T. A. Minelli, A. Vitturi and F. Zardi: A METHOD FOR THE ANALYTIC CONTINUATION OF THE S-MATRIX FOR CUT-OFF POTENTIALS.
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SUMMARY.

The \( \ell \)-th partial wave S-matrix element for cut-off potentials is Taylor expanded in the energy and momentum variable. The expansion is based on a suitable finite-interval Green's function, by which the derivatives are obtained in a recursion form involving only repeated integrations of the Green's function itself. The Taylor series can be analytically continued by resorting to the Padé method; some results of a numerical experiment are quoted. In this paper, however, the emphasis is put on a rather indirect but rigorous procedure based on the Hadamard theory, which allows to determine, in principle, all the poles of the S-matrix starting from its momentum Taylor series. Numerical results are displayed.

1. - INTRODUCTION.

The scattering matrix element in a partial wave for a short-range central potential is a meromorphic function of the momentum in a strip along the real axis(3). In principle, it can be expanded in

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2. a Taylor series about any regular point; the analytic continuation theory assures then that this series determines completely the S-matrix element in the whole analyticity region. As a matter of fact, the actual pursuing of this statement is not straightforward since it involves the search of practical methods for the evaluation of the S-matrix momentum derivatives, and the use of suitable procedures in order to go outside the Taylor series convergence circle.

In the present work we point out some results concerning the cut-off potential scattering problem, which is of the greatest interest in the nuclear resonance problem; in the concluding remarks a hint for the generalization of the procedure is given.

The results displayed in the present paper can be summarized as follows.

For cut-off potentials the S-matrix element can be expressed in terms of a suitable Green's function defined in the interaction region only, and satisfying energy-dependent boundary conditions\(^{(4, 5, 6)}\) (in the following we refer to its as the finite interval Green's function, or \(G\)-function). In the present work such a Green's function is proved to satisfy a Fredholm-type integral equation relating two different energies; from this equation the momentum derivatives are obtained in a recursion form which involves only repeated integrations of the Green's function itself. The S-matrix Taylor series can be easily obtained from these. Similarities and basic differences with respect to the perturbative expansion are thoroughly discussed.

Concerning the analytic continuation of the S-matrix Taylor expansion, various approaches have been used. A possible choice is to resort to the Padé approximant method\(^{(7)}\); although the numerical results so obtained (part of which are displayed in the present work and in Ref. (1)) are quite satisfactory, the problem of giving complete and rigorous theorems on the convergence of the approximants has not been solved in general.

In the present work, therefore, we prefer to put the emphasis on a procedure which—although rather indirect—gives a complete and mathematically rigorous answer to the analytic continuation problem.

The solution we propose is based on the following considerations. It is well known that for cut-off potentials the only singularities of the S-matrix in the whole momentum plane are poles. Now, in the Ning Hu representation the S-matrix is expressed in a factorized form involving only the position of the poles\(^{(3)}\), so that the analytic continuation amounts to the determination of the pole affixes. In this connection we resorted to a method due to Hadamard\(^{(8)}\), devised for the determination of the polar singularities of a meromorphic function starting from its Ta
Taylor expansion about a regular point. More rigorously, the method allows, in principle, to determine the affixes of all the poles lying within the meromorphism circle (the largest circle centered in the expansion point and containing only poles); in the problem we are dealing with this circle coincides with the momentum plane.

In Section 2 the essentials of the finite interval Green's function formalism are recalled in a self-consistent form, which should make it unnecessary to refer back to the original papers. Section 3 is devoted to the introduction of the Fredholm-type integral equation for energy variation of the finite interval Green's function, and to the deduction of its Taylor series. In Section 4 the analytic continuation methods we use are briefly discussed; the results of some numerical experiments concerning the fit of a resonance-exhibiting cross section by the Padé method, and the pole affixes evaluation by the Hadamard theory are displayed as well.

2. - THE FINITE INTERVAL GREEN'S FUNCTION AND THE SCATTERING MATRIX.

It is well known that the solution of any quantum mechanical problem with a cut-off potential requires the actual solution of the Schrödinger equation in the interaction region only. A formulation of this problem in terms of a Green's function defined in the sole interaction region has been given by Bloch(4); the analytic continuation of this algorithm in the momentum and energy plane has been considered by the authors in a previous work concerning the pole expansion of the S-matrix(6).

This Section is devoted to a self-consistent outline of the $G_f$-function formalism in the notation more suitable for the purpose of the present work.

2.1. - The Finite Interval Green's Function.

We first consider the scattering of two spinless particles interacting through a non-singular short range central potential. Let $M$ be the reduced mass and $E = \frac{\hbar^2 k^2}{2M}$ the energy in the c.m. reference frame. The physical solution $\psi^{(+)}_\ell(k, r)$ in the $\ell$-th partial wave is defined by the equation

$$H_\ell \psi^{(+)}_\ell(k, r) = E \psi^{(+)}_\ell(k, r)$$

(1)

together with the boundary conditions
\[ \psi_{\ell}^{(+)}(k, 0) = 0, \quad \psi_{\ell}^{(+)}(k, r) \rightarrow \frac{i}{2} \left[ I_{\ell}(kr) - S_{\ell}(k) 0_{\ell}(kr) \right] \]

the partial wave Hamiltonian operator \( H_\ell \) is defined by the relation

\[
H_\ell = -\frac{\hbar^2}{2M} \left[ \frac{d^2}{dr^2} - \frac{\ell(\ell+1)}{r^2} \right] + V(r) = H_\ell^1 + V(r);
\]

\( I_{\ell}(kr) \) and \( 0_{\ell}(kr) \) are the ingoing and outgoing solutions of the unperturbed Hamiltonian \( H_\ell^1 \), characterized by the following asymptotic behaviour

\[
I_{\ell}(kr) \rightarrow e^{-i(kr - \frac{l\pi}{2})}, \quad 0_{\ell}(kr) \rightarrow e^{i(kr - \frac{l\pi}{2})}
\]

Here we quote also the regular solution \( \varphi_{\ell}^{(r)}(k, r) \) and the outgoing Jost solution \( f_{\ell}(k, r) \), which satisfy eq. (1) and the following conditions (x)

\[
(3a, b) \quad \lim_{r \to 0} r^{-l-1} \varphi_{\ell}^{(r)}(k, r) = 1, \quad \lim_{r \to \infty} f_{\ell}(k, r) = \lim_{r \to \infty} 0_{\ell}(kr);
\]

the Jost function \( \mathcal{J}_{\ell}(k) \) is defined as the Wronskian of \( \varphi_{\ell}^{(r)}(k, r) \) and \( f_{\ell}(k, r) \)

\[
\mathcal{J}_{\ell}(k) = f_{\ell}(k, r) \frac{d}{dr} \varphi_{\ell}(k, r) - \varphi_{\ell}(k, r) \frac{d}{dr} f_{\ell}(k, r)
\]

