ANNALES DE L'I. H. P., SECTION A

S. N. M. RUIJSENAARS
P. J. M. BONGAARTS

Scattering theory for one-dimensional step potentials

Annales de l'I. H. P., section A, tome 26, nº 1 (1977), p. 1-17
<http://www.numdam.org/item?id=AIHPA_1977__26_1_1_0>

Ann. Inst. Henri Poincaré,
Vol. XXVI, n° 1, 1977, p. 1-17.

Section A :
Physique théorique.

Scattering theory for one-dimensional step potentials

by

S. N. M. RUIJSENAARS and P. J. M. BONGAARTS
Instituut-Lorentz, University of Leiden,
Leiden, The Netherlands

ABSTRACT. — We treat the scattering theory for the one-dimensional Dirac equation with potentials that are bounded, measurable, real-valued functions on the real line, having constant values, not necessarily the same, on the left and on the right side of a compact interval. Such potentials appear in the Klein paradox. It is shown that appropriately modified wave operators exist and that the corresponding S-operator is unitary. The connection between time-dependent scattering theory and time-independent scattering theory in terms of incoming and outgoing plane wave solutions is established and some further properties are proved. All results and their proofs have a straightforward translation to the one-dimensional Schrödinger equation with the same class of step potentials.

1. INTRODUCTION

The mathematical theory of potential scattering has been developed to a considerable extent in the last twenty years. Three-dimensional Schrödinger operators are treated in a monograph by Simon [*1*], while recent results and references on Dirac operators can be found in papers by Eckardt [*2*] and Guillot/Schmidt [*3*]. In both cases the investigated potentials go to zero at infinity in some sense. In this paper we consider scattering theory for potentials not having this property. For these potentials the usual techniques (cf. [*1*]) are no longer easily applicable. It therefore seems appropriate to treat this problem first in one space dimension. More in particular, we study the scattering of wave packets, described by the one-dimensional Dirac equation, at potentials that are bounded, measurable, real-valued functions on the real line, having constant values, not necessarily the same, on the left and on the right side of a compact interval.

Such potentials occur in the well-known Klein paradox. Rigorous scattering theory for the c-number Dirac equation with such potentials is a necessary preliminary for the discussion of this paradox in a second-quantized setting. This will be undertaken in a separate publication [*4*].

In § 2 we introduce a modification of the usual definition of wave operators. Using a lemma on the free evolution we then prove that these modified wave operators exist. In § 3 the existence of incoming and outgoing solutions is proved. In § 4 we establish the connection between these solutions and the wave operators and prove that the S-operator is unitary. The main result of § 5 is the asymptotic completeness of the wave operators. The paper ends with a summary of the changes which should be made to obtain analogous results for the Schrödinger equation with the same potentials.

2. PRELIMINARIES. A LEMMA ON THE FREE EVOLUTION. THE WAVE OPERATORS.

As an evolution equation in the Hilbert space of square-integrable two-component spinors $\mathscr{H} \equiv L^2(\mathrm{R})^2$, the free one-dimensional Dirac equation reads

$$i\frac{d}{dt}\psi(t, \cdot) = \mathrm{H}_0\psi(t, \cdot) \tag{2.1}$$

where

$$\mathrm{D}(\mathrm{H}_0) = \{ \phi \in \mathscr{H} \mid \phi_j(x) \ \text{ absolutely continuous}, \ \ j = 1, 2, \phi'(\cdot) \in \mathscr{H} \} \tag{2.2}$$

and

$$\mathrm{H}_0 = \frac{\alpha}{i}\frac{d}{dx} + \beta m\,. \tag{2.3}$$

In (2.3) $m > 0$; α and β are 2×2 matrices satisfying

$$\alpha = \alpha^* \qquad \beta = \beta^* \qquad \alpha\beta + \beta\alpha = 0 \qquad \alpha^2 = \beta^2 = 1\,. \tag{2.4}$$

It easily follows that H_0 is self-adjoint. We choose the representation

$$\alpha = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{2.5}$$

It is easily seen that our results are representation-independent.

We have occasion to use a spectral representation for H_0 generated by the unitary operator

$$\mathrm{V}_0 : \mathscr{H}^0 \equiv L^2(e)^2 \to \mathscr{H} \qquad e \equiv (-\infty, -m] \cup [m, \infty) \tag{2.6}$$

satisfying

$$(V_0 f)(x) \equiv \underset{N\to\infty}{\mathrm{l.i.m.}} \sum_{i=1}^{2} \int_{e\cap(-N,N)} dE V_i^0(x, E) f_i(E) \tag{2.7}$$

$$(V_0^{-1}\phi)_i(E) = \underset{N\to\infty}{\mathrm{l.i.m.}} \int_{-N}^{N} dx \overline{V_i^0}(x, E) . \phi(x) \tag{2.8}$$

where

$$V_j^0(x, E) \equiv \psi_j(E) \exp\left((-)^{j+1} i \frac{E}{|E|} p_E x\right) \tag{2.9}$$

$$\psi_j(E) \equiv (4\pi)^{-\frac{1}{2}} \begin{pmatrix} C_E \\ (-)^{j+1} C_E^{-1} \end{pmatrix}, C_E \equiv \left(\frac{E+m}{E-m}\right)^{\frac{1}{4}}, p_E \equiv (E^2 - m^2)^{\frac{1}{2}} . \tag{2.10}$$

One has

$$(V_0^{-1} H_0 \phi)_i(E) = E(V_0^{-1}\phi)_i(E) \qquad \forall\phi \in D(H_0) . \tag{2.11}$$

The straightforward proofs of the unitarity of V_0 and of (2.8) and (2.11) are omitted. We denote the projections of H_0 and the momentum operator $\left(\text{i. e. the operator } \frac{1}{i}\frac{d}{dx} \text{ on } D(H_0)\right)$ on $(-\infty, 0)((0, \infty))$ by $P_-(P_+)$ resp. $F_-(F_+)$.
We then define

$$G_1 = P_+F_+ + P_-F_- \qquad G_2 = P_+F_- + P_-F_+ . \tag{2.12}$$

Note that

$$(V_0^{-1} G_j \phi)_i(E) = \delta_{ij}(V_0^{-1}\phi)_j(E) \qquad \forall\phi \in \mathscr{H} . \tag{2.13}$$

