EXACT ANALYTIC SOLUTIONS IN CONFIGURATION SPACE FOR SCATTERING WAVEFUNCTIONS AND T MATRICES FOR A CLASS OF SEPARABLE NONLOCAL POTENTIALS

DISSERTATION

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by

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TABLE OF CONTENTS

TABLE OF CONTENTS (continued)

LIST OF FIGURES

CHAPTER I

INTRODUCTION

In most of the literature of physics the description of interacting particleshas been formulated in terms of static, local potentials. However, the most general potential that can be written is a nonlocal potential, such a potential being the spatial representative of an arbitrary potential operator. Consider the Schrödinger equation

$$(H_0 - E)\,|\Psi\rangle = -V\,|\Psi\rangle$$

Operating with the bra $\langle \vec{r}\,|$ and writing $\langle \vec{r}\,|\Psi\rangle \equiv \Psi(\vec{r})$ we get

$$\left(\frac{\hbar^2}{2m}\,\nabla^2 + E\right)\Psi(\vec{r}) = \int \langle \vec{r}\,|V|\vec{r}'\rangle\,\Psi(\vec{r}')\,d\vec{r}' \qquad (1)$$

The kernel $\langle \vec{r}\,|V|\vec{r}'\rangle$ [also often written $V(\vec{r}|\vec{r}')$] of the integro-differential Eq. (1) is called a nonlocal potential, as the potential energy of the system at point $\vec{r}$ depends on the behaviour of the wavefunction at neighbouring points $\vec{r}'$.

If we put $\langle \vec{r}|\,V|\vec{r}'\rangle = \delta(\vec{r}-\vec{r}')\,V(\vec{r})$, Eq. (1) reduces to

$$\left(\frac{\hbar^2}{2m}\,\nabla^2 + E\right)\Psi(\vec{r}) = V(\vec{r})\,\Psi(\vec{r})$$

which is the usual Schrödinger equation with a local potential $V(\vec{r})$. Thus the local potential $V(\vec{r})$ that is generally used is nothing but a special case of a nonlocal potential.[1]

Nonlocality of a potential in configuration space is equivalent to its dependence on the average momentum and, as such, nonlocal potentials are also called momentum (or velocity) dependent potentials. This dependence has been shown by Mulligan[2] and Hoshikazi and Machida[3]. We will discuss this using a simpler method, due to Tamagaki and Watari[4]. In terms of Fourier transforms we can write

$$\langle \vec{r}|V|\vec{r}'\rangle = \left(\frac{1}{2\pi}\right)^6 \int\int \langle \vec{p}|V|\vec{p}'\rangle \, e^{i(\vec{p}\cdot\vec{r} - \vec{p}'\cdot\vec{r}')} \, d\vec{p}\, d\vec{p}' \qquad (2)$$

where we have used $\langle \vec{r}|\vec{p}\rangle = \left(\frac{1}{2\pi}\right)^3 e^{i\vec{p}\cdot\vec{r}}$

Rewriting Eq. (2) with variables

$\vec{P} = (\vec{p} - \vec{p}')$ (momentum transfer) and

$\vec{Q} = (\vec{p} + \vec{p}')/2$ (average momentum) and

remembering that the Jacobian is unity, we have

$$\langle \vec{r}|V|\vec{r}'\rangle = \left(\frac{1}{2\pi}\right)^6 \int\int V(\vec{P},\vec{Q}) \, e^{i[\vec{Q}\cdot(\vec{r}-\vec{r}')+\vec{P}\cdot(\vec{r}+\vec{r}')/2]} \, d\vec{P}\, d\vec{Q}$$

where $V(\vec{P},\vec{Q}) \equiv \langle \vec{p}|V|\vec{p}'\rangle$

If $V(\vec{P},\vec{Q})$ is independent of $\vec{Q}$, namely a function of the momentum transfer $\vec{P}$ only, i.e., if

$$V(\vec{P}) \equiv V(\vec{P},\vec{Q}), \text{ then}$$

$$\langle \vec{r}|V|\vec{r}' \rangle = \delta(\vec{r}-\vec{r}') \left(\frac{1}{2\pi}\right)^3 \int V(\vec{P})\, e^{i\vec{P}\cdot(\vec{r}+\vec{r}')/2}\, d\vec{p}$$

$$= \delta(\vec{r}-\vec{r}')\, V(\vec{r})$$

where $V(\vec{r}) = \left(\frac{1}{2\pi}\right)^3 \int V(\vec{P})\, e^{i\vec{P}\cdot\vec{r}}\, d\vec{P}$

This means that $\vec{Q}$ (average momentum) dependence of $V(\vec{P},\vec{Q})$ causes nonlocality in configuration space.

Interest in calculations involving nonlocal potentials is of very recent origin, in spite of their being the more general spatial representation of the arbitrary potential operator V. The reason probably is the success of local potentials such as the Coulomb potential in many diverse quantum mechanical calculations. Also, it seems that one can 'visualize ' a local potential such as a square well potential, whereas the nonlocal potential may seem to be 'unphysical'. However, the importance of nonlocal potentials was realized as early as 1937 by Wheeler.[5] Not much work was done till 1941, when Buckingham and Massey [6] used a nonlocal potential to explain the data on neutron-deuteron scattering. Almost another thirteen years passed before further work was published. In 1954

a pair of articles was published by Yamaguchi [7] to show the usefulness of a nonlocal separable potential in fitting nucleon-nucleon (N-N) scattering data.

Again there was almost no work done in this field until 1958, when Feshbach [8] demonstrated that the nucleon-nucleus optical model-potential was in fact, nonlocal. The success of local optical models in fitting nuclear data suggested further work in understanding the effect of the nonlocality. Pioneering work in investigating the relationship between local and nonlocal potentials was done by Perey and Buck (1962) [9] and B. Mulligan (1964) [2]. Ghirardi and Rimini (1964) [10] and F. Tabakin (1964) [11] investigated other aspects of the use of nonlocal potentials. Still, the attention was so limited that in 1965 W. H. Nichols,Jr. [12] wrote in an article, " the separable nonlocal potential in quantum mechanics has been used little in either research or teaching since it seems so unphysical". But it was soon realized that a nonlocal potential can be used in many problems where it is reasonable to use a local potential and, in some instances, it is more convenient to use a nonlocal potential. In fact, after the work of Faddeev, [13] Lovelace, [14] and Mitra [15] on many particle scattering theory, where it was shown that a separable nonlocal potential reduces the many particle calculations to the level of two particle calculations, flurries of activities started in this field. Work on the

analytic properties of the radial Schrödinger equation for a nonlocal potential[16] now roughly parallels the earlier studies of the analytic properties of the radial Schrödinger equation for a local potential[17].

A nonlocal potential with no conditions attached to it except that it be Hermitian (to impose that energy eigenvalues be real) is mathematically extremely difficult to handle. The case is much simpler if the nonlocal potential is separable. The term separable indicates the fact that the interaction, which is assumed to be Hermitian, is characterized by structural features that allow it to be factored in a particular way. The interaction $V(\vec{r}|\vec{r}') = \lambda\, v(\vec{r})\, v^*(\vec{r}')$ is called a simple separable potential or a one-term or rank one separable nonlocal interaction. The most general nonlocal separable interaction, written in the operator formalism, is

$$V = \sum_{i,j=1}^{N} \lambda_{i\,j} |v_i\rangle\langle v_j|$$

In practice $V(\vec{r}|\vec{r}')$ is taken to be real, and the condition of Hermiticity follows once the individual terms are taken to be symmetric.

Since the publication of the classic papers by Yamaguchi[7] a number of separable potential models[18-25] have been proposed for the N-N interaction. These models came into the picture because of the basic assumption of current nuclear many-body theory that properties of nuclei such as level spectra and saturation of energy and density can be derived from a suitable N-N interaction. Since a local or 'static' potential requires

a hard core[26] in order to fit high energy data, and a hard core is a computational stumbling block, it is no wonder that many varieties of separable potentials have been used. Because the nucleon-nucleon phase shift data requires repulsion for very small distances and attraction for larger distances, almost all separable models use a rank two separable potential. The Yamaguchi potential, being of rank one, can fit the experimental data only at low energies. Out of all published separable potentials the only one-term potential which shows the change of sign of the phase shift characteristic of a local potential with a repulsive core coupled with a short-range attraction is that of Tabakin.[20] The form factor for this potential, however, is very complicated. The failure to get any polarization effect from the Yamaguchi potential with a tensor term[27] further suggests a reason for looking for a realistic potential among rank two or more separable potentials. In passing, it may be mentioned that Mongan [21] has done the most extensive separable potential fits to two-nucleon data and in doing so he has used four types (Case I-IV) of two-term separable potential models.

Most of the fitting with separable potentials has been done first by assuming a reasonable potential (as was done by Yamaguchi) and then adjusting the parameters to fit the required data. However, many theoretical investigations have been carried out on the inverse problem, i.e., the problem of finding a potential, expressible as a sum of a finite

number of separable terms, to fit certain characteristics such as phase shifts at all energies or the off-shell T matrices. Chadan[28], Mills and Reading[29], Tabakin[30], and Fiedeldey[31] have all approached the problem of phase shift fitting. Ernst, Shakin and Thaler[32] have presented a method which permits the construction of a rank-N separable potential which has the property that the resulting T matrix is exact both on the energy shell and half off the energy shell at N selected bound states and for continuum energies. They have applied the method to find a separable potential equivalent to a local square well potential.

Even before extensive fitting was done with nonlocal potentials, it was clear that certain properties of nonlocal potentials would be different from those of local potentials. After the publication of the Perey-Buck paper[9], Austern[33] found that eigenfunctions of the attractive nonlocal single particle Perey-Buck potential are always smaller inside the region of the potential than outside, with the inverse occuring for a repulsive potential of the same form. This is the so-called Perey effect. The Perey effect has been the subject of several recent papers.[34-39]

Later on other phenomena such as continuum bound states (CBS) and confusion about what constitutes an attractive or repulsive separable potential have required a development of methods involving a comparison between characteristics of separable potentials and the more familiar phenomenology of local potentials. At first, usual practice with regard to

the nucleon-nucleon interaction was to restrict the comparison to such features as the phase shifts or T matrix elements. But following Fiedeldey[40], Coz, Arnold and MacKellar[41] were able to define precisely an equivalent local potential (ELP) and show that a unique potential and solutions to an equivalent local equation can be obtained once two independent solutions of the nonlocal equation are known. Jost solutions[42] have become very prominent in this type of analysis. In fact, Arnold and MacKellar[43] have pointed out that the difference between a local and a nonlocal potential lies in the behaviour of the Wronskian of the two Jost solutions. This Wronskian is a constant for a local potential but is not constant for a nonlocal potential. Jost solutions are normalized so that the local potential Wronskian is everywhere unity, whereas the nonlocal potential Wronskian is found to approach unity at infinity. Thus deviation of the Wronskian from unity can be taken[43] to be a measure of the non-locality of a potential as a function of k and r.

In analyzing the ELP , Arnold and MacKellar also pointed out that a 'spurious' state exists for a nonlocal potential at energies where the Fredholm determinant goes to zero. It had already been shown by Gourdin and Martin[44] that one feature of the separable nonlocal potential is the possibility of wavefunctions in its spectrum which exist at positive energies yet behave asymptotically like bound states. These states have been labelled as positive energy bound states, positive energy degenerate

states, spurious bound states or simply continuum bound states (CBS). A CBS will always be characterized by a zero of the Fredholm determinant, but the spurious states shown by Arnold and MacKellar may also occur at energies other than those at which a CBS is found. By combining the Fredholm determinant technique with the ELP analysis these authors have also been able to show that both kinds of 'spurious' behaviour are characteristics only of nonlocal potentials. Chadan[28], while considering the inverse problem with a sum of separable potential plus a local potential, had noted that his local potential alone would not produce CBS. Work in this regard has been recently done by Krause and Mulligan[45]. Using a Green's function method they have shown that the presence of CBS is characteristic only of a nonlocal potential and arises when the Green's function is cancelled by the separable potential.

It is now generally accepted on the basis of theoretical arguments that the interaction between two nucleons is nonlocal[46]. Since the two-particle interaction is unknown, in recent years a number of separable models[18-25] have been used to fit the two nucleon data. These models are attractive because of the simplicity and ease they bring to the calculations, over and above their reasonably good fitting of the data. The two nucleon data is in principle inadequate to enable us to deduce a unique nucleon-nucleon potential, and each of these potential models implies a rather arbitrary off-shell extension of the two body scattering amplitude.

Unfortunately, however, there is practically no experimental data available on the off-shell T matrix elements. But Faddeev has shown that equations for three body scattering may be obtained in which the only input is the off-energy-shell T matrices for scattering of each of the three possible pairs of particles. It is, therefore, clear that to reduce the ambiguity in the two nucleon potential one must test it in three particle problem, in nuclear matter, and in general in nuclear structure calculations. Several separable potential models with a Yamaguchi form factor have already been used in finding the triton binding energy and in neutron-deuteron scattering[47]. Calculations with the triton have the advantage that they avoid Coulomb effects. It has been found[48] that triton binding energy is very sensitive to the parameters of the two nucleon separable potential.

Mitra has shown that quantum mechanical motion of three non-relativistic particles interacting via separable potentials can be reduced to a form not more complicated that that of the two body problem[48]. But since the three body calculations require two body off-shell T matrices, computationally the problem is still very difficult to solve. In the case of a separable potential, off-shell T matrices can be computed from the expressions given by Tabakin[11]. These expressions have been widely used even though they require the solution of a number of contour integrals. In the case of the Yamaguchi form factor these contour integrals can be handled quite easily; probably that is why the Yamaguchi form factor has been

used widely. These form factors, however, give a triton binding energy higher than the experimental value.

In short, looking at the situation of the two nucleon separable potential we see that what we need is a number of realistic separable potentials with a wide class of form factors which can be easily used in three or many particle calculations. This implies the desirability of a simple technique to get the off-shell T matrices. In this dissertation we take a reasonable class of nonlocal separable potentials of rank N (the Yamaguchi and Mongan case IV potentials are special cases of this class) and find analytic solutions in compact form in configuration space. We also obtain the irregular solutions and Jost solutions to determine analytic expressions for the equivalent local potentials. Next we find the off-shell T matrices for this class of potentials in a compact form which avoids contour integration. In so doing we hope these form factors can be easily applied in future many-particle calculations.

CHAPTER II

REGULAR SOLUTIONS FOR A CLASS OF POTENTIALS

In this chapter we consider a particular class of separable nonlocal potentials and demonstrate a technique by which analytic solutions for the wave functions in the coordinate representation can be found for all partial waves. Although the formalism which we shall present here refers to spinless particles and a spin-independent interaction, it is a simple matter to extend the technique to coupled channel calculation for which the coupling term is of exponential form.

The Schrödinger equation for a nonlocal potential in center of mass coordinates has been given as Eq. (1), and is

$$\frac{\hbar^2}{2m} \nabla^2 \Psi(\vec{r}) + E\Psi(\vec{r}) = \int \langle \vec{r} | V | \vec{r}' \rangle \Psi(\vec{r}') \, d\vec{r}' \tag{3}$$

in an obvious notation. To expedite the solution of Eq. (3), $\Psi(\vec{r})$ and $\langle \vec{r} | V | \vec{r}' \rangle$ (assumed to be rotationally invariant) are normally expanded in terms of partial waves:

$$\Psi(\vec{r}) = \sum_{\ell=0}^{\infty} \frac{u_\ell(r)}{r} P_\ell(\cos\theta)$$

$$\langle \vec{r} | V | \vec{r}' \rangle = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{+\ell} \frac{g_\ell(r|r')}{r r'} Y_\ell^m(\theta,\phi) \, Y_\ell^{m*}(\theta',\phi')$$

Substituting these expressions into Eq. (3) gives the nonlocal Schroedinger equation for each partial wave ℓ

$$\left[\frac{d^2}{dr^2} + k^2 - \frac{\ell(\ell+1)}{r^2}\right] u_\ell(r) = \frac{2m}{\hbar^2} \int_0^\infty g_\ell(r|r')\, u_\ell(r')\, dr' \qquad (4)$$

where $k^2 = \frac{2m}{\hbar^2} E$.

