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Some consequences of the Gel'fand–Levitan equations

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Abstract. The Gel'fand–Levitan equations for the solution of the inverse scattering problem are written in terms of the half-off-energy-shell matrix element. This element is given in terms of the phase shifts, by a double integral equation in which the kernel has simple poles. We also find an integral equation for the wave function. We include the effects of bound states, and find a relation between the large and small r behaviour of the bound-state wave function.

1. Introduction

It has been known for some time that, in the realm of potential theory, a knowledge of the phase shift for one angular-momentum state and all energies will determine the potential uniquely. Here we assume there are no bound states, and we return to the bound-state problem in § 4. A non-local potential can in general be written as $V = V(r^2, p^2, L^2)$, but if one assumes the form

$$V = V(r^2, L^2) \quad (1)$$

then a knowledge of the complete S matrix, phase shifts $\delta_l(k)$ for all l and for $0 < k < \infty$ determines V , by means of the equations of Gel'fand and Levitan (Newton 1960).

This theory is particularly interesting from the point of view of the two-nucleon interaction, where there is a considerable body of experimental and phenomenological data on the S matrix, and at the same time no simple and generally accepted theory of the interaction. However, there has been in recent years a change in emphasis in uses of the two-nucleon interaction. In dealing with inelastic problems such as three-body reactions (Aaron *et al.* 1964) and photon emission in two-body reactions (Cromer and Sobel 1966) the quantities actually required are the off-energy-shell elements of the two-body scattering matrix. A phenomenological potential is, of course, required to calculate these elements, but the potential itself is not directly required in calculating the reaction amplitudes. We propose, then, to express the Gel'fand–Levitan equations in a form which gives the half-off-shell matrix element in terms of the phase shift. This is an integral equation, which is found in § 3. In § 2 we find an integral equation for the wave function, which in turn leads to the result for the matrix element. The effects of bound states are considered in § 4 and we find an interesting condition on the bound-state wave function. In the appendix we summarize the basic equations for the inverse scattering problem and define our notation.

It should be noted that the actual two-nucleon interaction does not necessarily take the form of equation (1). Experiment does not, at this time, provide enough information to determine the nature of a general non-local potential, and there are several different models which are in adequate agreement with experiment. However, the models (Hamada and Johnston 1962, Lassila *et al.* 1962) which are generally considered most 'realistic' (in the sense of agreement with experiment) do take the form of (1).

2. Wave functions

In the Gel'fand–Levitan equation (A6), let us take $V^{(1)} = 0$. Thus we have

$$\phi_l^{(1)}(k, r) = rk^{-l}j_l(k, r) \quad (2)$$

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and $|f_i^{(1)}(k)| = 1$. Taking the Fourier transform† of (A9) we find

$$K_i(r, k) = \frac{1}{2}\pi\xi_i(k)k^{l+1}\phi_i(k, r). \tag{3}$$

Here

$$\xi_i(k) = \frac{2}{\pi} \left\{ 1 - \frac{1}{|f_i(k)|^2} \right\} \tag{4}$$

and the important point is that ξ is determined by the phase shift. If we use equation (A8) and write $\bar{K}_i(r, r')$ in terms of $K_i(r, k')$, we find the equation for ϕ_i :

$$\phi_i(k, r) = rk^{-l}j_l(k, r) + k^{-l-1} \int_0^\infty dk' \xi_i(k')k'^{l+1}\mathcal{F}_i(k, k'; r)\phi_i(k', r) \tag{5}$$

where

$$\mathcal{F}_i(k, k'; r) = \frac{1}{k'^2 - k^2} \left[k'rj_l(k'r) \frac{d}{dr} \{krj_l(k, r)\} - krj_l(k, r) \frac{d}{dr} \{k'rj_l(k'r)\} \right]. \tag{6}$$

Equation (5) is a single integral equation for the wave function, and the kernel \mathcal{F}_i is non-singular. An important characteristic of equation (5) is that the kernel is essentially an analytic function, which increases the practicality of a solution by numerical means. This is in contrast to (A6) where the kernel $g(r'', r')$ must be evaluated as an integral for each r'' and r' .

