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Properties of the scattering amplitude for electron-atom collisions

by

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ABSTRACT. — For the scattering of an electron by an atom finiteness of the amplitude at non treshold energies is proved in the framework of the N-body Schrödinger equation. It is also shown that both the direct and exchange amplitudes have analytic continuations for complex values of incident momentum, with pole or cut singularities on the imaginary axis.

RÉSUMÉ. — Pour la diffusion d'un électron par un atome, on démontre, dans le cadre de l'équation de Schrödinger à N corps, la finitude de l'amplitude pour les énergies différentes des seuils. On démontre aussi que les amplitudes directe et d'échange admettent des prolongements analytiques pour des valeurs complexes du moment incident, possédant des pôles ou des coupures sur l'axe imaginaire.

I. INTRODUCTION

The scattering of electrons from atoms has been studied throughout the history of atomic physics, both experimentally and theoretically. Neverthe-

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less it is only recently that progress has been made concerning the existence of scattering amplitudes for such systems and their analytic continuation into the complex energy plane. In the present work we consider the elastic forward scattering of an electron from an atom in its ground state in the Born-Oppenheimer approximation (fixed nucleus in the origin). We also neglect spin contributions to the Hamiltonian, so that we are left with a many-particle Coulomb problem. In the scattering channel we are interested in we are dealing with two fragments of which one is electrically neutral. As a consequence the wave-operators exist in the standard sense. Then the corresponding scattering amplitude exists in an average sense ([*1*], [*2*]) but their pointwise existence as a function of energy E does not follow from this result. In fact there is no general physical necessity for the latter since scattering amplitudes are related to probability densities rather than probabilities themselves. Nevertheless it is commonly believed that the elastic electron-atom amplitude exists pointwise and this has recently been demonstrated [*3*], [*4*] for energies below the three-fragment break-up energy of the system. Nutall and Singh have also found [*5*] that partial wave amplitudes have analytic continuation below the physical part of the real axis for energies in the above region. In the present work we show that the amplitude under consideration in fact exists for all E not equal to excitation or break-up threshold energies and also that analytic continuation is possible above the physical real axis. This fact is of importance for a proof of dispersion relations for electron-atom scattering as formulated by E. Gerjuoy and N. A. Krall [*6*]. (See also [*7*]).

The scattering amplitudes that we are interested in can be expressed in terms of the (inter) channel transition operators

$$T_{\alpha\beta}(z) = V_\alpha + V_\alpha(H - z)^{-1}V_\alpha \tag{1.1}$$

where H is the full Hamiltonian (without the center-of-mass term since we have adopted the Born-Oppenheimer approximation), V_α the interaction between the fragments in channel α and z the complex energy. In positron-atom scattering only one channel enters into the formalism, i. e. $\alpha = \beta$.

Because of the necessary anti-symmetrization this is different for electron-atom scattering, the full scattering amplitude now being a linear combination of a direct part f^d and a rearrangement part f^r. The total number of electrons is N so that the nuclear change in $Z = N - 1$. We use units such that $\hbar = e^2 = 1$ and m, the electron mass, is $\frac{1}{2}$. The electronic position vectors $\underline{x}_j$ (associated momenta p_j) have the nucleus as origin. The full Hamiltonian

$$H = H^N = \sum_{j=1}^{N} p_j^2 - \sum_{j=1}^{N} \frac{Z}{x_j} + \sum_{i>j} |\underline{x}_i - \underline{x}_j|^{-1} \tag{1.2}$$

then acts in the Hilbert space $\mathscr{H} = L^2(\mathbb{R}^{3N})$ after spin has been removed from the formalism. The interaction between electron j and the atom made up from the remaining particle is

$$V_j = \sum_{i \neq j} |\underline{x}_i - \underline{x}_j|^{-1} - \frac{Z}{x_j} = \sum_{i \neq j} \left\{ |\underline{x}_i - \underline{x}_j|^{-1} - \frac{1}{x_j} \right\} \tag{1.3}$$

For z outside $\sigma(H)$, the spectrum of H, the resolvent $(H - z)^{-1}$ is a bounded operator and for such z the direct and rearrangements parts of the offshell scattering amplitude can be defined as

$$\begin{aligned} f^d(k, z) &= -2\pi^2 \langle \hat{\psi}_{\underline{k}}^N | V_N | \hat{\psi}_{\underline{k}}^N \rangle - \langle \hat{\psi}_{\underline{k}}^N | V_N (H - z)^{-1} V_N \hat{\psi}_{\underline{k}}^N \rangle \\ &= f_B^d + \phi^d(k, z) \end{aligned} \tag{1.4}$$

and

$$\begin{aligned} f^r(k, z) &= -2\pi^2 \langle \hat{\psi}_{\underline{k}}^{N-1} | V_N | \hat{\psi}_{\underline{k}}^N \rangle - 2\pi^2 \langle \hat{\psi}_{\underline{k}}^{N-1} | V_{N-1} (H - z)^{-1} V_N | \hat{\psi}_{\underline{k}}^N \rangle \\ &= f_B^r(k) + \phi^r(k, z) \end{aligned} \tag{1.5}$$

Here is

$$\hat{\psi}_{\underline{k}}^j(\underline{x}_1, \ldots, \underline{x}_N) = (2\pi)^{-3/2} \exp(i\underline{k} \cdot \underline{x}_j) \varphi_0(\ldots, \underline{x}_{j-1}, \underline{x}_{j+1}, \ldots) \tag{1.6}$$

where $(2\pi)^{-3/2} \exp(i\underline{k} \cdot \underline{x}_j)$ is the relative motion plane wave state (with momentum $\underline{k}$, energy k^2) and φ_0 is the orbital part of the atomic ground-state. We assume φ_0 to be non degenerate, rotational invariant and symmetrized. Then the amplitudes f^d and f^r only depend on k instead of $\underline{k}$. The eigenvalues of the atomic Hamiltonian

$$H^{N-1} = \sum_{j=1}^{N-1} p_j^2 - \sum_{j=1}^{n} \frac{Z}{x_j} + \sum_{i<j} |\underline{x}_i - \underline{x}_j|^{-1} \tag{1.7}$$

are denoted by E_n^0 (so that E_0^0 corresponds with φ_0) and similarly the eigenvalues of H^{N-p-1}, the positive ion which charge p are denoted by E_n^p. It is not clear *a priori* that f^d and f^r exist. This, however, is indeed the case. For the Born parts f_B^d and f_B^r this follows directly from the exponential decay and spherical symmetry of φ_0 and for the non-Born parts ϕ^d and ϕ^r from the square integrability of $V_j \hat{\psi}_{\underline{k}}^j$. In fact each term on the right in (1.3) is square integrable in $\underline{x}_j$ with norm proportional to x_i. Since φ_0 has exponential decay in $\underline{x}_i$ it follows that

$$\psi_{\underline{k}}^j = V_j \hat{\psi}_{\underline{k}}^j \tag{1.8}$$

is square integrable. This argument break down for $Z \neq N - 1$ but in that case (1.4) itself is incorrect. We can now write ϕ^d and ϕ^r as inner products in $\mathscr{H}$:

$$\phi^d(k, z) = -2\pi^2 (\psi_{\underline{k}}^N, (H - z)^{-1} \psi_{\underline{k}}^N) \tag{1.9}$$

$$\phi^r(k, z) = -2\pi^2 (\psi_{\underline{k}}^{N-1}, (H - z)^{-1} \psi_{\underline{k}}^N) \tag{1.10}$$

From (1.4) and (1.5) the physical amplitudes are obtained by substituting $z = E(k) + i\varepsilon = k^2 + E_0^0 + i\varepsilon$ and taking the limit $\varepsilon \downarrow 0$. Thus in order to show that the physical amplitudes exist we have to prove that (1.9) and (1.10) have limits for $\varepsilon \downarrow 0$. This matter is considered in section 2 where we find that this limit indeed exists for $E(k)$ not equal to a threshold energy for excitation or break-up processes. The method used there also applies to a non-forward scattering. If we want to make an analytic continuation for complex $k = |\underline{k}|$ we run into the problem that the exponentials $\exp(i\underline{k} \cdot \underline{x}_j)$ in (1.6) blow up. It is therefore convenient to make a unitary scale transformation and consider the transformed Hamiltonian [8]

$$H(k) = k^2 \sum_{j=1}^{n} p_j^2 - k \sum_{j=1}^{N} \frac{Z}{x_j} + k \sum_{i>j} |\underline{x}_i - \underline{x}_j|^{-1}$$

This family extends for complex k to an analytic family. Furthermore after this transformation is performed on $\psi_{\underline{k}}^j$ one obtains a square integrable function even for complex k's as long as $|\operatorname{Arg} k| < \frac{\pi}{2}$. So the possible singular behaviour comes from $(H(k) - z)^{-1}$ for $z = E(k) + i\varepsilon$ in the limit $\varepsilon \downarrow 0$. In section III we show that also in the case of complex k the limit $\varepsilon \downarrow 0$ can be taken for $0 < \operatorname{Arg} k < \frac{\pi}{2}$. By reflection symmetry this is also true for $\frac{\pi}{2} < \operatorname{Arg} k < \pi^2$. Since dilation analyticity techniques do not apply for $\operatorname{Arg} k = \frac{\pi}{2}$ we use as an auxiliary method, the so-called boost transformation [9]. Finally we find that for the direct amplitude there is an analytic continuation domain in k in the upper half-plane with poles on the imaginary axis corresponding to bound state energies; for the exchange amplitude however there is an additional cut $i[\omega_0, +\infty)$ where ω_0 is the square root of the ionization energy of the atom. We also show that a meromorphic continuation exists below the physical real axis for energies smaller than the first excited state of the atom.

