W_{\pm}(H, H_0, J_{\pm})$, where

$$(J_{\pm}f)(x) = (2\pi)^{-d/2} \int_{\mathbb{R}^d} \psi_{\pm}(x, \xi) \zeta_{\pm}(x, \xi) \hat{f}(\xi) d\xi$$

and the functions $\psi_{\pm}(x, \xi)$ are defined by formula (4.5). Compared to the previous lecture, there are two important differences in the construction of the operators J_{\pm} . First, we cannot neglect high energies and therefore have to control the dependence on ξ in all estimates. Second, for the proof of the existence and completeness of the wave operators, it was sufficient to take $b_{\pm} = 1$ in (4.5). On the contrary, now $b_{\pm} = b_{\pm}^{(N)}$ is an approximate solution of the transport equation (4.8) depending on the parameter N , which allows us to obtain an arbitrary good approximation $\psi_{\pm} = \psi_{\pm}^{(N)}$ to solutions of the Schrödinger equation.

Writing T_{\pm} for the effective perturbation,

$$T_{\pm} = HJ_{\pm} - J_{\pm}H_0,$$

we have (see [12, 34, 36])

$$S(\lambda) = S_0(\lambda) + S_1(\lambda),$$

where

$$\begin{aligned} S_0(\lambda) &= -2\pi i \Gamma_0(\lambda) J_+^* T_- \Gamma_0^*(\lambda), \\ S_1(\lambda) &= 2\pi i \Gamma_0(\lambda) T_+^* R(\lambda + i0) T_- \Gamma_0^*(\lambda). \end{aligned} \quad (4.10)$$

Note that T_{\pm} is a pseudodifferential operator of order -1 , so that precise meaning of (4.10) needs to be explained. The special reason why S_0 is correctly defined is that

the amplitude of the pseudodifferential operator $J_+^* T_-$ is zero in a neighbourhood of the set where \hat{x} is close to $\hat{\xi}$ or $-\hat{\xi}$ or, to put it differently, in a neighbourhood of the conormal bundle to every sphere $|\xi| = \sqrt{\lambda}$.

The term $S_1(\lambda)$ turns out to be negligible for large N .

THEOREM 4.2. *For all integer p , there is an $N = N(p)$ such that*

$$s_1^{(N)}(\omega, \omega', \lambda) \in C^p(\mathbb{S}^{d-1} \times \mathbb{S}^{d-1}),$$

and

$$\|s_1^{(N)}(\cdot, \cdot, \lambda)\|_{C^p} \leq C\lambda^{-p}.$$

The proof relies on propagation estimates (see [25, 14, 13]) following from the Mourre estimate (3.5). We give an example of such an estimate. Let again A be the generator of dilations. Then for all integers p

$$\| \langle x \rangle^p E_A(\mathbb{R}_-) R(\lambda + i0) E_A(\mathbb{R}_+) \langle x \rangle^p \| = O(\lambda^{-1}).$$

Thus, the interesting part of the scattering matrix is contained in the term $S_0(\lambda)$ of (4.10). It is very explicit representation, but has a drawback because it depends on the cutoffs ζ_{\pm} . So one has to transform the expression for $S_0(\lambda)$ to the invariant expression (4.9), which does not contain the cutoffs ζ_{\pm} . This is the least obvious part of the proof of Theorem 4.1.

Finally, we note that formula (3.18) for the diagonal singularity of the scattering amplitude can be obtained applying the stationary phase method to integral (4.9).

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