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Determination of a Perturbing Potential from Its Scattering Phase Shift and Bound States Energy Levels

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Determination of a Perturbing Potential from Its Scattering Phase Shift and Bound States Energy Levels*

By

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A potential function $U(r)$ determines the so-called phase shift $\xi_l(k)$, $0 \leqslant k \leqslant \infty$, $l = 0, 1, \ldots$. Conversely consider $\xi_l(k)$ given, the problem is to find a function $U(r)$ reproducing $\xi_l(k)$.

In the case of no bound states $U(r)$ is uniquely determined by the phase shift. In the case of one or more bound states the phase shift and the energy levels of the bound states do not give sufficient information of the potential so that phase shift and energy levels may be reproduced by different functions.

In the case of sufficiently large l there will be no bound states and the problem of uniqueness of $U(r)$ does not arise. In the present investigation we consider for simplicity the S-scattering, $l = 0$, which is the most favorable for formation of bound states. These are therefore taken into full account.

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1. Introduction

The author has treated the inverse scattering problem, i.e., calculation of a perturbing potential from some known asymptotic phase shift, in a former paper [1] from 15 years ago and shown that only the phase shift, $\xi_l(k)$, for a single azimutal quantum number is needed to determine the potential function $U(r)$. The idea of that paper was to produce a real working method by which calculation of the potential in actual cases could most conveniently be performed. The extension of the theory to the more general case of some bound states being present is given in this investigation, whereas for the sake of simplicity it has been restricted to the S-scattering and S-states.

In recent literature [2, 3] the former investigation appears forgotten (ref. [2]) or very little recognized (ref. [3]). From these references we are picking up only a few papers [4, 5, 6, 7, 8, 9] which obviously are considered particularly prominent.

The reason for the method presented here and in the former publication remaining non-recognized appears to be the overwhelming interest for existence and uniqueness problems. The latter leading to studies of ad hoc constructed phase shifts and corresponding potentials of a somewhat potological shape and hence, of restricted physical interest. As a whole at least the papers from later years may be considered similar and in mutual agreement in the sense that they are accepting the Gelfand–Levitan integral equation as a cornerstone of the whole inversion problem.

The most useful papers for comparison studies has for me been the investigations by Jost and Kohn, because of the explicite solutions found there. In fact the solutions I am pointing to, and which will be used here for comparison, are obtained independently of the Gelfand-Levitan equation and only shown (if proved to be correct) to lead to the particular form of that equation.

As has been proved in this paper the Jost–Kohn solution is only an alternative solution of that which is obtained straight forward from the present theory. This alternative solution follows, however, also from the present theory if the roles of the constituents Y' and Z of the biorthonormal functional system are interchanged.

This alternative solution unfortunately has serious disadvantages in comparison with the direct one as used here. The most characteristic feature of the difference is that the occurrence of asymptotic amplitudes $u(k)$ and $u(-k)$ separately in the Jost–Kohn solution requires a difficult

computation of these quantities, whereas in the straight forward solution the amplitudes themselves are not needed but only their ratio $u(-k)/u(k) = e^{2i\xi}$, i.e., the asymptotic phase itself.

Since the Jost–Kuhn solution is in accordance with the particular form in which so far the Gelfand–Levitan equation is appearing, it follows that—if the Gelfand–Levitan theory is to be used at all—it must be considered subject to modifications and should be presented in some more adequate form.

2. Reciprocal Vector Systems and Systems of Biorthonormal Function

At the time of my first investigations, on consulting prominent mathematicians (J. v. Neumann, H. Weyl, etc.), it appeared that the conception of biorthonormal functional systems was unknown in mathematical literature. It may therefore be suspected still to be so.* For this reason I want to give an exposition showing how simple and natural this conception is.

Consider in an n-dimensional space an orthonormal vector system $\mathbf{a}_i$, hence obeying the relations

$$\mathbf{a}_i \mathbf{a}_k = \delta_{ik}. \tag{1}$$

Let this system be expressed by its components in a coordinate system defined by another system of orthonormal vectors $\mathbf{e}_i$, $i = 1, 2, \ldots, n$, so that we are able to define a definite system of transposed vectors $\tilde{a}_i$, whose components are the columns of the matrix a, having as its rows the components of the vectors $\mathbf{a}_i$. Then from (1) we have the matrix equation

$$a\tilde{a} = 1 \tag{1a}$$

and from simple considerations also

$$\tilde{a}a = 1, \tag{2}$$

or

$$\tilde{\mathbf{a}}_i \tilde{\mathbf{a}}_k = \delta_{ik}. \tag{2a}$$

Eq. (1) is the orthonormality and (2a) the completeness relation. This is seen from putting for an arbitrary vector $\mathbf{r}$

$$\mathbf{r} = \sum_i r_i \mathbf{a}_i, \quad r_i = \mathbf{r}\mathbf{a}_i. \tag{3}$$

In order that these equations be true, we find on inserting the former in the latter that (1) is a necessary condition. Conversely, on inserting the latter in the former, using in between the notation $r_i' = \mathbf{r}\mathbf{e}_i$,

* Later on I have learnt from different sources that they are known and adopted by mathematicians under the above name, from what time I do not know.

$$\mathbf{r} = \sum_i (\mathbf{r}\mathbf{a}_i)\,\mathbf{a}_i = \sum_k \mathbf{e}_k \sum_i (\mathbf{r}\mathbf{a}_i)\,a_{ik} = \sum_k \mathbf{e}_k \sum_j r'_j \sum_i a_{ij} a_{ik} = \sum_{kj} \mathbf{e}_k r'_j \tilde{\mathbf{a}}_j \tilde{\mathbf{a}}_k = \sum_k r'_k \mathbf{e}_k, \quad (4)$$

if eq. (2a) holds. Hence also this relation is a necessary condition for eqs. (3) to be both true.

Similarly for an orthonormal functional system $y_n(r)$,

$$\int y_m(r)\, y_n(r)\, dr = \delta_{mn} \quad (5)$$

we expect the following expansion theorem for an arbitrary function $F(r)$

$$F(r) = \sum_n F_n y_n(r), \quad F_n = \int F(r)\, y_n(r)\, dr. \quad (6)$$

Again inserting the former equation in the latter, the equations are true only if the orthonormality condition of eq. (5) holds. Conversely, inserting the latter in the former we find the result

$$\int dr'\, F(r') \sum_n y_n(r)\, y_n(r') = F(r) \quad (7)$$

to be true only on the condition that

$$\sum_n y_n(r)\, y_n(r') = \delta(r - r'), \quad (8)$$

which is the *completeness relation.*

The difference between an n-dimensional vector and a functional space of an infinite number of dimensions is that in the former case the completeness relation follows immediately from the orthonormality relation, whereas in the functional space the completeness relation may or may not be true for an orthonormal system. The expansion theorem presupposes the validity of the completeness relation.

