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T. A. Minelli and F. Zardi : SOLUTION OF THE STANDING WAVE INTEGRAL EQUATION AND APPLICATIONS. -



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SUMMARY. -

The coordinate representation of the standing wave integral equation is considered in the complex momentum plane. This equation is solved, and the solution is used to inquire about some properties of the reactance matrix. As illustrative application, the pole expansion of the reactance matrix and the two potential problem are then investigated.

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## 1. - INTRODUCTION. -

A long-far recognized hindrance in the reactance matrix approach to the scattering theory is the fact that the integral equation for the principal value wave function has a kernel which is not an operator valued analytic function of the energy[1÷3]. As a matter of fact, this prevents from employing in the framework of the K-matrix the powerful methods of functional analysis in a general and systematic fashion; whether these methods have been proved useful in carefully defining the reactance matrix and in elucidating its operatorial meaning relative to the S-matrix, they have produced no direct result concerning

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intrinsic properties of the K-matrix itself.

In this paper we resort to ordinary calculus and to the Green function methods, in the form they have been used in the study of the S-matrix properties for the potential scattering problem(x). Also the present work is concerned with the potential scattering problem; many features, however, open the path for extension to proper reactions.

From the mathematical view-point, the features characterizing our approach are the following:

- whenever possible, we put into evidence and take benefit of several results which have been obtained in connection with the study of the S-matrix; in particular we shall see that also in the reactance matrix theory the regular solution, the two linearly independent Jost solutions, and the related Jost functions are likely to play a fundamental role;
- we make a systematic use of two relations which hold between suitably defined Green functions that are not kernels of the resolvent; these relations are similar in form to well-known relations which hold between resolvents; in the problem we are dealing with, however, they cannot be proved by functional analysis techniques.

In Sect. 2 the standing wave integral equation is analytically continued in the momentum plane and is solved; the apparatus of the Jost solutions and Jost functions is widely used to give compactness and systematicity to the derivations. Two examples of the application of our formalism are dealt with in the next Sections. More precisely, in Sect. 3 we shall be concerned with the comparison of our formalism with the reactance matrix resonance theory given by Humblet(4); in Sect. 4 the additive interaction problem is analysed: this analysis, besides the implications concerning perturbation problems, is relevant to enlight the striking differences in the structure of the S matrix- and the K matrix-theory.

## 2.- THE PRINCIPAL VALUE INTEGRAL EQUATION AND ITS SOLUTION.-

### 2.1.- The principal value integral equation.-

Let us consider the scattering of a spinless particle of mass M by a central potential, vanishing at infinity faster than $r^{-1}$,

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(x) - See ref. (1), Chapt. 12.

and less singular than $r^{-2}$ at the origin. We shall work in a partial wave of definite angular momentum $\ell$; in this connection the operator

$$(1) \qquad H = H_o + V = -\frac{\hbar^2}{2M}\left[\frac{d^2}{dr^2} - \frac{\ell(\ell+1)}{r^2}\right] + V(r)$$

will be simply called the Hamiltonian, while $H_o$ will be called the unperturbed Hamiltonian (the symbol $\ell$ will be omitted when it is a mere label).

Now we consider the function $\psi^P(k,r)$, defined as a solution of the equation

$$(2) \qquad H\,\psi^P(k,r) = E\,\psi^P(k,r)$$

($k$ is the momentum and $E=\hbar^2k^2/2M$ is the energy), with the following boundary conditions

$$(3) \qquad \psi^P(k,0) = 0, \qquad \psi^P(k,r) \underset{r\to\infty}{\longrightarrow} F(kr)+K(k)G(kr);$$

in the above relations F and G are the Riccati-Bessel and the opposite of the Riccati-Neumann functions respectively, which are characterized by the asymptotic behaviour

$$(4) \qquad F(kr) \underset{r\to\infty}{\longrightarrow} \sin(kr-\ell\pi/2), \qquad G(kr) \underset{r\to\infty}{\longrightarrow} \cos(kr-\ell\pi/2).$$

For later reference we quote here the unperturbed ingoing and outgoing wave functions, defined by the relations

$$(5) \qquad \begin{aligned} I(kr) = G(kr)-iF(kr) &\underset{r\to\infty}{\longrightarrow} e^{-i(kr-\ell\pi/2)} \\ O(kr) = G(kr)+iF(kr) &\underset{r\to\infty}{\longrightarrow} e^{+i(kr-\ell\pi/2)}. \end{aligned}$$

The wave function defined by eq. (2) and eq. (3) is the well-known standing wave solution, which satisfies the following integral equation(o)

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(o) - See ref. (1), Chapts 7 and 11.

$$(6) \qquad \psi^{P}(k,r) = F(kr) + \int_{0}^{\infty} G_{o}^{P}(E;r,r')\, V(r')\, \psi^{P}(k,r')\, dr' .$$

In the above equation $G_{o}^{P}(E;r,r')$ is the kernel pertaining to the "principal value Green function", which is defined by the following relation

$$(7) \qquad G_{o}^{P}(E) = PG_{o}(E) = \lim_{\varepsilon \to 0} \frac{1}{2} \left[ \frac{1}{E+i\varepsilon - H_{o}} + \frac{1}{E-i\varepsilon - H_{o}} \right]$$

in terms of the resolvent $G_{o}(E)$ of the unperturbed Hamiltonian $H_{o}$. The operator $G_{o}^{P}(E)$ has a meaning of its own for $E > 0$, while for $E < 0$ it is trivially coincident with $G_{o}(E)$; no meaningful analytic continuation of the standing wave integral equation can be obtained starting from this definition.

The kernel of $G_{o}(E)$ is (x)

$$(8) \qquad G_{o}(k;r,r') = -\frac{2M}{\hbar^2} \frac{F(kr_{<})\, 0(kr_{>})}{W[0,F]} ,$$

where k is that determination of $(2ME/\hbar^2)^{1/2}$ which has $Imk \geq 0$; according to this prescription one must take

$$\lim_{\varepsilon \to 0} \left(\frac{2M}{\hbar^2}\right)^{1/2} (E \pm i\varepsilon)^{1/2} = \lim_{\varepsilon \to 0} \left(\pm k + \frac{i\varepsilon}{2k}\right) = \pm k , \qquad k > 0 .$$

From this one easily gets

$$(9) \qquad G_{o}^{P}(k;r,r') = \frac{1}{2}\left[G_{o}(k;r,r') + G_{o}(-k;r,r')\right] = -\frac{2M}{\hbar^2} \frac{F(kr_{<})\, G(kr_{>})}{k} , \qquad k > 0 .$$

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(x) - The wronskian of any two function m(r) and n(r) is defined by the relation $W[m(r), n(r)] = m(r)n'(r) - m'(r)n(r)$, where the prime stands for radious derivative.