II. FINITENESS OF THE SCATTERING AMPLITUDE FOR REAL INCIDENT MOMENTA

In the section we show that the non-Born parts of the scattering amplitudes $\phi^d(z)$ and $\phi^r(z)$ as given by (1.9) and (1.10) have boundary values when $z = E(k) + i\varepsilon$ and we let ε tend to zero. The main mathematical difficulty comes from the fact that since $E(k)$ belong to the spectrum of H the operators $(H - E(k) - i\varepsilon)^{-1}$ have no limit as a bounded operator on $L^2(R^n)$.

The most recent contribution to this problem is due to P. Perry, I. Sigal, B. Simon [10]. They extend to a very general class of many body systems including those considered here some, some results of S. Agmon [11]; T. Ikebe, Y. Saito [12] et E. Mourre [13]. To state their result in the present case let us introdûce the weighted L^2-spaces:

$$L_s^2 = \{ u \in L_{loc}^2, (1 + X^2)^{s/2} u \in L^2 \}$$

$\left(X^2 = \sum_{i=1}^{N} x_i^2\right)$ and the set Σ of « thresholds » of the system i. e. in our situation [14] the union of 0 and the set of eigenvalues of ionized atoms hamiltonians H^{N-1}, H^{N-2}, ... Then ([10]) the following limits exist in the norm topology of $\mathscr{L}(L_s^2, L_{-s}^2)$, the space of bounded linear operators from L_s^2 to L_{-s}^2:

$$(H - E \pm i0)^{-1} = \lim_{\varepsilon \downarrow 0} (H - E \pm i\varepsilon)^{-1}$$

for all $s > \frac{1}{2}$ and $E \notin \Sigma \cup \sigma_p(H)$ where $\sigma_p(H)$ denotes the point spectrum of H. Existence of the limit when $E \in \Sigma$ remains to our knowledge an open problem. This result will be referred to as PSS; it does not apply directly to the analysis of (1.9) and (1.10) since $\psi_{\underline{k}}^N$ and $\psi_{\underline{k}}^{N-1}$ are not in L_s^2 for some $s > \frac{1}{2}$; this is due to the long-range character of the Coulomb forces. To overcome this difficulty we will need to use the explicit structure of these states.

Let us first introduce

$$H_{0,j} = H - V_j \tag{2.1}$$

with V_j given by (1.3). It is clear that $H_{0,j}$ is the Hamiltonian of a system consisting of an $(N - 1)$ electron-atom and an electron j not interacting with it. It will be useful to have in mind the tensorial structure (with 1 the identity operator);

$$H_{0,j} = H^{N-1} \otimes 1 + 1 \otimes p_j^2 \tag{2.2}$$

acting on

$$\mathscr{H} = L^2\left(\mathbb{R}^{3N}, \prod_{i=1}^{N} d\underline{x}_i\right) = L^2\left(\mathbb{R}^{3(N-1)}, \prod_{i \neq j} d\underline{x}_i\right) \otimes L^2(\mathbb{R}^3, dx_j) \tag{2.3}$$

We will denote by $\sigma(\cdot)$, $\sigma_{ess}(\cdot)$ the spectrum and essential spectrum of a given closed operator. By the HVZ theorem [14] one has $\sigma_{ess} = [E_0^0, +\infty)$. In $(-\infty, E_0^0)$ the spectrum of H consists of isolated eigenvalues with finite multiplicities corresponding to the N-electron negative ion stable states. One also has $\sigma(H_{0,j}) = \sigma_{ess}(H_{0,j}) = [E_0^0, +\infty)$ by general results [14] on the spectrum of operators of tensorial sum type like (2.2).

Let $G(z) = (H - z)^{-1}$, $G_{0,j}(z) = (H_{0,j} - z)^{-1}$; we will often use the resolvent equation

$$G(z) = G_{0,j}(z) - G(z)V_jG_{0,j}(z),\ z \notin \sigma_p(H) \tag{2.4}$$

or its iterate

$$G(z) = G_{0,i}(z) - G_{0,i}(z)V_iG_{0,j}(z) - G_{0,i}(z)V_iG(z)V_jG_{0,j}(z) \tag{2.5}$$

In the analysis presented here the analytic structure of the states $\psi_{\underline{k}}^j$ given by (1.8) plays a very important role. One has denoting by $\mathscr{F}$ the Fourier transform on L^2

$$\mathscr{F}\psi_{\underline{k}}^j(\underline{k}_1, \dots, \underline{k}_N) = \frac{1}{|\underline{k}_i - \underline{k}_j|^2} \sum_{i \neq j} [\mathscr{F}\varphi_0^j(\dots, \underline{k}_i + \underline{k}_j - \underline{k}, \dots) - \mathscr{F}\varphi_0^j(\dots, \underline{k}_i, \dots)] \tag{2.6}$$

where φ_0^j is the atomic ground state wave-function involving the electrons different from j.

It is well-known that $\mathscr{F}\varphi_0^j$ is analytic in all its variables in a complex neighbourhood of $\mathbb{R}^{3(N-1)}$ (see for example Lemma 1, § III.2 below for an equivalent statement). So obviously $\mathscr{F}\psi_{\underline{k}}^j$ only has a singularity at $\underline{k}_j = \underline{k}$. In order to isolate this singular part we introduce a C^∞ function χ such that $0 \leqslant \chi \leqslant 1$, $\chi(q) = 0$ if $|q^2 - k^2| > \frac{1}{2}(E_1^0 - E_0^0)$ and $\chi(q) = 1$ if $|q^2 - k^2| < \frac{1}{4}(E_1^0 - E_0^0)$. We denote by χ_j the operator acting as multiplication by the function $\chi(\underline{k}_j)$ in momentum representation. Then one has a splitting

$$\begin{aligned} \psi_{\underline{k}}^j &= \chi_j + (1-\chi)\psi_{\underline{k}}^j \\ &\stackrel{\text{def}}{=} {}_1\psi^j + {}_2\psi^j \end{aligned} \tag{2.7}$$

(since we are now dealing with a fixed $\underline{k}$ we will drop this index in the notation of ψ's).

Notice that $\mathscr{F}_2\psi^j$ is infinitely differentiable in $L^2(R^{3N})$ so that ${}_2\psi^j$ is in L_s^2 for all $s \in R$.

We further decompose

$$\begin{aligned} {}_1\psi^j &= P_{j_1}\psi^j + Q_{j_1}\psi^j \\ &\stackrel{\text{def}}{=} {}_0\psi^j + {}_\perp\psi^j \end{aligned} \tag{2.8}$$

where $P_j = \varphi_0^j \rangle \langle \varphi_0^j \otimes 1$ in accordance with the decomposition (2.3) and $Q_j = 1 - P_j$. One has

$$\begin{aligned} \mathscr{F}_0\psi^j(\underline{k}_1, \dots, \underline{k}_N) &= \chi(\underline{k}_j)\mathscr{F}\varphi_0^j(\dots, \underline{k}_{j-1}, \underline{k}_{j+1}, \dots) \times \int \prod_{i \neq j} d\underline{q}_i \\ &\times \mathscr{F}\varphi_0^j(\dots, \underline{q}_{j-1}, \underline{q}_{j+1}, \dots)\mathscr{F}\psi_{\underline{k}}^j(\dots, \underline{q}_{j-1}, \underline{k}_j, q_{j+1}, \dots) \end{aligned} \tag{2.9}$$

Since φ_0 is rotation invariant and its Fourier transform is analytic the singularity $\frac{1}{|\underline{k} - \underline{k}_j|^2}$ in $\mathscr{F}\psi^j_{\underline{k}}$ disappears when integrations around $\underline{q}_i = \underline{k} - \underline{k}_j$ are performed. Accordingly $\mathscr{F}_0\psi^j$ is infinitely differentiable in all its variables in L^2 hence $_0\psi^j$ is L^2_s for all $s \in \mathbb{R}$.

So clearly in order to apply the Perry-Sigal-Simon theory to the scattering amplitudes (1.9) and (1.10) it remains to investigate the contributions from $_\perp\psi^j$, $j = N$ or $N - 1$. For this we need some intermediate results.

LEMMA II.1. — $\lim_{\varepsilon \downarrow 0^+} G_{0,j}(E(k) + i\varepsilon)_\perp\psi^j \in L^2$.

Proof. — Consider the subspace containing $_\perp\psi^j$:

$$\mathscr{M}_j = \text{Range of } Q_j\chi_j$$

It reduces $H_{0,j}$ since Q_j and χ_j commute with $H_{0,j}$. Let $H_{0,\mathscr{M}_j}$ denote the restriction of $H_{0,j}$ to $\mathscr{M}_j$; then $G_{0,j}(z)\psi = (H_{0,\mathscr{M}_j} - z)^{-1}\psi$ for $\psi \in \mathscr{M}_j$, and z in the connected domain $\text{Re } z < E^0_0$ or $\text{Im } z \neq 0$. So it is enough to show that $E^0_0 + k^2$ is not in $\sigma(H_{0,\mathscr{M}_j})$. Using the tensorial structure (2.2) one can write

$$H_{0,\mathscr{M}_j} = H^{N-1}Q_j \otimes 1 + 1 \otimes p_j^2\chi_j$$

and accordingly [*14*] :

$$\sigma(H_{0,\mathscr{M}_j}) = \sigma(H^{N-1}Q_j) + \sigma(p_j^2\chi_j)$$

By the construction of χ this set is contained in $\left[\frac{E^0_0 + E^1_0}{2} + k^2, + \infty\right)$ which concludes the proof since $E^1_0 > E^0_0$.