From the above definitions the following integral representation for the physical solution can be derived

\[
\psi_{\ell}^{(+)}(k, r) = F_{\ell}(kr) + \int_{0}^{\infty} dr' G_{\ell}^{(+)}(k; r, r') V(r') F_{\ell}(kr') dr',
\]

where \( G_{\ell}^{(+)}(k; r, r') \) is the complete outgoing Green's function, defined by the expression

(x) - The solution \( f(k, r) \) differs from the Jost solution \( f_{\ell}^{(+)}(k, r) \) of Newton (3) for the constant factor \( e^{-i\ell \pi/2} \).
(5) \[ G^{(+)}(k;r,r') = \frac{-2M}{\hbar^2} \frac{\varphi_e^+(k,r) f_\ell(k,r')}{\mathcal{F}_\ell(k)} \]

and

\[ F_\ell(kr) = \frac{i}{2} \left[ 1_\ell(kr) - \mathcal{F}_\ell(kr) \right] \]

is the Riccati-Bessel function. From now onward the symbol \( \ell \) will be omitted when it is a mere label.

For a cut-off potential \( V(r) \equiv 0 \) for \( r < a \) it appears from eq. (4) that, in order to evaluate \( \psi^{(+)}(k,r) \) in the interaction region - which determines completely the external behaviour and the S-matrix - it is enough to know \( G^{(+)}(k;r,r') \) in the square interval \( 0 \leq r, r' \leq a \).

We define now in this interval the kernel (6)

\[ G(k,r,r') = \frac{-2M}{\hbar^2} \frac{\varphi(k,r) f^k(k,r)}{\mathcal{F}^k(k)} \quad 0 \leq r, r' \leq a, \]

where \( f^k(k,r) \) is defined by the conditions

(6a) \[ (H-E) f^k(k,r) = 0 \quad 0 \leq r \leq a \]

(6b) \[ f^k(k,a) = 0 \quad (ka) \]

\[ \frac{d}{dr} f^k(k,r) \bigg|_{r=a} = L(k) f^k(k,a), \]

where

\[ L(k) = \frac{d}{dr} 0(kr) \bigg|_{r=a} \]

\[ 0(ka) \]

the function \( \mathcal{F}^k(k) \) is the Wronskian of \( \varphi(k,r) \) and \( f^k(k,r) \). The kernel \( g(k;r;r') \), which is defined in the interaction region only, is there coincident with \( G^{(+)}(k;r,r') \) since the boundary condition (6b) is the mere transposition at \( r = a \) of the asymptotic condition (3b) for the Jost solution. The kernel \( g(k;r,r') \) can be identified with the kernel of the problem of Kapur and Peierls (4, 5).
2.2. - Analytic Continuation of the \( \mathcal{G} \)-Function. The S-Matrix.

As it is apparent from eqs. (6a) and (6b) \( \mathcal{G}(k;r,r') \) depends on the momentum in two different ways: through the energy which appears in the Schrödinger equation and through the boundary conditions. The general form of the analytic continuation is therefore

\[
(7) \quad \mathcal{G}(k;r,r') = -\frac{2M}{\hbar^2} \frac{\varphi(k,r_<) \mathcal{F}(k,r_>)}{\mathcal{F}(k)} \quad 0 \leq r, r' \leq a
\]

where \( \mathcal{F}(k) \) is defined by the conditions

\[
(H-\mathcal{E}) \mathcal{F}(k) = 0
\]

\[
\mathcal{F}(k,a) = 0 \quad (k,a)
\]

\[
\left. \frac{d}{dr} \mathcal{F}(k,r) \right|_{r=a} = L(k) \mathcal{F}(k,a)
\]

and \( \mathcal{F}(k) \) is the Wronskian

\[
\mathcal{F}(k) = W[f(k,r), \varphi(k,r)]
\]

(we use the symbol \( k \) to denote any complex momentum - in particular \( k \) can be real - and \( \mathcal{E} \) to denote its related energy \( \mathcal{E} = \hbar^2 k^2 / 2M \); the symbols \( k \) and \( E \) are reserved for real values of the momentum and energy). If \( k' = k \), one gets \( \mathcal{G}_{k'}(k,r) = \mathcal{G}(k,r) \) and \( \mathcal{F}(k') = \mathcal{F}(k) \), where \( \mathcal{F}(k) \) is the Jost solution and the Jost function previously introduced. The analytic continuation of \( \psi^+(k,r) \) with continued boundary conditions (2) is clearly obtained through the Green's function

\[
(8) \quad \mathcal{G}(k;r,r') = \mathcal{G}_{k}(k;r,r') = -\frac{2M}{\hbar^2} \frac{\varphi(k,r_<) \mathcal{F}(k)}{\mathcal{F}(k)} \quad 0 \leq r, r' \leq a
\]

Although eq. (8) and the considerations from which it is deduced seem to be quite obvious, we preferred to introduce it as a particularization of the general form (7), to stress the fact that in any case the boundary conditions are momentum-dependent.

Since \( \varphi(k,r) \) and \( \mathcal{F}(k) \) are entire functions of \( k \), it follows that \( \mathcal{G}(k;r,r') \) is a meromorphic function whose poles are the zeros of \( \mathcal{F}(k) \); these poles are coincident with the S-matrix ones (3).

Most of the deductions we are going to make in the next Sections are obtained by considering the \( \mathcal{G} \)-function as a direct function of the
energy. In order to render \( g(E; r, r') \) a univocal function of the energy it will be considered on a single sheet of the energy Riemann surface.

The kernel \( g(E; r, r') \) coincides with the analytic continuation of the outgoing Green's function (5) for \( 0 \leq r, r' \leq a \), but it is not a resolvent kernel; in fact, because of the energy-dependence of the boundary conditions, at each energy the \( g \)-function is related to a different inversion of \( (E-H) \). This will not prevent us from writing an integral equation relating different energies, and obtaining the derivatives in a recursion form.