Now let us turn to a non-orthonormal system of vectors $\mathbf{a}_i$, $i = 1, 2, \ldots, n$. Just as in the three-dimensional case of $\mathbf{b}_1 = (\mathbf{a}_2 \times \mathbf{a}_3)/\Delta$, $\Delta = \mathbf{a}_1(\mathbf{a}_2 \times \mathbf{a}_3)$ a vector $\mathbf{b}_i$ may be found which is orthogonal to any vector $\mathbf{a}_k$, $k \neq i$ and whose scalar product with $\mathbf{a}_i$ is 1. Hence we may find a vector system $\mathbf{b}_i$, which is said to be reciprocal to the system $\mathbf{a}_i$ (and vice versa). The two systems form what may be called a biorthonormal system, instead of reciprocal systems, having the orthonormality property

$$\mathbf{a}_i \mathbf{b}_k = \delta_{ik}. \quad (9)$$

The expansion theorem now reads

$$\mathbf{r} = \sum_i r_i \mathbf{a}_i, \quad r_i = \mathbf{r}\mathbf{b}_i, \tag{9a}$$

and eq. (9) follows on inserting the former equation in the latter. Conversely, as before inserting the latter in the former we deduce the completeness relation,

$$\tilde{\mathbf{a}}_i \tilde{\mathbf{b}}_k = \delta_{ik}. \tag{10}$$

The generalization of these results to a functional space of infinite dimensions is the expansion theorem

$$F(r) = \sum_n F_n z_n(r), \quad F_n = \int F(r)\, y_n(r)\, dr, \tag{11}$$

the correctness of which requires the orthonormality and completeness relations

$$\int y_n(r)\, z_m(r)\, dr = \delta_{nm}, \quad \sum_n y_n(r')\, z_n(r) = \delta(r - r'). \tag{11a}$$

For functions with a continuous parameter k, instead of the discrete n, and with the expansion formulae

$$F(r) = \int F_k z_k(r)\, dk, \quad F_k = \int F(r)\, y_k(r)\, dr, \tag{12}$$

the analogous relations are

$$\int y_k(r)\, z_{k'}(r)\, dr = \delta(k - k'), \quad \int y_k(r')\, z_k(r)\, dk = \delta(r - r'). \tag{12a}$$

Only in the case of, say, $y_k(r)$ forming by itself an orthogonal system, which can easily be modified into an orthonormal system, the two systems $y_k(r)$ and $z_k(r)$ become identical systems.

If therefore for an unknown function $F(r)$ we have an integral equation

$$F_k = \int F(r)\, y_k(r)\, dr, \tag{13}$$

where F_k is known as a function of k and where the functional system is non-orthogonal, we shall first have to look for another system $z_k(r)$ forming together with $y_k(r)$ a biorthonormal system, as expressed in the first eq. (12a). Then the solution is

$$F(r) = \int F_k z_k(r)\, dk, \tag{13a}$$

provided the completeness relation of the second eq. (12a) is also valid.

This is just the main point of the present investigation that the equation connecting phase shift ξ and potential $U(r)$ in scattering theory presents itself in the form (13). Therefore the introduction and construction of biorthonormal systems of functions is suggested by the inversion problem itself. As far as my spare information reaches this is the first application of biorthonormal functional systems to quantum mechanical problems.

3. Wave Equations, Definitions and Notations. Auxiliary Potential Functions and Wave Equation

Consider in the regions $0 \leqslant r \leqslant \infty$, $0 \leqslant k \leqslant \infty$ the wave equation

$$\left\{\frac{d^2}{dr^2} + k^2 + U(r)\right\} y = 0, \tag{14}$$

it will possess independent solutions uniquely determined by the asymptotic values

$$\left.\begin{array}{l} y_1(0) = 0, \\ \left.\begin{array}{l} y_1(r) \to \sin(kr + \xi), \\ y_2(r) \to \cos(kr + \xi), \end{array}\right\} \quad (r \to \infty) \end{array}\right\} \tag{14a}$$

where $\xi = \xi(k)$ or ξ_k is the asymptotic phase.

For convenience we introduce another set of independent solutions with given asymptotic values

$$y = u(\pm k, r) \to e^{\pm ikr} \quad (r \to \infty) \tag{15}$$

by means of which we may write

$$y_1(r) = \frac{1}{2i}\,[u(k, r)\, e^{i\xi} - u(-k, r)\, e^{-i\xi}], \tag{15a}$$

$$y_2(r) = \tfrac{1}{2}[u(k, r)\, e^{i\xi} + u(-k, r)\, e^{-i\xi}]. \tag{15b}$$

With the abbreviated notations $u(\pm k, 0) = u(\pm k)$ we find from the requirement $y_1(0) = 0$,

$$S(k) = e^{2i\xi} = \frac{u(-k)}{u(k)}, \tag{16}$$

$$e^{\pm i\xi} = \frac{u(\mp k)}{|u(k)|}. \tag{16a}$$

The asymptotic values of the solutions at $r=0$, hence are

$$y_2(0) = |u(k)|,$$
$$y_1(r \to 0) = \frac{kr}{|u(k)|} \tag{17}$$

the latter value following from the Wronskian

$$W(y_1, y_2) = y_1' y_2 - y_1 y_2' = k, \tag{17a}$$

as seen from the asymptotic values (14a).

We now introduce an auxiliary potential $V(r)$ and a corresponding wave equation,

$$\left\{\frac{d^2}{dr^2} + k^2 + V(r)\right\} z = 0, \tag{18}$$

and define solutions z_1 and z_2, $v(k, r)$ and $v(-k, r)$ and a phase shift η as in the preceeding equations. Then by combination of (13) and (18), using asymptotic expressions, the following relation is obtained,

$$\sin(\xi - \eta) = \int_0^\infty (U - V)\, Y_k(r)\, dr = \int_0^\infty F(r)\, Y_k'(r)\, dr, \tag{19}$$

with $\quad F(r) = \int_r^\infty (U - V)\, dr, \quad U - V = -F'(r), \quad Y_k(r) = \frac{1}{k} y_1 z_1. \quad$ (19a)

Here our first problem is to find a functional system $Z_k(r)$, forming together with $Y_k'(r)$ an orthonormal system

$$\int Y_k'(r)\, Z_{k'}(r)\, dr = \delta(k - k'). \tag{20}$$

A function leading to relation (19) is

$$F(r) = \int \sin(\xi - \eta)_k Z_k(r)\, dk. \tag{21}$$

On inserting (19) in (21) it is found, however, that the equation is true only on the condition that

$$\int Y_k'(r')\, Z_k(r)\, dk = \delta(r - r'), \tag{22}$$

the completeness relation, holds.

4. The Function $Z_k(r)$ and the Inversion Formula

The asymptotic form of the function $Y'_k(r)$ is

$$Y'_k(r) \to \sin(2kr + \xi_k + \eta_k). \tag{23}$$

Hence, in order that eq. (20) be true it is necessary that

$$Z_k(r) \to \frac{4}{\pi} \sin(2kr + \xi_k + \eta_k). \tag{23a}$$

Because of the non-orthonormality of the system $Y'_k(r)$ we cannot take $Z_k(r) = (4/\pi) Y'_k(r)$. There is however another very simple way of obtaining (23a), namely by putting

$$Z_k(r) = \frac{4}{\pi} [y_1 z_2 + y_2 z_1], \tag{24}$$

as easily seen from the asymptotic formula (14a).

It is essential now to prove that this choice satisfies the orthonormality condition (20). The simplest way is maybe to prove the equation

$$4(k^2 - k'^2) Y'_k Z_{k'} + \frac{d}{dr} W(Y'_k, Z_{k'}) = \frac{d}{dr} R, \tag{25}$$

with the definition (17a) of the Wronskian, and with R being an expression in $y_{1k}, z_{1k}, y_{1k'}, y_{2k'}, z_{1k'}, z_{2k'}$ and their derivatives which vanishes identically at $r=0$ and as $r \to \infty$, as explained in detail in ref. [1].

Since $Y'_k(0) = 0$ and $Z_{k'}(0) = 0$ the Wronskian vanishes at $r \to \infty$ and its asymptotic value is easily found. The result is that

$$\int_0^R Y'_k Z_{k'} dr = \frac{1}{\pi(k^2 - k'^2)} [(k + k') \sin(2(k - k') R + \xi_k + \eta_k - \xi_{k'} - \eta_{k'})$$
$$- (k - k') \sin(2(k + k') R + \xi_k + \eta_k + \xi_{k'} + \eta_{k'})] \to \delta(k - k') - \delta(k + k') \tag{25a}$$

as $R \to 0$.