LEMME II.2. — $V_jG_{0,j}(E(k))_\perp\psi^j \in L^2_s$ for all real s with $s \leqslant 1$.

Proof. — Let us first show that $G_{0,j}(E(k))_\perp\psi^j$ is in the domain of the operators

$$B_j(\underline{\tau}) = \exp(i\Sigma\underline{x}_l \cdot \underline{\tau}_l),\ \underline{\tau} = (\underline{\tau}_1, \ldots, \underline{\tau}_N) \in \mathbb{C}^{3N},\ \underline{\tau}_j = 0,$$

for $|\text{Im } \underline{\tau}|^2 = \sum_l |\text{Im } \underline{\tau}_l|^2$ small enough. Since $_\perp\psi^j$ does by the enponential decay properties of φ_0 ([*9*]) we only have to show that if $_\perp\psi^j(\underline{\tau}) = B_j(\underline{\tau})_\perp\psi^j$ and $H_{0,j}(\underline{\tau}) = B_j(\underline{\tau})H_{0,j}B_j^{-1}(\tau)$, $\underline{\tau} \in \mathbb{R}^{3N}$, then

$$(H_{0,j}(\underline{\tau}) - E(k))^{-1}{}_\perp\psi^j(\underline{\tau}) = B_j(\underline{\tau})(H_{0,j} - E(k))^{-1}{}_\perp\psi^j$$

has an analytic continuation under this type of condition on $|\text{Im } \underline{\tau}|$. By the tensorial structure (2.2), (2.3) one has

$$H_{0,j}(\underline{\tau}) = H^{N-1}(\underline{\tau}) \otimes 1 + 1 \otimes p_j^2$$

This family is analytic of type A in $\underline{\tau}$ ([*15*]) and the spectral analysis of $H^{N-1}(\underline{\tau})$ (see [*9*] or ch. III below) shows that its essential spectrum consists of parabolas and their interior centered around the thresholds $E_0^0, E_1^0 \dots$ of H^{N-1}, whose size depends on $|\operatorname{Im} \tau|$. Furthermore the point spectrum is the same as for H^{N-1} with the exception of those eigenvalues absorbed by the parabolas. Consider now the restriction $H_{0,\mathcal{M}_j}(\underline{\tau})$ of $H_{0,j}(\underline{\tau})$ to the subspace $\mathcal{M}_j(\underline{\tau}) = \text{Range } \chi_j Q_j(\underline{\tau})$ where $Q_j(\underline{\tau}) = 1 - P_j(\underline{\tau})$ and

$$P_j(\underline{\tau}) = B_j(\underline{\tau}) P_j B_j(\underline{\tau})^{-1}$$

(see Lemma III.1 below for the properties of $P_j(\underline{\tau})$) Then one shows as in Lemma II.1 that the spectrum of $H_{0,\mathcal{M}_j}(\underline{\tau})$ lies entirely in the domain $\operatorname{Re} z > \dfrac{E_0^0 + E_1^0}{2} + k^2$. Also for any $\psi \in \mathcal{M}_j(\underline{\tau})$, $\operatorname{Re} z < E_0^0$, one has $(H_{0,\mathcal{M}_j}(\underline{\tau}) - z)^{-1}\psi = (H_{0,j}(\underline{\tau}) - z)^{-1}\psi$. Accordingly in this domain $(H_{0,j}(\underline{\tau}) - z)^{-1}$ is analytic in $\underline{\tau}$ for $|\operatorname{Im} \underline{\tau}|$ small enough; by a standard argument [*15*] $(H_{0,\mathcal{M}_j}(\underline{\tau}) - E(k))^{-1}$ also is since $E(k)$ and $\{ z \in \mathbb{C}, \operatorname{Re} z < E_0^0 \}$ belong to a common connected component of the resolvent set of $H_{0,\mathcal{M}_j}$. So finally $B_j(\underline{\tau})(H_{0,j} - E(k))^{-1} {}_{\perp}\psi^j = (H_{0,\mathcal{M}_j}(\underline{\tau}) - E(k))^{-1} {}_{\perp}\psi^j$ is analytic for $|\operatorname{Im} \underline{\tau}|$ small enough which implies $G_{0,j}(E(k))_{\perp}\psi^j$ is in the domain of any polynômial in the x_i's, $i \neq j$.

Now coming back to the definition (1.3) of V_j and using $x_j \leqslant |\underline{x}_i - \underline{x}_j| + x_i$ it is clear that $V_j G_{0,j}(E(k))_{\perp}\psi^j \in \mathcal{D}(x_j)$ hence finally belongs to L_1^2 (we omit here the problem linked to the unbounded character of V which can be solved by a « relative boundedness » argument ([*15*]).

We are now in position to prove our first main result.

THEOREM II.1. — The scattering amplitudes

$$f^d(k) = f_B^d + \lim_{\varepsilon \downarrow 0} \phi^d(k, E(k) + i\varepsilon) \tag{2.10}$$

and

$$f^r(k) = f_B^r(k) + \lim_{\varepsilon \downarrow 0} \phi^r(k, E(k) + i\varepsilon) \tag{2.11}$$

exist and are continuous on the complement in R^+ of the set

$$\{ k \in \mathbb{R}^+, E(k) \in \Sigma \cup \sigma_p(H) \}.$$

Proof. — We will investigate separately the various contributions to the amplitudes coming from the decompositions (2.7) and (2.8) when $E(k) \notin \Sigma \cup \sigma_p(H)$. Let us look at $f^d(k)$ first; the non Born part of the amplitude is the limit when ε tend to zero of

$$\langle {}_0\psi^N + {}_{\perp}\psi^N + {}_2\psi^N, G(E(k) + i\varepsilon)_0\psi^N + {}_{\perp}\psi^N + {}_2\psi^N \rangle .$$

Since ${}_0\psi^N$ and ${}_2\psi^N$ are in L_s^2 for all $s \in R$ they give finite contributions according to PSS.

So we only need to look at those terms involving ${}_{\perp}\psi^N$. Using the resolvent equation (4) one gets first, with $\delta = 0$ or 2 :

$$\begin{aligned}({}_\delta\psi^N, G(E(k) + i\varepsilon)_{\perp}\psi^N) &= ({}_\delta\psi^N, G_{0,N}(E(k) + i\varepsilon)_{\perp}\psi^N) \\ &+ ({}_\delta\psi^N, G(E(k) + i\varepsilon)V_N G_{0,N}(E(k) + i\varepsilon)_{\perp}\psi^N)\end{aligned} \tag{2.12}$$

By Lemma 1 the first term on the right-hand side has a finite limit as $\varepsilon \downarrow 0$. With a little extra argument it is easy to show from Lemma II.2 that $V_N G_{0,N}(E(k) + i\varepsilon)_{\perp}\psi^N$ converges in L_1^2 to $V_N G_{0,N}(E(k))\psi_N^{\perp}$ so that another application of PSS gives existence of the limit for the second term on the r. h. s. of (2.12). It remains to look at $({}_{\perp}\psi^N, G(E(k) + i\varepsilon)_{\perp}\psi^N)$; by equation (2.5) with $i = j = N$ one has

$$\begin{aligned}({}_{j}\psi^N, G(E(k) + i\varepsilon)_{\perp}\psi^N) &= ({}_{\perp}\psi^N, G_{0,N}(E(k) + i\varepsilon)_{\perp}\psi^N) \\ &- (G_{0,N}(E(k) - i\varepsilon)_{\perp}\psi^N, V_N G_{0,N}(E(k) + i\varepsilon)\psi_{\perp}^N) \\ &+ (V_N G_{0,N}(E(k) - i\varepsilon)\psi_{\perp}^N, G(E(k) + i\varepsilon)V_N G_{0,N}(E(k) + i\varepsilon)_{\perp}\psi^N)\end{aligned}$$

The first two terms on the r. h. s. of this equality have finite limits by Lemma II.1 and a relative boundedness argument in order to deal with the unboundedness of V_N. As to the third term existence of the limit follows again from lemma II.2 and PSS. Let us now look at $f^r(k)$. Here again it is enough to look at contributions like

$$({}_{\delta}\psi^{N-1}, G(E(k) + i\varepsilon)_{\perp}\psi^N), \; ({}_{\perp}\psi^{N-1}, G(E(k) + i\varepsilon)_{\delta}\psi^N),$$

or $({}_{\perp}\psi^{N-1}, G(E(k) + i\varepsilon)_{\perp}\psi^N)$. Terms of the first type are analysed as before with the help of eq. (4) with $j = N$ or $N - 1$. The term of the second type is analysed with eq. (2.12) in which one takes $i = N - 1$, $j = N$; then Lemma II.2 and PSS provide again the existence of the limit as $\varepsilon \downarrow 0$.