The class of potentials $g_\ell(r|r')$ for which we are able to obtain exact analytic solutions is defined by

$$g_\ell(r|r') = \frac{\hbar^2}{2m} \sum_\nu e^{-\alpha_\nu (r+r')} (rr')^{n_\nu} \sum_{g=0}^{K_\nu} \sum_{i=0}^{J_\nu} \Lambda^\nu_{gi}\, P^\nu_g(r) P^\nu_i(r') \qquad (5)$$

where the Λ^ν_{gi} are constants; the n_ν are, for simplicity, taken to be integers and $P^\nu_i(r)$ is an arbitrary polynomial in r of order i. That is

$$P^\nu_i(r) = \sum_{j=0}^{i} b^{(i,\nu)}_j\, r^j . \qquad (6)$$

Note that the potential of Eq. (5) will be Hermitian only if $\Lambda^\nu_{gi} = \Lambda^\nu_{ig}$ and $K_\nu = J_\nu$. The solution to the potential given in Eq. (5) can be constructed by taking advantage of the linear nature of the integro-differential equation, Eq. (4). This allows us to base our discussion on a solution of Eq. (4) for which $g_\ell(r|r')$ assumes the simple separable form

$$g_\ell(r|r') = \frac{\hbar^2}{2m} \lambda\, q(r)\, q(r') \qquad (7)$$

with

$$q(r) = A\, e^{-\alpha r}\, r^n \qquad (8)$$

For convenience, the subscript ℓ has been suppressed on both λ and $q(r)$.

For a potential of the form given by Eq. (7), Eq. (4) can be written as

$$\left[\frac{d^2}{dr^2} + k^2 - \frac{\ell(\ell+1)}{r^2}\right] u_\ell(r) = \lambda\, q(r) \int_0^\infty q(r')\, u_\ell(r')\, dr'. \tag{9}$$

For later purposes, it is also convenient to introduce the constant C, defined by

$$\int_0^\infty q(r')\, u_\ell(r')\, dr' = C. \tag{10}$$

Thus we see that the basic equation to be solved for a given partial wave is

$$\left[\frac{d^2}{dr^2} + k^2 - \frac{\ell(\ell+1)}{r^2}\right] u_\ell(r) = \lambda C q(r) \tag{11}$$

subject to the condition (10).

Equation (11) has been treated by several investigators in several different ways. In particular, Cassola and Koshel[49] and Moiseiwitsch[50] have shown that the use of Green's function allows one to write down explicit expressions for the phase shifts and wave functions for any ℓ for an arbitrary potential function $q(r)$. While these expressions are of use for numerical calculations, they lead to analytic results for wave-functions and phase shifts only if the necessary integrals can be performed.

1. The Method of Solution

The structure of Eq. (11) differs significantly, depending upon whether $n \geq \ell$ or $n < \ell$. Comparison with Schroedinger equations for non-singular local potentials shows that the case $n \geq \ell$ will correspond most closely to results which might be expected from calculations with a local potential. The conclusions presented in this chapter are thus restricted to values of $n \geq \ell$.

The potential function of Eq. (8) was discussed as early as 1941 by Buckingham and Massey,[6] who obtained explicit solutions of Eq. (9) in the case $\ell = 0$. Hussain and Ali[51] have suggested a simplification of the method of Cassola and Koshel, and have recalculated Buckingham and Massey's results as an example of the use of their procedure. Neither group of investigators, however, has attempted the analytic solution of Eq. (9) for arbitrary ℓ.

The technique which we have found useful in obtaining solutions of Eq. (9) with the potential function (8), and which can be used to obtain exact analytic solutions for the potential (5), is that of introducing into (9) for $u_\ell(r)$ the product $e^{-\alpha r}$ times a power series in r. We are able to find the solution in terms of this series, and then, in turn, are able to sum the series to put the solution into a compact form.

For the potential function (8), Eq. (9) becomes

$$\left[\frac{d^2}{dr^2} + k^2 - \frac{\ell(\ell+1)}{r^2}\right] u_\ell(r) = De^{-\alpha r} r^n \tag{12}$$

where $D = \lambda CA$. Equation (12) is basically an inhomogeneous spherical Bessel equation, but subject to the subsidiary condition (10) which assures the homogeneity of the original integro-differential equation. Inserting into Eq. (12) a solution of the form

$$u_\ell(r) = D\, e^{-\alpha r} r^{n+2} \sum_{m=0}^{\infty} a_m r^m , \tag{13}$$

we find the following recurrence relation for the coefficients a_m

$$a_m = \frac{2\alpha(m+n+1)}{(m+n+2+\ell)(m+n+1-\ell)} a_{m-1} - \frac{\alpha^2 + k^2}{(m+n+2+\ell)(m+n+1-\ell)} a_{m-2} \tag{14}$$

The homogeneity of the integro-differential equation imposes the additional conditions that

$$a_0 = \frac{1}{(n+2+\ell)(n+1-\ell)} \tag{15}$$

$$a_1 = \frac{(2n+4)\,\alpha}{(n+3+\ell)(n+2-\ell)} \alpha_0 \tag{16}$$

In order to find an expression for a_m consistent with conditions (15) and (16), it is necessary to treat Eq. (14) by difference equation techniques. The general solution to a second order difference equation contains two arbitrary constants. The two arbitrary constants which appear in the general solution of Eq. (14) can be evaluated so as to give

for a_o and a_1 the values demanded in (15) and (16). There is no general procedure for solving a second order difference equation with variable coefficients [see, for example, Ref. (52)]. The case of $\ell = 0$, however, is fairly simple, and since it suggests the difficulties to be overcome for $\ell \neq 0$, we present it in the following section as a separate case.

In passing, we point out that in an earlier paper Luke[53] has solved an equation similar to Eq. (12). However, in his case, the operator appearing on the left-hand side was that of a modified Bessel equation, and resulted in a two term recurrence relation (a first order difference equation) which could be solved by standard techniques.

2. Solution for $\ell=0$

The case $\ell = 0$ is simple because under this condition Eq. (14) can be converted into an equation with constant coefficients by using the substitution

$$a_m = \frac{b_m}{(m+n+2)!} \tag{17}$$

The difference equation for b_m is

$$b_m - 2\alpha b_{m-1} + (\alpha^2 + k^2) b_{m-2} = 0 \tag{18}$$

Using the standard technique for solving a difference equation with constant coefficients,[54] we get

$$b_m = C_1 (\alpha+ik)^m + C_2 (\alpha-ik)^m \tag{19}$$

Equation (12) contains only real terms and it is the real solution to this equation which we wish to obtain. This can be accomplished by the usual proper choice of the constants C_1 and C_2 in terms of real constants F and G. The general real expression for a_m can be put into the form

$$a_m = \frac{(\alpha^2+k^2)^{\frac{m+n+2}{2}}}{(m+n+2)!} [F \cos(m+n+2)\theta + G \sin(m+n+2)\theta] \tag{20}$$

where

$$\theta = \arctan \frac{k}{\alpha} \tag{21}$$

The constants F and G determined from Eqs. (15) and (16) are:

$$F = - \frac{n! \sin(n+1)\theta}{k(\alpha^2+k^2)^{\frac{n+1}{2}}} \tag{22a}$$

$$G = \frac{n! \cos(n+1)\theta}{k(\alpha^2+k^2)^{\frac{n+1}{2}}} \tag{22b}$$

Equation (20) for a_m then reduces to

$$a_m = \frac{n!(\alpha^2+k^2)^{\frac{1}{2}(m+1)}}{k(m+n+2)!} \sin(m+1)\,\theta \tag{23}$$

and we have

$$\sum_{m=0}^{\infty} a_m r^m = \frac{n!\, r^{-n-2}}{k(\alpha^2+k^2)^{\frac{n+1}{2}}} \sum_{m=0}^{\infty} \frac{(\alpha^2+k^2)^{\frac{m+n+2}{2}} \sin(m+1)\,\theta\, r^{m+n+2}}{(m+n+2)!} \tag{24}$$

The series in Eq. (24) can be evaluated by replacing $\sin(m+1)\,\theta$ in Eq. (24) by $e^{i(m+n+2)\,\theta}$, summing, multiplying by $e^{-i(n+1)\,\theta}$, and taking the imaginary part. Multiplying by $De^{-\alpha r} r^{n+2}$, we get as a particular solution $u_o^P(r)$ the result

$$u_o^P(r) = \frac{n!\, De^{-\alpha r}}{k(\alpha^2+k^2)^{\frac{n+1}{2}}} \left\{ e^{\alpha r} \sin[kr-(n+1)\theta] + \sum_{s=0}^{n} \frac{(\alpha^2+k^2)^{s/2}}{s!} r^s \sin(n+1-s)\theta \right\} \tag{25}$$

The general solution of Eq. (12) is the particular solution $u_o^P(r)$ plus the general solution of the homogeneous part, namely M sin kr + N cos kr. In specifying M and N we make use of two conditions which the wave function $u_o(r)$ must satisfy. The first is that $u_o(r)$ be zero at r = 0. Since the particular solution $u_o^P(r)$ is zero at r = 0, we must choose N = 0. The second condition will determine the normalization of $u_o(r)$. In this chapter

we have followed the convention standard in the discussion of Jost solutions,[55] and normalized the regular solution $u_o(r)$ to unit slope at the origin. This requires that $M = 1/k$. The reader should note that this choice for M results in wave functions which are not normalized to $\delta(k-k')/k^2$, another standard normalization.

With the boundary conditions specified above we find that

$$u_o(r) = \frac{\sin kr}{k} + \frac{D\, n!\, \cos(n+1)\,\theta}{k(\alpha^2 + k^2)^{\frac{n+1}{2}}} \sin kr - \frac{D\, n!\, \sin(n+1)\,\theta}{k(\alpha^2 + k^2)^{\frac{n+1}{2}}} \cos kr$$

$$+ \frac{n!\, D\, e^{-\alpha r}}{k(\alpha^2 + k^2)^{\frac{n+1}{2}}} \sum_{s=0}^{n} \frac{(\alpha^2 + k^2)^{\frac{s}{2}}}{s!}\, r^s \sin(n+1-s)\,\theta. \qquad (26)$$

The constant D can be evaluated by substituting expression (26) for $u_o(r)$ into Eq. (10). We get

$$D = \frac{\lambda A^2 n!\, \sin(n+1)\,\theta}{k\Delta(\alpha^2 + k^2)^{\frac{n+1}{2}}} \qquad (27a)$$

where

$$\Delta = 1 - \frac{\lambda A^2\, n!}{k(\alpha^2+k^2)^{\frac{n+1}{2}}} \sum_{s=0}^{n} \frac{(n+s)!\,(\alpha^2+k^2)^{\frac{s}{2}}\, \sin(n+1-s)\,\theta}{s!\,(2\alpha)^{n+s+1}} \quad . \qquad (27b)$$

It is interesting to note that Δ is the same as the Fredholm determinant appropriate to this potential, which has been discussed extensively elsewhere.[43] In particular, the zeros of $\Delta(k)$ are known to correspond to so-called spurious solutions of Eq. (12). The solution of Eq. (12) given in Eq. (26) is not valid at the energies for which $\Delta(k) = 0$.

The phase shift δ_0 also follows from Eq. (12) once D is known, with $\tan\delta_0$ given by

$$\tan\delta_0 = -\frac{n!\, D \sin(n+1)\theta}{(\alpha^2+k^2)^{\frac{n+1}{2}} + n!\, D\cos(n+1)\theta}$$

$$= -\frac{\lambda A^2 (n!)^2 \sin^2(n+1)\theta}{k(\alpha^2+k^2)^{n+1} + \lambda A^2 n!\left[\frac{n!}{2}\sin(2n+2)\theta - \sum_{s=0}^{n} \frac{(n+s)!\,(\alpha^2+k^2)^{\frac{n+s+1}{2}}}{s!(2\alpha)^{n+s+1}}\sin(n+1-s)\theta\right]} \tag{28}$$

For the case λ=1, n = 1, A = λ, the phase shift δ_0 given by Eq. (28) agrees with that presented in Mott and Massey.[56]

3. Solution for Arbitrary ℓ

For $\ell > 0$, the difference equation (14) cannot be solved by standard procedures. To find the general expression for a_m, to which we can apply conditions (15) and (16), we multiply Eq. (14) by r^m and sum over m. We find that the function

$$y = \sum_{m=0}^{\infty} a_m r^m \tag{29}$$

satisfies the differential equation

$$r^2 y'' + [(2n+4)r - 2\alpha r^2\ ]\ y' + [(n^2+3n+2-\ell-\ell^2) - 2\alpha(n+2)r + (\alpha^2+k^2)\ r^2\ ]\ y = 0 \tag{30}$$

The general solution of Eq. (30) is

$$y(r) = e^{\alpha r} r^{-n-1} [C_1 h_\ell(kr) + C_2 h_\ell^*(kr)\ ] \tag{31}$$

where

$$h_\ell(kr) = i^{-\ell-1}(kr)^{-1} e^{ikr} \sum_{s=0}^{\ell} \frac{(\ell+s)\,!}{s!(\ell-s)\,!} (-2ikr)^{-s} \tag{32}$$

Expanding y(r) in a power series in r gives as the general solution for a_m

$$a_m = C_1 (-i)^{\ell+1} \sum_{s=0}^{\ell} \frac{(\ell+s)\,!}{s!(\ell-s)\,!} (-2ik)^{-s} \frac{(\alpha+ik)^{m+n+s+2}}{(m+n+s+2)\,!}$$

$$+ C_2\, i^{\ell+1} \sum_{s=0}^{\ell} \frac{(\ell+s)\,!}{s!(\ell-s)\,!} (2ik)^{-s} \frac{(\alpha-ik)^{m+n+s+2}}{(m+n+s+2)}\ . \tag{33}$$

The constants C_1 and C_2 can be so chosen as to put this solution into a real form. We get

$$a_m = \sum_{s=0}^{\ell} B_s \frac{(\alpha^2+k^2)^{\frac{m+s+n+2}{2}}}{(m+s+n+2)} \{F\cos[(m+s+n+2)\theta+(s-\ell-1)\pi/2] + G\sin[(m+s+n+2)\theta+(s-\ell-1)\pi/2]\} \quad (34)$$

where

$$B_s = \frac{(\ell+s)!}{s!(\ell-s)!(2k)^s} \quad (35)$$

and θ is as defined in Eq. (23).

The choices for F and G are fixed by Eqs. (15) and (16), and are

$$F = \frac{1}{x(n+1-\ell)(n+2+\ell)} \sum_{s=0}^{\ell} E_s \left[\sin\{(s+n+3)\theta + (s-\ell-1)\pi/2\} - \frac{(2n+4)(s+n+3)}{(n+2-\ell)(n+3+\ell)} \cos\theta \sin\{(s+n+2)\theta + (s-\ell-1)\pi/2\}\right] \quad (36)$$

$$G = \frac{1}{x(n+1-\ell)(n+2+\ell)} \sum_{s=0}^{\ell} E_s \left[\frac{(2n+4)(s+n+3)}{(n+2-\ell)(n+3+\ell)} \cos\theta \cos\{(s+n+2)\theta + (s-\ell-1)\pi/2\} - \cos\{(s+n+3)\theta + (s-\ell-1)\pi/2\}\right] \quad (37)$$

where

$$E_s = \frac{(\ell+s)!(\alpha^2+k^2)^{\frac{s+n+3}{2}}}{s!(\ell-s)!(s+n+3)!(2k)^s} \quad (38)$$

and

$$x = \sum_{s=0}^{\ell}\sum_{t=0}^{\ell} \frac{(\ell+s)!(\ell+t)!(\alpha^2+k^2)^{\frac{2n+s+t+5}{2}} \sin\{(t-s+1)\theta + (t-s)\pi/2\}}{s!(\ell-s)!\,t!(\ell-t)!(2k)^{s+t}(s+n+2)!(t+n+3)!} \quad (39)$$

The series $\sum_{m=0}^{\infty} a_m r^m$ can be easily evaluated in the same way as in the $\ell = 0$ case. As a particular solution $u_\ell^P(r)$ we get the result

$$u_\ell^P(r) = F\,D\,krj_\ell(kr) + G\,D\,krn_\ell(kr)$$

$$- D\,e^{-\alpha r} \sum_{s=0}^{\ell} \sum_{t=0}^{n+s+1} \frac{(\ell+s)!(\alpha^2+k^2)^{t/2} r^{t-s}}{t!s!(\ell-s)!(2k)^s} [F\cos\{t\theta+(s-\ell-1)\pi/2\}$$

$$+ G \sin\{t\theta+(s-\ell-1)\pi/2\} \qquad (40)$$

Adding the general homogeneous solution and applying the appropriate boundary conditions[8] gives

$$u_\ell(r) = \frac{(2\ell+1)!!}{k^{\ell+1}} krj_\ell(kr) + F\,D\,kr\,j_\ell(k4) + G\,D\,krn_\ell(kr)$$

$$-D\,e^{-\alpha r} \sum_{s=0}^{\ell} \sum_{t=0}^{n+s+1} \frac{(\ell+s)!(\alpha^2+k^2)^{t/2} r^{t-s}}{t!s!(\ell-s)!(2k)^s} [F\cos\{t\theta+(s-\ell-1)\pi/2\}$$

$$+ G \sin\{t\theta+(s-\ell-1)\pi/2\}]. \qquad (41)$$

The constant D can be evaluated by substituting expression (41) for $u_\ell(r)$ into Eq. (10). We get

$$D = \lambda A^2 \frac{(2\ell+1)!!}{k^{\ell+1}} \sum_{s=0}^{\ell} B_s (n-s)!(\alpha^2+k^2)^{\frac{s-n-1}{2}} \cos\{(n-s+1)\theta+(s-\ell-1)\pi/2\}/\Delta \qquad (42a)$$

where

$$\Delta = 1 - \lambda A^2 \sum_{s=0}^{\ell} B_s (n-s)!(\alpha^2+k^2)^{\frac{s-n-1}{2}} [G\sin\{(n-s+1)\theta+(s-\ell-1)\pi/2\}$$

$$+F\cos\{(n-s+1)\theta+(s-\ell-1)\pi/2\}]$$

$$+\lambda A^2 \sum_{s=0}^{\ell} \sum_{t=0}^{s+n+1} \frac{B_s(n+t-s)!(\alpha^2+k^2)^{t/2}}{t!(2\alpha)^{n+t-s+1}} [F\cos\{t\theta+(s-\ell-1)\pi/2\}$$

$$+G\sin\{t\theta+(s-\ell-1)\pi/2\}] \qquad (42b)$$

and B_s is given by Eq. (35).