Through the analytic continuation of the \( g \)-function various expressions of the analytic continuation of the S-matrix can be derived\((5, 6)\). The relation that came out to be the most fruitful for the purposes of the present work is easily obtained by the matching of the internal and the external solution at \( r=a \). One obtains

\[
S(k_a) = \frac{I(k_a)}{0(k_a)} + 2i \frac{\psi^+ (k_a, a)}{0(k_a)};
\]

the finite interval Green's function is now introduced by using the proportionality relation between \( \psi^+ (k, r) \) and the regular solution \( \varphi (k, r) \); one gets

\[
\psi^+ (k_a, a) = k_a \frac{\varphi (k_a, a)}{S(k_a)} = -\frac{\hbar^2}{2M} k_a G(k_a, a, a) \frac{0(k_a)}{0(k_a)}
\]

From eqs. (9) and (10) one gets finally\((4, 5, 6)\)

\[
S(k) = \frac{I(k_a)}{0(k_a)} \left[ 1 - 2i k_a \frac{\hbar^2}{2M} \frac{G(k_a; a, a)}{I(k_a) 0(k_a)} \right] = \frac{I(k_a)}{0(k_a)} S_{\text{Res}}(k)
\]

Equation (11) is worth a few comments. We first observe that the above procedure leads to a separation of the hard sphere scattering from the so-called resonant scattering. This separation does not introduce any spurious feature in the analytic structure of the S-matrix. In particular, one can easily verify that \( S(k) \) and the \( Q \)-function have the same poles. Furthermore, from eq. (11) it appears that all information about \( S(k) \) is contained in the \( Q \)-function since \( I(k_a) \) and \( O(k_a) \) are known functions of the energy; because of this the next Section is devoted to the study of the \( Q \)-function.
3. - THE ENERGY AND MOMENTUM TAYLOR EXPANSION FOR THE FINITE INTERVAL GREEN'S FUNCTION.

In this Section a Fredholm-type equation is derived, which relates the finite interval Green's function at two different energies (Sect. 3.1); this equation enables us to deduce a recursion formula for its energy and momentum derivatives (Sect. 3.2). In Section 3.3, an interpretation of the above results in terms of the regularization procedure is analysed.

3.1. - The Integral Equation.

In order to stress the mathematical peculiarities of our formalism and to enlight the differences with respect to problems in which resolvent kernels are involved, two preliminary examples are discussed.

We consider the well-known general relation which connects the inverses of two differential operators associated to the same boundary conditions

\[ \frac{1}{z - \Omega} - \frac{1}{z' - \Omega'} = \frac{1}{z - \Omega} \left[ (z' - z) - (\Omega' - \Omega) \right] \frac{1}{z' - \Omega'} , \]

where \( z \) and \( z' \) are complex numbers in the resolvent set of the operators \( \Omega \) and \( \Omega' \).

This relation can be used in order to connect the unperturbed Green's function \( G^{(+)}(\Omega^2;E;r,r') \) and the Green's function \( G^{(+)}(\Omega^1;E;r,r') \) pertaining to the description of the scattering by a potential \( \lambda \in (r) \); one obtains the Fredholm integral equation

\[ G^{(+)}(\Omega^1;E;r,r') = G^{(+)}(\Omega^2;E;r,r') + \lambda \int_0^\infty G^{(+)}(\Omega^2;E;r,r'')V(r'')G^{(+)}(\Omega^1;E;r'',r')dr'' . \]

Solving this equation by the iterative method one gets a power series in the coupling parameter, i.e.

\[ G^{(+)}(\Omega^1;E;r,r') = \sum_{n=0}^\infty Q_n(E;r,r') \lambda^n \]

where the coefficients are given in the recursion form

\[ Q_0(E;r,r') = G^{(+)}_0(E;r,r'), \quad Q_n(E;r,r') = \int_0^\infty G^{(+)}_0(E;r,r'')V(r'')Q_{n-1}(E;r'',r')dr'' \]

\[ n \geq 1 \]
Comparison of eq. (13) with the Taylor series, owing to the independence of $Q_n(E; r, r')$ on the coupling parameter, leads to the identification

\begin{equation}
\frac{d^n}{d\lambda^n} G^{(+)}(\lambda; E; r, r') \bigg|_{\lambda=0} = n! Q_n(E; r, r').
\end{equation}

Relation (12) can be applied also to the problem of connecting the Green's function $G^{(+)}(E; r, r')$ at two different energies in the upper momentum plane, in which the analytic continuation of the outgoing Green's function (5) is a true resolvent kernel; one gets

\begin{equation}
G^{(+)}(E; r, r') = G^{(+)}(E; r, r') - \int_{E_o}^{E} G^{(+)}(E; r, r'') G^{(+)}(E; r', r'') dE''
\end{equation}

Also in this case the iterative series is directly connected to the Taylor expansion by a relation similar to eq. (14).

This standard procedure cannot be utilized in the framework of the finite interval Green's function owing to the energy-dependence of the boundary conditions; there are however other ways to deduce an integral equation for energy variation. The most direct is suggested by the Bloch representation of the $G$-function, which embodies explicitly the boundary conditions in the inverse operator.

By putting

\[ L(E) = \frac{\hbar^2}{2M} \left[ \frac{d}{dr} - L(E) \right] \delta(r-a) \]

one gets (4, 9)

\[ G(E; r, r') = \langle r | G(E) | r' \rangle = \langle r | \frac{1}{E - L(E) - H} | r' \rangle. \]

In this connection formula (12) has been generalized to include inverse operators related to different boundary conditions (9, 10). In the problem we are dealing with this procedure leads to the relation

\begin{equation}
\frac{1}{E - L(E) - H} - \frac{1}{E_o - L(E_o) - H} = \frac{1}{E - L(E) - H} \left[ E_o - E + \frac{\hbar^2}{2M} \delta(r-a) \left\{ L(E) - L(E_o) \right\} \right] \frac{1}{E - L(E) - H};
\end{equation}

\[ E \neq E_o \]
a somewhat hybrid notation has been used to evidence the fact that
the boundary condition variation originates an energy-dependent sur-
face term.

In the coordinate representation the above relation writes

\[ G(\mathcal{E}; r, r') = G(\mathcal{E}_o; r, r') - \mathcal{E} - \mathcal{E}_o \int_0^a G(\mathcal{E}_o; r, r'') \cdot \]

\[ 1 + \frac{\hbar^2}{2M} \delta(r - a) \left( \frac{\mathcal{L}(\mathcal{E}) - \mathcal{L}(\mathcal{E}_o)}{\mathcal{E} - \mathcal{E}_o} \right) \right] G(\mathcal{E}; r'', r') \, dr''. \]

In Appendix an alternative derivation of the relation (17), is given
which avoids the introduction of the symbolic boundary condition ope-
rators, and is based on standard analysis. We must remark, however,
that eq. (16) is formally valid also for rearrangement collisions, with
a suitable modification of the boundary condition operator(4, 9).