If equation (5) is written for large r , we obtain two conditions on the phase shifts. Using the asymptotic forms for ϕ_i (equation (A2)) and j_l , we may equate coefficients of $\cos kr$ and $\sin kr$, to find

$$\begin{aligned} |f_i(k)| \cos \delta_i(k) &= 1 - \frac{1}{2} \int_0^\infty dk' \xi_i(k') |f_i(k')| \sin \delta_i(k') \frac{k'}{k'^2 - k^2} \\ |f_i(k)| \sin \delta_i(k) &= \frac{1}{2} \int_0^\infty dk' \xi_i(k') |f_i(k')| \cos \delta_i(k') \frac{k}{k'^2 - k^2}. \end{aligned} \tag{7}$$

These are, of course, highly non-linear, and not of much practical value.

3. Off-energy-shell matrix elements

The half-off-shell matrix element is proportional to the momentum-space wave function. Hence we will want the Fourier transform of (5), or the double transform of (A6). It has been shown (Noyes 1965) that the full off-shell element is given by an integral over a product of half off-shell elements, so that $K_i(k, k')$ may be regarded as the fundamental quantity in describing scattering. From (5) it is easy to deduce

$$K_i(k, k') = \left(\frac{1}{2}\pi\right)^2 \xi_i(k)\delta(k - k') + \frac{1}{2}\pi\xi_i(k') \int_0^\infty d\beta \int_0^\infty d\beta' K_i(\beta, \beta') F_i(k, k'; \beta, \beta') \tag{8}$$

where

$$F_i(k, k'; \beta, \beta') = \left(\frac{2}{\pi}\right)^2 \int_0^\infty dr(kr) j_l(kr)(\beta r) j_l(\beta r) \mathcal{F}_i(k', \beta'; r).$$

† Our notation is $f(k) = \int_0^\infty dr(kr)j_l(kr)f(r)$. To avoid an excess of symbols we denote a function and its Fourier transform by the same letter. The meaning will be indicated by the argument, k 's and β 's for momenta and r 's for positions.

For $l = 0$ the kernel F is

$$\begin{aligned}
 F_0(k, k'; \beta, \beta') &= -\frac{1}{\pi^2} \left\{ \frac{1}{(\beta' - k')^2 - (\beta - k)^2} - \frac{1}{(\beta' - k')^2 - (\beta + k)^2} \right. \\
 &\quad \left. - \frac{1}{(\beta' + k')^2 - (\beta - k)^2} + \frac{1}{(\beta' + k')^2 - (\beta + k)^2} \right\} \\
 &= \frac{32}{\pi^2} \frac{\beta\beta'kk'(k^2 - k'^2 + \beta^2 - \beta'^2)}{\{\beta'^2 - (k' + k + \beta)^2\}\{\beta'^2 - (k' + k - \beta)^2\}} \\
 &\quad \times \{\beta'^2 - (k' - k + \beta)^2\}\{\beta'^2 - (k' - k - \beta)^2\}^{-1}.
 \end{aligned} \tag{9}$$

The second form is written to show that there should be no difficulty about convergence of the integral equation (8) at $\beta, \beta' \rightarrow \infty$. For $l > 0$ we have not found a simple general form for the function F_l but for any particular low l value one can always find a straightforward analytic expression, and it will have properties similar to F_0 . In any case, in a practical solution of (8), one will certainly first deal with S waves, which are best known and most important.