Another way of proving the result is to write

$$Y'_k(r) Z_{k'}(r) = \frac{1}{2} W(Y_k, Z_{k'}) + \frac{1}{2} \frac{d}{dr} (Y_k Z_{k'}) \tag{26}$$

and integrate the latter term from $r=0$ to $r=R$, where R is large enough for the asymptotic expressions to be valid. We first find that

$$\int_0^R \frac{1}{2}\frac{d}{dr}(Y_k Z_{k'})\,dr = \frac{2}{\pi} Y_k(R)\sin(2k'R+\xi_{k'}+\eta_{k'})$$

$$= [\cos(\xi_k-\eta_k)-\cos(2kR+\xi_k+\eta_k)]\frac{k'}{k}\delta(k'). \quad (26\,\mathrm{a})$$

On the other hand, it is found that

$$\frac{1}{2}W(Y_k, Z_{k'}) = \frac{2}{\pi k(k^2-k'^2)}\left\{\frac{d}{dr}\{W(y_{1k'}, y_{1k})\,W(z_{1k}, z_{2k'})\right.$$

$$\left. + W(z_{1k'}, z_{1k})\,W(y_{1k}, y_{2k'})\}\right\}. \quad (26\,\mathrm{b})$$

Integrating the expression and using asymptotic formulae it is found that

$$\int_0^R \frac{1}{2}W(Y_k, Z_{k'})\,dr = \frac{1}{\pi}\left[\frac{k+k'}{2k}\,\frac{\sin\{2(k-k')R+\xi_k+\eta_k-\xi_{k'}-\eta_{k'}\}}{k-k'}\right.$$

$$-\frac{k-k'}{2k}\,\frac{\sin\{2(k+k')R+\xi_k+\eta_k+\xi_{k'}+\eta_{k'}\}}{k+k'}$$

$$\left.-\frac{1}{k}\cos(\xi_k-\eta_k)\sin(2k'R+\xi_{k'}+\eta_{k'})\right]. \quad (26\,\mathrm{c})$$

Adding the asymptotic expressions (26 a) and (26 c) we just have the result (25 a).

The only possible solution of the inversion problem in the case of no bound states is now that of formula (21). It is easily seen that for real k we may write

$$Z_k(r) = \frac{2}{i\pi}[uve^{i(\xi+\eta)} - u^* v^* e^{-(\xi+\eta)}] \quad (27)$$

and, since ξ and η are antisymmetric in k and $u^* = u(-k, r)$ etc., it is readily found that

$$F(r) = \int_0^\infty \sin(\xi-\eta)_k Z_k(r)\,dk = -\frac{1}{\pi}\int_{-\infty}^\infty [e^{2i\xi} - 2^{2i\eta}]\,uvdk, \quad (27\,\mathrm{a})$$

or,

$$F(r) = -\frac{1}{\pi}\int_{-\infty}^\infty \left[\frac{u(-k)}{u(k)} - \frac{v(-k)}{v(k)}\right] u(k, r)\,v(k, r)\,dk, \quad (28)$$

using the phase shift equation (16) and the corresponding $e^{2i\eta} = v(-k)/v(k)$.

5. The Inversion Problem Including Potentials with Bound States

Writing (15a) by means of (16a) in the form

$$y_1(r) = \frac{1}{2i\,|u(k)|}\{u(-k)\,u(k,r) - u(k)\,u(-k,r)\}, \tag{29}$$

it is seen, by putting $k = i\varkappa$, $u(\pm k, r) \to e^{\mp \varkappa r}$, that the condition for stationary states to exist is

$$u(k) = 0, \quad k = i\varkappa, \tag{29a}$$

and correspondingly for the potential $V(r)$,

$$v(k) = 0, \quad k = k' = i\varkappa'. \tag{29b}$$

Because of the denominator $|u(k)| = [u(k)\,u(-k)]^{\frac{1}{2}}$ eq. (29) provides no more a suitable expression for $y_1(r)$. Nevertheless forgetting for a while about the normalization and considering, after deletion of the last term, only $u(-k)\,u(k,r)$ it is seen to have the proper asymptotic form at $r = 0$ as well as when $r \to \infty$.

We now suggest the inversion formula (28) to be replaced by

$$F(r) = -\frac{1}{\pi}\int_C \left[\frac{u(-k)}{u(k)} - \frac{v(-k)}{v(k)}\right] u(k,r)\,v(k,r)\,dk, \tag{30}$$

where C is a path of integration in the complex k-plane not following the real axis all the way, but avoiding by loops possible zeros of $u(k)$ and $v(k)$ on the positive imaginary axis, i.e., keeping those zeros to the right, however all other possible singularities on the positive imaginary axis to the left.

Retracting again our path of integration to the real k-axis we have

$$F(r) = -\frac{1}{\pi}\int_{-\infty}^{\infty} \left[\frac{u(-k)}{u(k)} - \frac{v(-k)}{v(k)}\right] u(k,r)\,v(k,r)\,dk$$
$$+ \sum_n \frac{2iu(-k_n)}{\dot{u}(k_n)}\,(uv)_{k_n} - \sum_m \frac{2iv(-k'_m)}{\dot{v}(k'_m)}\,(ub)_{k'_m}, \tag{31}$$

the sums being by hypotheses (30) the contributions from the bound states of $U(r)$ and $V(r)$, respectively. The k-values $k_n = i\varkappa_n$, $k'_m = i\varkappa'_m$, $n = 1, 2, \ldots, N$, $m = 1, 2, \ldots, M$ are the zeros of $u(k)$ and $v(k)$, respectively, and the dots denote derivation with respect to k. It should be noted that the admitted inconvenience of the factor $|u(k)|$ in the denominator of (29) has disappeared owing to the presence of the same

factor in $\sin(\xi-\eta)$. This gives a product $u(k)\,u(-k)$ which produces simple poles in the integrand and by complex integration these poles are replaced by their residua. The inclusion of bound states necessitates however a redefinition of the functions Y and Z.

Consulting when needed the detailed notation of eq. (31) we may venture to use some simplified notations. For instance we write

$$Z = uv, \tag{32}$$

which in either case has the asymptotic values

$$Z(0)=0, \quad Z_{k_n}(r)\to e^{-2\varkappa_n r}, \quad Z_{k'_m}(r)\to e^{-2\varkappa'_m r}. \tag{32 a}$$

Next we take the forms

$$Y_{k_n}(r)=\frac{u\bar{z}}{N_{k_n}}, \quad Y_{k'_m}(r)=\frac{\bar{y}v}{M_{k'_m}} \tag{33}$$

requiring for definiteness that $\bar{z}(0)=0$, $\bar{y}(0)=0$, and

$$W(\bar{z},v)=2, \quad W(u,\bar{y})=-2. \tag{33 a}$$

This means that

$$\begin{aligned} \bar{z} &= \frac{1}{\varkappa}\left[v(-k,r)-\frac{v(-k)}{v(k)}\,v(k,r)\right], \\ \bar{y} &= \frac{1}{\varkappa}\left[u(-k,r)-\frac{u(-k)}{u(k)}\,u(k,r)\right], \end{aligned} \tag{33 b}$$

since with $k=i\varkappa$

$$W(v^*,v)=-2ik=2\varkappa, \quad W(u,u^*)=2ik=-2\varkappa. \tag{33 c}$$

Now if we require for any pair Y, Z that

$$\int_0^\infty Y'Z\,dr=1 \tag{34}$$

we have

$$N_{k_n}=\int_0^\infty [u^2 v\bar{z}'+uu'v\bar{z}]\,dr=\tfrac{1}{2}\int_0^\infty u^2 W(\bar{z},v)\,dr=\int_0^\infty u^2\,dr \tag{34 a}$$

and correspondingly

$$M_{k'_m}=\int_0^\infty v^2\,dr. \tag{34 b}$$

Using the results as presented in eq. (25) or eqs. (26) one easily finds that any Z_{k_n} or $Z_{k'_m}$ belonging to the closed system is orthogonal to any Y', whether belonging to the open or the closed system, except its counterpartner Y'_{k_n} or $Y'_{k'_m}$, and vice versa.