Equation (17) is a Fredholm-type integral equation, which can
be solved by the iterative method; however the iterative series, be-
cause of the energy-dependence contained in the surface term, cannot
be interpreted as an energy-power expansion.

3.2.- The Taylor Series.-

The energy derivatives can still be obtained in a recursion
form from the integral equations (16) or (17) by the following procedure.
In the operator representation (16) the first derivative (in the regular
point \( \mathcal{E}_o \)) is

\[ G^{(1)}(\mathcal{E}_o) = \frac{dG(\mathcal{E})}{d\mathcal{E}} \bigg|_{\mathcal{E} = \mathcal{E}_o} = \lim_{\mathcal{E} \to \mathcal{E}_o} \left( \frac{G(\mathcal{E}) - G(\mathcal{E}_o)}{\mathcal{E} - \mathcal{E}_o} \right) = \]

\[ = -G(\mathcal{E}_o) \left[ 1 + \frac{\hbar^2}{2M} \delta(r - a) L^{(1)}(\mathcal{E}_o) \right] G(\mathcal{E}_o) \]

where \( L^{(1)}(\mathcal{E}_o) \) is the first energy derivative of \( L(\mathcal{E}) \). By derivation
of eq. (18) one gets immediately for the second derivative the expression

\[ G^{(2)}(\mathcal{E}_o) = -2G^{(1)}(\mathcal{E}_o) G^{(1)}(\mathcal{E}_o) - 2G^{(1)}(\mathcal{E}_o) \left[ \frac{\hbar^2}{2M} \delta(r - a) L^{(1)}(\mathcal{E}_o) \right] G(\mathcal{E}_o) - \]

\[ -G(\mathcal{E}_o) \left[ \frac{\hbar^2}{2M} \delta(r - a) L^{(2)}(\mathcal{E}_o) \right] G(\mathcal{E}_o) \]
It can be shown\(^\text{(11)}\) that iteration of the above procedure leads to the general expression

\[ g^{(n)}(E_o) = -n g^{(n-1)}(E_o) g(E_o) - \frac{\hbar^2}{2M} \sum_{i=0}^{n-1} \frac{n!}{i!(n-i)!} x \]

\[ x g^{(i)}(E_o) \left[ \delta(r-a) L^{(n-i)}(E_o) \right] g(E_o), \]

with \( g^{(0)}(E_o) = g(E_o) \). It is clear from the coordinate representation of \( g^{(n)}(E_o) \) that the evaluation of the n-th derivative starting from the n-l lower order derivatives requires one actual integration only. It is worth noting that also the derivatives of \( L(E) \), can be given a recursion form\(^\text{(11)}\), so that the n-th order energy derivative evaluation can be reduced to the knowledge of \( g(E_o) \).

In a similar way, starting again from eq. (17), the following general expression for the n-th momentum derivative \( g^{(n)}(k_o; r, r') \) is obtained (\( k_o \) is a regular point)

\[ g^{(1)}(k_o; r, r') = \frac{\hbar^2}{M} k_o \int_0^a g(k_o; r', r'') g(k_o; r''; r') dr'' - \frac{\hbar^2}{2M} L^{(1)}(k_o) g(k_o; r, a) g(k_o; a, r'); \]

\[ g^{(n)}(k_o; r, r') = -n \frac{\hbar^2}{M} k_o \int_0^a g^{(n-1)}(k_o; r', r'') g^{(n-2)}(k_o; r', r'') dr'' - \frac{n(n-1) \hbar^2}{2M} \int_0^a g^{(n-2)}(k_o; r', r'') g^{(n-3)}(k_o; r', r''' dr''' - \frac{\hbar^2}{2M} \sum_{i=0}^{n-1} L^{(n-i)}(k_o) g^{(i)}(k_o; r, a) g(k_o; a, r') \quad n \geq 2 \]
It can be concluded that we have succeeded in giving an operative prescription in order to obtain the coefficients of the Taylor series

$$G(\xi) = \sum_{n=0}^{\infty} \frac{G^{(n)}(\xi)}{n!}(\xi - \xi_0)^n, \quad G(k) = \sum_{n=0}^{\infty} \frac{G^{(n)}(k)}{n!}(k - k_0)^n.$$

The S-matrix Taylor series could be now obtained from eq. (11) by the use of the above expansions of the $G$-function; in fact it contains, besides the $G$-function, only known functions of the momentum. However, since the S-matrix and the $G$-function have the same analytic structure (in particular both are meromorphic functions in the whole momentum plane and have the same poles; see Section 2.2), the properties of S we are interested in can be inferred directly from the $G$-function expansion, avoiding the cumbersome complete procedure.

3.3. - Discussion of the Mathematical Structure of the Formalism.

A noteworth feature of the finite interval Green's function is that it allows one to treat in a quite symmetrical way all the (regular) points of the momentum plane. We recall, on the other hand, that in the upper part of the momentum plane the function $G^{(+)}(\xi;r, r')$ is a resolvent kernel and that there it satisfies the integral equation (15). Since $G^{(+)}(\xi;r, r')$ and $G^{(n)}(\xi;r, r')$ coincide in the square interval $0 \leq r, r' \leq a$ (see Sect. 2.2), eq. (15) must coincide with eq. (17) there.

This can be easily proved.

By taking into account representation (5), in the square interval $0 \leq r, r' \leq a$ eq. (15) can be put in the form

$$G^{(+)}(\xi;r, r') - G^{(+)}(\xi_0;r, r') = - (\xi - \xi_0) \int_0^a G^{(+)}(\xi_0;r, r'')G^{(+)}(\xi;r'', r') dr'' -$$

$$-(\xi - \xi_0) \left[ \frac{2M}{\hbar^2} \phi(k_0, r') \psi(k, r') \int_a^{\infty} 0(k_0 r'')0(kr'') d\theta'' \right].$$

From the Green's theorem we get \{note that $0(kr) \longrightarrow 0$ for $\text{Im} k \rightarrow 0$\}

$$\frac{(k - k_0)}{\hbar^2} \int_a^{\infty} 0(k_0 r)0(kr) dr = \frac{\pi^2}{2M} \left[ L(\xi) - L(\xi_0) \right].$$
we have therefore

\[
G^{(+)}(\mathcal{E}_0;r,r')-G^{(+)}(\mathcal{E}_0;r',r')=-(\mathcal{E}_0-\mathcal{E})\int_0^a G^{(+)}(\mathcal{E}_0;r,r'')x \\
xG^{(+)}(\mathcal{E};r'',r')dr''\frac{\hbar^2}{2M}L(\mathcal{E})L(\mathcal{E}_0)G^{(+)}(\mathcal{E}_0;r,a)G^{(+)}(\mathcal{E};a,r') \quad 0 \leq r, r' \leq a
\]

which coincides with eq. (17).