Equation (8) has both a δ -function singularity and a simple pole at $k = k'$. These singularities are actually present in K_l because $K_l(r, k')$ does not go to zero at $r \rightarrow \infty$. However, we may subtract from $K_l(r, k')$ its asymptotic form, as given by (3) and (A2), and define

$$U_l(r, k) \equiv K_l(r, k) - \frac{1}{2}\pi kr \{c_l(k)j_l(kr) - s_l(k)n_l(kr)\} \tag{10}$$

where

$$\begin{aligned}
 c_l(k) &= \xi_l(k)|f_l(k)| \cos \delta_l(k) \\
 s_l(k) &= \xi_l(k)|f_l(k)| \sin \delta_l(k).
 \end{aligned} \tag{11}$$

Then $U_l(r, k) \rightarrow 0$ as $r \rightarrow \infty$ and $U_l(k, k')$ is finite at $k = k'$. It obeys the integral equation

$$\begin{aligned}
 U_l(k, k') &+ (\frac{1}{2}\pi)^2 \{c_l(k) - \xi_l(k)\} \delta(k - k') - \frac{1}{2}\pi k s_l(k') \left(\frac{k}{k'}\right)^l \frac{1}{k'^2 - k^2} \\
 &= \frac{1}{2}\pi \xi_l(k') \int_0^\infty d\beta' \int_0^\infty d\beta \left\{ U_l(\beta, \beta') + (\frac{1}{2}\pi)^2 c_l(\beta) \delta(\beta - \beta') - \frac{1}{2}\pi \beta s_l(\beta') \right. \\
 &\quad \left. \times \left(\frac{\beta}{\beta'}\right)^l \frac{P}{\beta'^2 - \beta^2} \right\} F_l(kk', \beta\beta').
 \end{aligned} \tag{12}$$

Here P denotes the principal values, and, since U_l is real, one may take the principal value for the poles in F_l as well. One could multiply the equation by $k' - k$ and write an equivalent equation for $\bar{U}(k, k') = (k' - k) \times U(k, k')$, thereby eliminating the singularity at $k = k'$. This equation would have the undesirable features of requiring the *ad hoc* boundary condition $\bar{U}(k, k) = 0$, and of having an inhomogeneous term which does not obey the boundary condition. Preferably one can subtract from both sides the quantity $(k' - k)^{-1}R$ where R is the residue at $k' = k$. This eliminates the pole but leaves the δ -function. In fact there are also terms in $\delta(k - k')$ appearing in the inhomogeneous terms on the right-hand side of (12). These appear when the singularities (in F_l and the factor $(\beta'^2 - \beta^2)^{-1}$) coincide,† and we may isolate all these singular terms. Then they may simply be dropped, as will be apparent shortly.

To find the relation between $U_l(k, k')$ and the half-off-shell matrix element we first define the latter as $t_l(k)\eta(k, k')$. Here $t_l(k) = k^{-1} \sin \delta_l(k) \exp\{i\delta_l(k)\}$ is the on-shell element, and $\eta(k, k) = 1$. Then it is well known (Noyes 1965) that

$$\eta_l(k, k') = \left(\frac{k'}{k}\right)^l + (k'^2 - k^2) \int_0^\infty dr kr^2 j_l(k'r) \{n_l(kr) - \cot \delta_l(k) j_l(kr) - u_l(k, r)\} \tag{13}$$

† We use the relation $\int_{-\infty}^{\infty} dt \{(t-s)(t-s')\}^{-1} = 2\pi^2 \delta(s-s')$.

where u_l is the radial wave function that goes asymptotically as $n_l(kr) - \cot \delta_l(k) j_l(kr)$. By comparing the normalization of u_l with that of ϕ_l and using (3), we find

$$U_l(k, k') = \frac{1}{2} \pi s_l(k') k \frac{\eta_l(k', k) - (k/k')^l}{k^2 - k'^2}. \quad (14)$$