We will consider a perturbed Dirac Hamiltonian

$$H = H_0 + V ; \quad V(x) \equiv \begin{cases} 0 & x \leq -R \\ U & x \geq R \\ \text{bounded, measurable, real-valued } |x| < R. \end{cases} \tag{2.14}$$

In (2.14) $R > 0$ and $U \geq 0$. Results for the case of arbitrary real values on both sides of $|x| < R$ can be easily obtained by adding a constant and/or using the parity operator

$$(P\phi)(x) \equiv \beta\phi(-x) . \tag{2.15}$$

Besides P we will also use the (Wigner) time reversal operator

$$(T\phi)(x) \equiv \beta\bar{\phi}(x) . \tag{2.16}$$

Note that

$$\begin{aligned} (V_0^{-1} P\phi)_{\substack{1\\2}}(E) &= (V_0^{-1}\phi)_{\substack{2\\1}}(E) \\ (V_0^{-1} T\phi)_{\substack{1\\2}}(E) &= (\overline{V_0^{-1}\phi})_{\substack{2\\1}}(E) . \end{aligned} \tag{2.17}$$

LEMMA 2.1 (On the free evolution). — Let

$$D \equiv \{ \phi \in \mathscr{H} \mid (V_0^{-1}\phi)_j \in C_0^\infty, \pm m \notin \operatorname{supp} (V_0^{-1}\phi)_j, j = 1, 2 \}. \quad (2.18)$$

For any $\phi \in D$ and $a \in R$ there are $C_n > 0$ ($n \in N^+$) such that

$$\| \chi_{[a,\infty)} \exp(- iH_0 t) G_{\frac{1}{2}} \phi \|^2 \leq C_n |t|^{-n} \qquad \forall t \lessgtr 0 \quad (2.19)$$

where χ_I is the operator of multiplication by the characteristic function of I.

Proof. — Setting

$$\theta_\varepsilon(x) \equiv \chi_{[a,\infty)}(x) \exp\left(-\frac{\varepsilon}{2}(x-a)\right) \quad (2.20)$$

one has, by dominated convergence,

$$\| \chi_{[a,\infty)} \exp(- iH_0 t) G_1 \phi \|^2 = \lim_{\varepsilon \downarrow 0} \| \theta_\varepsilon \exp(- iH_0 t) G_1 \phi \|^2 \equiv \lim_{\varepsilon \downarrow 0} M_\varepsilon(t). \quad (2.21)$$

Clearly,

$$\begin{aligned} M_\varepsilon(t) &\leq 2 \sum_{\delta = +,-} \| V_0^{-1} \theta_\varepsilon \exp(- iH_0 t) P_\delta F_\delta \phi \|^2 \\ &= \sum_{\delta=+,-} \iint_{\delta m}^{\delta\infty} dEdE' g_\delta(E, E') \exp(i(E - E')t)(\varepsilon + i\delta(p_E - p_{E'}))^{-1} \\ &= \int dpdp' h(p, p') \exp(i(E_p - E_{p'})t)(\varepsilon + i(p - p'))^{-1} \end{aligned} \quad (2.22)$$

where
$$E_k \equiv (k^2 + m^2)^{\frac{1}{2}} \quad (2.23)$$

and $h(p, p')$ is a C_0^∞ function with $\operatorname{supp} h \subset [b, c] \times [b, c]$, $0 < b < c$. Introducing

$$\begin{aligned} y &\equiv (E_p - E_{p'})(p - p')^{-1} = (p + p')(E_p + E_{p'})^{-1} \\ v &\equiv p - p' \end{aligned} \quad (2.24)$$

one easily sees that this is a $1 - 1$ C^∞ map from $(0, \infty) \times (0, \infty)$ to $(0, 1) \times R$ with inverse

$$p = \frac{1}{2}v + \frac{1}{2}(v^2y^2 + 4m^2y^2(1 - y^2)^{-1})^{\frac{1}{2}} \qquad p' = p - v. \quad (2.25)$$

As the inverse is C^∞ the Jacobian is non-zero and C^∞. Thus,

$$M_\varepsilon(t) = \int dydv F(y, v) \exp(iyvt)(\varepsilon + iv)^{-1} = \int dy \int_{-\infty}^{yt} dx \hat{F}(y, x) \exp(\varepsilon(x - yt)) \quad (2.26)$$

where

$$\hat{F}(y, x) \equiv \int dv F(y, v) \exp(ivx) \quad (2.27)$$

and $F(y, v)$ is a C_0^∞ function with supp $F \subset [y_1, y_2] \times [v_1, v_2]$, $0 < y_1 < y_2 < 1$, $-\infty < v_1 < v_2 < \infty$. Hence, there exist $C'_n > 0$ $(n \in \mathrm{N}^+)$ such that

$$|\hat{F}(y, x)|\,|x|^{n+1} \leq C'_n \qquad \forall (y, x) \in \mathrm{R}^2. \tag{2.28}$$

It follows that

$$M_\varepsilon(t) \leq C'_n(y_2 - y_1)n^{-1}(-y_1 t)^{-n} \qquad \forall t < 0. \tag{2.29}$$

Thus, the upper relation of (2.19) holds. Since

$$\|\chi_{[a,\infty)} \exp(-iH_0 t)G_2\phi\| = \|\chi_{[a,\infty)} \exp(iH_0 t)G_1 T\phi\| \tag{2.30}$$

the lower one holds as well. ■

It easily follows from this lemma that for any $\phi \in \mathscr{H}$ and $a \in \mathrm{R}$

$$\lim_{t\to\pm\infty} \|\chi_{[a,\infty)} \exp(-iH_0 t)G_{\substack{2\\1}}\phi\|^2 = \lim_{t\to\pm\infty} \|\chi_{(-\infty,a]} \exp(-iH_0 t)G_{\substack{1\\2}}\phi\|^2 = 0. \tag{2.31}$$

(Use P to obtain the second relation.) Thus, if $\phi \in G_1\mathscr{H}$ resp. $G_2\mathscr{H}$ then $\exp(-iH_0 t)\phi$ is a wave packet which moves from left to right resp. right to left. (In particular one infers that a negative energy wave packet moves in a direction opposite to its average momentum.)