The last member of eq. (9) is capable of an obvious analytic continuation in the momentum plane; this continuation however is not related to the operator $G_o^P(E)$ not even for $E<0$, where one has $G_o^P(k;r,r') \equiv G_o(k;r,r')$ with k imaginary positive. We shall call $\Gamma_o(k;r,r')$ the analytic continuation of the kernel (9), i.e. we put identically

$$\Gamma_o(k;r,r') \equiv -\frac{2M}{\hbar^2}\,\frac{F(kr_<)G(kr_>)}{k} \tag{10}$$

for any complex value of the momentum; the meaning of $\Gamma_o(k;r,r')$ and its relation with $G_o(k;r,r')$ will be discussed in Appendix A.

From the above definition it follows that the equation

$$\psi^P(k,r) = F(kr) + \int_o^\infty \Gamma_o(k;r,r')\,V(r')\,\psi^P(k,r')\,dr' \tag{11}$$

defines a solution of eq. (2) with the boundary conditions (3) in the complex momentum plane. By comparison of eq. (11) with the second of eqs. (3) it follows that K(k) is given by the relation

$$K(k) = -\frac{2M}{\hbar^2 k}\int_o^\infty F(kr)\,V(r)\,\psi^P(k,r)\,dr\,. \tag{12}$$

In order to make easy the comparison with the Humblet theory[4] which we shall discuss in Sect. 3, we give here an alternative expression for the reactance matrix. We first recall the well-known definitions of the regular solution $\varphi(k,r)$ and Jost solutions $f_\pm(k,r)$; they are solutions of eq. (2) with the following conditions(x)

$$\varphi(k,r) \underset{r\to 0}{\longrightarrow} r^{\ell+1};\quad f_-(k,r) \underset{r\to\infty}{\longrightarrow} I(kr),\quad f_+(k,r) \underset{r\to\infty}{\longrightarrow} O(kr); \tag{13}$$

the Jost functions are defined by the identity

$$\mathcal{J}_\pm = W\left[f_\pm, \varphi\right]. \tag{14}$$

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(x) - We explicitly remark that our definition of the Jost solutions differs by a phase factor with respect to the standard definition (compare with the definitions in ref. (1), Capt. 12).

Now, since both solutions $\varphi(k,r)$ and $\psi^P(k,r)$ vanish at the origin, they are proportional; by expressing $\varphi$ and $\psi^P$ as a linear combination of the Jost solutions, and comparing their asymptotic behaviour, one obtains

$$\psi^P(k,r) = \frac{2k\varphi(k,r)}{\mathcal{F}_+(k) + \mathcal{F}_-(k)} \tag{15}$$

while the reactance matrix is expressed by the relation

$$K(k) = i\frac{\mathcal{F}_+(k) - \mathcal{F}_-(k)}{\mathcal{F}_+(k) + \mathcal{F}_-(k)}. \tag{16}$$

The identity of the second members of eq. (12) and eq. (16) is easily checked: one expresses the standing wave solution in eq. (12) through the relation (15), and represents the regular solution by means of the Jost solutions; the integrals so obtained are then compared with the integral representation of the Jost functions.

2.2.- The Green functions and their relations.-

In this Subsection we shall introduce in full generality the Green functions in which we shall be interested in the following, and establish some relations between them.

Let us consider the partial wave Hamiltonian

$$H_i = H_o + V_i = -\frac{\hbar^2}{2M}\left[\frac{d^2}{dr^2} - \frac{\ell(\ell+)}{r^2}\right] + V_i(r),$$

where i is a label which identifies a generic potential of the type specified in the previous Subsection; when we shall consider more potentials together we use the labels $i_1, i_2 \ldots$. We define now two classes of solutions of the equation

$$H_i\,\psi_i = E\,\psi_i, \tag{17}$$

by specifying the boundary conditions at the origin and at infinity respectively:

- the solutions which we shall call $\varphi_i(k,r)$ satisfy eq. (17) and the regularity condition at the origin

$$\varphi_i(k,r) \xrightarrow[r\to 0]{} r^{\ell+1};$$

- the solutions which we shall call $\chi_i^{\alpha}(k,r)$ satisfy eq. (17), and conditions at infinity of the type

$$\chi_i^{\alpha}(k,r) \xrightarrow[r\to\infty]{} h^{\alpha}(k,r) \tag{18}$$

where $h^{\alpha}(k,r)$ is an assigned solution of the unperturbed equation: the label $\alpha$ identifies the solution; when we shall need more solutions at once, we shall label them as $\alpha_1$, $\alpha_2$.....

By means of these solutions we construct the Green function

$$G_i^{\alpha}(k;r,r') = -\frac{2M}{\hbar^2}\frac{\varphi_i(k,r_<)\,\chi_i^{\alpha}(k,r_>)}{W\left[\chi_i^{\alpha},\varphi_i\right]}\ ; \tag{19}$$

it is well known that a Green function of this type can be associated with the resolvent of $H_i$ only for very particular boundary conditions; so that, in general, eq. (19) does not define a resolvent. As a consequence, we cannot resort to standard functional analysis to state relations between such a type of Green functions.

In Appendix B the following relations will be proved:

a) the difference of two Green functions defined by the same asymptotic boundary conditions and belonging to different potentials $V_{i_1}$ and $V_{i_2}$ is given by

$$G_{i_1}(k;r,r')-G_{i_2}(k;r,r') = \int_0^{\infty} dr''\left[G_{i_1}(k;r,r'')\left\{V_{i_1}(r'')-V_{i_2}(r'')\right\}G_{i_2}(k;r'',r')\right] \tag{20a}$$

(the label $\alpha$ has been omitted, since it is the same in both Green functions).

b) The difference of the two Green functions pertaining to the same potential and to the different asymptotic conditions is given by

$$G^{\alpha_1}(k;r,r')-G^{\alpha_2}(k;r,r')=\frac{2M}{\hbar^2}\varphi(k,r)\varphi(k,r')\frac{W\left[\chi^{\alpha_1},\chi^{\alpha_2}\right]}{W\left[\chi^{\alpha_1},\varphi\right]W\left[\chi^{\alpha_2},\varphi\right]} \tag{20b}$$

(the index i has been omitted, since it is the same in both Green functions).