We now need only the integral over $F(r)Y'_k(r)$ to establish our inversion formula. The integral is found to be

$$\int_0^\infty F(r)Y'_k(r)\,dr = \int_0^\infty [U(r)-V(r)]\,Y_k(r)\,dr = \frac{1}{N_k}W(\bar{z},u)_0^\infty = \frac{2}{N_k}, \tag{35}$$

and similarly

$$\int_0^\infty F(r)Y'_{k'}(r)\,dr = \frac{1}{M_{k'}}W(v,\bar{y})_0^\infty = -\frac{2}{M_{k'}}. \tag{35a}$$

Subtracting from $F(r)$ in (31) the contribution $F_c(r)$ from the continuum and calling the difference $F_d(r)$, we have

$$F_d(r) = \sum_n \frac{2}{N_{k_n}} u(k_n,r)\,V(k_n,r)\,v(k_n,r) - \sum_m \frac{2}{M_{k'_m}} u(k'_m,r)\,v(k'_m,r), \tag{36}$$

provided
$$N_{k_n} = \frac{\dot{u}(k_n)}{iu(-k_n)}, \quad M_{k'_m} = \frac{\dot{v}(k'_m)}{iv(-k'_m)}. \tag{36a}$$

This is just the result which follows from (35) and (35a) for normalized biorthogonal functions Y'_k and Z_k as defined according to (32), (33) and (34).

Eqs. (36a) are evidently true, but experience is better than logic, so we rather give a direct proof. The proof is most easily obtained by using the following equation for $\dot{u}(k,r)$ as obtained from our wave equation by differentiation with respect to k,

$$\left\{\frac{d^2}{dr^2}+k^2+U(r)\right\}\dot{u}+2ku=0. \tag{36b}$$

Combining it with the undifferentiated equation we find

$$\int_0^\infty u^2\,dr = \frac{1}{2k}W(u,\dot{u})_0^\infty = -\frac{1}{2k}u'(k,0)\,\dot{u}(k,0) = \frac{\dot{u}(k,0)}{iu(-k,0)} = \frac{\dot{u}(k)}{iu(-k)} = N_k, \tag{36c}$$

since from $W(u,u^*)=2ik$ we have

$$u'(k)\,u(-k)=2ik. \tag{36d}$$

Hence the true meaning of N_{k_n} and similarly of $M_{k'_m}$ in (36a) is clear.

The procedure is now to guess at some convenient potential $V(r)$ giving solutions $v(\pm k,r)$ with $e^{2i\eta}=v(-k)/v(k)$ as near as possible to $e^{2i\xi}$,

or, with $\eta = \arg v(-k)$ possibly nearest to ξ. Simultaneously one should want the $k'_m = i\varkappa'_m$ as near as possible to $k_n = i\varkappa_n$. When that is not accurately obtained $F(r) \neq 0$ and $U(r) \neq V(r)$. For the difference $U(r) - V(r)$ we can however obtain only an approximation, since $u(k, r)$ is unknown and must be replaced by $v(k, r)$. This approximate difference serves to find an approximate potential $U_1(r)$, which by repetition of the process is used for a better auxiliary potential $V_1(r)$.

Since any $N_{k_n} = \dot{u}(k_n)/iu(-k_n)$ is unknown from the measurement of $\xi(k)$ and the $E_n = -\varkappa_n^2$, there is for each stable state a parameter N_k at disposal, each of them allowing for an infinity of solutions of the problem.

Consider now the case of two potentials $U(r)$ and $V(r)$ giving the same phase shifts $\eta(k) = \xi(k)$ and the same binding energies, i.e., $k'_n = k_n$. Still $F(r)$ may be different from zero,

$$F(r) = \sum_n \left[\frac{2iu(-k_n)}{\dot{u}(k_n)} - \frac{2iv(-k_n)}{\dot{v}(k_n)}\right] u(k_n, r)\, v(k_n, r), \tag{37}$$

the potential difference hence being

$$U(r) - V(r) = -\sum_n \left[\frac{2}{N_{k_n}} - \frac{2}{M_{k_n}}\right] [u(k_n, r)\, v(k_n, r)]'. \tag{37 a}$$

This result has been observed by the author in 1948 and published in a less accessible journal [10].

6. Applications to Elementary Potentials

The general inversion formula (30) has been checked by some simple potentials of the short range type. In particular its validity for the following potentials has been proved [11].

Example 1.

$$U(r) = \lambda(\lambda+1)\,\alpha^2(1 - \operatorname{tgh}^2 \alpha r), \quad V(r) = \mu(\mu+1)\,\beta^2(1 - \operatorname{tgh}^2 \beta r). \tag{38}$$

Example 2.

$$U(r) = \frac{\lambda^2 \alpha^2 e^{-\alpha r}}{1 - e^{-\alpha r}}, \quad V(r) = \frac{\mu^2 \beta^2 e^{-\beta r}}{1 - e^{-\beta r}}. \tag{38 a}$$

These examples provide a great variety of potential curves. The former give curves of a finite, however arbitrary depth together with arbitrary

range. The latter has an infinite depth, a pole at the origin, and reminds very much of the Yukawa potential. Its strength as well as its range can be regulated at will by the two parameters λ and α (or μ and β) and hence can have an arbitrary number of closed states.

The demonstration is however lengthy and we shall be satisfied by proving the simpler case

$$V(r)=0, \quad v(k,r)=e^{ikr} \tag{39}$$

for which the inversion formula, with $U(r)=-F'(r)$, turns into

$$F(r)=-\frac{1}{\pi}\int_C\left[\frac{u(-k)}{u(k)}-1\right]u(k,r)\,e^{ikr}\,dk. \tag{40}$$

Next, we shall make a further simplification in choosing in the first example $\alpha=1$ and in the second example $\alpha=2$.

Example 1.

$$U(r)=\lambda(\lambda+1)\,(1-\operatorname{tgh}^2 r), \quad F(r)=\lambda(\lambda+1)\,(1-\operatorname{tgh} r). \tag{41}$$

We shall write the solution in two versions, by means of hypergeometric series

$$u(k,r)\,e^{ikr}\left(\frac{1-\operatorname{tgh} r}{2}\right)^{ik}=F\left(-ik-\lambda,\,-ik+\lambda+1,\,-ik+1,\,\frac{1-\operatorname{tgh} r}{2}\right) \tag{41 a}$$

$$=F\left(-\frac{ik}{2}-\frac{\lambda}{2},\,-\frac{ik}{2}+\frac{\lambda+1}{2},\,-ik+1,\,1-\operatorname{tgh}^2 r\right), \tag{41 b}$$

the former being used in (40) and the latter to obtain the asymptotic amplitudes

$$u(k)=\frac{2^{ik}(-ik)!\,(-\frac{1}{2})!}{\left(-\frac{ik}{2}+\frac{\lambda}{2}\right)!\left(-\frac{ik}{2}-\frac{\lambda+1}{2}\right)!}, \quad u(-k)=\frac{2^{-ik}(ik)!\,(-\frac{1}{2})!}{\left(\frac{ik}{2}+\frac{\lambda}{2}\right)!\left(\frac{ik}{2}-\frac{\lambda+1}{2}\right)!} \tag{41 c}$$

The poles of $u(-k)$ are evenly distributed along the positive imaginary axis, $k=in$, $n=1,2,\ldots,\infty$, and with

$$s_n=\frac{(\lambda+n)!}{(n-1)!\,n!\,(\lambda-n)!} \tag{41 d}$$

where is_n are the residua of $u(-k)/u(k)$ at the above poles of $u(-k)$. Hence

$$F(r)=\sum_{n=1}^{\infty}\frac{2(\lambda+n)!}{(n-1)!\,n!\,(\lambda-n)!}\left(\frac{1-\operatorname{tgh} r}{2}\right)^n F\left(n-\lambda, n+\lambda+1, \frac{1-\operatorname{tgh} r}{2}\right). \tag{41 e}$$