It is physically quite plausible that the usual wave operators do not exist if $U > 0$ (we shall prove this in section 5). Indeed, the potential then has (had) a persistent effect on wave packets moving to (coming from) the right, which is reflected in an extra oscillating factor $\exp(-iUt)$ as compared to the corresponding free wave packet. However, a moment's consideration suggests that this factor can be neutralized if one defines

$$H_0^+ = (H_0 + U)G_1 + H_0 G_2 \qquad H_0^- = H_0 G_1 + (H_0 + U)G_2 \tag{2.32}$$

and compares the perturbed evolution $\exp(-iHt)$ with the two « almost free » evolutions $\exp(-iH_0^\pm t)$ (for $t \to \pm\infty$) instead of the free evolution $\exp(-iH_0 t)$. The next theorem shows that this indeed happens.

THEOREM 2.2. — The (modified) wave operators

$$W_\pm = \mathop{s.\lim}_{t\to\pm\infty} \exp(iHt)\exp(-iH_0^\pm t) \tag{2.33}$$

exist.

Proof. — Since

$$T\exp(iHt)\exp(-iH_0^+ t) = \exp(-iHt)\exp(iH_0^- t)T \tag{2.34}$$

it suffices to prove that W_- exists. This will follow if for any $\phi \in D$

$$f(t) \equiv \|(H - H_0^-)\exp(-iH_0^- t)\phi\| \tag{2.35}$$

belongs to $L^1((-\infty, -1])$ (cf. e. g. [5]). To show this we note that

$$f(t) \leq \|(V_1 - UG_2)\exp(-iH_0^- t)\phi\| + \|V_2 \exp(-iH_0^- t)\phi\| \tag{2.36}$$

where

$$V_1(x) \equiv U\chi_{[0,\infty)}(x) \tag{2.37}$$

and $V_2(x)$ has compact support. Hence, setting $e \equiv \exp(-iH_0t)$,

$$f(t) \leq \| (V_1 - U)eG_2\phi \| + \| V_1eG_1\phi \| + \sum_i \| V_2eG_i\phi \|$$

$$= \| V_1eG_1P\phi \| + \| V_1eG_1\phi \| + \| V_2eG_1\phi \| + \| PV_2PeG_1P\phi \| . \quad (2.38)$$

The statement now easily follows from (2.19). ■

In the sequel we will need spectral representations for $H_0^{\pm}$, generated by the unitary operators

$$V_{\pm} : \mathscr{H}^{\pm} \equiv \sum_{j=1}^{2} L^2(e_j^{\pm}) \to \mathscr{H} \qquad \bar{e}_1 = e_2^{+} \equiv e \qquad \bar{e}_2 = e_1^{+} \equiv e + U \quad (2.39)$$

defined by

$$(V_{\pm} f^{\pm})(x) = \underset{N\to\infty}{\mathrm{l.i.m.}} \sum_{i=1}^{2} \int_{e_i^{\pm} \cap (-N,N)} dE V_i^{\pm}(x, E) f_i^{\pm}(E) \quad (2.40)$$

where

$$\begin{aligned} V_1^{-}(x, E) &\equiv V_1^0(x, E) \qquad & V_2^{-}(x, E) &\equiv V_2^0(x, E - U) \\ V_1^{+}(x, E) &\equiv V_1^0(x, E - U) \qquad & V_2^{+}(x, E) &\equiv V_2^0(x, E) . \end{aligned} \quad (2.41)$$

Evidently,

$$(V_{\pm}^{-1} H_0^{\pm} \phi)_i(E) = E(V_{\pm}^{-1}\phi)_i(E) \qquad \forall \phi \in D(H_0) \quad (2.42)$$

and

$$V_{+} = TV_{-}L \quad (2.43)$$

where $L : \mathscr{H}^{+} \to \mathscr{H}^{-}$ is the conjugation defined by

$$(Lf)_{\substack{1\\2}}(E) = \bar{f}_{\substack{2\\1}}(E) . \quad (2.44)$$

3. INCOMING AND OUTGOING SOLUTIONS.

We shall consider absolutely continuous (a. c.) solutions of the differential equation

$$\left(\frac{\alpha}{i}\frac{d}{dx} + \beta m + V(x) - \lambda\right)U(x, \lambda) = 0 \qquad \text{a. e.} \quad (3.1)$$

with the boundary condition

$$U(a, \lambda) = C(\lambda) \qquad a \in R \quad (3.2)$$

where λ belongs to a domain $0 \subset C$ in which C_1 and C_2 are analytic.

THEOREM 3.1. — For any $\lambda \in 0$ (3.1) has a unique a. c. solution $U(x, \lambda)$ satisfying (3.2). It is

a) analytic in $\mathcal{O}$, uniformly for x in a bounded subset of R;
b) jointly continuous on $\mathrm{R} \times \mathcal{O}$;
c) differentiable w. r. t. x on a set K_V depending only on V and the complement of which has measure zero, uniformly for λ in a compact subset of $\mathcal{O}$.

Proof. — Existence of an a. c. solution of (3.1-2) is clearly equivalent to existence of a continuous solution of the integral equation

$$U(x, \lambda) = C(\lambda) + \int_a^x ds M(s, \lambda) U(s, \lambda) \tag{3.3}$$

where

$$M(x, \lambda) \equiv -i\alpha\beta m - i\alpha V(x) + i\alpha\lambda. \tag{3.4}$$

We will first prove that (3.3) has a unique solution in the Banach space B of two-component complex-valued continuous functions on a compact interval I ($a \in \mathrm{I}$) with the norm $\|F\| \equiv \sum_{i=1}^{2} \sup_{x \in \mathrm{I}} |F_i(x)|$. Defining a Volterra integral operator on B by

$$(\Phi(\lambda)F)(x) \equiv \int_a^x ds M(s, \lambda) F(s), \tag{3.5}$$

(3.3) can be regarded as an equation in B:

$$(1 - \Phi(\lambda))U(\cdot, \lambda) = C(\lambda). \tag{3.6}$$

It easily follows that (3.6) has the unique solution

$$U(\cdot, \lambda) = \sum_{j=0}^{\infty} \Phi(\lambda)^j C(\lambda). \tag{3.7}$$

Existence and unicity of the solution on R now follows from an easy continuation argument.