In the scattering theory, relations of the type (20) are well known when they can be obtained in the framework of functional analysis.

2.3.- Solution of the standing wave integral equation.-

We now return to the specific problem of the standing wave integral equation, and consider the operator

$$G^P(E) = \lim_{\varepsilon \to 0} 1/2 \left[ \frac{1}{E+i\varepsilon - H} + \frac{1}{E-i\varepsilon - H} \right]. \tag{21}$$

As it is well known, this Green function does not solve the standing wave equation(x). It will be briefly investigated here in order to compare it with the operator $\Gamma(k;r,r')$ we introduce below; explicit use of $G^P(E)$ will be made in Section 4.

Now, to the operator (21) we associate the kernel

$$G^P(k;r,r') = \frac{1}{2}\left[G(k;r,r') + G(-k;r,r')\right], \tag{22}$$

where

$$G(k;r,r') = -\frac{2M}{\hbar^2} \frac{\varphi(k,r_<) f_+(k,r_>)}{\mathcal{F}_+(k)} \tag{23}$$

is the Green function pertaining to the complete Hamiltonian (1). From this one has

$$G^P(k;r,r') = -\frac{1}{2}\frac{2M}{\hbar^2}\varphi(k,r_<)\frac{\mathcal{F}_-(k) f_+(k,r_>) + \mathcal{F}_+(k) f_-(k,r_>)}{\mathcal{F}_+(k)\mathcal{F}_-(k)} =$$

$$= -\frac{2M}{\hbar^2}\frac{\varphi(k,r_>) g(k,r_<)}{W[g,\varphi]} \tag{24}$$

where

$$g(k,r) = \frac{1}{2}\left[\mathcal{F}_-(k) f_+(k,r) + \mathcal{F}_+(k) f_-(k,r)\right].$$

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(x) - See ref. (1), Chapt. 7.

From the above definition one sees that g(kr) is a solution of the complete Schrodinger equation; for positive real energies its asymptotic behaviour is the following

$$g(k,r) \underset{r\to\infty}{\longrightarrow} \mathcal{J}_+(k)\, e^{i\,\delta(k)} \cos\{kr + \delta(k) - \ell\pi/2\}\,; \tag{25}$$

the phase shift is related to the Jost functions by the relation $\mathcal{J}_-(k)/\mathcal{J}_+(k) = e^{2i\,\delta(k)}$. It appears evident from this that $G^P(k;r,r')$ cannot give rise to a solution characterized by conditions (3).

Then we consider the kernel $\Gamma(k;r,r')$ defined by the following relation

$$\Gamma(k;r,r') = -\frac{2M}{\hbar^2}\,\frac{\varphi(k,r_<)\,\gamma(k,r_>)}{W[\gamma,\varphi]}\,, \tag{26}$$

where it has been introduced the function

$$\gamma(k,r) = \frac{1}{2}\left[f_+(k,r) + f_-(k,r)\right] \tag{27a}$$

which is a solution of the Schodinger equation and has the following asymptotic behaviour

$$\gamma(k,r) \underset{r\to\infty}{\longrightarrow} G(kr) \underset{r\to\infty}{\longrightarrow} \cos(kr - \ell\pi/2) \tag{27b}$$

(compare defs (13) and (5)). It follows that the kernel (26) solves the integral equation (6) and gives the solution in the form

$$\psi^P(k,r) = F(kr) + \int_0^\infty \Gamma(k;r,r')\,V(r')\,F(kr')\,dr'\,. \tag{28}$$

By putting this solution into eq. (12) we get for the reactance matrix the expression

$$K(k) = -\frac{2M}{\hbar^2 k}\left[\int_0^\infty F(kr)\,V(r)\,F(kr)\,dr + \right.$$

$$\left. + \int_0^\infty dr \int_0^\infty dr'\,F(kr)\,V(r)\,\Gamma(k;r,r')\,V(r')\,F(kr')\right]. \tag{29}$$

This may be viewed as the matrix element of the operator

$$R = V + V \Gamma V ,$$

evaluated between the unperturbed states F(kr). We note that an operator endowed with this property is usually defined through the integral equation[1÷3]

$$R = V + V G_o^P R . \tag{30}$$

What is the relation between $\Gamma_o(k;r,r')$ and $\Gamma(k;r,r')$? It can be obtained from the relation (20a) by putting $V_{i_1}=0$ and $V_{i_2}=V$: one immediately gets

$$\Gamma = \Gamma_o + \Gamma_o V \Gamma . \tag{31}$$

(We observe that this relation could be obtained also by comparison of the standing wave integral equation [eq. (16)] with its formal solution [eq. (27)]; however, since $\Gamma_o$ and $\Gamma$ have been defined independently of each other, we ought to prove that relation (31) is consistent with the definitions).

We remember that Tobocman and Nagarajan[3] have also achieved a relation formally coincident with our eq. (31), although they operated in a quite different conceptual framework. They started from eq. (30) and summed formally the series that can be obtained by iterating that equation; in this fashion, a formal solution is achieved in the form

$$R = V + G_o^P (1 - V G_o^P)^{-1} V .$$

Then they defined

$$\bar{\Gamma} = G_o^P (1 - V G_o^P)^{-1} ; \tag{32}$$

from this definition an equation for $\bar{\Gamma}$ coincident with eq. (31) for $E > 0$ is obtained: for positive energies one has therefore $\bar{\Gamma} = \Gamma$. We remark that while in ref. (3) eq. (31) is taken as the definition of $\bar{\Gamma}$, in our derivation eq. (31) is a relation between independently defined operators.

We finally observe that eq. (31) can be iterated and a Born-type expansion of K can be obtained.