By a similar procedure the derivatives of \( G^{(+)}(\mathcal{E};r,r') \) obtained from the integral equation (15) can be proved to coincide with the \( \mathcal{G}(\mathcal{E};r,r') \) derivatives. For example, we get for the first derivative

\[
(24) \quad G^{(+)(1)}(\mathcal{E}_0;r,r')=-\int_0^\infty G^{(+)}(\mathcal{E}_0;r,r'')G^{(+)}(\mathcal{E}_0;r'',r')dr'' \quad 0 \leq r, r' \leq \infty.
\]

If \( r \) and \( r' \) are in the interaction region one gets

\[
G^{(+)(1)}(\mathcal{E}_0;r,r')=-\int_0^\infty G^{(+)}(\mathcal{E}_0;r,r'')G^{(+)}(\mathcal{E}_0;r'',r')dr'' - \left[ \frac{2M}{\hbar^2} \right]^2 \frac{(\kappa_0, r)}{(\kappa_0, r')} \int_0^\infty 0^2(\kappa_0 r'')dr'' \quad 0 \leq r, r' \leq a;
\]

the last integral can be obtained from eq. (22): one gets

\[
\int_0^a 0^2(\kappa r)dr = \frac{\hbar^2}{2M} 0^2(\kappa a) L^{(1)}(\kappa).
\]

At this stage the identification of eqs. (24) and (18) for \( \text{Im} \kappa > 0 \) is immediate.

On the converse, equation (15) can be neither deduced in the unphysical energy sheet (lower part of the momentum plane), since \( G^{(+)}(\mathcal{E};r,r') \) is not a resolvent kernel there, nor directly analytically continued because the integral is not convergent there.

If, however, we limit our interest to the square interval \( 0 \leq r, r' \leq a \), the analytic continuation of eq. (15) can be done on the ground of the representation (23).
Alternatively the integral equation (15) itself can be continued, provided a suitable prescription is given on the handling of the non convergent integral. This can be achieved by the "regularization" of the integral, which amounts to define\(^{(12)}\)

\[
\int_0^\infty g(r) \, dr = \lim_{a \to 0} \int_0^\infty e^{-ar^2} g(r) \, dr;
\]

with this prescription the tail contribution of eq. (15) becomes identical with the surface contribution of eq. (23) also in the lower part of the momentum plane. We can assert, therefore, that prescription (25) realizes the correct analytic continuation of the right hand member of eq. (15).

All this leads to the following interpretation of the \(Q\)-function: it can be viewed as a compact formalism by which one can obtain in the whole momentum plane the results that are obtainable directly in the framework of the resolvent kernel in the sole upper part of the plane.

4. - THE ANALYTIC CONTINUATION OF THE S-MATRIX. -

The convergence limitations of the Taylor series render it a useless tool just in connection with the most interesting features of the cut-off potential, namely the poles of the S-matrix and the related resonant regions. An example of these shortcomings can be found in ref. (1).

In Section 4.1, the structure of the S-matrix is briefly analysed, in order to point out the methods which, in the authors' opinion, are the most suitable to derive information concerning the S-matrix in the whole momentum plane starting from its Taylor expansion about a regular point. In Section 4.2, some results we have obtained in the framework of the Padè approximation are briefly commented. Sections 4.3, and 4.4, are devoted to the application of the Hadamard method, which leads, in principle, to a rigorous and complete solution to the analytic continuation of the S-matrix; some numerical results obtained in this framework are displayed.

4.1.- The Analytic Structure of the S-Matrix. -

Specific procedures for the analytic continuation of the scattering matrix are related to the framework in which the S-matrix itself is considered.
In a first instance the S-matrix can be considered as a function of the momentum, without any other specification; in this connection the Padé approximant method has been used.

Alternative descriptions of the S-matrix are given in terms of a suitable denumerably infinite set of parameters; in this connection the analytic continuation of the S-matrix amounts to the determination of these parameters. Some parametrizations can be viewed as the generalization of the one-level formula, which is a natural representation of the S-matrix in the neighbouring of a pole $k_n$ with residue $\phi_n$.

\begin{equation}
S(k) = \frac{\phi_n}{k - k_n} + \psi_n(k).
\end{equation}

Such a generalization leads, in the cut-off potential problem, to a complete expansion of the S-matrix in partial fraction series in which all the poles and their related residues are involved\(^{(3,13)}\). One the converse the generalization of the one pole-one zero formula

$$S(k) = B(k) \frac{k - k_n}{k - k_n}$$

where \(B(k)\) is a unitary background function, leads to the Ning Hu product representation\(^{(3)}\)

$$S(k) = e^{-2i\bar{\kappa}a} \prod_n \frac{k - k_n}{k - k_n}$$

in which only the pole positions are involved.

Now, the Hadamard method, which is described in Sections 4.3 and 4.4, allows, in principle, to determine the affixes of all the poles of a meromorphic function starting from its Taylor expansion about a regular point. It can be asserted, therefore, that through the Ning Hu representation, this method determines the S-matrix in the whole momentum plane. As a by-product the residue of the nearest pole is immediately obtained; the evaluation of the other residues is much more involved. Because of this, in the present work formula (26) will be briefly considered as an introductory example; the complete expansion in partial fractions will be considered in a forthcoming paper.
4.2.- The Padé Approximant Method.-

A standard procedure for the analytic continuation of a Taylor series is given by the Padé approximant method. Although this method lacks a general mathematical foundation, it has been successfully employed in many fields of theoretical physics\(^7\). We recall here only the basic definition. The approximant of order \([N, M]\) to a function \(f(z)\) of which we know the Taylor expansion

\[
f(z) = \sum_{n=0}^{\infty} a_n (z-z_0)^n
\]

is defined as the ratio of two polynomials \(P^M(z-z_0)\) and \(Q^N(z-z_0)\) of degree \(M\) and \(N\) respectively with the prescription that

\[
f[N, M](z-z_0) = \frac{P^M(z-z_0)}{Q^N(z-z_0)} = f(z) + O((z-z_0)^{M+N+1})
\]