Since $\Phi(\lambda)$ is an entire function with values in $\mathscr{L}(\mathrm{B})$ all terms in the sum are analytic in $\mathcal{O}$. It then easily follows from the Weierstrass theorem that $U(\cdot, \lambda)$ is analytic in $\mathcal{O}$. Thus, since

$$\left| \frac{U_i(x, \lambda) - U_i(x, \lambda_0)}{\lambda - \lambda_0} - \left(\frac{d}{d\lambda} U\right)_i (x, \lambda_0) \right| \leq \left\| \frac{U(\cdot, \lambda) - U(\cdot, \lambda_0)}{\lambda - \lambda_0} - \left(\frac{d}{d\lambda} U\right)(\cdot, \lambda_0) \right\| \tag{3.8}$$

a follows. Evidently, *b* follows from *a*. To prove *c* we define

$$A(x) = \int_0^x ds V(s). \tag{3.9}$$

By the fundamental theorem of calculus there exists a set K_V having the required properties and such that

$$\frac{d}{dx}A(x) = V(x) \qquad \forall x \in K_V . \tag{3.10}$$

Using (3.3) and b it then easily follows that

$$\frac{d}{dx}U(x, \lambda) = M(x, \lambda)U(x, \lambda) \qquad \forall x \in K_V , \tag{3.11}$$

uniformly for λ in a compact subset of 0. ■

We note that if U_1, U_2 are a. c. solutions of (3.1) then

$$F(U_1, U_2) \equiv (U_1(x))_1(U_2(x))_2 - (U_1(x))_2(U_2(x))_1 \tag{3.12}$$

is a constant. Indeed,

$$\begin{aligned}\frac{d}{dx}F(U_1, U_2) &= \frac{d}{dx}U_1(x)\beta\alpha U_2(x)\\ &= (M(x, \lambda)U_1(x))\beta\alpha U_2(x) + U_1(x)\beta\alpha M(x, \lambda)U_2(x) = 0 \quad \forall x \in K_V\end{aligned} \tag{3.13}$$

(cf. (2.4-5)). We further observe that if $U(x)$ satisfies (3.1) with $\lambda \in R$ then $(TU)(x)$ also does. In the next theorem we use the following intervals on the E-axis:

$$\begin{array}{rl} \text{I.} & E > m + U \\ \text{II.} & \max(m, -m + U) < E < m + U \\ \text{III.} & m < E < -m + U \quad \text{if} \quad U > 2m; \qquad \text{otherwise empty} \\ \text{IV.} & -m < E < \min(m, -m + U) \\ \text{V.} & E < -m. \end{array} \tag{3.14}$$

THEOREM 3.2. — For $\lambda = E$ real (3.1) admits solutions of the following form:

1. $E \in$ I, III, V.

$$U_1^-(x, E) = \begin{cases} V_1^-(x, E) + r_1(E)V_2^+(x, E) \\ t(E)V_1^+(x, E) \end{cases}$$

$$U_2^-(x, E) = \begin{cases} t(E)V_2^+(x, E) & x \leq -R \\ V_2^-(x, E) + r_2(E)V_1^+(x, E) & x \geq R \end{cases} \tag{3.15}$$

where

$$t(E)\bar{r}_1(E) + r_2(E)\bar{t}(E) = 0 \qquad |t(E)|^2 + |r_i(E)|^2 \qquad i = 1, 2 . \tag{3.16}$$

2. $E \in$ II.

$$U_1^-(x, E) = \begin{cases} V_1^-(x, E) + r(E)V_2^+(x, E) \\ g(E)V_2(x, E - U) \end{cases}$$

$$U_2(x, E) = \begin{cases} V_2^-(x, E) & x \leq -R \\ a_1(E)V_1(x, E - U) + a_2(E)V_2(x, E - U) & x \geq R \end{cases} \tag{3.17}$$

E ∈ IV.

$$U_1(x, E) = \begin{cases} a_2(E)V_1(x, E) + a_1(E)V_2(x, E) \\ V_1^-(x, E) \end{cases}$$

$$U_2^-(x, E) = \begin{cases} g(E)V_1(x, E) & x \leq -R \\ V_2^-(x, E) + r(E)V_1^+(x, E) & x \geq R \end{cases} \quad (3.18)$$

where

$$V_{\substack{1\\2}}(x, E) \equiv (4\pi)^{-\frac{1}{2}}\begin{pmatrix} d_E \\ \mp i d_E^{-1} \end{pmatrix} \exp(\pm (m^2 - E^2)^{\frac{1}{2}} x),$$

$$d_E \equiv \left(\frac{m + E}{m - E}\right)^{\frac{1}{4}}, \qquad |E| < m \quad (3.19)$$

and

$$r(E) = g(E)\bar{g}(E)^{-1} \qquad a_1(E) = -ig(E)^{-1}$$
$$\bar{a}_2(E)a_1(E) - \bar{a}_1(E)a_2(E) = -i. \quad (3.20)$$

3. $U < 2m$ and $-m + U < E < m$.

$$U_1(x, E) = \begin{cases} a(E)V_2(x, E) + b(E)V_1(x, E) \\ V_2(x, E - U) \end{cases}$$

$$U_2(x, E) = \begin{cases} V_1(x, E) & x \leq -R \\ a(E)V_1(x, E - U) + c(E)V_2(x, E - U) & x \geq R. \end{cases} \quad (3.21)$$

The functions $a(E)$, $b(E)$ and $c(E)$ are real-valued and $a(E)$ has a finite number of zeros in any closed interval belonging to $(-m + U, m)$.

If $[a, b]$ is a subset of any of the above-mentioned 6 energy intervals then there exists an $\varepsilon > 0$ such that all functions of E in (3.15-21) which are defined on $[a, b]$ have analytic continuations to the closed rectangle $Q \in C$ with corners $a \pm i\varepsilon$, $b \pm i\varepsilon$. The analytic continuations of the functions $U_i^{(-)}(x, E)$ which correspond to $[a, b]$ have the properties a, b and c from Th. 3.1 on Q.