Also, once D is known, we can write

$$\tan\delta_\ell = -\,G\,D \Big/ \left[\frac{(2\ell+1)!!}{k^{\ell+1}} + F\,D\right] \tag{43}$$

where F and G are given by Eqs. (36) and (37) and D by Eq. (42a). It can easily be shown that the equations for arbitrary ℓ reduce to those given in the previous section for $\ell = 0$.

Several types of numerical calculations were performed to check the equations of this and the previous section for algebraic errors. First, ℓ=0 phase shifts were calculated independently and compared with those from Eq. (28). Next, numerical values of a_m given by Eq. (34) were shown to satisfy Eq. (14). Finally, phase shifts for ℓ and n from 0 to 4 were obtained by numerical integration of Eq. (12) and were found to agree with those given by Eq. (43).

4. The Solution for the General Separable Potential

Before presenting the solution for the general potential given by Eq. (5), we will discuss two less complicated examples. These examples are of interest in that they give additional insight into the formulation of the solution with the general potential, and will be discussed in the next section, which deals with the inversion problem. We consider first a potential of the form of Eq. (5) for which α is fixed (no summation over ν). That is, we consider the potential

$$g_\ell(r|r') = \frac{\hbar^2}{2m}\, e^{-\alpha(r+r')}(rr')^n \sum_{i=0}^{J} \lambda_i P_i(r)\, P_i(r') \quad . \tag{44}$$

For this potential, the differential equation for the radial function $u_\ell(r)$ becomes

$$\left[\frac{d^2}{dr^2} + k^2 - \frac{\ell(\ell+1)}{r^2}\right] u_\ell(r) = \sum_{i=0}^{J} \sum_{j=0}^{i} \sum_{k=0}^{i} \lambda_i b_j^{(i)} b_k^{(i)} C_k^{(n)} e^{-\alpha r} r^{n+j} \tag{45}$$

where

$$C_k^{(n)} = \int_0^\infty e^{-\alpha r} r^{n+k} u_\ell(r)\, dr \tag{46}$$

As mentioned earlier, because of the linearity of the nonlocal Schroedinger equation, we can immediately write a particular solution of Eq. (45) as

$$u_\ell^P(r) = \sum_{i=0}^{J} \sum_{j=0}^{i} \sum_{k=0}^{i} \lambda_i b_j^{(i)} b_k^{(i)} C_k^{(n)} \left[F_j^{(n)} kr\, j_\ell(kr) + G_j^{(n)} kr\, n_\ell(kr) \right.$$

$$\left. - e^{-\alpha r} \sum_{p=0}^{\ell} \sum_{q=0}^{p+n+j+1} \frac{(\ell+p)!(\alpha^2+k^2)^{q/2} r^{q-p}}{p!(\ell-p)!q!(2k)^p} \left\{ F_j^{(n)} \cos\left[q\theta + (p-\ell-1)\frac{\pi}{2}\right] \right.\right.$$

$$\left.\left. + G_j^{(n)} \sin\left[q\theta + (p-\ell-1)\frac{\pi}{2}\right] \right\} \right] \tag{47}$$

where $F_j^{(n)}$ and $G_j^{(n)}$ are given by the expressions for F and G as defined in Eqs. (36) and (37) but with n replaced by n + j. Adding the general homogeneous solution and applying the same boundary conditions as before, we get as the solution for Eq. (45)

$$u_\ell(r) = \frac{(2\ell+1)!!}{k^{\ell+1}} kr\, j_\ell(kr) + \sum_{i=0}^{J} \sum_{j=0}^{i} \sum_{k=0}^{i} \lambda_i b_j^{(i)} b_k^{(i)} C_k^{(n)} \Bigg[F_j^{(n)} kr\, j_\ell(kr)$$

$$+ G_j^{(n)} kr\, n_\ell(kr) - e^{-\alpha r} \sum_{p=0}^{\ell} \sum_{q=0}^{p+n+j+1} \frac{(\ell+p)!(\alpha^2+k^2)^{q/2} r^{q-p}}{p!q!(\ell-p)!(2k)^p}$$

$$\times \left\{ F_j^{(n)} \cos\left[q\theta + (p-\ell-1)\frac{\pi}{2} \right] + G_j^{(n)} \sin\left[q\theta + (p-\ell-1)\frac{\pi}{2} \right] \right\} \Bigg] \qquad (48)$$

The function $u_\ell(r)$ given by Eq. (48) is completely determined once the constants $C_k^{(n)}$ are known. To obtain $C_k^{(n)}$, Eq. (48) for $u_\ell(r)$ can be substituted back into Eq. (46), and the order of summation rearranged to give an easily solvable expression of the form

$$C_m^{(n)} = \sum_{j=0}^{J} R_{mj}^{(n)} C_j^{(n)} + U_m^{(n)} \qquad (49)$$

where

$$R_{mj}^{(n)} = -\sum_{i=j}^{J} \sum_{k=0}^{i} \lambda_i b_j^{(i)} b_k^{(i)} \sum_{p=0}^{\ell} \sum_{q=0}^{p+n+k+1} \frac{(\ell+p)!(\alpha^2+k^2)^{q/2}(m+n+q-p)!}{p!q!(\ell-p)!(2k)^p (2\alpha)^{m+n+q-p+1}}$$

$$\times \left\{ F_k^{(n)} \cos\left[q\theta + (p-\ell-1)\frac{\pi}{2} \right] + G_k^{(n)} \sin\left[q\theta + (p-\ell-1)\frac{\pi}{2} \right] \right.$$

$$\left. - \sum_{t=0}^{\ell} \frac{(\ell+t)!(m+n-t)!(\alpha^2+k^2)^{-\frac{1}{2}(m+n-t+1)}}{t!(\ell-t)!(2k)^t} \right.$$

$$\left. \times \left\{ F_k^{(n)} \cos\left[(m+n-t+1)\theta + (t-\ell-1)\frac{\pi}{2} \right] + G_k^{(n)} \sin\left[(m+n-t+1)\theta + (t-\ell-1)\frac{\pi}{2} \right] \right\} \right.$$

(50)

and

$$U_m^{(n)} = \frac{(2\ell+1)!!}{k^{\ell+1}} \sum_{t=0}^{\ell} \frac{(\ell+t)!(m+n-t)!(\alpha^2+k^2)^{-\frac{1}{2}(m+n-t+1)}}{t!(\ell-t)!(2k)^t}$$

$$\times \cos\left[(m+n-t+1)\,\theta + (t-\ell-1)\,\frac{\pi}{2}\right] \tag{51}$$

The phase shift δ_ℓ can be determined immediately from Eq. (48), and is

$$\tan\delta_\ell = -\frac{\sum_{i=0}^{J}\sum_{j=0}^{i}\sum_{k=0}^{i}\lambda_i b_j^{(i)} b_k^{(i)} C_k^{(n)} G_j^{(n)}}{\frac{(2\ell+1)!!}{k^{\ell+1}} + \sum_{i=0}^{J}\sum_{j=0}^{i}\sum_{k=0}^{i}\lambda_i b_j^{(i)} b_k^{(i)} C_k^{(n)} F_j^{(n)}} \tag{52}$$

As expected, Eqs. (48) and (52) reduce to Eqs. (41) and (43) for J=0 and $b_o^{(o)} = A$.

The second example which we will consider is the potential given by Eq. (5) with the summation over ν retained, but without polynomial terms $P_i^{\nu}(r)$; that is

$$g_\ell(r,r') = \frac{\hbar^2}{2m} \sum_{\nu} \Lambda^{\nu} e^{-\alpha_\nu (r+r')} (rr')^{n_\nu} . \tag{53}$$

For this potential, Eq. (4) reduces to

$$\left[\frac{d^2}{dr^2} + k^2 - \frac{\ell(\ell+1)}{r^2}\right] u_\ell(r) = \sum_{\nu} \Lambda^{\nu} e^{-\alpha_\nu r} r^{n_\nu} C^{\nu} \tag{54}$$

where

$$C^{\nu} = \int_0^{\infty} e^{-\alpha_\nu r} r^{n_\nu} u_\ell(r)\, dr . \tag{55}$$

The solution is

$$u_\ell(r) = \frac{(2\ell+1)!!}{k^{\ell+1}} kr\, j_\ell(kr) + \sum_\nu \Lambda^\nu C^\nu \left[F^\nu kr\, j_\ell(kr) + G^\nu kr\, n_\ell(kr) \right.$$

$$\left. - e^{-\alpha_\nu r} \sum_{s=0}^{\ell} \sum_{t-0}^{n_\nu+s+1} \frac{(\ell+s)!(\alpha^2+k^2)^{t/2} r^{t-s}}{t!s!(\ell-s)!(2k)^s} \left\{ F^\nu \cos\left[t\theta_\nu + (s-\ell-1)\frac{\pi}{2} \right] \right.\right.$$

$$\left.\left. + G^\nu \sin\left[t\theta_\nu + (s-\ell-1)\frac{\pi}{2} \right] \right\} \right] \tag{56}$$

where F^ν and G^ν are given by Eqs. (36) and (37) with n replaced by n_ν and with $\theta_\nu = \arctan \frac{k}{\alpha_\nu}$.

As before, it is necessary to specify the constants C_ν in terms of an equation involving known quantities. We get

$$C^\nu = \sum_{\nu'} R^{\nu\nu'} C^{\nu'} + U^\nu \tag{57}$$

where

$$R^{\nu\nu'} = \Lambda^{\nu'} \sum_{t=0}^{\ell} \frac{(\ell+t)!(n_\nu - t)!(\alpha_\nu^2 + k^2)^{-\frac{1}{2}(n_\nu - t+1)}}{t!(\ell-t)!(2k)^t}$$

$$\times \left[F^{\nu'} \cos\left\{ n_\nu - t+1)\theta_\nu + (t-\ell-1)\frac{\pi}{2} \right\} + G^{\nu'} \sin\left\{ (n_\nu - t+1)\theta_\nu + (t-\ell-1)\frac{\pi}{2} \right\} \right]$$

$$- \sum_{s=0}^{\ell} \sum_{t=0}^{n'_{\nu'}+s+1} \frac{(\ell+s)!(n_{\nu'}+t-s)!(\alpha^2_{\nu'}+k^2)^{t/2}}{t!s!(\ell-s)!(2k)^s (\alpha_\nu + \alpha_{\nu'})^{n'_{\nu'}+t-s+1}}$$

$$\times \left[F^{\nu'} \cos\left\{ t\theta_{\nu'} + (s-\ell-1)\frac{\pi}{2} \right\} + G^{\nu'} \sin\left\{ t\theta_{\nu'} + (s-\ell-1)\frac{\pi}{2} \right\} \right] \tag{58}$$

and

$$U^{\nu} = \frac{(2\ell+1)!!}{k^{\ell+1}} \sum_{t=0}^{\ell} \frac{(\ell+t)!(n_\nu-t)!(\alpha_\nu+k^2)^{-\frac{1}{2}(n_\nu-t+1)}}{t!(\ell-t)!(2k)^t}$$

$$\times \cos\left[(n_\nu-t+1)\,\theta_\nu+(t-\ell-1)\,\frac{\pi}{2}\right] . \tag{59}$$

The phase shift is given by

$$\tan\delta_\ell = -\frac{\sum_\nu \Lambda^\nu C^\nu G^\nu}{\frac{(2\ell+1)!!}{k^{\ell+1}}+\sum_\nu \Lambda^\nu C^\nu F^\nu} . \tag{60}$$

The wave function and phase shift appropriate to the general potential given by Eq. (5) combine aspects of both of these examples. The final results are

$$u_\ell(r) = \frac{(2\ell+1)!!}{k^{\ell+1}} kr\, j_\ell(kr)+\sum_\nu \sum_{g=0}^{K_\nu}\sum_{i=0}^{J_\nu}\sum_{m=0}^{g}\sum_{j=0}^{i} \Lambda^\nu_{gi} b^{(g,\nu)}_m b^{(i,\nu)}_j C^\nu_j$$

$$F^\nu_m kr\, j_\ell(kr)+G^\nu_m kr\, n_\ell(kr) - e^{-\alpha_\nu r}\sum_{p=0}^{\ell}\sum_{q=0}^{p+n_\nu+m+1} \frac{(\ell+p)!(\alpha_\nu^2+k^2)^{q/2} r^{q-p}}{p!q!(\ell-p)!(2k)^p}$$

$$\times\left\{F^\nu_m \cos\left[q\theta_\nu+(p-\ell-1)\,\frac{\pi}{2}\right]+G^\nu_m \sin\left[q\theta_\nu+(p-\ell-1)\,\frac{\pi}{2}\right]\right\} \tag{61}$$

and

$$\tan\delta_\ell = -\frac{\sum_\nu \sum_{g=0}^{K_\nu}\sum_{i=0}^{J_\nu}\sum_{m=0}^{g}\sum_{j=0}^{i} \Lambda^\nu_{gi} b^{(g,\nu)}_m b^{(i,\nu)}_j C^\nu_j F^\nu_m}{\frac{(2\ell+1)!!}{k^{\ell+1}}+\sum_\nu \sum_{g=0}^{K_\nu}\sum_{i=0}^{J_\nu}\sum_{m=0}^{g}\sum_{j=0}^{i} \Lambda^\nu_{gi} b^{(g,\nu)}_m b^{(i,\nu)}_j C^\nu_j G^\nu_m} . \tag{62}$$

where F_m^ν and G_m^ν are given by Eqs. (36) and (37) with n replaced by $n_\nu + m$ and α replaced by α_ν.