Thus $U_l(k, k')$ is directly related to the half-off-shell element. Furthermore, we note from (14) that U_l is undefined at $k = k'$ to the extent of a term in $\delta(k - k')$. So, if we want to make the obvious choice

$$U_l(k, k) = \lim_{k' \rightarrow k} U_l(k, k')$$

it is correct to drop all δ -functions which appear in (12). We write the result for $l = 0$. If

$$\tilde{U}_l(k, k') \equiv \frac{U_l(k, k')}{\frac{1}{2} \pi \xi_l(k')}$$

and

$$\tilde{F}_l(k, k'; \beta, \beta') \equiv \frac{1}{2} \pi \xi_l(\beta') F_l(k, k'; \beta, \beta')$$

then

$$\tilde{U}_0(k, k') = u_0(k, k') + \int_0^\infty d\beta \int_0^\infty d\beta' \tilde{U}_0(\beta, \beta') \tilde{F}_0(k, k'; \beta, \beta') \quad (15)$$

where

$$\begin{aligned} u_0(k, k') &= \gamma_0(k', k)^{(1)} + \frac{1}{8} c_0(k) \frac{1}{k' - k} \ln \left(1 + \frac{k' - k}{2k} \right) \\ &- \frac{1}{16} \int_0^\infty d\beta \frac{c_0(\beta) - c_0(k)}{\beta - k} \frac{1}{\beta - \frac{1}{2}(k + k')} + \frac{1}{2} \frac{k' - k}{k' + k} \int_0^\infty d\beta c_0(\beta) \frac{1}{(2\beta)^2 - (k' - k)^2} \\ &- \frac{1}{16} \int_0^\infty d\beta \frac{c_0(\beta)}{\beta + k} \frac{1}{\beta + \frac{1}{2}(k + k')} + \int_0^\infty d\beta \gamma_+(\beta, \beta') \frac{1}{k' - k} \ln \frac{\beta + k' - k}{\beta} \\ &- \int_0^\infty d\beta \int_0^\infty d\beta' \gamma_+^{(1)}(\beta', \beta) \frac{1}{\beta' - (\beta + k' - k)} \\ &- \int_0^\infty d\beta \gamma_-(\beta, \beta') \frac{1}{k' - k} \ln \frac{\beta - k' + k}{\beta} \\ &- \int_0^\infty d\beta \int_0^\infty d\beta' \gamma_-^{(1)}(\beta', \beta) \frac{1}{\beta' - (\beta - k' + k)} \\ &+ \frac{1}{2\pi} \int_0^\infty d\beta \int_0^\infty d\beta' \frac{1}{\beta'^2 - \beta^2} \beta s_0(\beta') \\ &\times \left\{ \frac{1}{(\beta' - k')^2 - (\beta + k)^2} + \frac{1}{(\beta' + k')^2 - (\beta - k)^2} \right\}. \quad (16) \end{aligned}$$

Here

$$\begin{aligned} \gamma_0(k', k) &= \frac{k}{k' + k} \frac{s_0(k')}{\xi_0(k')} \\ \gamma_\pm(\beta', \beta) &= \frac{1}{2\pi} \frac{\beta s_0(\beta')}{\beta' + \beta} \frac{1}{\beta - \{\pm(k' + k) - \beta\}} \end{aligned}$$

and we use the notation, for any function $\chi(x, y)$

$$\chi^{(1)}(x, y) \equiv \frac{\chi(x, y) - \chi(y, y)}{x - y}.$$

Thus we have a double integral equation in which the kernel has simple poles; the kernel is a simple algebraic expression. What is the possibility of a practical solution, by numerical means, of (15)? It is hard to say, but this type of equation is perhaps about at the limit of present computers' capabilities. In any case, the point would not be to calculate off-shell matrix elements by this method as they are needed in a calculation of some other process. Rather, off-shell elements could be computed once and for all (to be revised, of course, as phase-shift analyses are improved) and once found possibly fitted by a simple analytic formula. This would constitute a parameterization of the two-body interaction to replace the customary parameterization by means of a potential model. It would have the advantage of being more closely related to the uses to which it would be put. Moreover, the possibility of using experimental data on nucleon-nucleon bremsstrahlung to determine half-off-shell elements has recently been investigated (Cromer and Sobel, to be published) and this further argues for the new parameterization.

4. Bound states

In the case of n_l bound states of angular momentum l we expect to find an equation for the off-shell elements which has n_l free parameters, and involves the binding energies $-\kappa_n^2$, and the phase shifts. In what follows we take for simplicity $n_l = 1$; if there are several bound states only minor algebraic modifications occur.