We will now deduce the relation between the K matrix expressed in the form (12), (29) and the S matrix element defined by

$$S(k)=1-\frac{4iM}{\hbar^2 k}\int_0^\infty F(kr)V(r)\psi^{(+)}(k,r)dr=1-\frac{4iM}{\hbar^2 k}\left[\int_0^\infty F(k\,r)V(r)F(kr)dr+\right.$$

(33)

$$\left.+\int_0^\infty dr\int_0^\infty dr'\,F(kr)V(r)G^{(+)}(k;r,r')V(r')F(kr')\right];$$

in eq. (33) $\psi^{(+)}(k,r)$ is the physical solution pertaining to the complete Hamiltonian, and $G^{(+)}(k;r,r')$ is the analytical continuation in the complex momentum plane of the kernel $G(k;r,r')$ defined by eq. (23).

For this purpose we specialize eq. (20b) to the case in which $G^{\alpha_1}\equiv G^{(+)}$ and $G^{\alpha_2}\equiv \Gamma$. We have(x)

(34)

$$G^{(+)}(k;r,r')-\Gamma(k;r,r')=$$

$$=\frac{2M}{\hbar^2}\varphi(k,r)\varphi(k,r')\frac{W[f_+,\gamma]}{W[f_+,\varphi]\,W[\gamma,\varphi]}=-\frac{2M}{\hbar^2}\frac{i}{k}\psi^{(+)}(r)\psi^{P}(r')$$

We now multiply at the right and at the left by $V(r)F(kr)$ and integrate: we get

(35)

$$\int_0^\infty dr\int_0^\infty dr'\,F(kr)V(r)G^{(+)}(k;r,r')V(r')F(kr')-$$

$$-\int_0^\infty dr\int_0^\infty dr'F(kr)V(r)\,\Gamma(k;r,r')V(r')F(kr')=$$

$$=\frac{2M}{\hbar^2}\frac{i}{k}\left[\int_0^\infty F(kr)V(r)\psi^{(+)}(k,r)dr\right]\left[\int_0^\infty \psi^{P}(k,r')V(r')F(kr')dr'\right];$$

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(x) - In the last step of eq. (34) we use the relation (15) and the easily proved relations

$$(+)=\frac{k\varphi}{W[f_+,\varphi]},\qquad W[\gamma,\varphi]=\frac{1}{2}(\mathcal{F}_+-\mathcal{F}_-),\qquad W[\gamma,f_+]=ik$$

comparing the above equality with the definitions (12), (29) and (33) one gets

$$\frac{1-S}{2} + iK = \frac{i}{2}(1-S)K ,$$

and finally

$$S = \frac{1+iK}{1-iK} \tag{36}$$

which is the Heitler relation[1÷3]. The deduction now given is valid in every point of the complex plane in which the functions $\mathcal{F}_+(k)$ and $\mathcal{F}_-(k)$ are analytical.

For later reference we remember that for positive energy the standing wave solution and the pnysical solution can be given in the asymptotic region the following expression

$$(37)\quad \psi^P(k,r) \underset{r\to\infty}{\longrightarrow} \frac{\sin(kr+\delta-\ell\pi/2)}{\cos\delta}, \quad \psi^{(+)}(k,r) \underset{r\to\infty}{\longrightarrow} e^{i\delta}\sin(kr+\delta-\ell\pi/2)$$

in terms of the phase shift.

## 3. - POLES AND RESIDUES OF THE REACTANCE MATRIX. -

Recently Humblet proposed a nuclear resonance theory, based on the Cauchy expansion of the reactance matrix[4]. The pole expansion, which is valid for finite range interactions, is made starting from the expression of K which one may obtain by the wave function matching method. The merit of this theory is that it provides through the Heitler relation (36) a unitary resonant parametrization of the S-matrix; contrary to the R-matrix theory[5], in the Humblet approach the parameters describing a resonance are independent of the channel radii.

In this Section it will be shown that an alternative derivation of the results of the Humblet theory can be given in the framework of the integral representation of the reactance matrix given by eq. (29); and that this representation provides an alternative expression for the residues which will be commented on. An important part of Humblet work is devoted to the analysis of the location of the poles in the asymptotic momentum region, in order to verify that the conditions for the expansion convergence are satisfied. We shall see that the problem of the pole location has in our approach the same analytical formulation as in the Humblet formalism, so that this analysis will be not re-

peated here. In this Section finite range potentials are dealt with.

The reactance matrix element in the actual form analysed by Humblet can be easily obtained from the Jost function representation of K given by eq. (16); one may think of the Wronskians $\mathcal{F}_+$ which appear in that formula as evaluated at the point r = a: using the definitions (5) and (13) for the reactance matrix one immediately obtains the expression

$$K(k) = - \frac{W\left[\varphi, F; a\right]}{W\left[\varphi, G; a\right]} , \tag{38}$$

which is, apart from the notations, the expression analysed by Humblet(x)

Starting from eq. (38) the deduction of the poles and the residues goes as follows. Besides the K matrix, it is introduced the threshold matrix(4)

$$\mathcal{K} = -k^{-2\ell-1} K = (-1)^{\ell} \frac{k^{-\ell-1} W\left[\varphi, F; a\right]}{(-k)^{\ell} W\left[\varphi, G; a\right]} = (-1)^{\ell} \frac{w_+(k)}{w_-(k)} \tag{39}$$

where

$$w_+(k) = k^{-\ell-1} W\left[\varphi, F, a\right]; \qquad w_-(k) = (-k)^{\ell} W\left[\varphi, G; a\right] .$$

This matrix has the noteworth property of being meromorfic in the energy plane; it follows that half a plane in the momentum variable is equivalent to the full energy plane: on this ground a biunivocal correspondence between the energy and momentum variables can be stated.

Apart from the exceptional case (which will be here excluded) where k=0 is a pole, the poles of k are associated to the zeros of $w_-(k)$. Let $k_n$ be such a zero, so that for the residue of $\mathcal{K}$ we have the expression

$$\varrho_n = \lim_{E \to E_n} (E - E_n) \mathcal{K} = (-1)^{\ell} \frac{w_+(k)}{\frac{d}{dE}\left[w_-(k)\right]_{E=E_n}} . \tag{40}$$

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(x) - We note that the expression (16) lends in a natural fashion to the study of the analyticity properties of the K matrix for the wider class of potential for which the Jost functions can be defined.