The unknown C_j^ν's can be found from the condition

$$C_j^\nu = \sum_{\nu'} \sum_{j'=0}^{J_{\nu'}} R_{jj'}^{\nu\nu'} C_{j'}^{\nu'} + U_j^\nu \tag{63}$$

where

$$R_{jj'}^{\nu\nu'} = \sum_{i=j}^{J_{\nu'}} \sum_{g=0}^{K_{\nu'}} \sum_{m=0}^{g} \Lambda_{gi}^{\nu'} b_m^{(g,\nu')} b_j^{(i,\nu')} \sum_{t=0}^{\ell} \frac{(\ell+t)!(n_\nu+j-t)!}{t!(\ell-t)!(2k)^t}$$

$$\times (\alpha^2+k^2)^{-\frac{1}{2}(n_\nu+j-t+1)} \left\{ F_m^{\nu'} \cos\left[(n+j-t+1)\theta_\nu + (t-\ell-1)\frac{\pi}{2}\right] \right.$$

$$\left. + G_m^{\nu'} \sin\left[(n+j-t+1)\theta_\nu + (t-\ell-1)\frac{\pi}{2}\right] \right\}$$

$$- \sum_{p=0}^{\ell} \sum_{q=0}^{p+n_{\nu'}+m+1} \frac{(\ell+p)!(n_{\nu'}+j+q-p)!(\alpha_{\nu'}^2+k^2)^{q/2}}{\nu!p!(\ell-p)!(2k)^p(\alpha_\nu+\alpha_{\nu'})^{n_{\nu'}+j+q-p+1}}$$

$$\times \left\{ F_m^{\nu'} \cos\left[q\theta_{\nu'} + (p-\ell-1)\frac{\pi}{2}\right] + G_m^{\nu'} \sin\left[q\theta_{\nu'} + (p-\ell-1)\frac{\pi}{2}\right] \right\} \tag{64}$$

and

$$U_j^\nu = \frac{(2\ell+1)!!}{k^{\ell+1}} \sum_{t=0}^{\ell} \frac{(\ell+t)!(n_\nu+j-t)!(\alpha_\nu^2+k^2)^{-\frac{1}{2}(n_\nu+j-t+1)}}{t!(\ell-t)!(2k)^t}$$

$$\times \cos\left[(n_\nu-t+1)\theta_\nu + (t-\ell-1)\frac{\pi}{2}\right] . \tag{65}$$

5. Summary

The method presented in this chapter is closely related to those standardly employed in the solutions for wavefunctions and phase shifts for the scattering of particles by a local potential. To obtain an analytic solution for a local potential, one also normally expands the solution in a power series about the origin which results in a difference equation involving the coefficients of the power series. Because in the case of a local potential the difference equation is homogeneous, the regular solution follows directly from consideration of the indicial equation.

We have shown that in the case of a large class of separable nonlocal potentials a similar technique can be employed. Consideration of the indicial equation must be replaced by the task of obtaining the two independent solutions of the difference equation . The condition of homogeneity of the original integro-differential equation can then be imposed upon these solutions. The solutions presented here for the class of potentials under study are particularly simple, and could be so rearranged that the series expansion was identified as a combination of trigonometric functions.

The results which we have obtained provide an opportunity for calculations with the class of potentials discussed which totally avoid the

necessity of numerical integration of the integro-differential equation. This is particularly important, since numerical integration of an integro-differential equation requires complicated matrix methods or time consuming iterations. In the case of local potential the equation is differential in character, and numerical integration techniques present much less difficulty than in the case of a nonlocal potential. Although matrices appear in the expressions presented here, they can be handled in a trivial way. For the potentials we have considered the wavefunctions and phase shifts are in each case given in closed form by a single expression. For the single-term potential for the $\ell=0$ case, the wavefunction and phase shift are given by Eqs. (26) and (28) respectively. The corresponding equations for the wavefunction and phase shift for arbitrary ℓ are Eqs. (41) and (43). For the most general many-term potential given by Eq. (5), the wavefunction for arbitrary ℓ is given by Eq. (61), and the phase shift by Eq. (62). The only unknowns which appear in the expressions for the wavefunction and phase shift are the elements of the matrix $\mathbf{C}$. The matrix $\mathbf{C}$ will be of dimension equal to the number of terms employed in the potential and thus will usually be easy to invert. In dealing with a particular problem, one may wish to invert the matrix directly. If not, the matrix inversion involved is available as a standard subroutine package for any computer, such as GELG(R, A, M, N, EPS, IER) from the IBM library.

CHAPTER III

IRREGULAR SOLUTIONS AND EQUIVALENT LOCAL POTENTIALS

To develop a better understanding of nonlocal interactions it is logical that a comparison be made between the characteristics of nonlocal potentials and the more familiar phenomenology of local potentials. However, only recently have successful attempts been made to relate the nonlocal interaction to its 'equivalent' local form in coordinate space. It has been shown by Coz, Arnold and MacKellar[41] that a unique potential and solutions to an equivalent local equation can be obtained once two independent solutions of the nonlocal equation are known. The above authors used two independent Jost solutions to get an unique equivalent local potential (ELP) from a nonlocal potential. Instead of Jost solutions, the regular and irregular solutions can also be used to formulate the ELP. However, it is customary to find the irregular solution in terms of the Jost solution and Jost function, as it is more difficult to get the irregular solution from the boundary conditions. In this chapter, using the techniques developed in Chapter II, we will derive the irregular

solution and Jost solutions from the boundary conditions. Then closely following Coz, Arnold and MacKellar[41] we will obtain compact expressions for ELP for the class of separable nonlocal potentials for which we have been able to get exact solutions for the scattering wavefunctions.

1. Irregular and Jost Solutions

In this section we will obtain the irregular and Jost solutions in a number of steps, as was done in the previous chapter for regular solutions. First, we will consider the one term separable potential for the case $\ell=0$, and then extend the discussion to arbitrary ℓ. Next the more general case of the many term separable potential will be treated in three steps.

Case a: Solutions for the one-term separable potential for $\ell=0$:

Let us consider the case of the single term separable potential given by Eqs.(7) and (8), that is,

$$g(r|r') = \lambda\, q(r)\, q(r')$$

with

$$q(r) = A\, e^{-\alpha r}\, r^{n} \quad .$$

The regular solution for this potential is given by Eq. (26), which asymptotically reduces to the following form,

$$u_o(r) \xrightarrow[r \to \infty]{} Z \sin(kr+\delta) \tag{66}$$

where

$$Z = \left[\left(\frac{1}{k} + \frac{Dn!\cos(n+1)}{k(\alpha^2+k^2)^{\frac{n+1}{2}}}\right)^2 + \left(\frac{Dn!\sin(n+1)\theta}{k(\alpha^2+k^2)^{\frac{n+1}{2}}}\right)^2\right]^{\frac{1}{2}}, \tag{67}$$

$$\sin\delta = -\frac{Dn!\sin(n+1)\theta}{k(\alpha^2+k^2)^{\frac{n+1}{2}}} \Big/ Z \tag{68a}$$

$$\cos\delta = \frac{(\alpha^2+k^2)^{\frac{n+1}{2}} + Dn!\cos(n+1)\theta}{k(\alpha^2+k^2)^{\frac{n+1}{2}}} \Big/ Z, \tag{68b}$$

and D is evaluated from Eqs. (27a) and (27b).

The irregular solution does not go to zero at the origin, and is normally chosen,[17] so that it behaves asymptotically as

$$\theta_o(r) \xrightarrow[r \to \infty]{} -\frac{1}{kZ}\cos(kr+\delta) \tag{69}$$

The choice of normalization in Eq. (69) is such that the Wronskian $W(u_o, \theta_o)$ at infinity is unity. Sometimes this condition is slightly changed[40],[46] so that the asymptotic Wronskian is either -1 or k.

To incorporate the boundary conditions for the irregular solution, we add Msinkr + Ncoskr to the particular solution given by Eq. (25) and adjust M and N accordingly. We find

$$M = \frac{Dn!\ \cos(n+1)\,\theta}{k(\alpha^2 + k^2)^{\frac{n+1}{2}}} + \frac{1}{kZ}\sin\delta$$

and

$$N = \frac{Dn!\ \sin(n+1)\,\theta}{k(\alpha^2 + k^2)^{\frac{n+1}{2}}} - \frac{1}{kZ}\cos\delta$$

so that the irregular solution $\theta_o(r)$ can be put into the form

$$\theta_o(r) = -\frac{1}{kZ}\cos(kr+\delta) + \frac{D'n!\ e^{-\alpha r}}{k(\alpha^2+k^2)^{\frac{n+1}{2}}} \sum_{s=0}^{n} \frac{(\alpha^2+k^2)^{\frac{s}{2}} \sin(n+1-s)\theta r^s}{s!} \tag{70}$$

where

$$D' = \lambda A^2 \int_o^\infty e^{-\alpha r} r^n \theta_o(r)\, dr$$

$$= -\frac{\lambda A^2 n!\ \cos[(n+1)\,\theta+\delta]}{kz(\alpha^2+k^2)^{n+1}\,\Delta(k)} \tag{71}$$

with $\Delta(k)$ given by Eq. (27b).

Jost solutions $f_o^{\pm}(k,r)$, Jost functions $J_o^{\pm}(k)$, and the relationship between these and the regular and irregular solutions u_o and θ_o are discussed in the Appendix, where we have shown that

$$u_o(r) = \frac{1}{2ik}\left[J_o^-(k)\, f_o^+(k,r) - J_o^+(k)\, f_o^-(k,r)\right] \tag{72}$$

and

$$\theta_o(r) = -\tfrac{1}{2}\left[J_o^+(k)^{-1}\, f_o^+(k,r) + J_o^-(k)^{-1}\, f_o^-(k,r)\right]. \tag{73}$$

If we add $M\sin kr + N\cos kr$ to Eq. (25) and apply the boundary conditions for Jost solutions given in the Appendix, we get after some manipulation

$$f_o^{\pm}(k,r) = e^{\pm ikr} + \frac{D_{\pm}\, n!\, e^{-\alpha r}}{k(\alpha^2+k^2)^{\frac{n+1}{2}}} \sum_{s=0}^{n} \frac{(\alpha^2+k^2)^{s/2} \sin(n+1-s)\theta}{s!}\, r^s \tag{74}$$

where

$$D_{\pm} = \lambda A^2 \int_0^{\infty} e^{-\alpha r}\, r^n\, f_o^{\pm}(k,r)\, dr$$

$$= \frac{\lambda A^2\, n!\, e^{\pm i(n+1)\theta}}{(\alpha^2+k^2)^{\frac{n+1}{2}}\, \Delta(k)} \tag{75}$$

Since $J_o^{\pm}(k) = f_o^{\pm}(k,0)$ we have

$$J_o^{\pm}(k) = 1 + \frac{\lambda A^2 (n!)^2 \, e^{\pm i(n+1)\theta} \sin(n+1)\,\theta}{k(\alpha^2+k^2)^{n+1}\,\Delta(k)} \tag{76}$$

As a check we can substitute Eqs. (74) and (76) into Eqs. (72) and (73). We get back Eqs. (26) and (70), showing that Eqs. (72) and (73) are, indeed, equivalent to Eqs. (26) and (70) respectively.

Case b: Solutions for the one-term potential for arbitrary ℓ

For the one term potential given by Eq. (7), the asymptotic form of the regular solution given by Eq. (41) can be written as

$$u_\ell(r) \xrightarrow[r\to\infty]{} Z_\ell \sin(kr - \tfrac{1}{2}\ell\pi + \delta_\ell) \tag{77}$$

where

$$Z_\ell = \left[\left(\frac{(2\ell+1)!!}{k^{\ell+1}} + FD\right)^2 + (GD)^2\right]^{\frac{1}{2}}, \tag{78}$$

$$\sin\delta_\ell = -GD/Z_\ell \tag{79a}$$

$$\cos\delta_\ell = \left(\frac{(2\ell+1)!!}{k^{\ell+1}} + FD\right) / Z_\ell, \tag{79b}$$

and D is defined by Eq. (42a).

Adding $Mkrj_\ell(kr) + Nkrn_\ell(kr)$ to Eq. (40) and using the boundary condition

$$\theta_\ell(r) \xrightarrow[r\to\infty]{} -\frac{1}{kZ_\ell}\cos[kr - \tfrac{1}{2}\ell\pi + \delta_\ell] \tag{80}$$

we get

$$M = - FD + \frac{1}{kZ_\ell} \sin \delta_\ell \tag{81a}$$

$$N = - GD + \frac{1}{kZ_\ell} \cos \delta_\ell \tag{81b}$$

Hence the irregular solution $\theta_\ell(r)$ is

$$\theta_\ell(r) = \frac{1}{kZ_\ell} \sin \delta_\ell \, kr \, j_\ell(kr) + \frac{1}{kZ_\ell} \cos \delta_\ell \, kr \, n_\ell(kr)$$

$$- D' e^{-\alpha r} \sum_{s=0}^{\ell} \sum_{t=0}^{n+s+1} \frac{(\ell+s)!(\alpha^2+k^2)^{t/2} r^{t-s}}{s!(\ell-s)!\, t!(2k)^s} \left[F \cos\left\{t\theta+(s-\ell-1)\frac{\pi}{2}\right\}\right.$$

$$\left. + G \sin \left\{t\theta+(s-\ell-1) \frac{\pi}{2} \right\}\right] \tag{82}$$

where

$$D' = \lambda A^2 \int_0^\infty e^{-\alpha r} r^n \theta_\ell(kr) \, dr$$

$$= \frac{\lambda A^2}{kZ_\ell \Delta_\ell(k)} \left[\sum_{s=0}^{\ell} \frac{(\ell+s)!(n-s)!(\alpha^2+k^2)^{\frac{s-n-1}{2}}}{s!(\ell-s)!(2k)^s} \right.$$

$$\left. \sin\left\{(n+1-s)\theta + (s-\ell-1)\frac{\pi}{2} + \delta_\ell\right\}\right] \tag{83}$$

and

$$\Delta_\ell(k) = 1 + \lambda A^2 \sum_{s=0}^{\ell} \sum_{t=0}^{n+s+1} \frac{(\ell+s)!(n+t-s)!(\alpha^2+k^2)^{t/2}}{s!(\ell-s)!t!(2k)^s(2\alpha)^{n+t-s+1}}$$

$$\times \left[F \cos\left\{t\theta+(s-\ell-1)\frac{\pi}{2}\right\}+G \sin\left\{t\theta+(s-\ell-1)\frac{\pi}{2}\right\}\right]$$

(84)

To find the Jost solutions $f_\ell^{\pm}(k,r)$ we add $M^{\pm}kr\, j_\ell(kr) + N^{\pm}kr\, n_\ell(kr)$ to Eq. (40) and, using the boundary conditions for $f_\ell^{\pm}(k,r)$ given in the Appendix, we get

$$M^{\pm} = -\,FD + e^{\pm i(\ell+1)\pi/2} \tag{85a}$$

$$N^{\pm} = -\,GD + e^{\pm i(\ell+2)\pi/2} \tag{85b}$$

It follows that

$$f_\ell^{\pm}(k,r) = e^{\pm i(\ell+1)\,\pi/2} kr\, j_\ell(kr) + e^{\pm i(\ell+2)\,\pi/2}\, kr\, n_\ell(kr)$$

$$- D_{\pm}\, e^{-\alpha r} \sum_{s=0}^{\ell} \sum_{t=0}^{n+s+1} \frac{(\ell+s)!\,(\alpha^2+k^2)^{t/2}}{t!\; s!\; (\ell-s)!\,(2k)^s} \left[F \cos\left\{t\theta+(s-\ell-1)\frac{\pi}{2}\right\}\right.$$

$$\left. + G \sin\left\{t\theta+(s-\ell-1)\frac{\pi}{2}\right\}\right] \tag{86}$$

where

$$D_{\pm} = \lambda A^2 \int_0^{\infty} e^{-\alpha r}\, r^n\, f_\ell^{\pm}(k,r)\, dr$$

$$= \frac{\lambda A^2\, e^{\pm i(\ell+1)\pi/2}}{\Delta_\ell(k)} \sum_{s=0}^{\ell} \frac{(\ell+s)!\,(n-s)!\,(\alpha^2+k^2)^{\frac{s-n-1}{2}}}{s!\,(\ell-s)!\,(2k)^s}$$

$$\times\; e^{\mp i\left[(n+1-s)\theta+(s-\ell-1)\frac{\pi}{2}\right]} \tag{87}$$

and $\Delta_\ell(k)$ is given by Eq. (84).

Using the boundary conditions for Jost functions given in the Appendix we can immediately write from Eq. (86)

$$J_{\ell}^{\pm}(k) = - \frac{(2\ell+1)!!}{k^{\ell}} e^{\pm i(\ell+2)\pi/2} + \frac{(2\ell)! G D_{\pm}}{\ell!\ (2k)^{\ell}} \tag{88}$$

As shown in the Appendix, the regular solution $u_{\ell}(r)$ and the irregular solution $\theta_{\ell}(r)$ can be written in terms of the Jost solutions $f_{\ell}^{\pm}(k,r)$ and Jost functions $J_{\ell}^{\pm}(k)$, that is

$$u_{\ell}(r) = \frac{1}{2ik} [J_{\ell}^{-}(k)\ f_{\ell}^{+}(k,r) - J_{\ell}^{+}(k)\ f_{\ell}^{-}(k,r)] \tag{89}$$

and

$$\theta_{\ell}(r) = -\tfrac{1}{2} [J_{\ell}^{+}(k)^{-1}\ f_{\ell}^{+}(k,r) + J_{\ell}^{-}(k)^{-1}\ f_{\ell}^{-}(k,r)] \tag{90}$$

Case c: Many-term Separable Potential for arbitrary ℓ

Before presenting the irregular and Jost solutions for the potential given by Eq. (5), we will obtain solutions for two less complicated examples, as was done in Chapter II. We will then extend the results to the general potential given by Eq. (5).