This condition determines the two polynomials apart from an overall constant

\[
P^M(z-z_0) = a_{M-N+1} \begin{array}{cccc}
a_{M-N+1} & a_{M-N+2} & \cdots & a_{M+1} \\
\vdots & \vdots & \ddots & \vdots \\
a_{M} & a_{M+1} & \cdots & a_{M+N} \\
\sum_{j=N}^{M} a_{j-N}(z-z_0)^j & \sum_{j=N}^{M} a_{j-N-1}(z-z_0)^j & \cdots & \sum_{j=0}^{M} a_{j}(z-z_0)^j
\end{array}
\]

\[
Q^N(z-z_0) = \begin{array}{cccc}
a_{M-N+1} & a_{M-N+2} & \cdots & a_{M+1} \\
\vdots & \vdots & \ddots & \vdots \\
(z-z_0)^N & (z-z_0)^{N-1} & \cdots & 1
\end{array}
\]

Several numerical experiments have been carried out in order to reproduce the "resonant cross section" \{compare formula (11)\}
\[ k^2 \sigma_{\text{Res}}(k) = 1 - \text{Re} \mathcal{S}_{\text{Res}}(k) = \text{Im} \left[ \frac{kG(k; a, a)}{I(ka)} \right]. \]

Since \( I(ka) \) and \( O(ka) \) are known functions of the momentum, the Padé method has been applied to the Taylor expansion of \( G(k; a, a) \); a complete expansion of the \( S \)-matrix would be a useless complication.

In Fig. 1 the results obtained by various diagonal \((N=M)\) approximants are compared with the exact values obtained by a direct numerical solution; a square well characterized by the following parameters

\[
\begin{align*}
V(r) &= -30 \text{ MeV}, & 0 < r < a \\
V(r) &= 0, & r > a
\end{align*}
\]

\[ a = 4 \cdot 10^{-13} \text{ cm} \]

\[ \frac{2M}{\hbar^2} = 0.25 \cdot 10^{-26} \text{ (MeV)}^{-1} \text{ cm}^{-2} \] (\( M \geq 5 \) nucleon mass)

has been used; the p-wave has been chosen to avoid the peculiarities and oversimplifications of the s-wave. The four resonances exhibited by the exact cross section in the considered interval \( 1 \leq E \leq 100 \text{ MeV} \).
18.

are related to four poles located at energies

\[ E_1 = 8.36 - i3.11 \text{ MeV} \]
\[ E_2 = 30.41 - i6.88 \text{ MeV} \]
\[ E_3 = 57.30 - i10.61 \text{ MeV} \]
\[ E_4 = 89.21 - i14.40 \text{ MeV} \]

As one can see, the fit is very satisfactory; many other examples where also non diagonal approximations have been used can be found in refs. (1,11).

We have been stimulated by these good results to search a complete and rigorous justification of the applicability of the Padé method to our specific problem. For this purpose the authors are considering \( Q(k;a,a) \) both as a meromorphic function \{ on the line of the particular case examined by Baker(14) \}, and as a solution of the integral equation (15)(15). Preliminary results seem to be promising.

4.3.- The One-Level Formula.-

As an introduction to the Hadamard method(8) we consider in this Subsection the one-level formula (26).

Let

\[ f(z) = \sum_{n=0}^{\infty} a_n (z-z_0)^n \]

be the Taylor expansion of a function about a regular point \( z_0 \), and \( z_1 \) a simple pole of \( f(z) \); if any other singularity is more distant from \( z_0 \), the function can be usefully separated in the form

\[ f(z) = \frac{R_1}{z-z_1} + \varphi_1(z) \]

where \( R_1 \) is the residue. The point is that the function \( \varphi_1(z) \) can be Taylor expanded about \( z_0 \),

\[ \varphi_1(z) = \sum_{n=0}^{\infty} a_n'(z-z_0)^n \]

and this series converges also in \( z=z_1 \). Comparison between (27) and (28) gives

\[ 551 \]
\[(30) \quad a_m = -\frac{R_1}{(z-z_0)^{m+1}} + a'_m; \]

from this one gets

\[(31) \quad \lim_{m \to \infty} \frac{a_m}{a_{m+1}} = \lim_{m \to \infty} \frac{(z-z_0)^m}{m!} \frac{a(z-z_0)^m - R_1}{R_1} = z-z_0 \]

where one has taken into account that

\[(32) \quad \lim_{m \to \infty} a'(z-z_0)^m = 0 \]

because of the convergence of the series (29) at \(z=z_1\). Finally one gets for the pole affix the simple formula

\[z_1 = z_0 + \lim_{m \to \infty} \frac{a_m}{a_{m+1}}.\]

The residue is easily obtained by rewriting eq. (30) in the form

\[a_m (z-z_0)^{m+1} = -R_1 + a'(z-z_0)^{m+1}; \]

because of eq. (32) one gets

\[(33) \quad R_1 = \lim_{m \to \infty} a_m (z-z_0)^{m+1}. \]

We have so succeeded in determining the nearest pole affix and the related residue starting from the Taylor series of \(f(z)\) about \(z_0\); the coefficients of the Taylor expansion of the background function \(\varphi(z)\) can be determined from eq. (30).

The above analyticity hypothesis on the function to be expanded are in general verified for the S-matrix (difficulties are to be expected only if the expansion point is pure imaginary; this case is discussed in connection with the general Hadamard method outlined in the next Subsection). Starting from the \(G\)-function Taylor series (21) and formula (11), the above procedure allows one therefore to determine
the parameters of the one-level formula (26). Numerical results obtained by this method can be found in the next Subsection (Table I).

The procedure could now be applied to the function \( \varphi_1(z) \) which is explicitly known from eqs. (29) and (30) in order to determine the parameters of the two-level approximation formula

\[
f(z) = \frac{R_1}{z-z_1} + \frac{R_2}{z-z_2} + \varphi_2(z),
\]

and so on. The iterative procedure implies, however, that the first pole has been determined exactly, otherwise \( \varphi_1(z) \) has still a polar singularity in \( z = z_1 \). These difficulties can be avoided by resorting to the general Hadamard theory, displayed in the next Subsection.

4.4.- The General Hadamard Procedure for the Determination of the S-Matrix Poles.-

The procedure outlined in the previous Subsection for the determination of the nearest pole to the Taylor series expansion point \( z_o \) can be generalized (8, 16) in order to include all the poles lying in the meromorphism circle (namely the largest circle centered in \( z_o \) and including polar singularities only). Since to the authors' knowledge this analytic tool has not been previously used in quantum scattering theory, the essentials of the method will be sketched here.