A straightforward calculation shows that

$$(41)\qquad \frac{d}{dE}\left[(-k)^{\ell}\, W\left[\varphi, G; a\right]\right]_{E=E_n} = \frac{2M}{\hbar^2}(-k_n)^{\ell}\,\frac{G(k_n a)\;\nu_n}{\varphi(k_n, a)}$$

where

$$\nu_n = \int_0^a dr\,\varphi^2(k_n, r) + \frac{\hbar^2}{2M}\,\varphi^2(k_n, a)\,\frac{d}{dE}\left[\frac{G'(k\ a)}{G(k\ a)}\right]_{E=E_n}\ ;$$

in eq. (40) the numerator $w_+(k_n)$ can be simplified by taking into account that the condition $w_-(k_n)=0$ gives $\varphi'(k_n, a) = \varphi(k_n, a)\,G'(k_n a)/G(k_n a)$; then one gets for the residue the final expression

$$(42)\qquad \varrho_n = \frac{\hbar^2}{2M}\,\frac{k_n^{-2\ell}}{\nu_n}\left[\frac{\varphi(k_n, a)}{G(k_n a)}\right]^2 .$$

The residues of K are immediately obtained from eq. (39).

We deduce now the residues of K starting from the integral representation (29). The deduction can be done in several ways, on the line of a similar analysis the authors made in some previous paper concerning the pole expansion of the S matrix[6, 7]. For the potential scattering problem, in which we are concerned, it is enough to resort to the simplest method, described in ref. (6). Let us re-write the matrix element (29) by exploiting the finite range of the potential and evidencing the threshold factor; we get

$$K(k) = \mathcal{B}(k) + k^{2\ell+1}\mathcal{R}(k)$$

where B(k) is the Born integral, while

$$(43)\qquad \mathcal{R}(k) = \left(\frac{2M}{\hbar^2}\right)^2 \frac{1}{k^{2\ell+2}}\,\frac{1}{W\left[\gamma, \varphi\right]}\int_0^a F(kr)\,V(r)\,x$$

$$x\left\{\int_0^r \varphi(k, r')\,\gamma(k, r) + \int_r^a \gamma(k, r')\,\varphi(k, r)\right\} V(r')F(kr')\,dr\,dr'$$

is the resonant term. The analyticity properties of $\mathcal{R}(k)$ are quite simple; the only singularities one can have are the poles arising from

the zeros of $W[\gamma, \varphi]$, since the radial functions are analytic in the whole k plane, and the integration covers the finite square interval $0 \leq r,\ r' \leq a$ (we observe that by the same reasoning it comes that $\mathcal{B}(k)$ is an entire function). Because of the behaviour of $\gamma$ in the external region (cfr. eq. (27b)) one has

$$W[\gamma, \varphi] \quad W[\gamma, \varphi; a] = W[G, \varphi; a];$$

then it is verified that the integral representation and the matching method give the same pole location, as it must be.

As far as the residues of $\mathcal{R}(k)$ are concerned, we observe that for $k = k_n$ one has $W[\varphi(k_n), \gamma(k_n)] = 0$, so that one can put

$$\gamma(k_n, r) = b_n \varphi(k_n, r). \tag{44}$$

The integral in eq. (43) assumes then, for $k = k_n$, the simple form

$$b_n \left[ \int_0^a F(k_n r) V(r)\, \varphi(k_n, r)\, dr \right]^2 .$$

By the position

$$J(k_n) = \int_0^a F(k_n r) V(r)\, \varphi(k_n, r)\, dr$$

and using eqs. (41), (43) and (44) we have finally

$$\operatorname{res} \mathcal{R}(k_n) = \frac{2M}{\hbar^2} \frac{1}{k_n^{2\ell+2}} \frac{1}{\nu_n} J^2(k_n). \tag{45}$$

By a procedure similar to that used in ref. (6) we may prove the following identity

$$-\frac{\hbar^2}{2M} k_n \frac{\varphi(k_n, a)}{G(k_n a)} = J(k_n) \tag{46}$$

Taking into account this relation, a straightforward calculation proves that the residue (45) is identical to that given by eq. (42). Since also the pole location is the same, it follows that a pole expansion equivalent to the Humblet expansion can be given; in our case, the re

sidues would have the integral form given by eq. (45).

Relation (46) can also be used in order to give the residue a more homogeneous form, by eliminating from the denominator the boundary evaluated resonant state $\varphi(k_n, a)$. Advantages of using such an expression instead of the form arise in connection with approximate calculations; in fact, whereas formula (42) requires the knowledge of the resonant state in a critical point as the boundary, the integral form involves average properties of the resonant state, since it appears in an integral which smears point properties.

## 4. - THE ADDITIVE INTERACTIONS PROBLEM. -

We consider here a problem in which the whole interaction is separated into the sum of two terms, one of which is exactly accounted for, while the other is regarded, in the case, as a perturbation. Besides the practical implications concerning perturbation problems, this analysis is likely to be relevant to enlight the striking differences of the internal structure of the K matrix with respect to the S matrix.

Let us consider the Hamiltonian

$$H = H_o + V_1 + V_2 = -\frac{\hbar^2}{2M}\left[\frac{d^2}{dr^2} - \frac{\ell(\ell+1)}{r^2}\right] + V_1(r) + V_2(r). \tag{47}$$

Our purpose is to seek for a standing wave solution of the type(x)

$$\overline{\psi}^P(1,2;k,r) = \psi^P(1;k,r) + M(k,r);$$

this separatedform has been chosen in analogy to the expression one

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(x) - The notations we shall use in this Section are the following. For radius-dependent quantities, such as the wave functions and the Green functions, notations of the type $m(1;k,r)$, $n(1;k,r,r')\ldots$ or $m(1,2;k,r)$, $n(1,2;k,r,r')$ respectively, will be used, according as they are related to the Hamiltonian $H_1 = H_o + V_1$ or to the complete Hamiltonian H. Radially integrated quantities, such as matrix elements, will be denoted $M_1, N_1 \ldots$ or $M(1,2)$, $N(1,2)\ldots$, respectively, whether they are pertaining to the Hamiltonian $H_1$ or to the Hamiltonian H; notations of the type $M_2$, $N_2$, will be used for the so-called reduced quantities, i.e. for quantities which are properly combined with $M_1, N_1$ to give $M(1,2)$, $N(1,2)\ldots$.