Example I.

We consider a potential of Eq. (5) for which α is fixed (no summation over ν). We thus consider the potential given by Eq. (44), that is,

$$g_\ell(r|r') = \frac{\hbar^2}{2m}\, e^{-\alpha(r+r')}(rr')^n \sum_{i=0}^{J} \lambda_i P_i(r)\, P_i(r')$$

The regular solution for this potential is given by Eq. (48).

Asymptotically

$$u_\ell(r) \xrightarrow[r\to\infty]{} Z_\ell \sin(kr - \tfrac{1}{2}\ell\pi + \delta_\ell) \tag{91}$$

where

$$Z_\ell = \Bigg[\left(\frac{(2\ell+1)!!}{k^{\ell+1}} + \sum_{i=0}^{J}\sum_{j=0}^{i}\sum_{k=0}^{i} \lambda_i b_j^{(i)} b_k^{(i)} C_k^{(n)} F_j^{(n)}\right)^2$$

$$+\left(\sum_{i=0}^{J}\sum_{j=0}^{i}\sum_{k=0}^{i} \lambda_i\, b_j^{(i)} b_k^{(i)} C_k^{(n)} G_j^{(n)}\right)^2\Bigg]^{\frac{1}{2}}, \tag{92}$$

$$\sin\delta_\ell = \left(-\sum_{i=0}^{J}\sum_{j=0}^{i}\sum_{k-0}^{i} \lambda_i b_j^{(i)} b_k^{(i)} C_k^{(n)} G_j^{(n)}\right)/Z_\ell \tag{93a}$$

and

$$\cos\delta_\ell = \left(\frac{(2\ell+1)!!}{k^{\ell+1}} + \sum_{i=0}^{J}\sum_{j=0}^{i}\sum_{k=0}^{i} \lambda_i b_j^{(i)} b_k^{(i)} C_k^{(n)} F_j^{(n)}\right)\Big/ Z_\ell \tag{93b}$$

Following exactly case b, we can immediately write

$$\theta_\ell(r) = \frac{1}{kZ_\ell} \sin\delta_\ell \, kr\, j_\ell(kr) + \frac{1}{kZ_\ell} \cos\delta_\ell \, kr\, n_\ell(kr)$$

$$- e^{-\alpha r} \sum_{i=0}^{J} \sum_{j=0}^{i} \sum_{k=0}^{i} \lambda_i b_j^{(i)} b_k^{(i)} C_k^{(n)} \left[\sum_{p=0}^{\ell} \sum_{q=0}^{p+n+j+1} \frac{(\ell+p)!(\alpha^2+k^2)^{\frac{q}{2}} r^q}{p!(\ell-p)!q!(2k)^p} \right.$$

$$\left. \times \{F_j^{(n)} \cos[q\theta+(p-\ell-1)\tfrac{\pi}{2}] + G_j^{(n)} \sin[q\theta+(p-\ell-1)\tfrac{\pi}{2}]\} \right] \qquad (94)$$

where

$$C'^{(n)}_m = \int_0^\infty e^{-\alpha r} r^{n+m} \theta_\ell(r)\, dr$$

$$= \sum_{j=0}^{J} R'^{(n)}_{mj} C_j^{(n)} + U'^{(n)}_m \qquad (95)$$

with

$$R'^{(n)}_{mj} = - \sum_{i=j}^{J} \sum_{k=0}^{i} \lambda_i b_j^{(i)} b_k^{(i)} \left[\sum_{p=0}^{\ell} \sum_{q=0}^{p+n+k+1} \frac{(\ell+p)!(\alpha^2+k^2)^{q/2}(m+n+q-p)}{p!q!(\ell-p)!(2k)^p(2\alpha)^{m+n+q-p}} \right.$$

$$\left. \times \{F_k^{(n)} \cos[q\theta+(p-\ell-1)\tfrac{\pi}{2}] + G_k^{(n)} \sin[q\theta+(p-\ell-1)\tfrac{\pi}{2}]\} \right] \qquad (96a)$$

and

$$U'^{(n)}_m = \frac{1}{kZ_\ell} \sum_{t=0}^{\ell} \frac{(\ell+t)!(m+n-t)!(\alpha^2+k^2)^{-\frac{1}{2}(m+n-t+1)}}{t!(\ell-t)!(2k)^t}$$

$$\times \sin\{(m+n-t+1)\theta + (t-\ell-1)\tfrac{\pi}{2} + \delta_\ell\} \qquad (96b)$$

Similarly, the Jost solutions $f_\ell^{\pm}(k,r)$ can be written as

$$f_\ell^{\pm}(k,r) = e^{\pm i(\ell+1)\pi/2} kr\, j_\ell(kr) + e^{\pm i(\ell+2)\pi/2} kr\, \eta_\ell(kr)$$

$$-e^{-\alpha r} \sum_{i=0}^{J} \sum_{j=0}^{i} \sum_{k=0}^{i} \lambda_i b_j^{(i)} b_k^{(i)} C_k^{(n)\pm} \left[\sum_{p=0}^{\ell} \sum_{q=0}^{p+n+j+1} \frac{(\ell+p)!(\alpha^2+k^2)^{\frac{q}{2}} r^{q-p}}{p!(\ell-p)!q!(2k)^p} \right.$$

$$\left. \times \{ F_j^{(n)} \cos[q\theta + (p-\ell-1)\frac{\pi}{2}] + G_j^{(n)} \sin[q\theta + (p-\ell-1)\frac{\pi}{2}] \} \right] \tag{97}$$

where the unknown $C_k^{(n)\pm}$ can be found from

$$C_m^{(n)\pm} = \sum_{j=0}^{J} R'^{(n)}_{mj} C_j^{(n)\pm} + U_m^{(n)\pm} \tag{98}$$

with

$$U_m^{(n)\pm} = e^{\pm i(\ell+1)\pi/2} \sum_{t=0}^{\ell} \frac{(\ell+t)!(m+n-t)!(\alpha^2+k^2)^{-\frac{1}{2}(m+n-t+1)}}{t!(\ell-t)!(2k)^t}$$

$$\times e^{\pm i[(m+n-t+1)\theta + (t-\ell-1)\pi/2]} \tag{99}$$

and $R'^{(n)}_{mj}$ is given by Eq. (96a).

The Jost functions $J_\ell^{\pm}(k)$ are then

$$J_\ell^{\pm}(k) = -\frac{(2\ell+1)!!}{k\ell} e^{\pm i(\ell+2)\pi/2} + \sum_{i=0}^{J} \sum_{j=0}^{i} \sum_{k=0}^{i} \lambda_i b_j^{(i)} b_k^{(i)} C_k^{(n)\pm} \frac{(2\ell)!}{t!(2k)^\ell} G_j^{(n)} \tag{100}$$

Example II

The second example is the potential given by Eq. (5) with the summation over ν retained but without the polynomial terms $P_i^{\nu}(r)$, that is

$$g_{\ell}(r|r') = \frac{\hbar^2}{2m} \sum_{\nu} \Lambda^{\nu} e^{-\alpha_{\nu}(r+r')} (rr')^{n_{\nu}}$$

The regular solution for this potential is given by Eq. (56), which has the following asymptotic form

$$u_{\ell}(r) \underset{r \to \infty}{} Z_{\ell} \sin (kr - \tfrac{1}{2}\ell\pi + \delta_{\ell})$$

with

$$Z_{\ell} = \left[\left(\frac{(2\ell+1)!!}{k^{\ell+1}} + \sum_{\nu} \Lambda^{\nu} C^{\nu} F^{\nu} \right)^2 + \left(\sum_{\nu} \Lambda^{\nu} C^{\nu} G^{\nu} \right)^2 \right]^{\frac{1}{2}} \qquad (101)$$

$$\sin \delta_{\ell} = -\left(\sum_{\nu} \Lambda^{\nu} C^{\nu} G^{\nu} \right) / Z_{\ell} \qquad (102a)$$

$$\cos \delta_{\ell} = \left(\frac{(2\ell+1)!!}{k^{\ell+1}} + \sum_{\nu} \Lambda^{\nu} C^{\nu} F^{\nu} \right) \Big/ Z_{\ell} \qquad (102b)$$

and C^{ν} given by Eq. (57).

Following example I, the irregular solution can be immediately written as

$$\theta_{\ell}(r) = \frac{1}{kZ_{\ell}} [\sin \delta_{\ell} \, kr \, j_{\ell}(kr) + \cos \delta_{\ell} \, kr \, n_{\ell}(kr)]$$

$$- \sum_{\nu} \sum_{s=0}^{\ell} \sum_{t=0}^{n_{\nu}+s+1} \Lambda^{\nu} C'^{\nu} e^{-\alpha_{\nu} r} \frac{(\ell+s)! (\alpha^2+k^2)^{t/2} \, r^{t-s}}{t! \, s! \, (\ell-s)! (2k)^s}$$

$$\times \{F^{\nu} \cos[t\theta_{\nu} + (s-\ell-1)\tfrac{\pi}{2}] + G^{\nu} \sin[t\theta_{\nu} + (s-\ell-1)\tfrac{\pi}{2}]\} \qquad (103)$$

where

$$C'^{\nu} = \sum_{\nu'} R'^{\nu\nu'} C'^{\nu'} + U'^{\nu} \tag{104}$$

with

$$R'^{\nu\nu'} = -\Lambda^{\nu'} \sum_{s=0}^{\ell} \sum_{t=0}^{n_{\nu'}+s+1} \frac{(\ell+s)!(n_{\nu'}+t-s)!(\alpha_{\nu'}^2+k^2)^{t/2}}{t!\,s!(\ell-s)!(2k)^s(\alpha_\nu+\alpha_{\nu'})^{n_{\nu'}+t-s+1}}$$

$$\times \left[F^{\nu'} \cos\{t\theta_{\nu'}+(s-\ell-1)\frac{\pi}{2}\} + G^{\nu'} \sin\{t\theta_{\nu'}+(s-\ell-1)\frac{\pi}{2}\}\right] \tag{105a}$$

and

$$U'^{\nu} = \frac{1}{kZ_\ell} \sum_{t=0}^{\ell} \frac{(\ell+t)!(n_\nu-t)!(\alpha_\nu^2+k^2)^{-\frac{1}{2}(n_\nu-t+1)}}{t!(\ell-t)!(2k)^t}$$

$$\times \sin\{(n_\nu-t+1)\theta+(t-\ell-1)\frac{\pi}{2}+\delta_\ell\} \tag{105b}$$

The Jost solutions $f_\ell^{\pm}(k,r)$ for this potential can now be written as

$$f_\ell^{\pm}(k,r) = e^{\pm i(\ell+1)\pi/2} kr\, j_\ell(kr) + e^{\pm i(\ell+2)\pi/2} kr\, n_\ell(kr)$$

$$-\sum_{\nu} \sum_{s=0}^{\ell} \sum_{t=0}^{n_\nu+s+1} \Lambda^\nu C^{\nu\pm} e^{-\alpha_\nu r} \frac{(\ell+s)!(\alpha^2+k^2)^{t/2} r^{t-s}}{t!\,s!(\ell-s)!(2k)^s}$$

$$\times\{F^\nu \cos[t\theta_\nu+(s-\ell-1)\frac{\pi}{2}] + G^\nu \sin[t\theta_\nu+(s-\ell-1)\frac{\pi}{2}]\} \tag{106}$$

where

$$C^{\nu\pm} = \sum_{\nu'} R'^{\nu\nu'} C^{\nu'\pm} + U^{\nu\pm} \tag{107}$$

with

$$U^{\nu\pm} = e^{\pm i(\ell+1)\pi/2} \sum_{t=0}^{\ell} \frac{(\ell+t)!(n_\nu-t)!(\alpha_\nu^2+k^2)^{-\frac{1}{2}(n_\nu-t+1)}}{t!(\ell-t)!(2k)^t}$$

$$\times e^{\pm i[(n_\nu-t+1)\theta_\nu+(t-\ell-1)\pi/2]} \tag{108}$$

and $R'^{\nu\nu'}$ is given by Eq. (105a).

The Jost functions $J_\ell^{\pm}(k)$ can now be written as

$$J_\ell^{\pm}(k) = -\frac{(2\ell+1)!!}{k^{\ell+1}} e^{\pm i(\ell+2)\pi/2} + \sum_\nu \Lambda^\nu C^{\nu\pm} \frac{(2\ell)!}{\ell!(2k)^\ell} G^\nu \tag{109}$$

Example III

In this example we combine the results of Example I and Example II and derive the irregular and Jost solutions for the potential given by Eq. (5). The regular solution is given by Eq. (61) and the asymptotic form can be written as

$$u_\ell(r) \xrightarrow[r\to\infty]{} Z_\ell \sin[kr - \tfrac{1}{2}\ell\pi + \delta_\ell]$$

where

$$Z_\ell = \Bigg[\Bigg(\frac{(2\ell+1)!!}{k^{\ell+1}} + \sum_\nu \sum_{g=0}^{K_\nu} \sum_{i=0}^{J_\nu} \sum_{m=0}^{g} \sum_{j=0}^{i} \Lambda_{gi}^\nu b_m^{(g,\nu)} b_j^{(i,\nu)} C_j^\nu F_m^\nu\Bigg)^2$$

$$+ \Bigg(\sum_\nu \sum_{g=0}^{K_\nu} \sum_{i=0}^{J_\nu} \sum_{m=0}^{g} \sum_{j=0}^{i} \Lambda_{gi}^\nu b_m^{(g,\nu)} b_j^{(i,\nu)} C_j^\nu G_m^\nu\Bigg)^2\Bigg]^{\frac{1}{2}}, \tag{110}$$

$$\sin\delta_\ell = \Bigg(-\sum_\nu \sum_{g=0}^{K_\nu} \sum_{i=0}^{J_\nu} \sum_{m=0}^{g} \sum_{j=0}^{i} \Lambda_{gi}^\nu b_m^{(g,\nu)} b_j^{(i,\nu)} C_j^\nu G_m^\nu\Bigg) \Big/ Z_\ell \tag{111a}$$

and

$$\cos\delta_\ell = \left(\frac{(2\ell+1)!!}{k^{\ell+1}} + \sum_{\nu}\sum_{g=0}^{K_\nu}\sum_{i=0}^{J_\nu}\sum_{m=0}^{g}\sum_{j=0}^{i} \Lambda^{\nu}_{gi}\, b^{(g,\nu)}_{m} b^{(i,\nu)}_{j} C^{\nu}_{j} F^{\nu}_{m}\right) \Big/ Z_\ell \tag{111b}$$

The irregular solution $\theta_\ell(r)$ is then straightforward and is given by

$$\theta_\ell(r) = \frac{1}{kZ_\ell}\left[\sin\delta_\ell\, kr\, j_\ell(kr) + \cos\delta_\ell\, kr\, n_\ell(kr)\right]$$

$$- \sum_{\nu}\sum_{g=0}^{\nu}\sum_{i=0}^{J_\nu}\sum_{m=0}^{g}\sum_{j=0}^{i} \Lambda^{\nu}_{gi} b^{(g,\nu)}_{m} b^{(i,\nu)}_{j} C'^{\nu}_{j} e^{-\alpha_\nu r} \sum_{p=0}^{\ell}\sum_{q=0}^{p+n_\nu+m+1}$$

$$\frac{(\ell+p)!(\alpha_\nu^2 + k^2)^{q/2}\, r^{q-p}}{p!\, q!\, (\ell-p)!(2k)} \left\{F^{\nu}_{m} \cos\left[q\theta_\nu + (p-\ell-1)\frac{\pi}{2}\right]\right.$$

$$\left. + G^{\nu}_{m} \sin\left[q\theta_\nu + (p-\ell-1)\frac{\pi}{2}\right]\right\} \tag{112}$$

where

$$C'^{\nu}_{j} = \sum_{\nu'}\sum_{j'=0}^{J_{\nu'}} R'^{\nu\nu'}_{jj'} C'^{\nu'}_{j'} + U'^{\nu}_{j} \tag{113}$$

with

$$R'^{\nu\nu'}_{jj'} = -\sum_{\nu'}\sum_{i=j'}^{J_{\nu'}}\sum_{g=0}^{K_{\nu'}}\sum_{m=0}^{g}\sum_{p=0}^{\ell}\sum_{q=0}^{p+n_\nu+m+1} \Lambda^{\nu'}_{gi} b^{(g,\nu')}_{m} b^{(i,\nu')}_{j'} \frac{(\ell+p)!(n_\nu+j+q-p)!}{q!\,p!(\ell-p)!(2k)^p}$$

$$\times \frac{(\alpha_{\nu'}^2+k^2)^{q/2}}{(\alpha_\nu+\alpha_{\nu'})^{n_\nu+j+q-p+1}} \left\{F^{\nu'}_{m} \cos\left[q\theta_{\nu'} + (p-\ell-1)\frac{\pi}{2}\right]\right.$$

$$\left. + G^{\nu'}_{m} \sin\left[q\theta_{\nu'} + (p-\ell-1)\frac{\pi}{2}\right]\right\} \tag{114a}$$

and

$$U'^{\nu}_{j} = \frac{1}{kZ_{\ell}} \sum_{t=0}^{\ell} \frac{(\ell+t)!(n_{\nu}+j-t)!(\alpha_{\nu}^{2}+k^{2})^{-\frac{1}{2}(n_{\nu}+j-t+1)}}{t!(\ell-t)!(2k)^{t}}$$

$$\times \sin\{(n_{\nu}+j-t+1)\theta_{\nu} + (t-\ell-1)\frac{\pi}{2} + \delta_{\ell}\} \tag{114b}$$