First we suppose that the poles occur at increasing distance from the expansion point \( z_o \), i.e.

\[
|z - z_1| < |z - z_2| < \ldots < |z - z_p| < \ldots .
\]

In this case a theorem by Hadamard states that the \( p \)-th pole is determined starting from the Taylor (27) by the simple relation

\[
z_p = z_o + \lim_{m \to \infty} \frac{D_{m,p-1}}{D_{m+1,p-1}} \frac{D_{m+1,p-2}}{D_{m,p-2}}, \quad p \geq 2,
\]

where \( D_{\mu,\lambda} \) are the determinants

\[
D_{\mu,\lambda} = \begin{vmatrix}
a_{\mu} \cdots a_{\mu+\lambda} \\
\vdots & \ddots & \vdots \\
a_{\mu+\lambda} \cdots a_{\mu+2\lambda}
\end{vmatrix}
\]
The applicability of formula (35) is based on the assumption that relation (34) has been somehow ascertained. As a matter of fact, the Hadamard method is more general since it allows, in principle, to determine all the poles in the meromorphism circle however they are distributed. The general procedure consists of two different stages which can be summarized as follows.

In the former the radii $r_q$ of the circumferences on which poles do lie, and the number $m_q$ of poles on the general $q$-th circumference are determined (more precisely $m_q$ stays for the sum of the pole multiplicities). This is achieved through the evaluation of the superior limits

$$\ell_\lambda = \lim_{\mu \to \infty} \mu \left| \frac{1}{D^{\mu-\lambda}} \right|$$

and the study of the behaviour of the ratios $\ell_{\lambda+1} / \ell_\lambda$ (8, 16).

When only one pole lies on the $q$-th circumference ($m_q = 1$), the affixes are again determined by formula (35) where in this case one must put

$$p = m_1 + m_2 + \ldots + m_{q-1} + 1,$$

(the circumference have been ordered according to increasing radii). When $m_q \neq 1$, the affixes are obtained as the solutions of an equation of degree $m_q$, whose coefficients are determined through the Taylor series expansion coefficients $a_m$. The method allows also to determine the distance of the closest non-polar singularity. The method is not suitable for the determination of the poles lying outward the meromorophism circle.

The actual procedure to be applied in the S-matrix problem emerges from the following considerations. First the S-matrix for cut-off potentials is known to be a meromorphic function in the whole momentum plane; secondally, the hypothesis (34) is verified, save accidentally, for any $k_o$ not pure imaginary. For these reasons formula (35) can be safely applied and the cumbersome complete procedure avoided.

Formula (35), though formally rigorous, meets with numerical limitations. As it is apparent from eq. (31), one has that

$$\lim_{m \to \infty} \frac{a_m}{a_{m+1}} = \frac{z - z_o}{z - z_1} = \text{const;}$$
it follows from this that when $\mu \to \infty$ the rows of the determinant (36) tend to become proportional one to the other. It is evident that in such a connection the accuracy of the final result is strictly connected with an accurate knowledge of the coefficients $a_m$; in our problem this is ultimately connected with the accuracy of the numerical integration (20). In the present work, whose aim is to point out the feasibility of our general program, we have just carried out the integration with the simple trapezoidal rule with hundred points.

The numerical results we obtained are summarized in Table I. The experiment has been carried out on the same potential as described in Section 4.2, again in the $p$-wave; in Fig. 2 the exact poles in the

![Fig. 2](image)

FIG. 2 - Poles of the $S$-matrix in the momentum plane in the region $-5 \leq \operatorname{Re} k \leq 5$, and $-2.5 \leq \operatorname{Im} k \leq 2.5$ (units $10^{-13} \text{ cm}^{-1}$).

region $-5 \leq \operatorname{Re} k \leq 5$, and $-2.5 \leq \operatorname{Im} k \leq 2.5$ are displayed; the momentum $k$ is expressed in unit $10^{-13} \text{ cm}^{-1}$. As a general rule ten derivatives are enough to stabilize two poles, the nearest to the expansion point, to the values quoted in Table I; the third pole, which is obtained with an acceptable accuracy with a few low order derivatives, becomes then completely instable. These difficulties get more remarkable when the nearest pole has a large residue; in these cases only the nearest pole has been determined. In Table I the $S$-matrix residue of the first pole, evaluated by formula (33) is quoted too.

In a less general but more concrete perspective, the poles can be determined separately by a suitable choice of expansion points $\mathbf{p}_0$;
TABLE I