uses for the physical solution in the additive interaction problem

$$\bar{\psi}^{(+)}(1,2;k,r) = \psi^{(+)}(1;k,r) + N(k,r) .$$

The structure of $M(k,r)$ and $N(k,r)$ can be deduced by comparison of these expressions with the "direct solutions" $\psi^{P}(1,2;k,r)$ and $\psi^{(+)}(1,2;k,r)$, in the form they assume by putting $\delta(1,2) = \delta_1 + \delta_2$ in the solution (37) quoted in Sect. 2. The comparison shows an important difference in the asymptotic behaviour of $M(k,r)$ and $N(k,r)$: while $N(k,r)$ is ruled by $kr$, one immediately sees that $M(k,r)$ is ruled by $kr + \delta_1$. By introducing the reduced matrix $K_2 = \operatorname{tg} \delta_2$ and the reduced matrix $S_2 = e^{2i\delta_2}$ one has the following explicit expression

$$(48) \qquad \bar{\psi}^{P}(1,2;k,r) \xrightarrow[r\to\infty]{} \psi^{P}(1;k,r) + \frac{K_2}{\cos\delta_1} \cos(kr + \delta_1 - \ell\pi/2)$$

$$(49) \qquad \bar{\psi}^{(+)}(1,2;k,r) \xrightarrow[r\to\infty]{} \psi^{(+)}(1;k,r) + S_2 \frac{e^{2i\delta_1} - 1}{2i} e^{i(kr - \ell\pi/2)}$$

furthermore it is interesting to observe that the solution $\bar{\psi}^{(+)}(1,2)$ has the same normalization as $\psi^{(+)}(1,2)$ while $\bar{\psi}^{P}(1,2)$ satisfies the relation

$$(50) \qquad \bar{\psi}(1,2) = (1 - \operatorname{tg}\delta_1 \operatorname{tg}\delta_2)\, \psi^{P}(1,2) .$$

The standing wave solution $\bar{\psi}^{P}(1,2)$ satisfies the following integral equation

$$(51) \qquad \bar{\psi}^{P}(1,2;k,r) = \psi^{P}(1;k,r) + \int_0^\infty G^{P}(1;k,r,r') V_2(r')\, \bar{\psi}^{P}(1,2;k,r')\, dr' ,$$

where the kernel $G^{P}(1;k,r,r')$ is coincident with the kernel $G^{P}(k;r,r')$ defined in Sect. 2.3 (the notation has been modified here for uniformity with the symbolism of this Section). This equation can be solved by the techniques we used in Sect. 2. We define the kernel

$$(52) \qquad \Gamma(1,2;k,r,r') = -\frac{2M}{\hbar^2} \frac{\varphi(1,2;k,r_<)\, \gamma(1,2;k,r_>)}{W[\gamma(1,2), \varphi(1,2)]} ;$$

$\varphi(1,2)$ is the angular solution pertaining to the complete Hamiltonian, while the function $\gamma(1,2)$, which is also a solution of the complete Schrödinger equation defined by the relation

$$(53a) \qquad \gamma(1,2;k,r) = \frac{1}{2}\left[\mathcal{F}_-(1;k) f_+(1,2;f,r) + \mathcal{F}_+(1;k) f_-(1,2;k,r)\right] ,$$

is characterized by the following asymptotic behaviour

$$(53b) \qquad \gamma(1,2;k,r) \xrightarrow[r\to\infty]{} \mathcal{F}_+(1;k)\, e^{i\delta_1} \cos(kr + \delta_1 - \ell\pi/2).$$

It follows that

$$(54) \qquad \bar{\psi}^P(1,2;k,r) = \psi^P(1;k,r) + \int_0^\infty \Gamma(1,2;k,r,r') V_2(r')\, \psi^P(1;k,r')\, dr'$$

is the formal solution of the above integral equation. By the techniques examined in Subsection 2.2 the relation

$$(55) \qquad \Gamma(1,2) = G^P(1) + G^P(1) V_2\, \Gamma(1,2)$$

is immediately proved.

We are now in a position to make a precise comparison between the kernels which appear in the S matrix and those which appear in the K matrix. In the K-matrix problem, in order to define the equations which satisfy the standing wave functions $\psi^P(1)$ and $\bar{\psi}^P(1,2)$ (eqs. (11) and (51)), together with the formal solutions of these equations (eqs. (28) and (54)), we ought to introduce the four Green functions $\Gamma_o$, $G^P(1)$, $\Gamma(1)$ and $\Gamma(1,2)$; these kernels are connected by the unlinked relations (31) and (55). In the S-matrix theory, in order to define the integral equations for $\psi^{(+)}(1)$ and $\bar{\psi}^{(+)}(1,2)$ and their formal solutions, one needs the three kernels $G_o^{(+)}$, $G^{(+)}(1)$ and $G^{(+)}(1,2)$, which are connected by the symmetric relations

$$G^{(+)}(1) = G_o^{(+)} + G_o^{(+)} V_1 G^{(+)}(1), \qquad G^{(+)}(1,2) = G^{(+)}(1) + G^{(+)}(1) V_2 G^{(+)}(1,2).$$

These different properties of the Green functions are ultimately related to the different asymptotic behaviour characterizing the physical solution $\bar{\psi}^{(+)}(1,2)$ and the standing wave solution $\bar{\psi}^P(1,2)$ (compare eqs. (48) and (49)). A direct consequence of these facts is the striking

difference between the formulae which correlate the matrices S and $S_2$ on one hand and the matrices K and $K_2$ on the other, which are respectively

$$S = S_1 S_2, \qquad K = \frac{K_1 + K_2}{1 - K_1 K_2}$$

Another problem which is related to these properties of the Green functions is the relation between the reduced matrices $S_2$ and $K_2$. It is trivial to obtain on the ground of the definition of $S_2$ and $K_2$ in terms of the phase shift the Heitler-type relation

$$S_2 = \frac{1+iK_2}{1-iK_2} . \tag{56}$$

This relation will be here deduced in the frame work of our formalism, starting from their integral representation.