The first term gives in accordance with (41)

$$F(r)=\lambda(\lambda+1)\,(1-\operatorname{tgh} r) \tag{41 f}$$

and it is easily seen that higher terms in powers of $1-\operatorname{tgh} r$ cancel. For instance the coefficient of $(1-\operatorname{tgh} r)^2$ is

$$\tfrac{1}{4}\lambda(\lambda+1)\,(1-\lambda)\,(\lambda+2)+\tfrac{1}{4}(\lambda+2)\,(\lambda+1)\,\lambda(\lambda-1)=0. \tag{41 g}$$

Example 2. $$U(r)=4\lambda^2 e^{-2r}/(1-e^{-er}), \tag{42}$$

$$F(r)=2\lambda^2\log\left[1/(1-e^{-2r})\right]=2\lambda^2\left[e^{-2r}+\tfrac{1}{2}e^{-4r}+\tfrac{1}{3}e^{-6r}+\ldots\right]. \tag{42 a}$$

With the abbreviation $$l=\sqrt{\lambda^2+\left(\frac{ik}{2}\right)^2} \tag{42 b}$$

the solution writes

$$e^{-ikr}u(k,r)=F\left(-\frac{ik}{2}-l,\quad -\frac{ik}{2}+l,\quad -ik+1, e^{-2r}\right) \tag{42 c}$$

with the asymptotic amplitudes

$$u(k)=\frac{(-ik)!}{\left(-\frac{ik}{2}+l\right)!\left(-\frac{ik}{2}-l\right)!},\qquad u(-k)=\frac{(ik)!}{\left(\frac{ik}{2}+l\right)!\left(\frac{ik}{2}-l\right)!} \tag{42 d}$$

This gives for the residua is_n of $u(-k)/u(k)$ in the poles of $u(-k)$

$$s_n=\frac{\lambda^2}{(n-1)!\,n!}\left[\frac{\left(l_n+\frac{n}{2}-1\right)!}{\left(l_n-\frac{n}{2}\right)!}\right]. \tag{42 e}$$

The calculations are best illustrated explicitly by

$$F(r) = \sum_{n=1} 2s_n e^{-2nr} F\left(\frac{n}{2} - l_n,\ \frac{n}{2} + l_n,\ n+1,\ e^{-2r}\right)$$

$$= 2\lambda^2 \left\{ e^{-2r} - \frac{\lambda^2}{1\cdot 2} e^{-4r} + \frac{\lambda^2(\lambda^2-2)}{1\cdot 2\cdot 2\cdot 3} e^{-6r} - \dots \right.$$

$$+ \frac{\lambda^2+1}{1\cdot 2} e^{-4r} - \frac{2\lambda^2(\lambda^2+1)}{1\cdot 2\cdot 2\cdot 3} e^{-6r} + \dots$$

$$\left. + \frac{(\lambda^2+2)(\lambda^2+2)}{1\cdot 2\cdot 2\cdot 3} e^{-6r} - \dots \right.$$

$$= 2\lambda^2 \{ e^{-2r} + \tfrac{1}{2} e^{-4r} + \tfrac{1}{3} e^{-6r} + \dots \} \tag{42f}$$

in conformity with (42a).

7. Comparison with Other Theories

A full comparison with current theories is highly impeded by the great number of investigations from a 15 years period (refs. [2] and [3]), which, moreover, as a rule are of a fairly sophisticated mathematical form. To the extent of my knowledge, however, no serious mutual disagreement is found and they appear much alike in one respect, namely in accepting the Gelfand–Levitan equation the cornerstone of the theory. To my knowledge none of them follows the pattern of this work. Therefore it appears adequate to restrict the comparison to a few investigations of an accepted prominent character, of which the Jost–Kohn investigations (Ref. 6) are more explicit and hence afford the easiest basis for comparison. Using the simplification $V(r) = 0$ their inversion formula reads in our notation

$$U(r) = -\Phi'(r), \quad \Phi(r) = -\int_0^r U(r)\, dr, \tag{43}$$

$$\Phi(r) = \frac{1}{\pi} \int_C \left[\frac{1}{u(k)} - u(-k) \right] u(k, r) \left[e^{ikr} - e^{-ikr} \right] dk. \tag{43a}$$

This result looks indeed very different from (36) and one may wonder why the asymptotic amplitudes $u(\pm k)$ are now separately needed with their fairly formal and impractical deduction from the phase shift ξ, whereas in (40) we need only their ratio which is identical with the simple function $e^{2i\xi}$.

Apart from this objection from the point of view of convenience, the form of the function (r) does not appear quite proper, since in general

it will be a nonvanishing constant at infinity and hence not integrable. It appears advisable, therefore, to take the formula in the more direct form

$$U(r) = -\frac{1}{\pi}\int_C \left[\frac{1}{u(k)} - u(-k)\right] \frac{d}{dr}\{u(k,r)\,[e^{ikr} - e^{-ikr}]\}\,dk, \tag{43 b}$$

which in some sense might be thought of as applicable even to Example 2, eq. (42), for $r > 0$, for which (43) becomes meaningless.

If (40) and (43 b) are both to be true, there must be some logical connection between them allowing for the deduction of one of them from the other. It appears worth while, therefore, to try whether an interchange of the constituents of the binary orthonormal system might afford an explanation.

With $Z_k(r) = (4/\pi)\,(y_1 z_2 + y_2 z_1)$, and for simplicity $V(r) = 0$, $z_1 = \sin kr$, $z_2 = \cos kr$, consider therefore the integral

$$I = \int_0^\infty U(r)\, Z_k(r)\, dr, \tag{44}$$

From the wave equations and asymptotic expressions

$$\int_0^\infty U(r)\, y_1 z_2 dr = \lim_{R\to\infty} W(z_2, y_1)_0^\infty = -k\cos\xi + \frac{k}{|u(k)|}, \tag{44 a}$$

$$\int_0^\infty U(r)\, y_2 z_1 dr = \lim_{R\to\infty} W(z_1, y_2)_0^\infty = k\cos\xi - k\,|u(k)|, \tag{44 b}$$

hence

$$I = k\left[\frac{1}{|u(k)|} - |u(k)|\right]. \tag{44 c}$$

Relying now upon the completeness of the binary system

$$Z_k(r) \quad \text{and} \quad Y'_k(r) = \frac{1}{k}\frac{d}{dr}(y_1 z_1),$$

we have

$$\begin{aligned} U(r) &= \frac{4}{\pi}\int_0^\infty \left[\frac{1}{|u(k)|} - |u(k)|\right] \frac{d}{dr}(y_1 z_1)_k\, dk \\ &= -\frac{1}{\pi}\int_{-\infty}^\infty \left[\frac{1}{u(k)} - u(-k)\right] \frac{d}{dr}\{u(k,r)\,[e^{ikr} - e^{-ikr}]\}\, dk \end{aligned} \tag{44 d}$$

in the absence of bound state. In the same way as used before this formula must be generalized into (43 b) when bound states are present.

At the first sight the one formula (40) or (43 b) appears just as good as the other since $Y'_k(r)$ and $Z_k(r)$ have the same asymptotic shape both at $r=0$ and as $r\to\infty$. There is however a difference if, as in Example 2, the potential $U(r)$ has a pole in $r=0$, which of course is a most interesting case (cf. the Yukawa potential). In that case $F(r)$ is an integrable function down to $r=0$ whereas $U(r)$ is not.