Poles and residues of the S-Matrix evaluated by the Hadamard method

<table>
<thead>
<tr>
<th>Expansion point $k_0$ (units $10^{-13}$ cm$^{-1}$)</th>
<th>Exact Values (units $10^{-13}$ cm$^{-1}$)</th>
<th>Values obtained by the Hadamard method</th>
</tr>
</thead>
<tbody>
<tr>
<td>0. +i</td>
<td>I Pole 0. +i 1.222</td>
<td>0. +i 1.222</td>
</tr>
<tr>
<td></td>
<td>Residue 0. -4.05 x 10$^3$</td>
<td>0. -4.06 x 10$^3$</td>
</tr>
<tr>
<td></td>
<td>II Pole 0. + 2.100</td>
<td>Unstable</td>
</tr>
<tr>
<td>0. +i2</td>
<td>I Pole 0. +i 2.100</td>
<td>0. +i 2.100</td>
</tr>
<tr>
<td></td>
<td>Residue 0. -2.90 x 10$^6$</td>
<td>0. -2.91 x 10$^6$</td>
</tr>
<tr>
<td></td>
<td>II Pole 0. +i 1.222</td>
<td>Unstable</td>
</tr>
<tr>
<td>0. -i</td>
<td>I Pole 0. -i 1.688</td>
<td>0. -i 1.688</td>
</tr>
<tr>
<td></td>
<td>Residue 0. -6.82 x 10$^{-7}$</td>
<td>0. -6.83 x 10$^{-7}$</td>
</tr>
<tr>
<td></td>
<td>II Pole 0. -2.442</td>
<td>0. -2.441</td>
</tr>
<tr>
<td>0. -i2</td>
<td>I Pole 0. -i 1.688</td>
<td>0. -i 1.688</td>
</tr>
<tr>
<td></td>
<td>Residue 0. -6.82 x 10$^{-7}$</td>
<td>0. -6.83 x 10$^{-7}$</td>
</tr>
<tr>
<td></td>
<td>II Pole 0. -2.442</td>
<td>0. -2.441</td>
</tr>
<tr>
<td>1.</td>
<td>I Pole 1.471 -i 0.266</td>
<td>1.471 -i 0.266</td>
</tr>
<tr>
<td></td>
<td>Residue -1.65 x 10$^{-2}$ -i 7.84 x 10$^{-2}$</td>
<td>-1.64 x 10$^{-2}$ -i 7.82 x 10$^{-2}$ Unstable</td>
</tr>
<tr>
<td></td>
<td>II Pole 0. +i 1.222</td>
<td></td>
</tr>
<tr>
<td>2.</td>
<td>I Pole 1.471 -i 0.266</td>
<td>1.470 -i 0.265</td>
</tr>
<tr>
<td></td>
<td>Residue -1.65 x 10$^{-2}$ -i 7.84 x 10$^{-2}$</td>
<td>-1.45 x 10$^{-2}$ -i 7.91 x 10$^{-2}$ Unstable</td>
</tr>
<tr>
<td></td>
<td>II Pole 2.773 -i 6.312</td>
<td>2.769 -i 6.311</td>
</tr>
<tr>
<td>3.</td>
<td>I Pole 2.773 -i 0.312</td>
<td>2.772 -i 0.312</td>
</tr>
<tr>
<td></td>
<td>Residue -4.81 x 10$^{-2}$ -i 7.12 x 10$^{-2}$</td>
<td>-4.59 x 10$^{-2}$ -i 7.11 x 10$^{-2}$</td>
</tr>
<tr>
<td></td>
<td>II Pole 3.801 -i 0.349</td>
<td>3.800 -i 0.349</td>
</tr>
<tr>
<td>4.</td>
<td>I Pole 3.801 -i 0.349</td>
<td>3.800 -i 0.348</td>
</tr>
<tr>
<td></td>
<td>Residue -5.70 x 10$^{-2}$ -i 7.01 x 10$^{-2}$</td>
<td>-5.78 x 10$^{-2}$ -i 7.02 x 10$^{-2}$</td>
</tr>
<tr>
<td></td>
<td>II Pole 4.738 -i 0.380</td>
<td>4.735 -i 0.381</td>
</tr>
</tbody>
</table>

by this method all the poles in any finite region are singled out solving the Schrödinger equation in a finite number of points. An example of this is given by Table I itself.

5. - CONCLUDING REMARKS. -

It has been proved that the solution of the Schrödinger equation in an arbitrary (regular) point $k_0$, that is in any case necessary for the evaluation of $S(k_0)$, is endowed with much more information, since it allows to determine the S-matrix in the whole momentum plane. We believe that this fact is capable of a remarkable practical relevance in...
connection with problems for which a compact solution is not available and approximation schemes are to be used. As an example, the cumbersome perturbative procedure, which is often necessary for the evaluation of the S-matrix had to be repeatedly applied for each value of the energy: the method pointed out in the present work allows to focus all efforts on an (arbitrary) energy only. In principle, our procedure can be used also in the case of reaggregation collisions, for which expression (16) is still formally valid (see Sections 3.1 and 3.2).

Finally we observe that many results obtained in the present work for the cut-off potential can be extended to potentials for which the ingoing and outgoing Jost solutions are explicitly known for $r \geq a$; the previous results are directly generalized to this case by substituting the ingoing and outgoing unperturbed solutions with the Jost solutions in $r = a$.

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APPENDIX.

In this Appendix we give, in the framework of the standard analysis methods, an alternative derivation of the integral equation (17)

\[ (A.1) \]

\[
\frac{1}{\hbar^2} \left[ 1 + \frac{\hbar^2}{2M} \delta(r-a) \left( \frac{L(\xi)-L(\xi_0)}{\xi-\xi_0} \right) \right] \int_0^a \frac{\varphi(\xi; r, r'' \cdot \xi_0)}{\varphi(\xi; r, r' \cdot \xi_0) - \varphi(\xi_0; r, r' \cdot \xi_0)} \, d\xi
\]

relating the finite-interval Green's function at two different energies. The equality of the two members of equation (A.1) will be proved for \( r < r' \); for \( r > r' \) the procedure is quite analogous.

According to the explicit coordinate representation (8) of \( \varphi(\xi; r, r') \) the two members of equation (A.1) represented by I and II respectively, can be expressed in the form

\[ (A.2) \]

\[
I = \frac{2M}{\hbar^2} \frac{\varphi(\xi, r) \varphi(\xi, r') \mathcal{F}(\xi)}{\mathcal{F}(\xi) \mathcal{F}(\xi_0)} - \frac{\varphi(\xi, r) \varphi(\xi, r') \mathcal{F}(\xi)}{\mathcal{F}(\xi) \mathcal{F}(\xi_0)}
\]

and

\[ (A.3) \]

\[
II = \frac{2M}{\hbar^2} \left[ L(\xi) - L(\xi_0) \right] \frac{\varphi(\xi, r) \varphi(\xi, r') f(\xi, a) f(\xi_0, a)}{\mathcal{F}(\xi) \mathcal{F}(\xi_0)}
\]

\[
\int_0^r \varphi(\xi', r') \varphi(\xi, r'') d\xi'' + \varphi(\xi, r) f(\xi, r'') \varphi(\xi_0, r'') d\xi'' + \varphi(\xi, r) \varphi(\xi_0, r'') f(\xi_0, r'') d\xi''
\]

The value of the integrals appearing in (A.3) can be easily obtained by resorting to the Green's theorem: we obtain

\[ (A.4a) \]

\[
\int_0^r \varphi(\xi, r') \varphi(\xi_0, r'') d\xi'' = \frac{\hbar^2}{2M} \sqrt{\varphi(\xi, r) \varphi(\xi_0, r)}
\]
where we have used the notation $W(u_1(r), u_2(r))$ for the Wronskian of $u_1(r)$ and $u_2(r)$.

By inserting relations (A.4) in (A.3), and suitably collecting the terms, we get

\[
(A.5) \quad \Pi = \frac{2M}{\hbar^2} \frac{\varphi(\hat{k}, r) \mathcal{F}(\hat{k}_0) - \varphi(\hat{k}_0, r) \mathcal{F}(\hat{k})}{\mathcal{F}(\hat{k}) \mathcal{F}(\hat{k}_0)}
\]

Comparison of expressions (A.2) and (A.5) proves the validity of equation (A.1).
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