The reduced matrix element $K_2$ is easily obtained by comparing eq. (48) with eq. (51): one has

$$K_2 = - \frac{2M}{\hbar^2 k} \frac{e^{i\delta_1}}{\mathcal{F}_-(1)} \cos\delta_1 ( \varphi(1) V_2 \overline{\psi}^P(1,2)) \tag{57}$$

by putting in this the expression (54) for $\overline{\psi}^P(1,2)$, one gets the more explicit expression

$$K_2 = - \frac{2M}{\hbar^2 k} \frac{e^{i\delta_1}}{\mathcal{F}_-(1)} \cos\delta_1 \left[ ( \varphi(1) V_2 \psi^P(1)) + (\varphi(1) V_2 \Gamma(1,2) \psi^P(1)) \right] . \tag{58}$$

where the following compact notation

$$\int_0^\infty u(r)\, v(r)\, dr = (uv)$$

has been used. In order to make easy the comparison with $S_2$, it is useful to introduce the function $\psi(1;k,r)$ which is defined in the following way

$$\psi(1;k,r) = e^{-i\delta_1} \psi^{(+)}(1;k,r) \xrightarrow[r\to\infty]{} \sin(kr + \delta_1 - \ell\pi/2) .$$

With this notation $K_2$ assumes the form

$$K_2 = -\frac{2M}{\hbar^2 k}\cos\delta_1(\psi(1)V_2\bar{\psi}^P(1,2)) =$$

(59)

$$= -\frac{2M}{\hbar^2 k}\left[(\psi(1)V_2\psi(1))+(\psi(1)V_2\Gamma(1,2)V_2\psi(1))\right]$$

while $S_2$ can be written in the form

$$S_2 = 1 - \frac{4iM}{\hbar^2 k}e^{-i\delta_1}(\psi(1)V_2\psi^{(+)}(1,2)) =$$

(60)

$$= 1 - \frac{4iM}{\hbar^2 k}\left[(\psi(1)V_2\psi(1))+(\psi(1)V_2G^{(+)}(1,2)V_2'\psi(1))\right].$$

Now, by a straighforward calculation, one gets(x)

$$G^{(+)}(1,2;r,r')-\Gamma(1,2;r,r') = \frac{2M}{\hbar^2}\varphi(1,2;r)\,\varphi(1,2;r')\,x$$

$$x\,\frac{W\left[f_+(1,2),\,\gamma(1,2)\right]}{W\left[f_+(1,2),\,\varphi(1,2)\right]W\left[\gamma(1,2),\varphi(1,2)\right]} = -\frac{2iM}{\hbar^2 k}\psi^{(+)}(1,2;r)\,\bar{\psi}^P(1,2;r')e^{-i\delta_1}\cos\delta_1$$

By multiplying on the left and on the right the first and the third member of the above relation by $\psi(1)V_2$, and comparing with formulae (59) and (60), one immediately gets

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(x) - We only remember that because of relations (15) and (50), the regular solution $\varphi(1,2)$ and the standing wave solution $\psi^P(1,2)$, are connected by the relation

$$2k\varphi(1,2)\,\frac{1-\mathrm{tg}\,\delta_1\,\mathrm{tg}\,\delta_1}{\mathcal{F}_+(1,2)+\mathcal{F}_-(1,2)} = \bar{\psi}^P(1,2)$$

$$\frac{\hbar^2 k}{2M}\,\frac{1-S_2}{2i}+K_2=\frac{\hbar^2 k}{4M}(1-S_2)K_2$$

from which the relation (56) is obtained.

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APPENDIX A. -

It is immediate to see that the kernel $\Gamma_o$ defined in Subsect. 2.1 by the relation (10) is capable of the following representation

$$\Gamma_o(k;r,r') = \frac{1}{2}\left[G_o^{(+)}(k;r,r') + G_o^{(-)}(k;r,r')\right] , \tag{A.1}$$

where the kernels $G_o^{(\pm)}(k;r,r')$ are defined for any complex value of the momentum by the relations

$$G_o^{(+)}(k;r,r') = -\frac{2M}{\hbar^2}\,\frac{F(kr_<)0(kr_>)}{W[0,F]} ,$$

$$G_o^{(-)}(k;r,r') = -\frac{2M}{\hbar^2}\,\frac{F(kr_<)I(kr_>)}{W[I,F]} .$$

These kernels can be given the following interpretation. The outgoing wave kernel $G_o^{(+)}(k;r,r')$ is obtained from the resolvent of $H_o$ by taking the physical determination of $(2ME/\hbar_2)^{1/2}$; it follows that in the region $\mathrm{Im}k \geq 0$ the kernel $G_o^{(+)}(k;r,r')$ is coincident with $G_o(k;r,r')$, while for $\mathrm{Im}K < 0$ it is to be interpreted as the analytic continuation of this kernel: in this region $G_o^{(+)}(k;r,r')$ is not related to the resolvent, neither is it an Hilbert space operator. A symmetric definition holds for the ingoing wave kernel $G_o^{(-)}(k;r,r')$: for $\mathrm{Im}k \leq 0$ it is the kernel of the resolvent of $H_o$, while for $\mathrm{Im}k > 0$ it is the analytic continuation of this kernel. From the definition it follows that $\Gamma_o(k;r,r')$ is defined in any point of the momentum plane, but it is a resolvent for no value of the momentum, neither is it an Hilbert space operator; this fact causes no trouble, provided we avoid to resort to functional analysis.

A straighforward calculation proves that

$$G_o^{(-)}(k;r,r') = G_o^{(+)}(-k;r,r') ,$$

so that formula (A.1) can be written in the alternative form

$$\Gamma_o(k;r,r') = \frac{1}{2}\left[G_o^{(+)}(k;r,r') + G_o^{(+)}(-k;r,r')\right] , \tag{A.2}$$

which for $k>0$ is coincident with $G_o^P(k;r,r')$.