Using the quantity $\bar{\rho}_l$ from (A10), let us define $\bar{g}_l(r, r')$ and $\bar{K}_l(r, r')$ by (A5) and (A9) respectively, with ρ_l replaced by $\bar{\rho}_l$. Then \bar{K}_l is related to the wave function (as in (3)), and to the half-off-shell matrix element. Instead of (14) we have

$$\bar{U}_l(k, k') = \frac{1}{2}\pi s_l(k')k \frac{\eta_l(k', k) - (k/k')^l}{k^2 - k'^2} \quad (17)$$

and (A6) can be written in the form

$$\begin{aligned} \bar{K}_l(r, r') &= \bar{g}_l(r, r') + \int_0^r dr'' \bar{K}_l(r, r'') \bar{g}_l(r'', r') \\ &\quad - \frac{1}{N^2} \phi(r) \int_0^r \phi_l^{(1)}(-i\kappa, r'') \bar{g}_l(r'', r') dr''. \end{aligned} \quad (18)$$

Here $\phi(r)$ is the bound-state wave function, normalized as in (A1). It should be noted that, although N is independent of κ , any information about the bound-state wave function will determine N . For example, one might use the photodisintegration of the deuteron, in principle, to determine the constant N for nucleons.

To solve for the off-shell elements we must eliminate $\phi(r)$, for which purpose we write (A8) at $k = -i\kappa$:

$$\phi(r)D(r) = \phi^{(1)}(-i\kappa, r) + \int_0^r dr' \bar{K}_l(r, r') \phi^{(1)}(-i\kappa, r') \quad (19)$$

where

$$D(r) = 1 + \frac{1}{N^2} \int_0^r dr' \{\phi^{(1)}(-i\kappa, r')\}^2. \quad (20)$$

After some algebra we find from (19) and (20)

$$\begin{aligned} \bar{K}_l(k, k') &= (\frac{1}{2}\pi)^2 \xi_l(k) \delta(k - k') + \frac{1}{2}\pi \xi_l(k') \frac{1}{N^2} h(k, k') \\ &\quad + \frac{1}{2}\pi \xi_l(k') \int_0^\infty d\beta \int_0^\infty d\beta' \bar{K}_l(\beta, \beta') \left\{ F_l(k, k'; \beta, \beta') - \frac{1}{N^2} \Phi(k, k'; \beta, \beta') \right\} \end{aligned} \quad (21)$$

where

$$h(k, k') = \int_0^\infty dr(kr) j_l(kr) \phi^{(1)}(-i\kappa, r) R(k', r)$$

$$\Phi(k, k'; \beta, \beta') = \int_0^\infty dr(kr) j_l(kr) (\beta r) j_l(\beta r) D(r) R(k', r) R(\beta', r)$$

with

$$R(q, r) = D(r)^{-1} \int_0^r dr'(qr') j_l(qr') \phi^{(1)}(-i\kappa, r').$$

Thus (21) replaces (8) as a double integral equation for the half-off-shell matrix element. The singularities at $k = k'$ can be removed in a similar, but much more tedious way. Here the kernel unfortunately is not given analytically. The function Φ involves integrals which, although they involve elementary functions, cannot be done analytically (primarily because of the function $D(r)^{-1}$).

An interesting condition on the bound-state wave function is found by evaluating (19) for large r . The leading terms go as $\exp(\kappa r)$. Taking $\phi(r) \xrightarrow{r \rightarrow \infty} a_\phi e^{-\kappa r}$ and equating coefficients, we find that a_ϕ/N^2 equals a quantity involving the phase shifts alone. Put in terms of the ordinary wave function ψ , normalized by $\int_0^\infty dr \psi^2(r) = 1$, we find

$$ab = \frac{4\kappa^{l+2}}{(2l+1)!!} \left[1 + \frac{1}{2} \int_0^\infty dk c_l(k) (\kappa^2 + k^2)^{-1} \{ \kappa - k \tan \delta_l(k) \} \right] \tag{22}$$