Proof. — We first assume E ∈ I. Then, by Th. 3.1, (3.1) with $\lambda = E$ and the boundary condition

$$U(R, E) = V_1^+(R, E) \quad (3.22)$$

has a unique solution, satisfying

$$U(x, E) = \begin{cases} p(E)V_1^-(x, E) + q(E)V_2^+(x, E) & x \leq -R \\ V_1^+(x, E) & x \geq R. \end{cases} \quad (3.23)$$

Calculating F(U, TU) for $x \leq -R$ and $x \geq R$ it follows that

$$|p(E)|^2 = |q(E)|^2 + 1, \quad (3.24)$$

so we can set

$$U_1^-(x, E) \equiv U(x, E)p(E)^{-1}, \quad t_1(E) \equiv p(E)^{-1}, \quad r_1(E) \equiv q(E)p(E)^{-1}. \quad (3.25)$$

Using the boundary condition

$$U'(-R, E) = V_2^+(-R, E) \quad (3.26)$$

one analogously infers the existence of a solution $U_2^-(x, E)$ satisfying

$$U_2^-(x, E) = \begin{cases} t_2(E)V_2^+(x, E) & x \leq -R \\ V_2^-(x, E) + r_2(E)V_1^+(x, E) & x \geq R. \end{cases} \tag{3.27}$$

Calculating $F(U_i^-, TU_i^-)$, $F(U_1^-, U_2^-)$ and $F(U_1^-, TU_2^-)$ for $x \leq -R$ and $x \geq R$ one then obtains $t_1(E) = t_2(E) \equiv t(E)$ and (3.16).

If $[a, b] \subset I$ then $V_1^+(R, E)$ can obviously be analytically continued to the closed rectangle $Q \subset C$ with corners $a \pm i\varepsilon$, $b \pm i\varepsilon$ for any $\varepsilon > 0$. Thus by Th. 3.1 and (3.23) the same is true for the functions

$$p(E) \exp(ip_E x) \pm q(E) \exp(-ip_E x) \qquad x \leq -R \tag{3.28}$$

and, consequently, for $p(E)$ and $q(E)$ as well. Choosing now an $\varepsilon > 0$ such that the continuation of $p(E)$ is non-zero on Q it follows that $t(E)$, $r_1(E)$ and $U_1^-(x, E)$ can be analytically continued to Q and that the continuation of $U_1^-(x, E)$ has the properties a, b and c on Q. A similar argument shows that the same is true for $r_2(E)$ and $U_2^-(x, E)$ so we have proved the theorem for the case $E \in I$. The proof for the 5 remaining cases is analogous.

To prove finally the statement on $a(E)$ we assume that there are an infinite number of zeros in some closed interval $J \subset (-m + U, m)$. As $a(E)$ is analytic on J it then must be zero on it. However, H would then have an uncountable number of eigenvectors. ■

The functions denoted by $U_i^-(x, E)$ are the incoming solutions. The outgoing ones are defined by

$$U_{\substack{1\\2}}^+(x, E) = TU_{\substack{2\\1}}^-(x, E). \tag{3.29}$$

Defining an operator $\tilde{S} : \mathscr{H}^- \to \mathscr{H}^+$ by

$$(\tilde{S}f)_i(E) = \sum_{j=1}^{2} S_{ij}(E) f_j(E) \tag{3.30}$$

where

$$S_{ij}(E) \equiv \begin{pmatrix} t(E) & r_2(E) \\ r_1(E) & t(E) \end{pmatrix}, \ E \in I, III, V; \quad \equiv \begin{pmatrix} 0 & 0 \\ r(E) & 0 \end{pmatrix}, \ E \in II; \quad \equiv \begin{pmatrix} 0 & r(E) \\ 0 & 0 \end{pmatrix}, \ E \in IV \tag{3.31}$$

one clearly has

COROLLARY 3.3. — The operator $\tilde{S}$ is unitary. ■

4. THE CONNECTION BETWEEN $W_\pm$ AND THE INCOMING AND OUTGOING SOLUTIONS. THE S-OPERATOR.

We shall now show that the operators $W_\pm V_\pm$ are generalized integral operators, the kernels of which are the incoming and outgoing solutions.

THEOREM 4.1. — For any $f^{\pm} \in \mathscr{H}^{\pm}$

$$(\mathrm{W}_{\pm}\mathrm{V}_{\pm}f^{\pm})(x) = \underset{\mathrm{N}\to\infty}{\mathrm{l.i.m.}} \sum_{i=1}^{2} \int_{e_i^{\pm} \cap \Omega_{\mathrm{N}}} d\mathrm{E}\mathrm{U}_i^{\pm}(x, \mathrm{E}) f_i^{\pm}(\mathrm{E}) \tag{4.1}$$

where

$$\Omega_{\mathrm{N}} \equiv \{ \mathrm{E} \in \mathrm{R} \mid |\mathrm{E}| < \mathrm{N},\ |\mathrm{E} \pm m| > \mathrm{N}^{-1},\ |\mathrm{E} \pm m - \mathrm{U}| > \mathrm{N}^{-1} \}. \tag{4.2}$$

Proof. — In view of (3.29) and the relation

$$\mathrm{W}_{+}\mathrm{V}_{+} = \mathrm{T}\mathrm{W}_{-}\mathrm{V}_{-}\mathrm{L} \tag{4.3}$$

it suffices to prove that

$$(\mathrm{W}_{-}\mathrm{V}_{-}f)(x) = \sum_{i=1}^{2} \int_{e_i^{-}} d\mathrm{E}\mathrm{U}_i^{-}(x, \mathrm{E}) f_i(\mathrm{E}) \tag{4.4}$$

for any $f \in \mathscr{H}^{-}$ with compact support in J, where J = I, ..., V. We shall show this for the case that $\mathrm{M} \equiv \operatorname{supp} f \subset \mathrm{I}$ and $f_2 = 0$. The proof for the remaining cases is analogous.