So the limits (2.10) and (2.11) exist when $E(k) \notin \Sigma \cup \sigma_p(H)$. To show continuity in this open set we notice that all components ${}_0\psi^j$, ${}_2\psi^j$, and $V_j G_{0,j}(E(k))_{\perp}\psi^j$ have a continuous dependence in k as elements of L_s^2, $s < 1$. On the other hand the boundary values of $G(E(k) + i\varepsilon)$ as elements of $\alpha(L_s^2, L_{-s}^2)$ also vary continuously in k (see [*10*]). Thus $\lim_{\varepsilon \downarrow 0} \phi^d(k, E(k) + i\varepsilon)$ and $\lim_{\varepsilon \downarrow 0} \phi(k, E(k) + i\varepsilon)$ are continuous in a neighbourhood of each k such that $E(k) \notin \Sigma \cup \sigma_p(H)$. For the Born term $f_B(k)$ continuity follows from elementary arguments.

REMARKS II.1. — 1) A by-product of the previous result is the finiteness of the cross-section for the process under consideration.

2) We could as well have considered the non forward scattering amplitudes (see (1.4), (1.5))

$$f^d(\underline{k}_1, \underline{k}_2, z) = -2\pi^2[\langle \hat{\psi}_{\underline{k}_1}^N \mid V_N{}' \hat{\psi}_{\underline{k}_2}^N \rangle + \langle \hat{\psi}_{\underline{k}_1}^N \mid V_N(H - z)^{-1}V_N \mid \hat{\psi}_{\underline{k}_2}^N \rangle$$

$$f^r(\underline{k}_1, \underline{k}_2, z) = -2\pi^2[\langle \hat{\psi}_{\underline{k}_1}^{N-1}, V_N\hat{\psi}_{\underline{k}_2}^N \rangle + \langle \hat{\psi}_{\underline{k}_1}^{N-1} \mid V_N(H - z)^{-1}V_N \mid \hat{\psi}_{\underline{k}_2}^N \rangle$$

with $k_1 = k_2 = k$ in the limit $z = E(k) + i\varepsilon$, $\varepsilon \downarrow 0$. The same arguments apply to show that these limits exist and are continuous for $E(k) \notin \Sigma \cup \sigma_p(H)$.

3) There is an argument (see e. g. [*18*]) allowing to show that non threshold eigenvalues of H actually decouple from the scattering amplitude in the

sense that they do not give rise to singularities. We will not develop this point here since the mathematical proof is quite involved (although formally it is not difficult to convince oneself that e. g. $(\psi_{\underline{k}}^j, \psi) = 0$ if $H\psi = E(k)\psi$ for all $j \in (1, \ldots, n)$.

III. ANALYTIC CONTINUATION OF SCATTERING AMPLITUDES

III.1 Complex canonical transformations.

The problem of continuing analytically the scattering amplitudes for complex values of k has been discussed by one of us ([*7*], [*16*], [*17*]) in connection with the dispersion relations of Gerjuoy and Krall [*6*].

In the previous references the parameter ε in (2.10, 2.11) was kept fixed and non zero and the problem of taking the limit was left open. The method of complex canonical transformations developped by Combes and Thomas [*9*] and already used in [*3*], [*4*], [*7*], [*16*], [*17*] appears as very well adapted to this type of analysis. It has already been used successfully to prove analyticity in the one-body problem [*18*]. However the method leads to transformed Hamiltonian operators which are no more self-adjoint and are not covered by the PSS theorem. Nevertheless it turns out that using the connected integral equations of Weinberg-Van Winter [*14*] one can still reach the on-shell limit $\varepsilon = 0$. This is due to the fact that for complex k, the canonical transformations separate the singularities of the resolvent and for the problems considered here only those coming from the ground-state channels need to be investigated; but, this reduces essentially the difficulty to a one-body problem. We introduce two families of unitary transformations. The group of dilation operators is defined by

$$\mathfrak{U}(\lambda)\phi(\underline{x}_1, \ldots, \underline{x}_N) = \lambda^{\frac{3N}{2}} \phi(\lambda\underline{x}_1, \ldots, \lambda\underline{x}_n), \ \lambda \in \mathbb{R}^+$$

The group of boosts (or translations in momentum space) has been already used in the previous section and is given by

$$B(\underline{\tau})\phi(\underline{x}_1, \ldots, \underline{x}_N) = \exp\left(i \sum_l \underline{x}_l \cdot \underline{\tau}_l\right)\phi(\underline{x}_1, \ldots, \underline{x}_N)$$

$$\underline{\tau} = (\underline{\tau}_1, \ldots, \underline{\tau}_N) \in \mathbb{R}^{3N}$$

These groups act in the following way on the kinetic energy operator

$$\mathfrak{U}^{-1}(\lambda)H_0\mathfrak{U}(\lambda) = \lambda^2 H_0$$

whereas

$$B^{-1}(\underline{\tau})H_0B(\underline{\tau}) = H_0(\underline{\tau})$$

where

$$H_0(\underline{\tau})\mathscr{F}\phi(\underline{k}_1, \ldots, \underline{k}_N) = \sum_l (\underline{k}_l + \underline{\tau}_l)^2 \mathscr{F}\phi(\underline{k}_1, \ldots, \underline{k}_N)$$

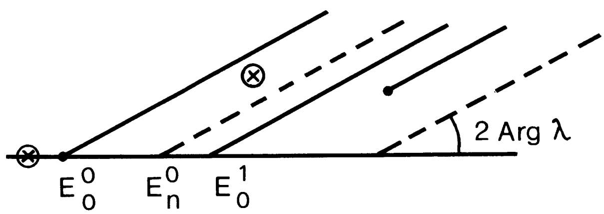
As for the potentials they transform under the dilation group as :

$$\mathfrak{U}^{-1}(\lambda)\frac{1}{|\underline{x}_i - \underline{x}_j|}\mathfrak{U}(\lambda) = \frac{\lambda}{|\underline{x}_i - \underline{x}_j|}$$

and they are invariant under the boost group. The main idea of complex canonical transformations is to make the parameters λ and τ complex. Then one gets families $H(\lambda)$ and $H(\tau)$, which are analytic of type A [*15*] in these parameters, whose spectrum has the following structure [*8*] : $\sigma_{ess}(H(\lambda)) = \lambda^2\mathbb{R}^+ + \Sigma(\lambda)$ where the set of thresholds $\Sigma(\lambda)$ is defined as

$$\Sigma(\lambda) = \bigcup_D \left(\sum_{C \in D} \sigma_p^C(\lambda)\right)$$

Here the union is over all fragmentations D of the system electrons + nuclei into disjoint clusters $D = \{ C_1, \ldots, C_l \}$, $1 < l \leqslant N + 1$ and the set $\sigma_p^C(\lambda)$ is the union of zero and the set of eigenvalues of the hamiltonian for the subsystem C (so that in particular it reduces to zero if C has no bound state; this occurs if and only if C contains only electrons). Since for λ real the set $\sigma_p^C(\lambda)$ is independent of λ one sees that $\sigma(H_N(\lambda))$ consists of a set of parallel half-lines, the leftmost ones originating at the eigenvalues $E_0^0, E_1^0, \ldots$ of H^{N-1}.

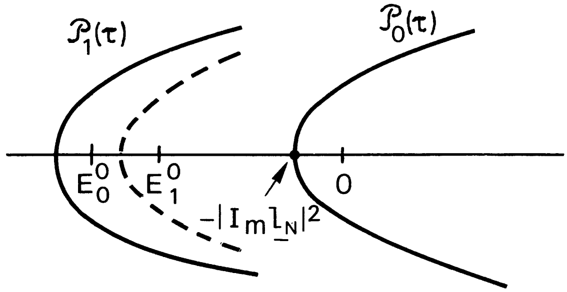


In addition to this spectrum $\sigma(H(\lambda))$ contains the same real eigenvalues as H $\left(\text{for } |\operatorname{Arg}\lambda| < \frac{\pi}{2}\right)$ and possibly in addition some complex eigenvalues and cuts in the domain $\{ z \in \mathbb{C}, 0 < \operatorname{Arg}(z - E_0^0) < 2\operatorname{Arg}\lambda \}$.

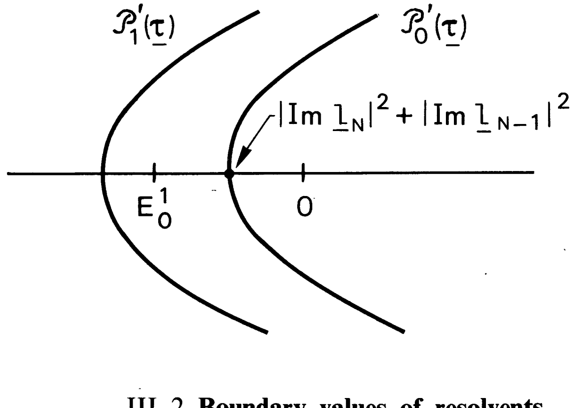
Concerning the spectrum of $H(\tau)$ one has ([*9*])

$$\sigma_{ess}(H(\underline{\tau})) = \bigcup_D \left(\sigma_0^D(\underline{\tau}) + \sum_{C \in D} \sigma_p^C\right)$$

Here $\sigma_0^D(\underline{\tau})$ is the spectrum of $H_0^D(\underline{\tau})$ where H_0^D is the kinetic energy operator for the centers-of-mass of the clusters C. As an illustration let us consider the decomposition with 2 clusters consisting of the electron N and the remaining atom. Then $H_0^D(\underline{\tau}) = (\underline{P}_N + \underline{\tau}_N)^2$ which has as spectrum the interior of parabola $\mathscr{P}_0(\tau)$; it has to be shifted over the eigenvalues of the atomic Hamiltonian $E_0^0, \ldots$ giving parabolas $\mathscr{P}_1(\tau), \ldots$ The decomposition in which electrons are interchanged gives the same type of contributions to $\sigma_{ess}(H(\underline{\tau}))$.