The Jost solutions $f^{\pm}_{\ell}(k,r)$ can now be written as

$$f^{\pm}_{\ell}(k,r) = e^{\pm i(\ell+1)\pi/2} kr\, j_{\ell}(kr) + e^{\pm i(\ell+2)\pi/2} kr\, n_{\ell}(kr)$$

$$- \sum_{\nu} \sum_{g=0}^{K_{\nu}} \sum_{i=0}^{J_{\nu}} \sum_{m=0}^{g} \sum_{j=0}^{i} \Lambda^{\nu}_{gi}\, b^{(g,\nu)}_{m}\, b^{(i,\nu)}_{j}\, C^{\nu\pm}_{j}\, e^{-\alpha_{\nu} r} \sum_{p=0}^{\ell} \sum_{q=0}^{p+n_{\nu}+m+1}$$

$$\frac{(\ell+p)!(\alpha_{\nu}^{2}+k^{2})^{q/2}\, r^{q-p}}{p!q!(\ell-p)!(2k)^{p}} \{F^{\nu}_{m} \cos[q\theta_{\nu} + (p-\ell-1)\frac{\pi}{2}]$$

$$+ G^{\nu}_{m} \sin[q\theta_{\nu} + (p-\ell-1)\frac{\pi}{2}]\} \tag{115}$$

where

$$C^{\nu\pm}_{m} = \sum_{\nu'} \sum_{j=0}^{J_{\nu'}} R'^{\nu\nu'}_{jj'}\, C^{\nu'\pm}_{j'} + U^{\nu\pm}_{j} \tag{116}$$

with

$$U^{\nu\pm}_{j} = e^{\pm i(\ell+1)\pi/2} \sum_{t=0}^{\ell} \frac{(\ell+t)!(n_{\nu}+j-t)!(\alpha_{\nu}^{2}+k^{2})^{-\frac{1}{2}(n_{\nu}+j-t+1)}}{t!(\ell-t)!(2k)^{t}}$$

$$\times e^{\pm i[(n_{\nu}+j-t+1)\theta_{\nu} + (t-\ell-1)\pi/2]} \tag{117}$$

and $R'^{\nu\nu'}_{jj'}$ given by Eq. (114a).

The Jost functions $J_\ell^{\pm}(k)$ are now seen to be

$$J_\ell^{\pm}(k) = -\frac{(2\ell+1)!!}{k^{\ell+1}} e^{\pm i(\ell+2)\pi/2} + \sum_{\nu} \sum_{g=0}^{K_\nu} \sum_{i=0}^{J_\nu} \sum_{m=0}^{g} \sum_{j=0}^{i} \Lambda_{gi}^{\nu} b_m^{(g,\nu)} b_j^{(i,\nu)}$$

$$\times C_j^{\nu\pm} \frac{(2\ell)!}{\ell!(2k)^{\ell}} G_m^{\nu} \qquad (118)$$

2. Equivalent Local Potentials

In this section we develop expressions for equivalent local potential for the class of separable nonlocal potentials for which we have expressions for Jost solutions. We develop this by closely following Coz, Arnold and MacKellar.[41]

Let $f_N^{\pm}(k,r)$ be the Jost solutions to the nonlocal equation

$$\left[\frac{d^2}{dr^2} + k^2 - \frac{\ell(\ell+1)}{r^2}\right] f_N^{\pm}(k,r) = \int_0^{\infty} g_\ell(r|r')\, f_N^{\pm}(k,r')\, dr' \qquad (119)$$

and let $f_L^{\pm}(k,r)$ be the Jost solutions to the local equation

$$\left[\frac{d^2}{dr^2} + k^2 - \frac{\ell(\ell+1)}{r^2}\right] f_L^{\pm}(k,r) = V(r)\, f_L^{\pm}(k,r) \qquad (120)$$

The transformation function which relates the nonlocal solution to the local one is written as

$$f_N^{\pm}(k,r) = A(k,r)\, f_L^{\pm}(k,r) \qquad (121)$$

where A(k,r) is called the damping function. It may be noted that Eq. (121) must be satisfied by both of the independent solutions, whereas a 'trivially' equivalent local potential applies only for one solution.

If we now define

$$\mathcal{J}(k,r) = -\frac{1}{2tk}\left[f^{+}(k,r)\, f^{-\prime}(k,r) - f^{-}(k,r)\, f^{+\prime}(k,r)\right] \tag{122}$$

then $\mathcal{J}_N(k,r)$ will be unity necessarily only at infinity and at the origin and $\mathcal{J}_L(k,r)$ will be unity everywhere. Taking advantage of this property, and remembering that $\mathcal{J}(k,r)$ is a normalized Wronskian, we can use Eqs. (121) and (122) to write

$$\mathcal{J}_N(k,r) = A^2(k,r) \tag{123}$$

Also, if we substitute Eq. (121) into Eq. (119) and use Eq. (120) and Eq. (122) to subtract the local equation, we get

$$\left[V(r) + \frac{A''}{A} - 2\left(\frac{A'}{A}\right)^2\right] f_N^{\pm}(k,r) + 2\left(\frac{A'}{A}\right) f_N^{\pm\prime}(k,r) = \int_0^{\infty} g_{\ell}(r \mid s)\, f_N^{\pm}(k,s)\, ds \tag{124}$$

where the prime denotes differentiation with respect to r.

To get an expression for V(r), we multiply Eq. (124) by $f_N^{\pm'}(k,r)$ and subtract the two resulting equations. We then have

$$V(r) = -\frac{A''}{A} + 2\left(\frac{A'}{A}\right)^2 + \frac{1}{2ikA^2}\left[f_N^{\pm'}(k,r)\int_0^\infty g_\ell(r|s) \times f_N^-(k,s)\,ds - f_N^{-'}(k,r)\int_0^\infty g_\ell(r|s)\, f_N^+(k,s)\,ds\right] \qquad (125)$$

Since compact expressions for $f_N^{\pm}(k,r)$ have been given in Section I, using Eqs. (125) and (122), the ELP V(r) can be calculated. Note that the integrals of $f_N^{\pm}(k,r)$ with the potential which occur in Eq. (125) have already been evaluated in Section I.

3. Summary

In this chapter the technique developed in Chapter II is extended to obtain irregular and Jost solutions for the same class of separable nonlocal potentials discussed there. The irregular wavefunction for the many-term separable potential defined by Eq. (5) is given by Eq. (112), whereas Jost solutions are given by Eq. (115). As in Chapter II, the only unknowns are the elements of the matrix $\mathbb{C}$. For the irregular solution the elements of this matrix can be found by solving Eq. (113) and for Jost solutions these can be found by solving Eq. (116). Since Eqs. (113) and (116) are simple matrix

equations, the solution involves only straightforward matrix inversion. As before, a standard subroutine package like GELG or double precision DGELG from the IBM Subroutine Library can be used.

In passing it may be mentioned that Jost solutions are important not only in finding the Equivalent Local Potential (ELP), but are also useful in a variety of contexts. Examples of other important applications of Jost solutions are given by Newton.[17]

CHAPTER IV

T MATRICES

The calculation of off-shell T matrices has been the subject of numerous investigations.[32,57-62] One of the factors which have created interest in off-shell T matrices has been the work of Faddeev, who has shown that the only input necessary in the equation for three-body scattering is the off-shell T matrix of each of the three possible pairs of particles. The formal calculation of T matrices is particularly simple for the case of a separable nonlocal potential. Watson[63] pointed this out and gave an expression for the separable T matrix for a one-term separable potential. Later on, Tabakin[18] obtained expressions for the off-shell T matrix for a rank two separable nonlocal potential in terms of the matrix elements of the free particle Green's function between the form factors of the potential. Tabakin's procedure can be extended to a potential of arbitrary rank. However, the difficulty with such an extension lies in the increasingly large number of contour integrals which must be evaluated.

Earlier we obtained exact analytic solutions for the wavefunctions and phase shifts for a class of separable nonlocal potentials. In this chapter, we present a method by which the off-shell T matrix can be obtained for the same class of separable nonlocal potentials without the necessity of evaluating any integrals involving Green's functions. In particular, when calculating a T matrix by the technique which we shall outline, an increase in the rank of the potential does not result in as significant an increase in computational effort as with the method of Tabakin. The expressions are in compact form, and given for all partial waves.

To show why the approach presented here can be advantageous for the class of potentials to which it can be applied, it is necessary to briefly review the construction of off-shell T matrices for a separable nonlocal potential of arbitrary rank. We then apply the method to a one-term separable potential before extending the analysis to the class of potentials for which we already have given the exact solutions in configuration space. In all of the calculations in this chapter, we have taken $\hbar^2/2m=1$.

1. T Matrix Calculations with a Separable Nonlocal Potential

The equation for the T matrix is given in terms of the potential V and the off-shell energy ω by

$$T = V + V\,(\omega - K - V + i\epsilon)^{-1}\,V \quad . \tag{126}$$

Let us consider the momentum space elements of the matrix T for the rank J+1 separable nonlocal potential defined by

$$V = \sum_{i,j=0}^{J} \Lambda_{ij} |v_i\rangle\langle v_j| \ . \tag{127}$$

We get

$$\langle k'|T(\omega)|k\rangle = \sum_{i,j,m=0}^{J} \langle k'|v_i\rangle \Lambda_{im} \Big[\delta_{mj} + \sum_{s=0}^{J} \langle v_m|(\omega-K-V+i\epsilon)^{-1}|v_s\rangle \Lambda_{sj}\Big]\langle v_j|k\rangle \ . \tag{128}$$

Because the potential V has been taken to be separable, we see that it is possible to write Eq.(128) for $\langle k'|T(\omega)|k\rangle$ in the form

$$\langle k'|T(\omega)|k\rangle = \sum_{i=0}^{J} \langle k'|v_i\rangle \, W_i(k|\omega) \tag{129}$$

where

$$W_i(k|\omega) = \sum_{j=0}^{J} \Gamma_{ij}(\omega)\langle v_j|k\rangle \tag{130}$$

and $\Gamma_{ij}(\omega)$ are the elements of the matrix $\boldsymbol{\Gamma}(\omega)$ defined by

$$\boldsymbol{\Gamma}(\omega) = \boldsymbol{\Lambda}\,[\mathbf{I} + \langle v|(\omega-K-V+i\epsilon)^{-1}|v\rangle\,\boldsymbol{\Lambda}\,] \ . \tag{131}$$

That is, not only does the T matrix separate as described in Eq.(129), but the function W_i can be written as a matrix with elements Γ_{ij}, which is a function of ω only, multiplied with the transformation function $\langle v_j|k\rangle$ which is a function of k only. It is this feature of the off-shell T matrix which is crucial to the method which we shall employ.

As an initial step, we compare Eq. (129) with $\omega = k^2$ with the half-off-shell T matrix obtained when solving for the stationary state $|\Psi_k^+\rangle$ with outgoing scattered wave appropriate to the potential of Eq. (127). The state $|\Psi_k^+\rangle$ will be the solution of the Lippman-Schwinger equation

$$|\Psi_k^+\rangle = |k\rangle + \sum_{i,j=0}^{J} (k^2 - K + i\epsilon)^{-1} |v_i\rangle \Lambda_{ij} \langle v_j|\Psi_k^+\rangle \quad . \tag{132}$$

To obtain an explicit expression for $|\Psi_k^+\rangle$, we multiply Eq. (132) by $\langle v_m|$

$$\langle v_m|\Psi_k^+\rangle = \langle v_m|k\rangle + \sum_{i,j=0}^{J} \langle v_m|(k^2 - K + i\epsilon)^{-1} |v_i\rangle \Lambda_{ij} \langle v_j|\Psi_k^+\rangle \quad . \tag{133}$$

Equation (133) can be solved for the coefficients $\langle v_m|\Psi_k^+\rangle$. We get

$$\langle v_m|\Psi_k^+\rangle = \sum_{j=0}^{J} M_{mj} \langle v_j|k\rangle \tag{134}$$

where the matrix M is defined by

$$M = [I - \langle v|(k^2 - K + i\epsilon)^{-1} |v\rangle \Lambda]^{-1} \quad . \tag{135}$$

The state $|\Psi_k^+\rangle$ is given by substituting Eq. (134) back into Eq. (132),

$$|\Psi_k^+\rangle = |k\rangle + \sum_{i,j,m=0}^{J} (k^2 - K + i\epsilon)^{-1} |v_i\rangle \Lambda_{im} M_{mj} \langle v_j|k\rangle \quad . \tag{136}$$

The half-off-shell T matrix also follows from a knowledge of the coefficients $\langle v_m|\Psi_k^+\rangle$, and is

$$\langle k'|T(k^2)|k\rangle = \sum_{i=0}^{J} \langle k'|v_i\rangle W_i(k|k^2) \tag{137}$$

where

$$W_i(k|k^2) = \sum_{m=0}^{J} \Lambda_{im} \langle v_m | \Psi_k^+ \rangle \ , \tag{138a}$$

or using Eq. (134)

$$W_i(k|k^2) = \sum_{j,m=0}^{J} \Lambda_{im} M_{mj} \langle v_j | k \rangle \ . \tag{138b}$$

Comparison of Eqs. (130) and (138b) shows that

$$\Gamma_{ij} = \sum_{m=0}^{J} \Lambda_{im} \, M_{mj} \ . \tag{139}$$

Equation (139) establishes the fact that if we know the matrix $\mathbb{M}$ we can calculate the matrix $\mathbb{\Gamma}$. But since off of the energy shell $\mathbb{\Gamma}$ is a function of ω only (and not k), expression (139) for $\mathbb{\Gamma}$ can be continued off the energy shell. Off-shell matrix elements $\langle k' | T(\omega) | k \rangle$ will be given in terms of the $\mathbb{\Gamma}$ thus obtained by Eqs. (129) and (130).

The procedure suggested by Tabakin substitutes the computation of the matrix elements of $\mathbb{M}$ for those of $\mathbb{\Gamma}$. In this dissertation we discuss an alternate method of obtaining the matrix $\mathbb{\Gamma}$ as defined by Eq. (139) which avoids the integration usually necessary to the construction of the elements of $\mathbb{M}$.

2. Expressions for Off-Shell T Matrices for a Rank One Potential

In Chapter II we have presented a method for obtaining analytic solutions for the wavefunction for scattering from a class of separable nonlocal potentials. Here we consider the general symmetric potential $g_\ell(r|r')$ defined by

$$g_\ell(r|r') = \sum_\nu e^{-\alpha_\nu (r+r')} (rr')^{n_\nu} \sum_{g=0}^{J_\nu} \sum_{i=0}^{J_\nu} \Lambda^\nu_{gi} P^\nu_g(r) P^\nu_i(r') \qquad (140)$$

where Λ^ν_{gi} are constants and $P^\nu_i(r)$ is an arbitrary polynomial in r of order i, defined by Eq. (6). The potential of Eq. (140) is the same as that of Eq. (5), with $K_\nu = J_\nu$ and $\Lambda^\nu_{gi} = \Lambda^\nu_{ig}$. From Sec. 1 of this Chapter it is clear that the information necessary to the construction of the matrix Γ is implicit in these solutions. We thus concentrate here on using these solutions to obtain the off-shell T matrix for the class of potentials given by Eq. (140).

a. Off-Shell T Matrices for $\ell=0$

Let us consider first the single term separable potential given by Eqs. (7) and (8):

$$g_\ell(r|r') = \lambda q(r) q(r') \qquad (141)$$

with

$$q(r) = A e^{-\alpha r} r^n . \qquad (142)$$

We will also specialize for the time being to the case $\ell=0$. The normalization chosen for the $\ell=0$ wavefunctions presented earlier was $u_o(0)=0, u_o'(0)=1$.