Denoting the r. h. s. of (4.4) by $(\mathrm{U}_{-}f)(x)$ it easily follows from (3.15) and property *b* that

$$(\mathrm{U}_{-}f)(\cdot) \in \mathscr{H} \tag{4.5}$$

and that

$$\| \mathrm{U}_{-}f \| \leq \mathrm{C}_{\mathrm{M}} \| f \| \tag{4.6}$$

where C_{M} only depends on M. Using property *c*, dominated convergence and (3.11) one also infers that

$$\frac{d}{dx}(\mathrm{U}_{-}f)(x) = \int_{\mathrm{M}} d\mathrm{E}\mathrm{M}(x, \mathrm{E})\mathrm{U}_{1}^{-}(x, \mathrm{E}) f(\mathrm{E}) \qquad \forall x \in \mathrm{K}_{\mathrm{V}} \tag{4.7}$$

so

$$\left(\frac{d}{dx}\mathrm{U}_{-}f\right)(\cdot) \in \mathscr{H}. \tag{4.8}$$

Moreover, by (3.11) and Fubini's theorem,

$$(\mathrm{U}_{-}f)(x) = (\mathrm{U}_{-}f)(0) + \int_{0}^{x} dt \frac{d}{dt}(\mathrm{U}_{-}f)(t), \tag{4.9}$$

so $(\mathrm{U}_{-}f)(x)$ is a. c. Thus, $\mathrm{U}_{-}f \in \mathrm{D}(\mathrm{H})$ and, by (4.7),

$$\mathrm{H}\mathrm{U}_{-}f = \mathrm{U}_{-}\mathrm{T}_{\mathrm{E}}f \tag{4.10}$$

where T_{E} denotes multiplication by E. Therefore, by induction, $\mathrm{U}_{-}f \in \mathrm{D}(\mathrm{H}^{n})$ and

$$\sum_{n=0}^{\mathrm{N}} \frac{(-i\mathrm{H}t)^{n}}{n!}\mathrm{U}_{-}f = \mathrm{U}_{-}\sum_{n=0}^{\mathrm{N}} \frac{(-i\mathrm{T}_{\mathrm{E}}t)^{n}}{n!} f. \tag{4.11}$$

Using (4.6) we then infer that the limit $N \to \infty$ of the r. h. s. exists. Hence,

$$\exp(-iHt)U_- f = U_- \exp(-iT_E t)f. \tag{4.12}$$

We now assert that

$$\lim_{t \to -\infty} \| (U_- - V_-) \exp(-iT_E t) f \| = 0. \tag{4.13}$$

To prove this, we set

$$\delta(t, x) \equiv ((U_- - V_-) \exp(-iT_E t) f)(x). \tag{4.14}$$

Then, if $x \geq R$,

$$\delta(t, x) = \int_M dE(t(E)V_1^0(x, E - U) - V_1^0(x, E)) \exp(-iEt) f(E). \tag{4.15}$$

Regarding the r. h. s. as a function on R one easily sees, using (2.31), that

$$\lim_{t \to -\infty} \| \chi_{[R,\infty)} \delta(t, \cdot) \| = 0. \tag{4.16}$$

Similarly,

$$\lim_{t \to -\infty} \| \chi_{(-\infty,-R]} \delta(t, \cdot) \| = 0. \tag{4.17}$$

Moreover, from the Riemann-Lebesgue lemma and dominated convergence it follows that

$$\lim_{t \to -\infty} \| \chi_{(-R,R)} \delta(t, \cdot) \| = 0. \tag{4.18}$$

Thus,

$$\lim_{t \to -\infty} \| \delta(t, \cdot) \| = 0 \tag{4.19}$$

as asserted.

We finally conclude that

$$\begin{aligned} \| U_- f - W_- V_- f \| &= \lim_{t \to -\infty} \| \exp(-iHt) U_- f - \exp(-iH_0^- t) V_- f \| \\ &= \lim_{t \to -\infty} \| (U_- - V_-) \exp(-iT_E t) f \| = 0 \end{aligned} \tag{4.20}$$

where (4.12) has been used. ∎

COROLLARY 4.2. — For any $\phi \in \mathscr{H}$,

$$(V_\pm^{-1} W_\pm^* \phi)_i(E) = \underset{N \to \infty}{\text{l.i.m.}} \int_{-N}^{N} dx \overline{U_i^\pm}(x, E) . \phi(x) \qquad i = 1, 2. \ ∎ \tag{4.21}$$

Defining the S-operator by

$$S = W_+^* W_- \tag{4.22}$$

we now have

THEOREM 4.3. — S is unitary and

$$S = V_+ \tilde{S} V_-^{-1}. \tag{4.23}$$

Proof. — A straightforward computation, using (4.3), Th. 4.1, (3.30-31) and (3.15-20), proves that

$$W_+ V_+ \tilde{S} = W_- V_-. \tag{4.24}$$

Thus (4.23) holds. In view of Cor. 3.3 S is unitary. ■

COROLLARY 4.4. — Ran $W_- =$ Ran W_+. ■ (4.25)

THEOREM 4.5. — For any $\phi \in \mathscr{H}$ and $a \in \mathrm{R}$

$$\lim_{t \to -\infty} \| \chi_{\substack{(-\infty,a] \\ [a,\infty)}} \exp(-iHt)W_-\phi \|^2 = \int_{e^-_{\frac{1}{2}}} dE\, |(V_-^{-1}\phi)_{\substack{1\\2}}(E)|^2 \quad (4.26)$$

$$\lim_{t\to\infty} \| \chi_{\substack{[a,\infty) \\ (-\infty,a]}} \exp(-iHt)W_-\phi \|^2$$
$$= \int_{e^+_{\frac{1}{2}}} dE \left| \sum_{i=1}^{2} S_{\substack{1\\2}i}(E)(V_-^{-1}\phi)_i(E) \right|^2 . \quad (4.27)$$

Proof. — Clearly,

$$\chi_{(-\infty,a]} \exp(-iH_0^- t)\phi = \exp(-iH_0^- t)G_1\phi - \chi_{[a,\infty)} \exp(-iH_0^- t)G_1\phi + \chi_{(-\infty,a]} \exp(-iH_0^- t)G_2\phi. \quad (4.28)$$