The next decomposition is into three clusters, say electrons N and N − 1 and the remaining positive ion. Here $H_0^D = (\underline{P}_{N-1} + \underline{\tau}_{N-1})^2 + \underline{P}_N + \underline{\tau}_N)^2$ whose spectrum is also the interior of a parabola $\mathscr{P}_0'(\tau)$ which has to be shifted over the eigenvalues of the positive ion Hamiltonian $E_0^1, \ldots$ giving new parabolas $\mathscr{P}_1'(\tau), \ldots$ It has to be noticed that $|\mathrm{Im}\,\underline{\tau}_{N-1}| = (E_0^1 - E_0^0)^{1/2}$ the parabola $\mathscr{P}_1'(\underline{\tau})$ will absorb E_0^0; this corresponds exactly to the complement of the domain of analyticity of $\varphi_0^N(\underline{\tau}) = B(\underline{\tau})\varphi_0^N$ when $\underline{\tau} = (0, \ldots, \underline{\tau}_{N-1}, 0)$ ([*9*]), a fact which will be used later.



III.2 **Boundary values of resolvents.**

We now turn to the analysis of the Weinberg-van Winter equation [*14*] :

$$G(z) = D(z) + I(z)G(z)$$

where

$$D(z) = \sum_{D_{N+1} \supset D_N \ldots \supset D_l} G_{D_{N+1}}(z) V_{D_{N+1} D_N} G_{D_N}(z) \ldots V_{D_{l+1} D_l} G_{D_l}(z) \quad (3.1)$$

and

$$I(z) = \sum_{D_{N+1} \supset \ldots \supset D_2} G_{D_{N+1}}(z) V_{D_{N+1} D_N} G_{D_N}(z) \ldots G_{D_2}(z) V_{D_2 D_1} \quad (3.2)$$

with the following meaning for the notations : D_l is a decomposition of the system (nucleus + N electrons) into l clusters and $D_l \supset D_{l-1}$ means that D_{l-1} is obtained by linking together two clusters of D_l; $V_{D_l D_{l-1}}$ is the sum of the interactions between those particles in the new cluster of D_{l-1} which are not in the same clusters of D_l. For example if D_2 is the partition in which one cluster is electron j and the other the remaining $(N-1)$ electron-atom then $V_{D_2 D_1} = V_j$ as given by (1.3). Finally $G_D(z) = (H_D - z)^{-1}$ where H_D is the Hamiltonian for the non interacting clusters in D, i. e. H minus the sum of interactions between particles belonging to different clusters in D; in particular $G_{D_{N+1}}(z) = (H_0 - z)^{-1}$.

Obviously there is a similar set of equations for the transformed Hamiltonian $H(\lambda)$ or $H(\underline{\tau})$ involving the resolvents $G_D(\lambda)$ or $G_D(\underline{\tau})$ of the operators H_D transformed under $\mathfrak{U}(\lambda)$ or $B(\underline{\tau})$, and the transformed interactions. These equations allow to derive the structure of the spectrum of the transformed Hamiltonians as described above; one uses compactness of $I(z)$ and its transforms for z outside the spectra of all H_D's. Since the cluster Hamiltonians H_D are tensorial sums their spectrum can be analyzed inductively using Ichinose's lemma [*14*]. For further purposes let us notice that in the case where D_2 is the partition into electron j and the remaining atom one has $H_{D_2} = H_{0,j}$ as given by (2.1). Let us decompose

$$G_{0,j} = G_{0,j}^{(1)}(z) + G_{0,j}^{(2)}(z) \quad (3.3)$$

with

$$G_{0,j}^{(1)}(z) = G_{0,j}(z) P_j, \qquad G_{0,j}^{(2)}(z) = G_{0,j}(z) Q_j$$

(with notations of II and a similar decomposition for the transformed $H_{0,j}$ and P_j under the groups $\mathfrak{U}(\lambda)$ or $B(\underline{\tau})$. The point of interest in this decomposition is that one has eliminated in $G_{0,j}^{(2)}(z)$ the threshold E_0^0 so that either the half-line $E_0^0 + \lambda^2 \mathbb{R}^+$ in the case of dilations, or the parabola $\mathscr{P}_1$ in the case of boosts do not belong anymore to the singular set of $G_{0,j}^{(2)}(z)$. As to the part $G_{0,j}^{(1)}(z)$ it has the simple structure

$$G_{0,j}^{(1)}(z) = (p_j^2 + E_0^0 - z)^{-1} P_j \quad (3.4)$$

and a similar form involving the transformed p_j^2 when canonical transformations are performed. This will be particularly convenient to discuss the boundary values of $G_{0,j}(z)$ when z reaches the physical value $E(k)$. The next lemmas conclude these technical preliminaries.

LEMMA III.1. — *Let* $P_j(\lambda)=\mathfrak{U}^{-1}(\lambda)P_j\mathfrak{U}(\lambda)$, $\lambda\in\mathbb{R}^+$ *and* $P_j(\underline{\tau})=B(\underline{\tau})^{-1}P_jB(\underline{\tau})$, $\underline{\tau}\in\mathbb{R}^{3N}$, $\underline{\tau}_j=0$. *Then* $P_j(\lambda)$ *has an analytic continuation in* $0\leqslant|\operatorname{Arg}\lambda|<\frac{\pi}{2}$ *and* $P_j(\underline{\tau})$ *is analytic for* $E_0^0\notin\bigcup_D\sigma(H_D(\underline{\tau}))$.

For the proof of this lemma we refer to [*8*], [*9*] or [*14*].

LEMMA III.2. — *For all* $z\notin\sigma(H_{0,j})$ *the operator* $G_{0,j}^{(1)}(z)V_j$ *is a bounded linear operator from* L^2_{-s} *to* L^2_s *for all* $s\leqslant 1$. *The same property holds for the operators obtained from it by complex dilation or boost transformations satisfying the conditions of Lemma* II.1.

Proof. — It is enough to show that for each $i\neq j$ the operator

$$B_{ij}=X(p_j^2+E_0^0-z)^{-1}P_j\left(\frac{1}{|\underline{x}_i-\underline{x}_j|}-\frac{1}{x_j}\right)X$$

is bounded operator on L^2. Now φ_0^j decays exponentially in $(X^2-x_j^2)^{1/2}$; furthermore by using commutation relations between $\underline{x}_j$ and $\underline{p}_j$ it is quite easy to show that $x_j(p_j^2+E_0^0-z)^{-1}x_j^{-1}$ is bounded (see e. g. [*18*]). So it is enough to show that if $f\in L^2(\mathbb{R}^{3N}; d\underline{x}_jd\underline{y})$ the function

$$g(\underline{x})=x^2\int d\underline{y}\left(\frac{1}{|x_i-\underline{x}|}-\frac{1}{x}\right)\phi_j(y)f(\underline{x},\underline{y}) \tag{3.5}$$

with $\phi_j(\underline{y})=y\varphi_0^j(\underline{y})$ satisfies

$$\|g\|_{L^2}\leqslant C\|f\|_{L^2} \tag{3.6}$$

for some constant C independent of f. Without restricting generality we can assume $N=2$ and $\underline{y}=\underline{x}_i$. We now separate the integration region in (3.5) into $y\leqslant\frac{1}{2}x$ and $y\geqslant\frac{1}{2}x$. For $y\leqslant\frac{1}{2}x$ it is easy to see that

$$-\frac{2}{3}\frac{y}{x^2}\leqslant\frac{1}{|\underline{y}-\underline{x}|}-\frac{1}{x}\leqslant 2\frac{y}{x^2}$$

Thus

$$\begin{aligned}\left|\int_{y\leqslant\frac{1}{2}x}d\underline{y}\left(\frac{1}{|\underline{y}-\underline{x}|}-\frac{1}{x}\right)\phi(y)f(\underline{x},\underline{y})\right|&\\ \leqslant\frac{2}{x^2}\int_{y\leqslant\frac{1}{2}x}d\underline{y}y|\phi(y)|\,|f(\underline{x},\underline{y})|&\\ \leqslant\frac{2}{x^2}\left(\int d\underline{y}|f(\underline{x},\underline{y})|^2\right)^{1/2}\left(\int d\underline{y}y^2|\phi(y)|^2\right)^{1/2}&\end{aligned} \tag{3.7}$$

For $y > \frac{1}{2}x$ one can write

$$\left| \int_{y>\frac{1}{2}x} d\underline{y} \left(\frac{1}{|\underline{y} - \underline{x}|} - \frac{1}{x} \right) \phi(\underline{y}) f(\underline{x}, \underline{y}) \right|$$
$$\leqslant \sup_{y>\frac{1}{2}x} |\phi(y)|^{1/2} \left(\int d\underline{y} \left(\frac{1}{|\underline{x} - \underline{y}|^2} - \frac{1}{x} \right)^2 |\phi(y)|^2 \right)^{1/2} \cdot \left(\int d\underline{y} |f(\underline{x}, \underline{y})|^2 \right)^{1/2} \tag{3.8}$$

Now since ϕ has pointwise exponential decay [14] one has in particular $\sup_{y>\frac{1}{2}x} |\phi(y)|^{1/2} \leqslant C(1 + x^2)^{-1}$ for all $x \in \mathbb{R}^3$.