When $u(k)$ and $u(-k)$ are separated as in (43) and the zeros of $u(k)$ are to be avoided by the contour C it appears as though $u(k)$ might be deleted. This is true, however, only after the contour C has been closed by a large semi-circle in the upper half-plane of k. This can be done because of $u(\pm k)\to 1$ as $k\to\infty$, and now the contour C may be contracted into small circles around the poles of $u(-k)$, the residua being $is_n u(k_n)$. We first try

Example 2.
$$U(r)=\frac{4\lambda^2 e^{-2r}}{1-e^{-2r}}. \tag{45}$$

With the abbreviation

$$F_n=F\left(\frac{n}{2}-l_n,\ \frac{n}{2}+l_n,\ n+1,\ e^{-2r}\right)=1-\frac{\lambda^2 e^{-2r}}{1\cdot(n+1)}-\frac{\lambda^2[1\cdot(n+1)-\lambda^2]\,e^{-4r}}{1\cdot 2\ (n+1)\,(n+2)}, \tag{45 a}$$

we may write

$$U(r)=-\sum_{n=1}^{\infty}2s_n u(in)\frac{d}{dr}\{[e^{-2nr}-1]\,F_n\}, \tag{45 b}$$

where s_n is given before in (42 c) and

$$u(in)=\frac{n!}{\left(\frac{n}{2}+l_n\right)!\,\left(\frac{n}{2}-l_n\right)!}. \tag{45 c}$$

This formula is extremely difficult to use in general, owing to the more intricate form of $u(in)$ in comparison to s_n. There are no simplifications obtained by choosing particular values for λ except $\lambda=0$. In that case we have $u(in)=1$ and to the first order of λ^2

$$s_n=\frac{\lambda^2}{n}. \tag{45 d}$$

To that order also all F_n may be replaced by unity, and so from (45 b) we obtain

$$U(r) = 4\lambda^2 \sum_{n=1}^{\infty} e^{-2nr} \tag{45e}$$

in conformity with (45).

If we write
$$U(r) = 4\lambda^2 I(\lambda, r) \sum_{n=1}^{\infty} e^{-2nr} \tag{45f}$$

we have now $I(0, r) = 1$. It appears that $I(\lambda, r)$ considered a function of the variable λ—irrespective of its dependence of r—is an integral function. If in addition this function is regular even at infinity it is a constant, and to determine that constant only a single functional value as $I(0, r)$ is needed.

This is only a statement that the inversion formula (45b) may be correct. Note that $\lambda^2 I(\lambda, r)$ has a singularity at $\lambda = \infty$ and hence is no constant.

In Example 1, eq. (41) we have better luck, owing obviously to the accidental cancelling of an infinite number of poles and zeros in $u(-k)$ for integral λ. The inversion formula is found to be

$$U(r) = -\sum_{n=1}^{\infty} 2s_n u(in) \frac{d}{dr}\left\{\left[\left(\frac{1-\operatorname{tgh} r}{2}\right)^n - \left(\frac{1+\operatorname{tgh} r}{2}\right)^n\right] \times F\left(\frac{n-\lambda}{2}, \frac{n+1+\lambda}{2}, n+1, 1-\operatorname{tgh}^2 r\right)\right\}, \tag{46}$$

with
$$s_n u(in) = \frac{2^{-n}(\lambda+n)!\,(-\frac{1}{2})!}{(n-1)!\,(\lambda-n)!\,\left(\frac{n}{2}+\frac{\lambda}{2}\right)!\,\left(\frac{n}{2}-\frac{\lambda+1}{2}\right)!}. \tag{46a}$$

For integral λ we have finite sums, for $\lambda = 1$ we have $n = 1$, for $\lambda = 3$, $n = 1, 3$, etc., and similarly for $\lambda = 2, 4, 6, \ldots$, $n = 2$, $n = 2, 4$, $n = 2, 4, 6$. $\lambda = 1$ and $\lambda = 2$ are easily seen to give $2(1 - \operatorname{tgh}^2 r)$ and $6(1 - \operatorname{tgh}^2 r)$. For $\lambda = 3$ the terms $n = 1, 3$ and their sums are as follows,

$$-3[\tfrac{7}{2}(1-\operatorname{tgh}^2 r) - \tfrac{15}{4}(1-\operatorname{tgh}^2 r)^2] + 15[\tfrac{3}{2}(1-\operatorname{tgh}^2 r) - \tfrac{3}{4}(1-\operatorname{tgh}^2 r)^2] = 12(1-\operatorname{tgh}^2 r). \tag{46b}$$

The calculations are easily extended and show that the result is

$$U(r) = \lambda(\lambda+1)(1-\operatorname{tgh}^2 r)\, I(\lambda), \tag{47}$$

where $I(\lambda)$ is unity for positive integral λ. Replacing λ by $-(\lambda+1)$ formula (46) is unchanged and $I(\lambda)$ is unity for $\lambda = -2, -3, \ldots$. Finally as $\lambda \to 0$ (46a) becomes

$$s_n u(in) = \frac{\lambda + 1 - n}{(n-1)!\,(1-n)!} \tag{47a}$$

with the only term $s_1 u(i)$ being different from zero. Therefore as is easily seen also for $\lambda = 0$, and hence for $\lambda = -1$ the function $I(\lambda)$ is unity.

Since the expression (46a) has no singularity in the entire complex λ-plane and since, moreover, the series (46) appears convergent for any λ, the function $I(\lambda)$ must be an integral function of λ. If, moreover, it is regular at infinity, it is a constant whose value is unity.

This does not however mean that formula like (43b) and even less (43a)—usually referred to as based on the Gelfand–Levitan equation—are equivalent to formulae of the character (40). This is most clearly demonstrated by the simple dependence of $u(-k)/u(k)$ on the phase ξ and the usually only formally feasible calculation of the phase amplitudes $u(\pm k)$ from ξ. Therefore the Gelfand–Levitan equation appears to me having a somewhat ad hoc character, in particular through the unfortunate factor $1/u(k)\,u(-k) - 1$ as originating mainly from a particular normalization of the solutions of the basic wave equation. If at all needed a more suitable form of the Gelfand-Levitan theory might possibly be found.

As long as the conception of binary orthonormal systems is not applied, rational formulae for the inverse problem are not obtainable. It is as though expressing vectors in an oblique coordinate system, one would refuse to use the reciprocal system.

8. Remarks on Completeness Relation Proofs

The validity of all previous results rests on the supposition of fulfilment of one of the three conditions, which of course automatically implies the fulfilment of the other:

(1) An independent proof of the completeness of the system $Y'_k(r)$, $Z_k(r)$.

(2) $K(r, r')$ as used by Jost and Kohn and in the Gelfand–Levitan theory being a solution of the Gelfand–Levitan integral equation.

(3) $u(k, r)$ or $y_1(k, r)$ as expressed by means of a certain kernel $K(r, r')$ in form of an integral equation being a solution of the wave equation.

The latter verification has been tried by Jost and Kohn (Ref. 6). For the rest, completeness relation proofs are sparse and sometimes

doubtful. Even the proof of the completeness of the ordinary orthonormal system $y_1(k,r)$, $u(k_n,r)$, which for convenience may be written in the form

$$\frac{2}{\pi}\int_0^\infty y_1(k,r)\,y_1(k,r')\,dk+\sum_n \frac{1}{N_{k_n}}\,u(k_n,r)\,u(k_n,r')=\delta(r-r') \tag{48}$$

appears in the presentation given in ref. [3] (L. D. Faddeyev) fallacious. We give here the following analysis.

Consider a kernel $L(r,r')$ with the properties

$$\left\{\frac{d^2}{dr'^2}+k^2+U(r')\right\}L(r,r')=0, \tag{48 a}$$

$$\lim_{\varepsilon\to 0}\{L'(r,r-\varepsilon)-L'(r,r+\varepsilon)\}=1,\ L'(r,r')=\frac{\partial L}{\partial r'}, \tag{48 b}$$

and finally $L(r,0)=0$.