According to (2.31) the last 2 terms strongly go to 0 for $t \to -\infty$. Thus,

$$\| G_1\phi \|^2 = \lim_{t\to-\infty} \| \chi_{(-\infty,a]} \exp(-iH_0^- t)\phi \|^2 = \lim_{t\to-\infty} \| \chi_{(-\infty,a]} \exp(-iHt)W_-\phi \|^2 , \quad (4.29)$$

which proves (4.26). The proof of (4.27) is analogous. ■

The relations (4.26-27) can be interpreted as the connection between the matrix elements of $\tilde{S}$ and the probability that a one-dimensional wave packet which comes in from the right or the left, after having been scattered by the potential is « detected » at the right or the left. When e. g. only $f(E) \equiv (V_-^{-1}\phi)_1(E) \neq 0$, and $|f(E)|$ is sharply peaked around $E_0 \in I$, then the perturbed wave packet corresponding to ϕ (described by $\exp(-iHt)W_-\phi$ in the Schrödinger picture) came from the left in the far past; the probability that it will be detected in the far future on the right or on the left is then approximately equal to $T(E_0) \equiv |t(E_0)|^2$ resp. $R(E_0) \equiv |r_1(E_0)|^2$, i. e. the usual transmission and reflection coefficient. If $|f(E)|$ is sharply peaked around $E_0 \in II$ then the perturbed wave packet came from the left in the far past and will be detected on the left in the far future with probability one, etc.

5. COMPLETENESS OF THE WAVE OPERATORS. THE SCHRÖDINGER CASE.

The main result of this final section is that the range of the wave operators equals the orthocomplement of the bound states. We denote the spectral projection of H on the Borel set Ω by P_Ω, the resolvent of H by R_λ, and the 2×2 matrix with elements V_iU_j by $V \otimes U$. Note that

$$F(U_1, U_2)\beta\alpha = U_1 \otimes U_2 - U_2 \otimes U_1 . \quad (5.1)$$

LEMMA 5.1. — If $U \geq 2m$ H has no eigenvalues. If $U < 2m$ its eigenvalues belong to $(-m + U, m)$ and it has no essential spectrum in $(-m + U, m)$.

Proof. — The first two statements are obvious. To prove the last one we note that by (3.21) E_0 is an eigenvalue if and only if $a(E_0) = 0$, so the eigenvalues have multiplicity one and have no limit point in $(-m + U, m)$. Thus, it suffices to show that $P_{[a,b]} = 0$ for any $[a, b] \subset (-m + U, m)$ with $a(E) \neq 0$ on $[a, b]$. We shall prove this by means of Stone's formula:

$$P_{[a,b]}\phi = s.\lim_{\delta \downarrow 0} \phi_\delta \tag{5.2}$$

where

$$\phi_\delta \equiv (2\pi i)^{-1} \int_a^b dE(R_{E-i\delta} - R_{E+i\delta})\phi . \tag{5.3}$$

By Th. 3.2 $U_i(x, E)$ and $a(E)$ have analytic continuations $U_i(x, \lambda)$ resp. $a(\lambda)$ to a rectangle $Q \subset C$ with corners $a \pm i\varepsilon$, $b \pm i\varepsilon$, such that $a(\lambda) \neq 0$ on Q. We define for any $\phi \in \mathscr{H}$ and $\lambda \in Q$

$$(\tilde{R}_\lambda\phi)(x) = -2\pi a(\lambda)^{-1}\left(\int_{-\infty}^x dx' U_1(x, \lambda) \otimes U_2(x', \lambda) + \int_x^\infty dx' U_2(x, \lambda) \otimes U_1(x', \lambda)\right)\beta\phi(x') . \tag{5.4}$$

The integrals are clearly absolutely convergent. We assert that $\tilde{R}_\lambda = R_\lambda$. Indeed, if supp ϕ is compact one concludes that $(\tilde{R}_\lambda\phi)(\cdot) \in D(H)$ and that

$$((\lambda - H)\tilde{R}_\lambda\phi)(x) = 2\pi i a(\lambda)^{-1} F(U_1(x, \lambda), U_2(x, \lambda))\phi(x) . \tag{5.5}$$

Thus, since by (3.21)

$$F(U_1(x, E), U_2(x, E)) = (2\pi i)^{-1} a(E) \qquad \forall E \in (-m + U, m), \tag{5.6}$$

our statement follows. An easy argument now shows that for any $\phi \in \mathscr{H}$ (a. e.)

$$\begin{aligned} \phi_\delta(x) = i \int_a^b dE \Big[\int_{-\infty}^x & dx' (a(\bar{\lambda})^{-1} U_1(x, \bar{\lambda}) \\ & \otimes U_2(x', \bar{\lambda}) - a(\lambda)^{-1} U_1(x, \lambda) \otimes U_2(x', \lambda)) \\ + \int_x^\infty & dx' (a(\bar{\lambda})^{-1} U_2(x, \bar{\lambda}) \otimes U_1(x', \bar{\lambda}) \\ & - a(\lambda)^{-1} U_2(x, \lambda) \otimes U_1(x', \lambda)) \Big] \beta\phi(x') \end{aligned} \tag{5.7}$$

where $\lambda \equiv E + i\delta$ and $0 < \delta \leq \varepsilon$. Hence, assuming that supp ϕ is compact, one infers by dominated convergence that for a. e. x

$$\lim_{\delta \downarrow 0} \phi_\delta(x) = 0 . \tag{5.8}$$

It follows that $P_{[a,b]} = 0$. ■

We decompose $\mathscr{H}$ by setting

$$\mathscr{H} = \mathscr{H}_{ac} \oplus \mathscr{H}_{\text{sing}} \oplus \mathscr{H}_{pp} ; \tag{5.9}$$

the restriction of H to $\mathscr{H}_{ac}$ has a. c. spectrum, to $\mathscr{H}_{\text{sing}}$ continuous singular spectrum, and to $\mathscr{H}_{pp}$ pure point spectrum.