So finally from (3.7) and (3.8) one gets

$$g(x) \leqslant C\rho(x)$$

for some constant C and $\rho(x) = \left(\int d\underline{y} |f(\underline{x}, \underline{y})|^2 \right)^{1/2}$ from which (3.6) follows.

Similar arguments apply to the transformed operators since in the range imposed for the variation of the dilation or boost parameters the exponential decay argument remains valid whereas V_j is either multiplied by a constant in the case of dilations or left invariant by boosts.

We are now ready to prove the extension of the PSS theorem to the case of transformed Hamiltonians :

THEOREM III.1. — *Let* $E(\varepsilon, k) = E_0^0 + e^{i\varepsilon}k^2$, $0 < \text{Arg}\, k < \frac{\pi}{2}$; *then*

$$G_u^+(k) = \lim_{\varepsilon \downarrow 0} (H(k) - E(\varepsilon, k))^{-1}$$

exists in the norm topology of $\mathscr{L}(L_s^2, L_{-s}^2)$ *for all* $s > \frac{1}{2}$. *Furthermore* $G_u^+(k)$ *is analytic in k in this domain.*

If $\underline{\tau}_1(k) = (0, \ldots, 0, k\underline{\omega})$, $0 < \text{Arg}\, k < \frac{\pi}{2}$, *and* $\omega \in \mathbb{R}^3$, $\omega = 1$, *then:*

$$G_{B_1}^+(k) = \lim_{\varepsilon \downarrow 0} (H(\underline{\tau}_1(k)) - E(\varepsilon, k))^{-1}$$

enjoys the same properties as $G_u^+(k)$ *with however poles for those purely imaginary k's such that* $E(k) \in \sigma_p(H)$.

Proof. — We denote by $G(\lambda, z)$, $D(\lambda, z)$, etc. the operators involved in the Weinberg-van Winter equation under the action of the dilation group $\mathfrak{U}(\lambda)$, $\lambda \in \mathbb{R}^+$, and extend the notation to their analytic continuations for complex λ. These families are bounded analytic as elements of $\mathscr{L}(L^2, L^2)$ in both parameters λ and z provided z lie in in the resolvent set of the Hamiltonians involved. It is technically simple but lengthy to show that actually they also are analytic families in $\mathscr{L}(L_s^2, L_s^2)$ for all $s \in R$. Consider first $D(k, z)$; (3.1) involves those sequences of cluster decompositions with $l > 2$, the corresponding contributions to D have a singular set given by a set of half-lines and points lying at the right of $\Sigma_l + k^2\mathbb{R}^+$, where $\Sigma_l = \inf_{D_l} \sigma(H_{D_l})$, hence $\Sigma_l > E_0^0$.

So $z = E(\varepsilon, k)$ is in the analyticity domain of these terms for $0 \leqslant \varepsilon \leqslant \pi$. Hence the main problem comes from those terms in (3.1) with $l = 2$ and $G_{D_2} = G_{0,j}$ for some j (In fact if D_2 is the decomposition into the nucleus and the cluster formed of the N electrons then H_{D_2} is simply the N electron Hamiltonian with no nuclear attraction). This Hamiltonian has positive spectrum for $k \in \mathbb{R}$ whereas it is simply $k^2\mathbb{R}^+$ for general k. If we perform the decomposition (3.3) the part $G_0^{(2)}(k, z)$ has a singular set in z consisting of half-lines at the right of $E_1^0 + k^2\mathbb{R}^+$ so that here again the points $E(\varepsilon, k)$ are in the analyticity domain. Consider now

$$G_0^{(1)}(k, \varepsilon, k)) = k^{-2}(p_j^2 - e^{i\varepsilon})^{-1}P_j(k)\,;$$

then ([*11*], [*12*]) this operator has a norm limit in $\mathscr{L}(L_s^2, L_{-s}^2)$, $s > \frac{1}{2}$, as $\varepsilon \downarrow 0$; hence

$$D_{0,j}^{(1)}(k, z) = k^{N-1} \sum_{D_{N+1} \supset \ldots \supset D_2} G_{D_{N+1}}(k, z) \ldots V_{D_3D_2}G_{0,j}^{(1)}(k, z)$$

has a norm limit as $\varepsilon \downarrow 0$ for $z = E(\varepsilon, k)$ in $\mathscr{L}(L_s^2, L_{-s}^2)$ since the other resolvents in $D_0^{(1)}$ are bounded analytic in $\mathscr{L}(L_s^2, L_{-s}^2)$ (here again we skip the irrelevant arguments concerning the relative boundedness of the potentials).

We now apply similar arguments to $I(k, z)$. If D_2 in (3.2) is the decomposition into the nucleus and the cluster formed with N electrons then the spectral analysis of each of the resolvents in the corresponding terms of (3.2) contributing to $I(k, z)$ shows that $E(\varepsilon, k)$ is in the analyticity domain of these terms for $0 \leqslant \varepsilon \leqslant \pi$. When $G_{D_2} = G_{0,j}$, the same property holds for the contribution of $G_{0,j}^{(2)}$. To treat the part

$$G_{D_{N+1}}(k, z)V_{D_{N+1}D_N} \ldots V_{D_3D_2}G_{0,j}^{(1)}(k, z)V_j$$

it is enough to apply Lemma III.2 above. According to it this is a bounded operator from L_{-s}^2 to L_s^2 for $s \leqslant 1$ when $z = E(\varepsilon, k)$, $\varepsilon > 0$. Near the limit $\varepsilon = 0$ one has to use the first resolvent equation

$$G_{0,j}^{(1)}(k, E(\varepsilon, k)) = G_{0,j}^{(1)}(k, E(\varepsilon_0, k)) + (e^{i\varepsilon_0} - e^{i\varepsilon})(p_j^2 - e^{i\varepsilon})^{-1}G_{0,j}^{(1)}(k, E(\varepsilon_0, k))$$

where ε_0 is some fixed positive number, $\varepsilon_0 < \pi$.

From this and the basic Agmon's theory it follows that $G_{0,j}^{(1)}(k, E(\varepsilon, k))$ converges in norm of $\mathscr{L}(L_s^2, L_{-s}^2)$ as ε goes to zero for $\frac{1}{2} < s \leqslant 1$. Since the other factors leave L_{-s}^2 invariant one obtains that norm lim $I(k, E(\varepsilon, k))$

exists in $\mathscr{L}(L^2_{-s}, L^2_{-s})$. Now for each ε, $0 < \varepsilon < \pi$, $I(k, E(\varepsilon, k))$ is compact on L^2_{-s} for $0 < s \leqslant 1$ and accordingly $\forall s > \frac{1}{2}$.

Now analyticity in k of the $\varepsilon = 0$ limits of D and I follows from Ascoli's analytic theorem since analyticity holds for $\varepsilon > 0$. From

$$(H(k) - E(\varepsilon, k))^{-1} = (1 - I(k, E(\varepsilon, k))^{-1} D(k, E(\varepsilon, k))$$

and Fredholm analytic theorem [*14*], the limit $G_u^+(k)$ exists in $\mathscr{L}(L_s^2, L^2_{-s})$, $-\frac{1}{2} < s \leqslant 1$, which is meromorphic in $0 < \operatorname{Arg} k < \frac{\pi}{2}$. The existence of spurious solutions of the equations $(1 - I)u = 0$ requires some auxiliary discussion of the poles of $G_u^+(k)$. We postpone it up to the end of this proof.

We now turn to the discussion of $G_{B_1}^+(k)$. As before we need to look at the spectrum of the various $H_D(\tau_1(k))$'s involved in D and I. Inductively on the number of electrons and using the tensorial sum structure of H_D it is easy to show that if electron N belongs to a cluster C in D then the spectrum of $H_D(\underline{\tau}_1(k))$ is the interior of the parabola $\mathscr{P}_0$ shifted over Σ_C where Σ_C is the lowest threshold of cluster C. So if $H_D \neq H_{0,N}$ the points $E(\varepsilon, k)$ stay away from $\sigma(H_D(\underline{\tau}_1(k))$ for $\varepsilon > 0$ and small enough for all k with $0 < \operatorname{Arg} k < \pi$. If $H_D = H_{0,N}$ then again one decomposes $G_{0,N}$ according to (3.3); the part $G_{0,N}^{(2)}$ has spectrum consisting of the interior of $\mathscr{P}_0$ shifted over E_1^0 which does not contain $E(\varepsilon, k)$. So it is enough to investigate $G_{0,N}^{(1)}(\underline{\tau}_1(k), E(\varepsilon, k)) = ((P_N + k\underline{\omega})^2 - e^{i\varepsilon}k^2)^{-1}P_N$; the limit of this operator in $\mathscr{L}(L_s^2, L^2_{-s})$, $s > \frac{1}{2}$, follows from the extension of Agmon's theory to boosted Hamiltonians ([*18*]). So we can carry over all the arguments used in the dilation case.