where

$$\psi(r) \xrightarrow{r \rightarrow \infty} a e^{-\kappa r}$$

$$\psi(r) \xrightarrow{r \rightarrow 0} br^{l+1}.$$

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Appendix

Here we present the Gel'fand–Levitan equation for solving the inverse scattering problem, following the treatment and notation of Newton (1960), and at first neglecting bound states. Define $\phi_l(k, r)$ for momentum $k = \sqrt{E^\dagger}$ and angular momentum l , as the solution of the radial Schrödinger equation which goes as

$$\phi_l(k, r) \rightarrow \{(2l+1)!!\}^{-1} r^{l+1} \quad \text{as } r \rightarrow 0. \tag{A1}$$

For large r clearly ϕ_l goes as

$$\phi_l(k, r) \rightarrow |f_l(k)| k^{-l-1} \sin\{kr - \frac{1}{2}\pi l + \delta_l(k)\} \tag{A2}$$

where $\delta_l(k)$ is the phase shift. Provided the first and second moments of $V(r^2, l(l+1))$ are finite, one can show that

$$\ln |f_l(k)| = -\frac{1}{\pi} P \int_{-\infty}^\infty \frac{dk' \delta_l(k')}{k' - k}. \tag{A3}$$

Furthermore we define the spectral function

$$\frac{d\rho_l(E)}{dE} = \frac{1}{\pi} \frac{k^{2l+1}}{|f_l(k)|^2}. \tag{A4}$$

† We use units in which $\hbar = 2m = 1$.

Now to solve the problem one must use a potential $V^{(1)}$ whose phase shifts are known. A kernel function

$$g_i(r, r') = \int d\{\rho_i^{(1)}(E) - \rho_i(E)\} \phi_i^{(1)}(k, r) \phi_i^{(1)}(k, r') \quad (\text{A5})$$

is constructed, using the spectral function $\rho_i^{(1)}$ and wave function $\phi_i^{(1)}$ corresponding to $V^{(1)}$. Then one must solve the integral equation

$$K_i(r, r') = g_i(r, r') + \int_0^r dr'' K_i(r, r'') g_i(r'', r') \quad (\text{A6})$$

for K_i . The potential may be constructed from K_i by

$$V(r^2, l(l+1)) = V^{(1)}(r^2, l(l+1)) + 2 \frac{d}{dr} K_i(r, r). \quad (\text{A7})$$

The wave function ϕ_i is related to K_i by

$$\phi_i(k, r) = \phi_i^{(1)}(k, r) + \int_0^r dr' K_i(r, r') \phi_i^{(1)}(k, r') \quad (\text{A8})$$

which is essentially the Fourier transform of (A6), and

$$K_i(r, r') = \int d\{\rho_i^{(1)}(E) - \rho_i(E)\} \phi_i(k, r) \phi_i^{(1)}(k, r'). \quad (\text{A9})$$

If there are bound states at energies $E_n = -\kappa_n^2$ ($n = 1, \dots, n_i$) one does not find a unique potential. There is rather an n_i -parameter set of potentials. Equations (A5)–(A9) remain valid, but the spectral function is changed to

$$\frac{d\rho_i(E)}{dE} = \frac{1}{\pi} \frac{k^{2l+1}}{|f_i(k)|^2} + \sum_{n=1}^{n_i} \frac{\delta(E - E_n)}{N_n^2} = \frac{d\bar{\rho}_i(E)}{dE} + \sum_{n=1}^{n_i} \frac{\delta(E - E_n)}{N_n^2} \quad (\text{A10})$$

and (A3) becomes

$$\ln|f_i(k)| = -\frac{1}{\pi} P \int \frac{dk' \delta_i(k')}{k' - k} + \sum_{n=1}^{n_i} \ln \frac{E - E_n}{E}. \quad (\text{A11})$$

The N_n are free parameters.

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