Such a normalization corresponds to the convention standard in the discussion of Jost solutions. It has the advantage that the Fredholm determinant $\Delta(k)$ will always appear in the denominator of the expression for the scattered portion of the wavefunction. As discussed in the Introduction, in the case of nonlocal potentials, it is well known that the zeros of $\Delta(k)$ correspond to spurious solutions of the Schrödinger equation for $\psi(r)$, and we have pointed out that solutions presented in Chapter II are not valid for $\Delta(k)=0$.

The first step in solving for the off-shell T matrix is to renormalize the wavefunctions to a delta function. In keeping with usual practice, wavefunctions so normalized will be designated by the Dirac bra and ket notation. That is, we will define the wavefunction $\langle r|\Psi_k^o\rangle_o$ as that which satisfies the boundary conditions

$$\langle r|\Psi_k^o\rangle_o \xrightarrow[r\to 0]{} 0 \tag{143a}$$

$$\langle r|\Psi_k^o\rangle_o \xrightarrow[r\to\infty]{} \frac{2}{\pi} \sin(kr + \delta_o) \tag{143b}$$

The superscript o indicates that $|\Psi^o_k\rangle_o$ is the real solution of the radial equation, and the subscript o has been used to designate the $\ell=0$ partial wave. We get

$$\langle r|\Psi^o_k\rangle_o = \sqrt{\frac{2}{\pi}}\left[\frac{1}{N(k^2)} + \frac{Dn!\cos(n+1)\,\theta}{N(k^2)(\alpha^2+k^2)^{\frac{n+1}{2}}}\right]\sin kr$$

$$-\sqrt{\frac{2}{\pi}}\,\frac{Dn!\sin(n+1)\,\theta}{N(k^2)(\alpha^2+k^2)^{\frac{n+1}{2}}}\,\cos kr$$

$$+\sqrt{\frac{2}{\pi}}\,\frac{Dn!e^{-\alpha r}}{N(k^2)(\alpha^2+k^2)^{\frac{n+1}{2}}}\sum_{s=0}^{n}\frac{(\alpha^2+k^2)^{s/2}}{s!}\,r^s\sin(n+1-s)\,\theta \qquad (144)$$

where θ and $D(k^2)$ are given by Eqs. (21) and (27a), and $N(k^2)$ is given by

$$N(k^2) = \left[\left(1+\frac{Dn!\cos(n+1)\,\theta}{(\alpha^2+k^2)^{\frac{n+1}{2}}}\right)^2 + \left(\frac{Dn!\sin(n+1)\,\theta}{(\alpha^2+k^2)^{\frac{n+1}{2}}}\right)^2\right]^{\frac{1}{2}} \qquad (145)$$

It should be pointed out that in using the techniques discussed in Chapter II for obtaining wavefunctions normalized according to Eq. (143), it is both easier and more instructive to use the normalization of Chapter II and then renormalize to Eq. (143). In this way the Fredholm determinant Δ becomes explicit in the T matrix which we later obtain from that wavefunction. Equation (144) can be written in a simpler form in terms of the phase shift δ defined by Eq. (28), which is

$$\tan\delta_o = - \frac{n!\, D \sin(n+1)\,\theta}{(\alpha^2+k^2)^{\frac{n+1}{2}} + n!\, D \cos(n+1)\,\theta} \quad . \tag{146}$$

That is, we can write the expression for $\langle r|\Psi_k^o\rangle_o$ in the form

$$\langle r|\Psi_k^o\rangle_o = \sqrt{\frac{2}{\pi}}\ \sin(kr+\delta_o) + \sqrt{\frac{2}{\pi}}\ \frac{n!\, D\, e^{-\alpha r}}{N(k^2)(\alpha^2+k^2)^{\frac{n+1}{2}}} \sum_{s=0}^{n} \frac{(\alpha^2+k^2)^{s/2}}{s!}\, r^s \sin(n+1-s)\,\theta \ . \tag{147}$$

For the construction of the T matrix we need the wavefunction $\langle r|\Psi_k^+\rangle_o$ with outgoing scattered wave, which is related to the wavefunction $\langle r|\Psi_k^o\rangle_o$ by the condition

$$\langle r|\Psi_k^+\rangle_o = \langle r|\Psi_k^o\rangle_o\ e^{i\delta_o(k)} \tag{148}$$

We will also need the constant D, defined by

$$D = \lambda A \int_0^\infty q(r) u_o(r)\, dr \quad . \tag{149}$$

From Eq. (138a) we have

$$W(k|k^2) = \lambda \langle v|\Psi_k^+\rangle \quad . \tag{150a}$$

Using the relationships between $u_o(r)$, $\langle r|\Psi_k^o\rangle_o$, and $\langle r|\Psi_k^+\rangle_o$ we get

$$W(k|k^2) = \sqrt{\frac{2}{\pi}}\, \frac{k\, D(k^2)\, e^{i\delta_o(k)}}{A\, N(k^2)} \quad . \tag{150b}$$

The transformation function $\langle k|v\rangle \equiv \langle v|k\rangle$ is defined in the $\ell=0$ case by

$$\langle k|v\rangle_o = A\sqrt{\frac{2}{\pi}} \int_0^\infty \sin kr\, e^{-\alpha r}\, r^n dr. \tag{151}$$

This integral can be easily evaluated to give

$$\langle k|v\rangle_o = A\sqrt{\frac{2}{\pi}}\, \frac{n!\sin(n+1)\,\theta}{(\alpha^2 + k^2)^{\frac{n+1}{2}}} \tag{152}$$

Thus from Eqs. (137), (151) and (152) the half-off-shell T matrix for the potential of Eqs. (141) and (142) is

$$\langle k'|T(k^2)|k\rangle = \sqrt{\frac{2}{\pi}}\, \frac{n!\sin(n+1)\,\theta'}{(\alpha^2 + k'^2)^{\frac{n+1}{2}}} \left[\frac{kD(k^2)\, e^{i\delta_o(k)}}{N(k^2)}\right] \tag{153}$$

where θ' is given by Eq. (21) with k replaced by k'.

The function Γ necessary for writing the completely off-shell T matrix can be obtained by factoring $W(k|k^2)$ as given by Eq. (150b) into the form indicated by Eq. (138b). Making use of Eqs. (139), (27a) and (152) we see that

$$\Gamma(\omega) = \frac{\lambda e^{i\delta(\sqrt{\omega})}}{N(\omega)\Delta(\omega)} \,. \tag{154}$$

The completely off-shell T matrix is given by substituting Eq. (154) into Eqs. (129) and (130). We get

$$\langle k'|T(\omega)|k\rangle = \frac{2\lambda A^2 (n!)^2}{\pi} \frac{\sin(n+1)\,\vartheta'}{(\alpha^2+k'^2)^{\frac{n+1}{2}}} \frac{e^{i\delta(\sqrt{\omega})}}{N(\omega)\Delta(\omega)} \frac{\sin(n+1)\,\vartheta}{(\alpha^2+k^2)^{\frac{n+1}{2}}} \tag{155}$$

As a check on the accuracy of Eq. (155) we specialized to the case of the Yamaguchi form factor, n=0, for which the integrals necessary to the computation of the completely off-shell T matrix by the usual methods (that is, the direct evaluation of $\mathbb{M}$ using Eq. (135)) can be easily handled. Both by that procedure and from Eq. (155) we get

$$\langle k'|T(\omega)|k\rangle = \frac{2\eta}{\pi}\left\{1+\frac{\lambda A^2}{2\alpha\beta}\left[\left(\omega-\alpha^2-\frac{\lambda A^2}{2\alpha}\right) - i\,2\alpha\sqrt{\omega}\right]\right\} \tag{156}$$

where

$$\eta = \frac{\lambda A^2\, kk'}{(\alpha^2+k^2)(\alpha^2+k'^2)} \tag{157}$$

and

$$\beta = \left(\omega+\alpha^2-\frac{\lambda A^2}{2\alpha}\right)^2 + 2\alpha\lambda A^2 \,. \tag{158}$$

b. Off-Shell T Matrices for Arbitrary ℓ

The procedure outlined in the previous section can be applied equally easily using the expressions obtained for arbitrary ℓ in Chapter II. In this case the boundary conditions on $\langle r|\Psi^o_k\rangle$ are

$$\langle r|\Psi^o_k\rangle \xrightarrow[r\to 0]{} 0 \tag{159}$$

$$\langle r|\Psi^o_k\rangle \xrightarrow[r\to\infty]{} \sqrt{\frac{2}{\pi}} \sin\left[kr - \tfrac{1}{2}\ell\pi + \delta(k)\right] . \tag{160}$$

The relationship between the outgoing scattered wave and real solution is

$$\langle r|\Psi^+_k\rangle = \langle r|\Psi^o_k\rangle \; e^{i\delta(k)} \tag{161}$$

where $\delta(k)$ is given by Eq. (43). We can thus write for the real solution $\langle r|\Psi^o_k\rangle$ the expression

$$\langle r|\Psi^o_k\rangle = \sqrt{\frac{2}{\pi}} \frac{1}{N}\left[\left(1 + \frac{k^{\ell+1}}{(2\ell+1)!!} FD\right) krj_\ell(kr) + \frac{k^{\ell+1}}{(2\ell+1)!!} GDkrn_\ell(kr)\right]$$

$$-\sqrt{\frac{2}{\pi}} \frac{k^{\ell+1}}{(2\ell+1)!!} \frac{De^{-\alpha r}}{N} \sum_{s=0}^{\ell} \sum_{t=0}^{n+s+1} \frac{(\ell+s)!(\alpha^2+k^2)^{t/2} r^{t-s}}{s!t!(\ell-s)!(2k)^s}$$

$$\times \left[F\cos\left(t\theta + (s-\ell-1)\frac{\pi}{2}\right) + G\sin\left(t\theta + s - \ell - 1)\frac{\pi}{2}\right)\right] \tag{162}$$

where F, G and D are defined respectively by Eqs. (36), (37) and (42a), N is defined as

$$N = \left[\left(1 + \frac{k^{\ell+1} FD}{(2\ell+1)!!}\right)^2 + \left(\frac{k^{\ell+1} GD}{(2\ell+1)!!}\right)^2\right]^{\frac{1}{2}} \tag{163}$$

and θ is given by Eq. (21).

For arbitrary ℓ the transformation function $\langle k|v\rangle$ can be shown to be

$$\langle k|v\rangle = A\sqrt{\frac{2}{\pi}}\, Q \tag{164}$$

where

$$Q = \sum_{s=0}^{\ell} \frac{(\ell+s)!(n-s)!}{s!(\ell-s)!(2k)^s} (\alpha^2+k^2)^{\frac{s-n-1}{2}} \cos\left[(n-s+1)\theta + (s-\ell-1)\frac{\pi}{2}\right] \tag{165}$$

The half-off-shell T matrix is then given by

$$\langle k'|T(k^2)|k\rangle = \frac{2}{\pi} Q(k') \frac{k^{\ell+1} D(k^2)}{(2\ell+1)!!N(k^2)} e^{i\delta(k)} \tag{166}$$

To obtain the completely off-shell T matrix we must factor the expression for D. We get

$$D = \lambda A^2 \frac{(2\ell+1)!!}{k^{\ell+1}\Delta} Q \tag{167}$$

where Δ is the Fredholm determinant defined by Eq. (42b). Thus

$$\Gamma(\omega) = \frac{\lambda e^{i\delta(\sqrt{\omega})}}{N(\omega)\Delta(\omega)} \quad . \tag{168}$$

The expression for $\langle k'|T(\omega)|k\rangle$ becomes

$$\langle k'|T(\omega)|k\rangle = \frac{2}{\pi} A^2 Q(k')\Gamma(\omega)Q(k) \tag{169}$$

3. Off-Shell T Matrices for Many-Term-Separable Potentials

In this section we consider T matrices for three examples of many-term separable potentials.

Case a.

Let us consider first, as before, a potential of the form of Eq. (140) for which α is fixed (no summation over ν). That is, we will obtain the T matrix for the potential

$$g_\ell(r|r') = e^{-\alpha(r+r')}(rr')^n \sum_{i=0}^{J} \lambda_i P_i(r) P_i(r') \tag{170}$$

This potential is of the type defined in Eq. (127) with $\Lambda_{ij} = \lambda_i \delta_{ij}$:

$$V = \sum_{i=0}^{J} \lambda_i |v_i\rangle\langle v_i| \tag{171}$$

with

$$\langle r|v_i\rangle = \sum_{m=0}^{i} b_m^{(i)} e^{-\alpha r} r^{n+m} \tag{172}$$

In order to obtain the T matrix for the potential of Eq. (170) we will need an expression for $\langle v_i|\Psi_k^+\rangle$. From the solution u(r) for this potential, given as Eq. (48), and the phase shift, given by Eq. (52), it is possible to obtain $\langle v_i|\Psi_k^+\rangle$ directly.

$$\langle v_i|\Psi_k^+\rangle = \sqrt{\frac{2}{\pi}}\, \langle v_i|u\rangle\, \frac{k^{\ell+1} e^{i\delta(k)}}{(2\ell+1)!!N(k^2)} \tag{173}$$

where

$$N = \left[\left(1+\frac{k^{\ell+1}}{(2\ell+1)!!}\sum_{i=0}^{J}\sum_{j=0}^{i}\sum_{m=0}^{i}\lambda_i b_j^{(i)} b_m^{(i)} C_m^{(n)} F_j^{(n)}\right)^2\right.$$

$$\left.+\left(\frac{k^{\ell+1}}{(2\ell+1)!!}\sum_{i=0}^{J}\sum_{j=0}^{i}\sum_{m=0}^{i}\lambda_i b_j^{(i)} b_m^{(i)} C_m^{(n)} G_j^{(n)}\right)^2\right]^{\frac{1}{2}} \tag{174}$$

and $F_j^{(n)}$ and $G_j^{(n)}$ are defined by Eqs. (36) and (37), respectively, with n replaced by n+j. The transformation function $\langle v_i|u\rangle$ follows from Eq. (172) and the definition

$$C_m^{(n)} = \int_0^\infty e^{-\alpha r} r^{n+m} u(r)\,dr \tag{175}$$

and is

$$\langle v_i|u\rangle = \sum_{m=0}^{i} b_m^{(i)} C_m^{(n)} \quad . \tag{176}$$

From Eq. (138a) we see then that

$$W_i(k|k^2) = \lambda_i\sqrt{\frac{2}{\pi}}\,\frac{k^{\ell+1}e^{i\delta(k)}}{(2\ell+1)!!N(k^2)}\sum_{m=0}^{i} b_m^{(i)} C_m^{(n)} \, . \tag{177}$$

Since the potential $\langle r|v_i\rangle$ defined by Eq. (172) is expressed as a sum of terms, it is convenient to define subfunctions $[v_s|k]$ such that

$$\langle v_i|k\rangle = \sum_{s=0}^{i} b_s^{(i)} [v_s|k] \, . \tag{178}$$

The information necessary for obtaining an expression for $[v_s|k]$ has been given in Chapter II, since

$$[v_s|k] = \sqrt{\frac{2}{\pi}} \frac{k^{\ell+1}}{(2\ell+1)!!} \quad U_s^{(n)} \tag{179}$$

and $U_s^{(n)}$ is defined by Eq. (51). The half-off-shell T matrix for the potential of Eq. (170) will, therefore, be

$$\langle k'|T(k^2)|k\rangle = \frac{2}{\pi} \sum_{i=0}^{J} \lambda_i \left[\frac{(k')^{\ell+1}}{(2\ell+1)!!} \sum_{s=0}^{i} U_s(k')\right] \frac{k^{\ell+1}}{(2\ell+1)!!} \frac{e^{i\delta(k)}}{N(k^2)} \sum_{m=0}^{i} b_m^{(i)} C_m^{(n)} . \tag{180}$$