We conclude this proof with a standard argument [*8*] which shows that spurious solutions of the homogeneous equation $1 - I = 0$ do not give poles of $G_u^+(k)$ or $G_B^+(k)$. So the only possible poles of $G_B^+(k)$ are on the positive imaginary axis for those values of k such that $E(k)$ is an eigenvalue of H lying below the threshold E_0^0. Assume $G_u^+(k)$ or $G_{B_1}^+(k)$ has a pole at $k = k_0$; then for some Gaussian type function $\exp - (\underline{x} - \underline{a})^2 = f_{\underline{a}}(\underline{x})$ the expectation values $(f_{\underline{a}}, G_u^+(k)f_{\underline{a}})$ or $(f_{\underline{a}}, G_B^+(k)f_{\underline{a}})$ have a pole at $k = k_0$, since the set of $f_{\underline{a}}$'s, $\underline{a} \in \mathbb{R}^{3N}$, is a total set in L^2 for all $s \in R$. Since such functions have both dilation analyticity in $|\operatorname{Arg} \lambda| < \frac{\pi}{2}$ or boost analyticity in the whole complex plane it is possible to dilate or boost back from k or $\tau_1(k)$ to one or zero. Then one obtains that $(H - z)^{-1}$ has a pole for $z = E(k)$. Since for $\operatorname{Im} k > 0$ such poles can appear only at eigenvalues of H one obtains the desired result.

For the analysis of exchange amplitudes we will need to use the family of boosts :

$$\underline{\tau}_2(k) = (0, \dots 0, k\underline{\omega}, k\underline{\omega}), \ \underline{\omega} \in \mathbb{R}^3, \ \omega = 1 \tag{3.9}$$

The previous result is weakened to :

THEOREM III.2. — *Let* $k \in i(0, (E_0^1 - E_0^0)^{1/2})$ *be such that* $E(k) \notin \sigma_p(H)$, *then*

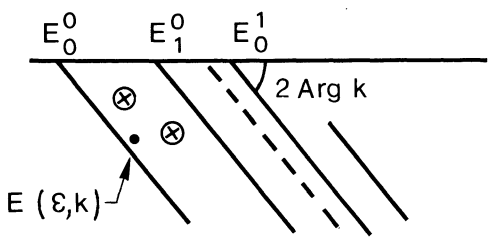
$$G_{B_2}^+(k) = \lim_{\varepsilon \downarrow 0} (H(\underline{\tau}_2(k)) - E(\varepsilon, k))^{-1}$$

exists in the norm operator topology $\mathscr{L}(L_s^2, L_{-s}^2)$ *for all* $s > \frac{1}{2}$ *and is meromorphic in a complex neighbourhood of such k's with poles for those purely imaginary values of k such that* $E(k) \in \sigma_p(H)$.

Proof. — Let us look at the spectrum of the various $H_D(\underline{\tau}_2(k))$'s. For any cluster decomposition D_l with $l > 3$ the points $E(\varepsilon, k)$ stay away from $\sigma(H_D(\underline{\tau}_2(k))$ since it consists of the interior of the parabola $\mathscr{P}_0'(\underline{\tau}_2(k))$ shifted over some threshold E_0^γ, $\gamma > 1$. This is also true if D is a three cluster decomposition different from the one, say D(N, N − 1), consisting of electrons N and N − 1 and the remaining positive ion. For D(N, N − 1) the spectrum $\mathscr{P}_1'(\underline{\tau}_2(k))$ whose leftmost point is $E_0^1 + 2\,|\,\mathrm{Im}\,k\,|^2$; it reaches $E(k)$ precisely for $k^2 = E_0^0 - E_0^1$. Let us look finally at two-cluster decompositions D_2; we need to consider only those decompositions where electron N or electron N − 1 is the isolated cluster. Then the spectrum is again $\mathscr{P}_1(\tau_1(k))$ leading to the same restriction $E(k) \notin \sigma_p(H)$.

The other statements of the theorem follow from the same type of arguments as in the previous theorem.

To conclude this section we briefly discuss some implications of the Balslev-Combes theory ([*8*], [*14*]) concerning analytic continuation of $G_u^+(k)$ in the unphysical sheets with Arg $k < 0$.



We refer to the recent review article by W. Reinhart [*19*] for the relevance of this theory to the discussion and numerical calculations of resonances energies in Atomic Physics. Since $H(\bar{k}) = H^\alpha(k)$ it is easy to apply our previous discussion of the transformed Weinberg-van Winter equations under the dilation group to the situation where $-\frac{\pi}{2} <$ Arg $k < 0$. However since now $E(\varepsilon, k)$ lies on the interior side of the cut $E_0^0 + k^2\mathbb{R}^+$ one has to take into account, in the discussion of the singular sets of D and I, the possible eigenvalues and cuts in the spectrum of the $H_D(k)$'s. Complex eigenvalues in the point spectrum of $H(k)$ are independent of k as long as they are not covered or uncovered by the cuts originating from the set of thresholds $\Sigma(k) = \bigcup_{D} \sum_{C \in D} \sigma_p^C(k)$. These complex eigenvalues are commonly interpreted as resonance energies; define

$$\sigma_{\text{res}} = \bigcup_{-\frac{\pi}{2} < \operatorname{Arg} k < 0} \{ \sigma_p(H(\lambda)) \cap \mathbb{C}^- \}$$

Then one can easily extend Theorem III.1 to

THEOREM III.3. — $G_u^+(k)$ *has a meromorphic continuation through* $(0, (E_1^0 - E_0^0)^{1/2})$ *in the domain* $\left\{ k \in \mathbb{C}, -\frac{\pi}{2} < \operatorname{Arg} k < 0 \right.$. *Its poles can only occur at those values of k such that*

i) $E(k) \in \sigma_{\text{res}}$

ii) $\operatorname{Arg}(E(k) - E_1^0) < 2 \operatorname{Arg} k$.

III.3 **Analyticity of the direct amplitude** (*).

In order to apply the previous results to the analytic continuation problem for f_k^d let us first rewrite the definitions (2.10, 2.11) under the form

$$(2\pi)^2 f^d(k) = f_B^d - \lim_{\varepsilon \downarrow 0} (\psi_{\underline{\omega}}^N(\bar{k}), (H(k) - E(\varepsilon, k))^{-1} \psi_{\underline{\omega}}^N(k)) \qquad (3.10)$$

where $\underline{k} = k\underline{\omega}$, $\omega = 1$, and

$$\psi_{\underline{\omega}}^j(k) = (2\pi)^{-3/2} k^{-\frac{1}{2}} \exp(i\underline{\omega} \cdot \underline{x}_j) V_j \varphi_0^j(k) \qquad (3.11)$$

$$\varphi_0^\gamma(\lambda) = \mathfrak{U}^{-1}(\lambda)\varphi_0^j, \ \lambda \in \mathbb{R}^+$$

Since the term f_B^d is independent of k the analytic continuation of $f^d(k)$ depends on the second term in the r. h. s. of (3.10). But since $\psi_{\underline{\omega}}^N(k)$ is now free of the diverging phase $\exp(i\underline{k} \cdot \underline{x}_j)$, and $\varphi_0^N(k)$ has an analytic continuation to $0 < \operatorname{Im} k < \frac{\pi}{2}$ with continuous boundary values for $\operatorname{Im} k = 0$ (Lemma III.1), the whole problem is now reduced to the analyticity of the resolvent $(H(k) - E(\varepsilon, k))^{-1}$ in the limit $\varepsilon = 0$. But due to Theorem III.1,

(*) The method presented here has already been discussed and used in [3], [7], [16], [17], [18]. We refer to these papers for more mathematical details.

we are now faced essentially with the same problem as for $\operatorname{Im} k = 0$ $\left(\text{since } \psi_{\underline{\omega}}^{N}(k) \text{ is not in } L_s^2 \text{ for some } s > \frac{1}{2}\right)$ and we will solve it in a similar (and in fact simpler) way. With the use of dilations and the first part of Theorem III.1, we will be able to obtain an analytic continuation in the sector $0 < \operatorname{Arg} k < \frac{\pi}{2}$. By reflexion symmetry this gives analyticity in $\frac{\pi}{2} < \operatorname{Arg} k < \pi$. However we cannot reach in this way the imaginary axis. This is why we need to supplement the previous analysis with the help of boosts writting now :

$$(2\pi^2)^{-1} f^d = f_B^d - \lim_{\varepsilon \downarrow 0} (\psi^N, (H(\underline{\tau}_1(k) - E(\varepsilon, k)^{-1}\psi^N) \tag{3.12}$$

with

$$\psi^j = (2\pi)^{-3/2} V_j \varphi_0^j$$

and $\underline{\tau}_1(k)$ as defined in Theorem III.1.

Obviously this provides the same analytic continuation as before (since this continuation is unique) in $0 < \operatorname{Arg} k < \frac{\pi}{2}$ but it allows now to reach the full domain $0 < \operatorname{Arg} k < \pi$. Our main result is

THEOREM III.4. — *The scattering amplitude $f^d(k)$ has a meromorphic continuation to the half-plane $\mathbb{C}^+ = \{ k, \operatorname{Im} k > 0 \}$ with possible poles at those imaginary values of k such that $E(k) \in \sigma_p(H)$. Furthermore it has a meromorphic continuation through $(0, (E_1^0 - E_0^0)^{1/2})$ in the domain*

$$\left\{ k \in \mathbb{C}, -\frac{\pi}{2} < \operatorname{Arg} k < 0 \right\}$$

whose poles can only occur for those value of k such that $E(k) \in \sigma_{res}$ and $\operatorname{Arg}(E(k) - E_1^0) < 2 \operatorname{Arg} k$.