Some words to enlight the relation between the kernel $\Gamma_o$ defined by eq. (A.2) and the kernel $G_o^P$. In our notations the kernel of $G_o^P(E)$ can be viewed as the average of $G_o^{(+)}(k;r,r')$ and $G_o^{(+)}(-k;r,r')$ where k can be only positive because of the condition $Im(\pm k)\geq 0$: our formula (A.2) can be interpreted as the generalization of this definition to any complex value of the momentum. As a final remark we observe that $G_o^P(E)$, because of its very definition, is capable of a spectral representation on the axis $-\infty < E < \infty$; on the converse, our definition involves $G_o^{(+)}(k;r,r')$ and $G_o^{(-)}(k;r,r')$ which are spectrally representable for $Imk \geq 0$ and $Imk \leq 0$ respectively. It follows that $\Gamma_o \times \Gamma_o(k;r,r')$ is capable of a spectral representation only on the axis $Imk = 0$, that is for $E>0$, and there the representation is coincident with the $G_o^P(E)$ representation.

APPENDIX B. -

We wish here to prove relations (20a) and (20b) of Sect. 3. To simplify the notations, the dependence on the momentum will not be explicitly written.

Let us call $\Delta G(r,r')$ the second member of eq. (20a), and consider it first for $r \leq r'$. By resorting to the definition (19) for $G_i$, one gets

$$\Delta G(r,r') = \left(\frac{2M}{\hbar^2}\right)^2 \frac{1}{W\left[\chi_{i_1}, \varphi_{i_1}\right] W\left[\chi_{i_2}, \varphi_{i_2}\right]} \left[ \int_o^r dr'' \varphi_{i_1}(r'') \chi_{i_1}(r) \left\{ V_{i_1}(r'') - V_{i_2}(r'') \right\} \varphi_{i_2}(r'') \chi_{i_2}(r') + \int_r^{r'} dr'' \chi_{i_1}(r'') \varphi_{i_1}(r) \left\{ V_{i_1}(r'') - V_{i_2}(r'') \right\} \chi_{i_2}(r') \varphi_{i_2}(r'') + \int_{r'}^{\infty} dr'' \varphi_{i_1}(r) \chi_{i_1}(r'') \left\{ V_{i_1}(r'') - V_{i_2}(r'') \right\} \varphi_{i_2}(r') \chi_{i_2}(r'') \right] \equiv$$

$$\equiv \left(\frac{2M}{\hbar^2}\right)^2 \frac{1}{W\left[\chi_{i_1}, \varphi_{i_1}\right] W\left[\chi_{i_2}, \varphi_{i_2}\right]} \left[ I(0,r) + I(r,r') + I(r',\infty) \right],$$

where $I(a,b)$ are the integrals appearing in the second member with the limits of integration there specified. Each of the terms, $I(a,b)$ will be handled as follows: the terms depending on r and r' are extracted, while the remaining is integrated by part. One easily obtains

$$I(0,r) = \frac{\hbar^2}{2M} \chi_{i_1}(r)\chi_{i_2}(r')\left[\varphi_{i_2}\varphi'_{i_1} - \varphi_{i_2}\varphi'_{i_2}\right]_0^r$$

$$I(r,r') = \frac{\hbar^2}{2M} \varphi_{i_1}(r)\chi_{i_2}(r')\left[\varphi_{i_2}\chi'_{i_1} - \varphi'_{i_2}\chi_{i_1}\right]_r^{r'}$$

$$I(r',\infty) = \frac{\hbar^2}{2M} \varphi_{i_1}(r)\varphi_{i_2}(r')\left[\chi_{i_2}\chi'_{i_1} - \chi'_{i_2}\chi_{i_1}\right]_{r'}^{\infty} .$$

We take into account now that the regular functions vanish at the origin and that $\chi_{i_1}$ and $\chi_{i_2}$ satisfy the same asymptotic conditions. The simplified expression we obtain from this is

$$\Delta G(r,r') = \frac{2M}{\hbar^2} \frac{1}{W\left[\chi_{i_1}, \varphi_{i_1}\right] W\left[\chi_{i_2}, \varphi_{i_2}\right]} \left[\varphi_{i_2}(r)\chi_{i_2}(r')\left\{\chi_{i_1}(r)\varphi'_{i_1}(r) - \right.\right.$$

$$\left.\left. - \chi'_{i_1}(r)\varphi_{i_1}(r)\right\} - \varphi_{i_1}(r)\chi_{i_1}(r')\left\{\chi_{i_2}(r')\varphi_{i_2}(r') - \chi'_{i_2}(r')\varphi_{i_2}(r')\right\}\right].$$

The terms in curl brakets are Wronskian, which can be simplified with the denominator. Then one obtains

$$\Delta G(r,r') = G_{i_1}(r,r') - G_{i_2}(r,r') \qquad r < r' .$$

For $r > r'$ one uses the same procedures. It follows that relation (20a) is proved.

We turn now to the relation (20b). From the definitions of the Green function $G^{\alpha}$ we have

$$G^{\alpha_1}(r,r') - G^{\alpha_2}(r,r') = \frac{2M}{\hbar^2} \varphi(r_<)\left[\frac{\chi^{\alpha_2}(r_>)}{W\left[\chi^{\alpha_2}, \varphi\right]} - \frac{\chi^{\alpha_1}(r_>)}{W\left[\chi^{\alpha_1}, \varphi\right]}\right]$$

Since the Wronskian has the same value for any value of r, we can write

$$G^{\alpha_1}(r,r')-G^{\alpha_2}(r,r')=\frac{2M}{\hbar^2}\frac{\varphi(r_<)}{W\left[\chi^{\alpha_2},\varphi\right]W\left[\chi^{\alpha_1},\varphi\right]}\Big[\chi^{\alpha_2}(r_>)\Big\{\chi^{\alpha_1}(r_>)\varphi'(r_>)-$$

$$\chi^{\alpha'_1}(r_>)\varphi(r_>)\Big\}-\chi^{\alpha_1}(r_>)\Big\{\chi^{\alpha_2}(r_>)\,\varphi'(r_>)-\chi^{\alpha'_2}(r_>)\,\varphi(r_>)\Big\}\Big]=$$

$$=\frac{2M}{\hbar^2}\varphi(r_<)\varphi(r_>)\frac{W\left[\chi^{\alpha_1}(r_>),\chi^{\alpha_2}(r_>)\right]}{W\left[\chi^{\alpha_2},\varphi\right]W\left[\chi^{\alpha_1},\varphi\right]}\;;$$

since $W\left[\chi^{\alpha_1},\chi^{\alpha_2}\right]$ is independent of r, formula (20b) is proved.

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