THEOREM 5.2. — $\mathscr{H}_{\text{sing}} = 0$; Ran $W_- =$ Ran $W_+ = \mathscr{H}_{ac}$. (5.10)

Proof. — In view of Cor. 4.4 and Lemma 5.1 it suffices to show that

$$W_-W_-^* = 1 \qquad U \geq 2m \tag{5.11}$$

$$W_-W_-^* = P_{(-\infty,-m+U]\cup[m,\infty)} \qquad U < 2m. \tag{5.12}$$

To prove (5.11-12) we will use Stone's formula as in the proof of Lemma 5.1 so as to obtain expressions for $P_I, \ldots, P_V$. We assume first $[a, b] \subset I$. By Th. 3.2 $U_i^-(x, E)$ and $t(E)$ have analytic continuations to a rectangle $Q \subset C$ with corners $a \pm i\varepsilon$, $b \pm i\varepsilon$, such that $t(\lambda) \neq 0$ on Q. Using the relation

$$F(U_1^-(x, E), U_2^-(x, E)) = -(2\pi)^{-1}t(E) \qquad \forall E \in I \tag{5.13}$$

one concludes as before that for any $\phi \in \mathscr{H}$ and $\lambda \in Q$ with $Im\,\lambda > 0$

$$(R_\lambda\phi)(x) = -2\pi i t(\lambda)^{-1}\left(\int_{-\infty}^{x} dx' U_1^-(x, \lambda) \otimes U_2^-(x', \lambda) + \int_x^\infty dx' U_2^-(x, \lambda) \otimes U_1^-(x', \lambda)\right)\beta\phi(x'). \tag{5.14}$$

As the analogue of (5.8) we then get

$$\lim_{\delta \downarrow 0} \phi_\delta(x) = \int_a^b dE \Bigg[\int_{-\infty}^{x} dx' (t(E)^{-1}\beta\overline{U_1^-}(x, E) \otimes \overline{U_2^-}(x', E) + t(E)^{-1}U_1^-(x, E) \otimes U_2^-(x', E)\beta)$$
$$+ \int_x^\infty dx' (\bar{t}(E)^{-1}\beta\overline{U_2^-}(x, E) \otimes \overline{U_1^-}(x', E) + t(E)^{-1}U_2^-(x, E) \otimes U_1^-(x', E)\beta)\Bigg]\phi(x') \tag{5.15}$$

where we used the relation $R_{\bar\lambda} = R_\lambda^*$. Since

$$\begin{aligned} \overline{U_1^-}(x, E) &= (\bar{t}(E)U_2^-(x, E) + \bar{r}_1(E)U_1^-(x, E))\beta \\ \overline{U_2^-}(x, E) &= (\bar{t}(E)U_1^-(x, E) + \bar{r}_2(E)U_2^-(x, E))\beta \end{aligned} \tag{5.16}$$

we conclude that

$$(P_{[a,b]}\phi)(x) = \int_a^b dE \int_{-\infty}^{\infty} dx' \sum_{i=1}^{2} U_i^-(x, E) \otimes \overline{U_i^-}(x', E)\phi(x'). \tag{5.17}$$

Thus, in view of (4.1) and (4.21)

$$P_{[a,b]} = W_-V_-\chi_{[a,b]}V_-^{-1}W_-^*. \tag{5.18}$$

The same arguments and formulas also lead to (5.18) if $[a, b] \subset$ III or V. Hence, by continuity,

$$P_J = W_-V_-\chi_J V_-^{-1}W_-^* \qquad J = I, III, V. \tag{5.19}$$

We now assume $[a, b] \subset$ II. Arguing as before and using the relation

$$F(U_1^-(x, E), U_2(x, E)) = -(2\pi)^{-1} \qquad \forall E \in II \tag{5.20}$$

one then infers that (5.14-15) hold true in the same sense if U_2^- is replaced by U_2 and t by 1. Since

$$\overline{U_1^-}(x, E) = \bar{r}(E)U_1^-(x, E)\beta, \ \overline{U_2}(x, E) = (U_1^-(x, E) - r(E)U_2(x, E))\beta \tag{5.21}$$

it follows that

$$(P_{[a,b]}\phi)(x) = \int_a^b dE \int_{-\infty}^{\infty} dx' U_1^-(x, E) \otimes \overline{U_1^-}(x', E)\phi(x') . \tag{5.22}$$

If $[a, b] \subset$ IV one also gets (5.22), with $U_1^- \to U_2^-$. Thus, (5.18) holds in both cases. Therefore

$$P_J = W_- V_- \chi_J V_-^{-1} W_-^* \qquad J = II, IV . \tag{5.23}$$

Since

$$P_{\{-m,m,-m+U,m+U\}} = 0 \tag{5.24}$$

we finally conclude that (5.11-12) hold true. ■

We are now in a position to exhibit a spectral representation of H. Let $\{\psi_n\}_{n=1}^K$ be a complete orthonormal family of eigenvectors of H with eigenvalues $E_n (K \leq \infty)$. For any $\phi \in \mathscr{H}$ we define

$$\alpha_n(\phi) = (\psi_n, \phi) \qquad n = 1, \ldots, K \tag{5.25}$$

$$\hat{\phi}_i(E) = (V_-^{-1}W_-^*\phi)_i(E) \qquad E \in e_i^- \qquad i = 1, 2 . \tag{5.26}$$

THEOREM 5.3. — *a*) If $U < 2m$: $E_n \in (-m + U, m)$, $n = 1, \ldots, K$. If $U \geq 2m$ H has no eigenvalues. *b*) For any $\phi \in \mathscr{H}$

$$\hat{\phi}_i(E) = \underset{N\to\infty}{\text{l.i.m.}} \int_{-N}^{N} dx \overline{U_i^-}(x, E) . \phi(x) \qquad i = 1, 2 . \tag{5.27}$$

c) If Λ is a Borel set then for any $\phi \in \mathscr{H}$

$$(\widehat{P_\Lambda\phi})_i(E) = \chi_\Lambda(E)\hat{\phi}_i(E) \qquad E \in e_i^- \qquad i = 1, 2 \tag{5.28}$$

$$\| P_\Lambda\phi \|^2 = \sum_{i=1}^{2} \int_{e_i^- \cap \Lambda} dE \, | \phi_i(E) |^2 + \tilde{\sum_n} | \alpha_n(\phi) |^2 \tag{5.29}$$

where $\tilde{\sum_n}$ denotes the sum over all n such that $E_n \in \Lambda$.

d) $\phi \in D(H)$ if and only if $\sum_{i=1}^{2} \int_{e_i^-} dE \, | E\hat{\phi}_i(E) |^2 < \infty$;

$$(\widehat{H\phi})_i(E) = E\hat{\phi}_i(E) \qquad \forall \phi \in D(H) . \tag{5.30}$$