Next consider a twice differentiable function $f(r)$ with the boundary value $f(0)=0$. Then from

$$\int_0^\infty f(r')\left[\frac{d^2}{dr'^2}+k^2+U(r')\right]L(r,r')\,dr'=0 \tag{49}$$

we obtain by partial integration

$$f(r)+\int_0^\infty L(r,r')\left[\frac{d^2}{dr'^2}+k^2+U(r')\right]f(r')\,dr'=0. \tag{49 a}$$

Multiplying the latter equation by $idk/k\pi$ and integrating over an infinitely large semi-circle C' in the upper half of the k-plane extending from $k=-\infty$ to $k=+\infty$ we need not care about the term

$$\left[\frac{d^2}{dr'^2}+U(r')\right]f(r')$$

which is finite since, as we shall see $L(r,r')$ is of the order of magnitude $1/|k|$. Hence,

$$f(r)=\frac{1}{\pi i}\int_{C'}dk\int_0^\infty kL(r,r')\,f(r')\,dr'. \tag{49 b}$$

The kernel is given by

$$ke^{-i\xi}L(r,r')=\begin{cases}u(k,r)\,y_1(k,r'), & (r'<r)\\ y_1(k,r)\,u(k,r'), & (r'>r).\end{cases} \tag{49 c}$$

To see the implication of (49 b), multiply (49 c) by $e^{i\xi} = u(-k)/|u(k)|$ and introduce $y_1(k, r)$ by its expression in terms of $u(k, r)$ and $u(-k, r)$ to obtain for $r' \lessgtr r$, respectively,

$$f(r) = -\frac{1}{2\pi} \int_{C'} dk \begin{Bmatrix} u(k, r) \left[\frac{u(-k)}{u(k)} u(k, r') - u(-k, r')\right] \\ u(k, r') \left[\frac{u(-k)}{u(k)} u(k, r) - u(-k, r)\right] \end{Bmatrix} f(r')\, dr'. \quad (49\,\mathrm{d})$$

Contracting the semi-circle C' down to the former C, forgetting about the singularities of $u(-k)$, and next down to the real axis, taking care of the zeros of $u(k)$, and finally transforming half the integral from $-\infty$ to 0 into a corresponding one from 0 to $+\infty$, the result would be the equation

$$f(r) = \frac{2}{\pi} \int_0^\infty dk \int_0^\infty y_1(k, r)\, y_1(k, r')\, f(r')\, dr' + \sum_n \frac{1}{N_{k_n}} \int_0^\infty u(k_n, r)\, u(k_n, r')\, f(r')\, dr', \quad (50)$$

which is equivalent to (48) in the domain of functions to which the arbitrary function $f(r)$ belongs.

What has been forgotten by this procedure is, however, in the case of simple poles of the asymptotic amplitude $u(-k)$ the in general infinite series

$$[f(r)]_{\mathrm{pol}} = \sum_m \frac{i \operatorname{Res} u(-k'_m)}{u(k'_m)} \int_0^\infty u(k'_m, r)\, u(k'_m, r')\, f(r')\, dr'. \quad (50\,\mathrm{a})$$

This series must be zero, which is difficult to prove, and it has not been proved as, moreover, the author has not been aware of it.

In the treatment given by Jost and Kohn the following integral equation appears, in our notation and with the simplification $V(r) = 0$,

$$|u(k)|\, y_1(r) = \sin kr + \int_0^r K(r, r') \sin kr'\, dr'. \quad (51)$$

It may be thought of as an integral equation for the kernel $K(r, r')$, but even if the kernel is known it remains an integral equation for $y_1(r)$ since $K(r, r')$ is expressed by means of $y_1(r)$.

The conditions for $y_1(r)$ to be equivalent with the former solution $y_1(r)$ of the wave equation are

$$\left\{\frac{\partial^2}{\partial r^2}-\frac{\partial^2}{\partial r'^2}+U(r)\right\}K(r,r')=0,\quad U(r)=-2\frac{dK(r,r)}{dr} \tag{51 a}$$

the correct asymptotic value of $y_1(r)$ as $r\to 0$ being already ensured by the form of (51).

Comparing with eq. (43 a), it is seen that the kernel is

$$K(r,r')=-\frac{1}{2\pi}\int_C\left[\frac{1}{u(k)}-u(-k)\right]u(k,r)\,[e^{ikr'}-e^{-ikr'}]. \tag{51 b}$$

It satisfies the first eq. (51 a) and it may satisfy the second. In particular this is true if eq. (51) is correct, so one may try to evaluate the integral in (51).

Since the zeros of $u(k)$ are avoided in (51 b) the evaluation of the first part of the integral (51) is simple. Using the asymptotic values $u(k)\to 1$, $u(k,r)\to e^{ikr}$ as $|k|\to\infty$ it gives $-\frac{1}{2}\sin kr$. In the second part of the integral the contour C may be drawn down to the real axis to give an integral

$$J=-\frac{1}{2\pi}\int_{-\infty}^{\infty}dk'u(-k')\,u(k',r)\cdot 2i\left\{\int_0^{\infty}dr'-\int_r^{\infty}dr'\right\}\sin k'r'\sin kr'=J_1+J_2. \tag{51 c}$$

It is easily seen that

$$\begin{aligned}J_1&=\frac{1}{2i}\int_{-\infty}^{\infty}dk'\,u(-k')\,u(k',r)\,[\delta(k-k')-\delta(k+k')]\\&=\frac{1}{2i}[u(-k)\,u(k,r)-u(k)\,u(-k,r)]=|u(k)|\,y_1(r).\end{aligned} \tag{51 d}$$

In the remaining part of the integral,

$$J_2=\int_r^{\infty}dr'\sin kr'\frac{1}{2\pi}\int_{-\infty}^{\infty}dk\,u(-k)\,u(k,r)\,[e^{ikr'}-e^{-ikr'}], \tag{51 e}$$

since $r'>r$, the path of integration for the latter part may be deformed into large semi-circle C'' in the lower half-plane, where $u(-k)\to 1$ and $u(k,r)\to e^{ikr}$, to give a contribution

$$-\int_r^{\infty}dr'\sin kr'\,\delta(r-r')=-\tfrac{1}{2}\sin kr. \tag{51 f}$$

In the first part of the integral the path of integration must be deformed into the former semi-circle C' in the upper half-plane to give

$$\int_r^\infty dr' \sin kr' \,\delta(r'+r) = 0. \tag{51 g}$$

To this, however, must be added the contributions from the poles $k_n = i\varkappa_n$ of $u(-k)$ with the net result that

$$\int_0^r K(r,r') \sin kr' \, dr' = |u(k)| \, y_1(r) - \sin kr + J_3, \tag{52}$$

$$J_3 = \sum_n i \operatorname{Res} u(-k_n) \, u(k_n, r) \int_r^\infty \sin kr' \, e^{ik_n r'} dr'$$

$$= \sum_n i \operatorname{Res} u(-k_n) \, u(k_n, r) \, \tfrac{1}{2} \left[\frac{e^{i(k_n+k)r}}{k_n+k} - \frac{e^{i(k_n-k)r}}{k_n-k} \right], \tag{52 a}$$

and it will be hard to prove that this expression is zero.

The Jost–Kohn procedure is somewhat different in performing first the integration in dr' in (51 c) to give

$$J = \frac{1}{2\pi i} \int_{-\infty}^\infty dk' \, u(-k') \, u(k', r) \left[\frac{\sin(k'-k)\, r}{k'-k} - \frac{\sin(k'+k)}{k'+k} \right], \tag{53}$$

or, to prepare a deformation of the contour into the upper half-plane

$$J = \frac{1}{2\pi i} \int_{-\infty}^\infty dk' \, [u(-k') \, u(k', r) - u(k') \, u(-k', r)]$$

$$\times \frac{1}{2i} \left[\frac{e^{i(k'-k)}}{k'-k} - \frac{e^{i(k'+k)}}{k'+k} \right]. \tag{53 a}$$

If k is slightly above or slightly below the real axis it is seen that on deforming the path of integration we have to pass a single pole in $k' = k$ or $k' = -k$ giving just the contribution $|u(k)| \, y(r)$. If k is on the axis we may before the integration in dr' make a loop to include, say, the pole $k = k'$ and exclude $k = -k'$ with the above result.