REMARKS. — 1) The residue at a pole $E(k_0)$ corresponding to a purely imaginary k_0 is given by

$$\lim_{k \uparrow k_0} (\psi^N, P_{k_0}(\underline{\tau}_1(k))\psi^N) \tag{3.13}$$

where P_{k_0} is the projection operator on the eigenspace of H associated to $E(k_0)$ and $P_{k_0}(\underline{\tau}) = B^{-1}(\underline{\tau}) P_{k_0} B(\underline{\tau})$. Exponential properties ([*9*], [*14*]) imply that $P_{k_0}(\underline{\tau})$ is analytic in the strip $|\operatorname{Im} \underline{\tau}| < (E(k_0) - E_0^0)^{1/2}$. Existence of the limit in (3.13) is accordingly a non-trivial by-product of Theorem III.4.

2) A stronger analytic continuation result on unphysical sheets has been obtained by Nutall and Singh [*5*]. They show that for partial waves such an analytic continuation exists through all the cuts having threshold in $(0, (E_0^1 - E_0^0)^{1/2})$.

Proof of Theorem III.4. — We investigate first the domain $0 < \text{Arg}\, k < \frac{\pi}{2}$; since we now have Theorem III.1 above available in place of the PSS result, we will be able to apply the arguments of Theorem II.1. According to (2.12) we need to investigate the boundary values of $(\psi^N, G(\underline{\tau}_1(k), E(k, \varepsilon))\psi^N)$. In analogy with (2.8) we decompose

$$\psi^N = P_N\psi^N + Q_N\psi^N \stackrel{\text{def}}{=} {}_0\psi^N + {}_\perp\psi^N$$

Then

$$\lim_{\varepsilon \downarrow 0} G_{0,N}(\underline{\tau}_1(k), E(k, \varepsilon))_\perp\psi^N = \lim_{\varepsilon \downarrow 0} G_{0,N}^{(2)}(\underline{\tau}_1(k), E(k, \varepsilon))\psi^N$$

is in L^2 since ψ^N does and $E(k)$ is not in the singular set of $G_{0,N}^{(2)}(\underline{\tau}_1(k), z)$. Also by arguments developped in the proof of Lemma II.2 we obtain that $V_N G_{0,N}(\underline{\tau}_1(k), E(k, \varepsilon))_\perp\psi^N$ is in L_s^2 for $s \leqslant 1$ uniformly in ε, $\varepsilon \geqslant 0$ and sufficiently small. On the other hand ${}_0\psi^N$ is in L_s^2 for all $s \in R$ (apply (2.9) for $k = 0$). We can now repeat the proof of Theorem II.1 (with the difference that here we do not have to make an initial cut-off on the momentum of electron N). Since the boundary values of the resolvent $G_{0,N}^{(l)}(\underline{\tau}(k), E(k, \varepsilon))$, $l = 1$ or 2 are analytic in $0 < \text{Arg}\, k < \pi$ and those of $G(\underline{\tau}_1(k), E(k, \varepsilon))$ are meromorphic one obtains the first statement of Theorem III.3. For the analytic continuation through (E_0^0, E_1^0) we use the form (3.10) of the amplitude and apply Theorem III.3 along the same lines as above namely with the decomposition

$$\begin{aligned} \psi_{\underline{\omega}}^N(k) &= P_N(k)\psi_{\underline{\omega}}^N(k) + Q_N(k)\psi_{\underline{\omega}}^N(k) \\ &\stackrel{\text{def}}{=} {}_0\psi_{\underline{\omega}}^N(k) + {}_\perp\psi_{\underline{\omega}}^N(k) \end{aligned} \tag{3.14}$$

In this decomposition both ${}_0\psi_{\underline{\omega}}^N(k)$ and ${}_\perp\psi_{\underline{\omega}}^N(k)$ are analytic in k in $0 < |\text{Arg}\, k| < \frac{\pi}{2}$ by Lemma III.1 hence singularities of the amplitude are those of $G_u^+(k)$.

To be complete one needs to show that the analytic function defined in this way in the lower and upper-half planes really is the analytic continuation of the physical scattering amplitude defined in § II. This follows from the remark that the property holds when the parameter ε in (3.10) is kept fixed and non-zero. Since on the other hand the scattering amplitude is continuous for real k (outside the set $E(k) \in \Sigma \cup \sigma_p(H)$) this remains true in the limit $\varepsilon = 0$ by Walsh's theorem.

III.4 **The exchange amplitude.**

In order to apply the same type of techniques to the non Born part of the exchange amplitude (1.5) we rewrite it alternatively as

$$f^r(k) = f_B^r(k) - \lim_{\varepsilon \downarrow 0} (\psi_{\underline{\omega}}^{N-1}(k), (H(k) - E(\varepsilon, k))^{-1}\psi_{\underline{\omega}}^N(k)) \tag{3.15}$$

with $\psi^j_{\underline{\omega}}(k)$ given by (3.11), or

$$= f^r_{B}(k) - \lim_{\varepsilon \downarrow 0} (\psi^{N-1}(-\bar{k}\underline{\omega}), (H(\underline{\tau}_2(k) - E(\varepsilon, k))^{-1}\psi^N(k\underline{\omega})) \quad (3.16)$$

with $\underline{\tau}_2(k)$ defined by (3.9) and

$$\psi^{N-1}(-\bar{k}\underline{\omega}) = (2\pi)^{-3/2} \exp(-i\bar{k}\underline{\omega}\cdot \underline{x}_N)V_{N-1}\psi_0^{N-1}$$
$$\psi^N(k\underline{\omega}) = (2\pi)^{3/2} \exp(ik\underline{\omega}\cdot \underline{x}_{N-1})V_N\varphi_0^N$$

From the first expression (3.15) one obtains as before analytic continuation in the domain $0 < |\operatorname{Arg} k| < \frac{\pi}{2}$. From the second one, it is possible to reach this part of the imaginary axis considered in Theorem III.2 provided one makes sure that both vectors $\psi^{N-1}(-k\underline{\omega})$ and $\psi^N(k\underline{\omega})$ are analytic in a neighbourhood of this domain. This is in fact precisely the case as follows from the previously mentioned results on exponential decay properties of φ_0^j ([*9*], [*14*]). Then one gets

THEOREM III.5. — The scattering amplitude $f^r(k)$ has a meromorphic continuation to the domain

$$\mathscr{D} = \{ k, \operatorname{Im} k > 0, \operatorname{Re} k \neq 0 \} \cup \{ k \in i[0, (E_0^1 - E_0^0)^{1/2}] \}$$

with possible poles when $E(k) \in \sigma_p(H)$. It also has a meromorphic continuation through $(0, (E_1^0 - E_0^0)^{1/2})$ as for $f^d(k)$.

Proof. — Since $\exp(ik\underline{\omega}\cdot \underline{x}_N)\varphi_0^{N-1}$ (resp. $\exp(ik\underline{\omega}\cdot \underline{x}_{N-1})\varphi_0^N$) is analytic in k and rapidly decreasing in all its variables for $|\operatorname{Im} k| < (E_0^1 - E_0^0)^{1/2}$ ([*9*] [*14*]) the analyticity of the Born term under this condition on $|\operatorname{Im} k|$ is easily shown. It can be extended to the full domain $\mathscr{D}$ using III.1. It remains to look at the non Born part of $f^r(k)$. Since $\psi^{N-1}(-k\underline{\omega})$ and $\psi^N(k\underline{\omega})$ also are analytic (as elements of $L^2(\mathbb{R}^{3N})$ for $|\operatorname{Im} k| < (E_0^1 - E_0^0)^{1/2}$) by Theorem III.2 and (3.16), the scattering amplitude is meromorphic in k in a neighbourhood of $L'(0, (E_0^1 - E_0^0)^{1/2})$. To reach the full domain $\mathscr{D}$ one uses the form (3.10) and Theorem III.1.

IV. CONCLUDING REMARKS

The results presented here can be extended in two directions namely when the atom is in an excited s-state or when the scattered electron is replaced by another atom or an ion.

Concerning excited atom corresponding to $E_p^0 < E_0^1$, in an s-state the arguments developped in chapter II to prove finiteness of the scattering amplitude can be extended with some minor modifications. However the dilation analyticity technique is not sufficient since once the complex dilation is performed the energy $E_p^0 + k^2$ lies below the half-lines $E_k^0 + k^2\mathbb{R}^+$, $k < p$ [3]. Then it is necessary to use local distortion techniques as those of Nutall and Singh [5], exploiting the full analyticity properties of the Fourier transforms of the states $\psi_{\underline{k}}$. For p-states it is easy to see that even the Born-term is not finite for real k and that all the arguments of § II and III break down.

The second remark concerns ion-atom scattering. The difficulty in extending our results to this situation is twofold. On one hand since it is not possible anymore to make the infinite nuclear mass approximation one has to deal with an extra book-keeping of the kinematics. Also the threshold analysis of the full Hamiltonian is not so simple. However both difficulties are of purely technical nature and our analysis can be applied in a similar way. It is not clear however that this would really be the right approach; it seems that a reformulation of the problem in a Born-Oppenheimer framework taking into account electronic levels of the clamped nuclei Hamiltonians would be more satisfying both physically and mathematically. This is presently under investigation.

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