In the part of (53 a) containing only $u(k')$ we may now pass to the semi-circle C', where $u(k') \to 1$ and $u(-k', r) \to e^{-ik'r}$. This gives the contribution

$$\frac{\sin kr}{2\pi i} \int_{C'} \frac{dk'}{k'} = -\frac{1}{2} \sin kr. \tag{53 b}$$

Forgetting about the poles of $u(-k')$ we get in a similar manner the contribution

$$-\frac{\sin kr}{2\pi i}\int_{C'}\frac{e^{2ik'r}\,dk'}{k'}=0. \tag{53c}$$

Again there remain the contributions from the poles of $u(-k')$, which is

$$J_3=\sum_n i\,\mathrm{Res}\,u(-k_n)\,u(k_n,r)\cdot\tfrac{1}{2}\left[\frac{e^{i(k_n+k)r}}{k_n+k}-\frac{e^{i(k_n-k)r}}{k_n-k}\right], \tag{53d}$$

the same expression as (52a).

9. Integral Equations Related to the Problem

The integral equation most frequently used for the inverse problem is that of the type (51) for the solution $y_1(r)$ of the wave equation. More in line with the present treatment is

$$u(k,r)=e^{ikr}-\int_r^\infty K(r,r')\,e^{ikr'}\,dr'. \tag{54}$$

We may at once presume that the kernel $K(r,r')$ obey the equation

$$\left\{\frac{\partial^2}{\partial r^2}-\frac{\partial^2}{\partial r'^2}+U(r)\right\}K(r,r'), \tag{54a}$$

which simply means that it is built up from products of solutions of the wave equation

$$\left\{\frac{d^2}{dr^2}+k^2+U(r)\right\}y=0 \tag{54b}$$

and corresponding circular or exponential functions with different arguments r and r' and summed or integrated over the parameter k.

It is found quite elementarily that

$$\left(\frac{d^2}{dr^2}+k^2\right)\int_r^\infty K(r,r')\,e^{ikr'}\,dr'=\frac{d^2}{dr^2}\int_r^\infty K(r,r')\,e^{ikr'}\,dr'-\int_r^\infty K(r,r')\,\frac{\partial^2 e^{ikr'}}{\partial r'^2}\,dr'$$

$$=-\frac{dK(r,r)}{dr}\,e^{ikr}+\frac{d}{dr}\int_r^\infty\frac{\partial K(r,r')}{\partial r}\,e^{ikr'}\,dr'+\int_r^\infty\frac{\partial K(r,r')}{\partial r'}\,\frac{\partial e^{ikr'}}{\partial r'}\,dr'$$

$$=-2\frac{dK(r,r)}{dr}\,e^{ikr}+\int_r^\infty\left[\frac{\partial^2 K(r,r')}{\partial r^2}-\frac{\partial^2 K(r,r')}{\partial r'^2}\right]e^{ikr'}\,dr'. \tag{54c}$$

Therefore from (54)

$$\left\{\frac{d^2}{dr^2}+k^2+U(r)\right\}u(k,r)=\left[U(r)+2\frac{dK(r,r)}{dr}\right]e^{ikr}, \tag{55}$$

and the condition that $u(k,r)$ becomes a solution of (54 b) is that

$$U(r)=-2\frac{dK(r,r)}{dr}. \tag{55 a}$$

If the formulae presented in this research are correct, as they are bound to be if our binary system is complete, the kernel in the case of $V(r)=0$ can be found from (27 a) or (40) as

$$\begin{aligned} K(r,r') &= \frac{2}{\pi}\int_0^\infty \sin\xi_k[y_1(r)\cos kr'+y_2(r)\sin kr']_k\,dk \\ &= -\frac{1}{2\pi}\int_C\left|\frac{u(-k)}{u(k)}-1\right|u(k,r)\,e^{ikr'}\,dk. \end{aligned} \tag{56}$$

The former expression of course is incorrect in the case of bound states and must be taken only formally.

We now introduce the simpler kernel

$$D(r,r')=-\frac{1}{2\pi}\int_C\left[\frac{u(-k)}{u(k)}-1\right]e^{ik(r+r')}\,dk. \tag{57}$$

Then if
$$K(r,r')=D(r,r')-\int_r^\infty K(r,r'')\,D(r'',r')\,dr'' \tag{57 a}$$

we find by elementary operations

$$\left\{\frac{\partial^2}{\partial r^2}-\frac{\partial^2}{\partial r'^2}\right\}K(r,r')=2\frac{dK(r,r)}{dr}K(r,r'). \tag{57 b}$$

If therefore two of the three equations (54 a), (55 a) and (57 a) are true, the third is also true.

Unfortunately, it is difficult to see how the correctness of (57 a) for $K(r,r')$ in (56) could be proved in any simple way. However, if the Gelfand–Levitan equation has so far proved to be of any practical use and not only a formalism, the same must be true for (57 a).

10. Calculation of Potentials for Small Perturbations

Let us write the wave equation in the form

$$\left\{\frac{d^2}{dr^2}+k^2+AU(r)\right\}y=0, \tag{58}$$

where $U(r)$ is a characteristic potential function and A a variable parameter giving the strength of the perturbation. Then we shall find a very interesting simplification in the case of $A\to 0$.

The general integral equation for $U(r)=-F'(r)$ or $F(r)$ now reads

$$\sin\xi = A\int_0^\infty U(r)\frac{1}{k}y_1(r)\sin kr\,dr = A\int_0^\infty F(r)\frac{1}{k}\frac{d}{dr}(y_1\sin kr)\,dr. \tag{58 a}$$

In the limit $A\to 0$ we may replace $y_1(r)$ by $\sin kr$ and have

$$\frac{1}{A}\sin\xi = \int_0^\infty F(r)\sin 2kr\,dr. \tag{59}$$

This equation can readily be inverted to give

$$AF(r)=\frac{4}{\pi}\int_0^\infty \sin\xi\,\sin 2kr\,dk. \tag{59 a}$$

Again, expressing $\sin\xi$ by means of the asymptotic amplitudes we have

$$AF(r)=-\frac{1}{\pi}\int_{-\infty}^\infty\left[\frac{u(-k)}{u(k)}-1\right]e^{2ikr}\,dk. \tag{59 b}$$

Let us now consider a potential function which can be expanded in a power series of $e^{-2\alpha r}$ or rather e^{-2r} such that

$$F(r)=\sum_{n=1} 2\sigma_n e^{-2nr}, \tag{60}$$

which, on being introduced in (59), gives

$$\frac{1}{A}\sin\xi=\tfrac{1}{2}\sum_n \sigma_n\left[\frac{1}{k-in}+\frac{1}{k+in}\right]. \tag{60 a}$$

Inserting in (59 a) we regain eq. (60) in the following way,

$$F(r) = \frac{2}{\pi} \int_0^\infty \sum_n \left[\frac{\sigma_n}{k - in} + \frac{\sigma_n}{k + in} \right] \sin 2kr\, dk$$

$$= \frac{1}{\pi i} \int_{-\infty}^\infty \sum_n \left[\frac{\sigma_n}{k - in} + \frac{\sigma_n}{k + in} \right] e^{2ikr}\, dk = \sum_{n=1}^\infty 2\sigma_n\, e^{-2nr}, \tag{60 b}$$

on closing the path of integration in the upper half-plane and contracting it around the poles.

On the other hand, for arbitrary A we would have from the general inversion formula

$$AF(r) = \sum_{n=1}^\infty 2s_n u(in, r)\, e^{-nr}, \tag{60 c}$$

where is_n is the residuum of $u(-k)/u(k)$ in the pole $k = in$. Hence we see that

$$s_n \to A\sigma_n \quad \text{as} \quad A \to 0, \tag{61}$$

where $2\sigma_n$ are the expansion coefficients of the integrated potential in (60).

This is a remarkable connection which may be of some use in the further discussion of the theory.

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