For the completely off-shell T matrix we must rewrite Eq. (177) for $W_i(k|k^2)$, as required by Eq. (138b). From Eq. (49) we have

$$C_m^{(n)} = \sum_{j=0}^{J} R_{mj}^{(n)} C_j^{(n)} + U_m^{(n)}$$

or, in matrix notation

$$[\mathbb{I} - \mathbb{R}] \underset{\sim}{C} = \underset{\sim}{U} \tag{181}$$

Let us for convenience define the matrix $\mathbb{L}$ by

$$\mathbb{L} = [\mathbb{I} - \mathbb{R}]^{-1} \tag{182}$$

Then

$$C_m^{(n)} = \sum_{j=0}^{J} L_{mj} U_j^{(n)} . \tag{183}$$

Substituting Eq. (183) into Eq. (176) gives

$$\langle v_i | u \rangle = \sum_{j=0}^{J} \left(\sum_{m=0}^{i} b_m^{(i)} L_{mj} \right) U_j^{(n)} \tag{184}$$

Putting this back into Eq. (177) for $W_i(k|k^2)$ and using Eq. (179) gives

$$W_i(k|k^2) = \lambda_i \frac{e^{i\delta(k)}}{N(k^2)} \sum_{s=0}^{J} \left(\sum_{m=0}^{i} b_m^{(i)} L_{ms} \right) [v_s|k] \ . \tag{185}$$

Equation (185) cannot be directly compared with Eqs. (138b) and (139) to determine Γ_{ij}. Introducing Eq. (178) into (138b) we get, after changing an order of summation

$$W_i(k|k^2) = \sum_{s=0}^{J} \sum_{m=0}^{J} \sum_{j=s}^{J} \Lambda_{im} M_{mj} b_s^{(j)} [v_s|k] \ . \tag{186}$$

Since the coefficients $b_s^{(j)}$ are constants, independent of either ω or k, Eq. (130) can be rewritten in the form

$$W_i(k|\omega) = \sum_{s=0}^{J} \gamma_{is}(\omega) [v_s|k] \tag{187}$$

where

$$\gamma_{is}(\omega) = \sum_{j=s}^{J} \Gamma_{ij}(\omega) b_s^{(j)} \ . \tag{188}$$

Comparing Eqs. (186) and (187) shows that

$$\gamma_{is} = \sum_{m=0}^{J} \sum_{j=s}^{J} \Lambda_{im} M_{mj} b_s^{(j)} \ . \tag{189}$$

It then follows that the off-shell T matrix is given by

$$\langle k' | T(\omega) | k \rangle = \frac{2}{\pi} \sum_{i=0}^{J} \sum_{t=0}^{i} \frac{(k')^{\ell+1}}{(2\ell+1)!!} b_t^{(i)} U_t^{(n)}(k') \gamma_{is}(\omega) \frac{k^{\ell+1}}{(2\ell+1)!!} U_s^{(n)}(k) \tag{190}$$

where, from Eq. (185),

$$\gamma_{is}(\omega) = \lambda_i \frac{e^{i\delta}}{N} \sum_{s=0}^{J} \left(\sum_{m=0}^{i} b_m^{(i)} L_{ms} \right) . \tag{191}$$

Case b.

As a second example, we consider the nonlocal potential

$$g_\ell(r|r') = \sum_{\nu=0} \Lambda^\nu e^{-\alpha_\nu (r+r')} (rr')^\nu \tag{192}$$

for which the wavefunction and phase shift were determined in Chapter II.

For $\langle v^\nu | \Psi_k^+ \rangle$ we get

$$\langle v^\nu | \Psi_k^+ \rangle = \sqrt{\frac{2}{\pi}} \frac{k^{\ell+1}}{(2\ell+1)!!} \langle v^\nu | u \rangle \frac{e^{i\delta(k)}}{N(k^2)} \tag{193}$$

where

$$N = \left[\left(1 + \frac{k^{\ell+1}}{(2\ell+1)!!} \sum_\nu \Lambda^\nu C^\nu F^\nu \right)^2 + \left(\frac{k^{\ell+1}}{(2\ell+1)!!} \sum_\nu \Lambda^\nu C^\nu G^\nu \right)^2 \right]^{\frac{1}{2}} . \tag{194}$$

The transformation function $\langle v^\nu | u \rangle$ is given by

$$\langle v^\nu | u \rangle = C^\nu = \int_0^\infty e^{-\alpha_\nu t} r^\nu u(r)\, dr . \tag{195}$$

From Eq. (138a) we see then that

$$W^{\nu}(k|k^2) = \sqrt{\frac{2}{\pi}} \frac{k^{\ell+1}}{(2\ell+1)!!} \frac{e^{i\delta(k)}}{N(k^2)} \Lambda^{\nu} C^{\nu} . \tag{196}$$

Since

$$\langle v^{\nu}|k\rangle = \sqrt{\frac{2}{\pi}} \frac{k^{\ell+1}}{(2\ell+1)!!} U^{\nu} , \tag{197}$$

where U^{ν} is given by Eq. (59), the half-off-shell T matrix for the potential of Eq. (170) will be

$$\langle k'|T(k^2)|k\rangle = \frac{2}{\pi} \sum_{\nu} \Lambda^{\nu} \frac{(k')^{\ell+1}}{(2\ell+1)!!} U^{\nu}(k') \frac{e^{i\delta(k)}}{N(k^2)} \frac{(k)^{\ell+1}}{(2\ell+1)!!} C^{\nu} \tag{198}$$

where C^{ν} can be determined using Eq. (57), namely

$$C^{\nu} = \sum_{\nu} R^{\nu\nu'} C^{\nu'} + U^{\nu} \tag{199}$$

and $R^{\nu\nu'}$ has been defined by Eq. (58).

From Eq. (198) it follows that

$$C^{\nu} = \sum_{\nu'} L^{\nu\nu'} U^{\nu'} \tag{200}$$

where

$$\mathbb{L} = [\mathbb{I} - \mathbb{R}]^{-1} . \tag{201}$$

Thus we get for the off-shell T matrix the expression

$$\langle k'|T(\omega)|k\rangle = \frac{2}{\pi} \sum_{\nu,\nu'} \frac{(k')^{\ell+1}}{(2\ell+1)!!} U^{\nu}(k') \Gamma^{\nu\nu'}(\omega) \frac{k^{\ell+1}}{(2\ell+1)!!} U^{\nu'}(k) \tag{202}$$

where

$$T^{\nu\nu'} = \frac{\Delta^{\nu} e^{i\delta}}{N} \; L^{\nu\nu'} \tag{203}$$

Case c.

As a final example we consider the T matrix associated with the general potential defined by Eq. (140). This potential can be written as

$$V = \sum_{\nu} \sum_{i,j=0}^{J_{\nu}} \Lambda_{ij}^{\nu} |v_i^{\nu}\rangle\langle v_j^{\nu}| \tag{204}$$

where

$$\langle r|v_i^{\nu}\rangle = e^{-\alpha_{\nu} r} \, r^{n_{\nu}} P_i^{\nu}(r) \; . \tag{205}$$

Such a potential is still of the general form defined in Eq. (127). In writing the potential as in Eq. (198), we have merely broken down the J+1 dimensional matrix Λ_{ij} into a set of square submatrices of dimensions $J_{\nu}+1$, ($\nu=0,1\ldots$), as indicated by the presence of the superscript ν, such that

$$J+1 = \sum_{\nu=0} (J_{\nu}+1) \tag{206}$$

Following the procedure used in I, we obtain the wavefunction and phase shift appropriate to the potential the expressions

Again it is convenient to write the transformation function in terms of subfunctions, in the following manner

$$\langle v_m^{\nu} | k \rangle = \sum_{j=0}^{m} b_j^{(m,\nu)} \, [v_j^{\nu} | k] \tag{207}$$

where the function $[v_j^{\nu} | k]$ will be given by

$$[v_j^{\nu} | k] = \sqrt{\frac{2}{\pi}} \, \frac{k^{\ell+1}}{(2\ell+1)!!} \, U_j^{\nu} \, . \tag{208}$$

Equation (129) for the off-shell T matrix becomes

$$\langle k' | T(\omega) | k \rangle = \sum_{\nu} \sum_{i=0}^{J_{\nu}} \langle k' | v_i^{\nu} \rangle W_i^{\nu}(k | \omega) \tag{209}$$

and, in analogy with Eqs. (187) and (188)

$$W_i^{\nu}(k | \omega) = \sum_{\nu'} \sum_{s=0}^{J_{\nu'}} \gamma_{is}^{\nu\nu'} \, [v_s^{\nu'} | k] \tag{210}$$

with

$$\gamma_{is}^{\nu\nu'} = \sum_{j=0}^{J_{\nu}} \Lambda_{ij}^{\nu} \sum_{t=s}^{J_{\nu'}} b_s^{(t,\nu)} \Big[\delta_{jt}^{\nu\nu'} + \sum_{m=0} \langle v_j^{\nu} | (\omega - k - V + i\epsilon)^{-1} | v_m^{\nu'} \rangle \, \Lambda_{mt}^{\nu'} \Big] . \tag{211}$$

For this potential, the expression for $\langle v_m^{\nu} | \Psi_k^{+} \rangle$ is given by

$$\langle v_m^{\nu} | \Psi_k^{+} \rangle = \langle v_m^{\nu} | u \rangle \, e^{i\delta(k)} \sqrt{\frac{2}{\pi}} \, \frac{k^{\ell+1}}{(2\ell+1)!! N(k^2)} \tag{212}$$

where the phase $\delta(k)$ was defined in Eq. (62) and

$$N = \left[\left(1 + \frac{k^{\ell+1}}{(2\ell+1)!!} \sum_{\nu} \sum_{i,g=0}^{J_\nu} \sum_{m=0}^{g} \sum_{j=0}^{i} \Lambda^{\nu}_{gi} b^{(g,\nu)}_{m} b^{(i,\nu)}_{j} C^{\nu}_{j} F^{\nu}_{m} \right)^2 \right.$$

$$\left. + \left(\frac{k^{\ell+1}}{(2\ell+1)!!} \sum_{\nu} \sum_{i,\, g=0}^{J_\ell} \sum_{m=0}^{g} \sum_{j=0}^{i} \Lambda^{\nu}_{gi} b^{(g,\nu)}_{m} b^{(i,\nu)}_{j} C^{\nu}_{j} G^{\nu}_{m} \right)^2 \right]^{\frac{1}{2}} \tag{213}$$

Since

$$\langle v^{\nu}_{m} | u \rangle = \sum_{j=0}^{m} b^{(m,\nu)}_{j} C^{\nu}_{j} , \tag{214}$$

it follows from Eq. (212) that

$$\langle v^{\nu}_{m} | \Psi^{+}_{k} \rangle = \sqrt{\frac{2}{\pi}} \frac{k^{\ell+1} e^{i\delta(k)}}{(2\ell+1)!!N(k^2)} \sum_{j=0}^{m} b^{(m,\nu)}_{j} C^{\nu}_{j} . \tag{215}$$

Thus, from the definition of the half-off-shell T matrix

$$\langle k' | T(k^2) | k \rangle = \sum_{\nu} \sum_{i,m=0}^{J_\nu} \Lambda^{\nu}_{im} \langle k' | v^{\nu}_{i} \rangle \langle v^{\nu}_{m} | \Psi^{+}_{k} \rangle \tag{216}$$

we have that

$$\langle k' | T(k^2) | k \rangle = \sum_{\nu} \sum_{i=0}^{J_\nu} \langle k' | v^{\nu}_{i} \rangle W^{\nu}_{i}(k | k^2) \tag{217}$$

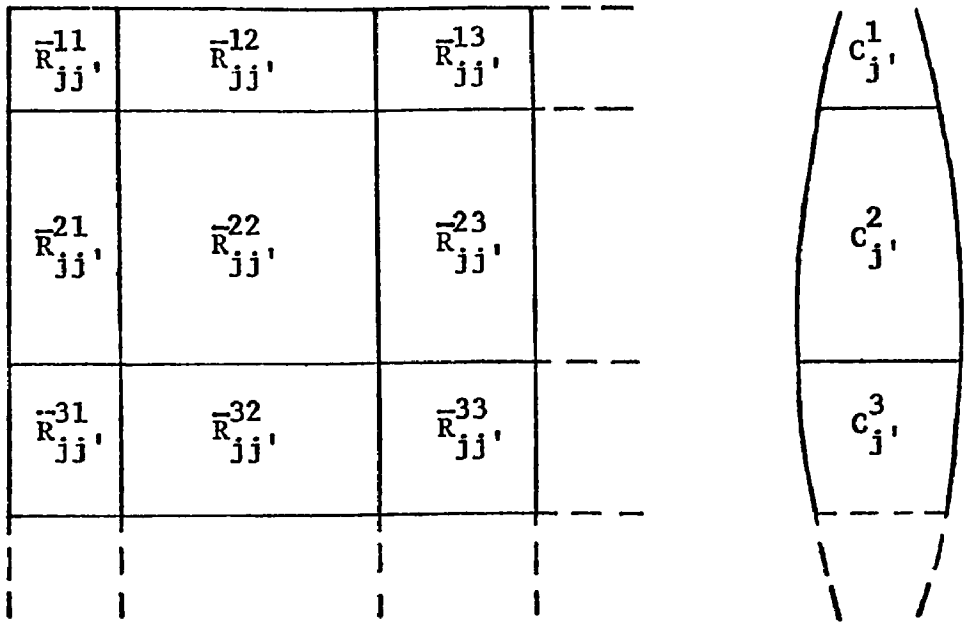
where

$$W^{\nu}_{i}(k | k^2) = \sum_{m=0}^{J_\nu} \Lambda^{\nu}_{im} \sqrt{\frac{2}{\pi}} \frac{k^{\ell+1} e^{i\delta(k)}}{(2\ell+1)!!N(k^2)} \sum_{j=0}^{m} b^{(m,\nu)}_{j} C^{\nu}_{j} . \tag{218}$$

To obtain the off-shell T matrix, it is necessary to factor Eq. (212) into a form which makes the expression for $\gamma_{is}^{\nu\nu'}$ explicit. For this purpose, we must transform Eq. (63) to a form which can be inverted for the unknowns C_j^{ν} in terms of the known quantities U_j^{ν}. As mentioned earlier, following the introduction of the single superscript ν in Eqs. (204) and (205), the addition of such a superscript merely breaks the matrix element Λ_{ij} into submatrices which lie along the diagonal. The double superscripts on R in Eqs. (63) and (64) indicate that the submatrices of which it is composed will not lie along the diagonal. Thus for the inversion process at hand we must consider the J+1 dimensional matrix $\bar{\mathbb{R}}$ with components $\bar{R}_{ij}$ composed of the submatrices $R_{jj'}^{\nu\nu'}$. The equation

$$[\mathbb{I} + \bar{\mathbb{R}}]\,\underset{\sim}{C} = \underset{\sim}{U} \tag{219}$$

will correspond to the usual rules for matrix multiplication if the matrix $\bar{\mathbb{R}}$ and the vector $\underset{\sim}{C}$ are constructed as follows



On this basis, Eq.(219) can be inverted to give

$$\underset{\sim}{C} = \bar{\mathbb{L}}\ \underset{\sim}{U} \tag{220}$$

or, breaking the larger matrix $\bar{\mathbb{L}}$ into submatrix formulation

$$C^{\nu}_{j} = \sum_{\nu'} \sum_{s=0}^{J_{\nu'}} L^{\nu\nu'}_{js}\ U^{\nu'}_{s} \tag{221}$$

Substituting Eq.(221) into Eq.(218), making use of Eq.(208), and changing an order of summation gives for $W^{\nu}_{i}(k|k^2)$ the result

$$W^{\nu}_{i}(k|k^2) = \sum_{s=0}^{J_{\nu'}} \gamma^{\nu\nu'}_{is}\ [v^{\nu}_{s}|k] \tag{222}$$

where

$$\gamma_{is}^{\nu\nu'} = \sum_{m=0}^{J_\nu} \sum_{j=0}^{m} \Lambda_{im}^{\nu} \frac{e^{i\delta(k)}}{N(k^2)} b_j^{(m,\nu)} L_{js}^{\nu\nu'} . \tag{223}$$

It then follows that the off-shell T matrix is given by

$$\langle k' | T(\omega) | k \rangle$$

$$= \frac{2}{\pi} \sum_{\nu,\nu'} \sum_{i=0}^{J_\nu} \sum_{s=0}^{J_{\nu'}} \sum_{t=0}^{i} \frac{k'^{\ell+1}}{(2\ell+1)!!} b_t^{(i,\nu)} U_t^{\nu}(k') \gamma_{is}^{\nu\nu'}(\omega) \frac{k^{\ell+1}}{(2\ell+1)!!} U_s^{\nu'}(k) \tag{224}$$

where $\gamma_{is}^{\nu\nu'}(\omega)$ is given by Eq. (223) with k replaced by $\sqrt{\omega}$.

4. Summary

For local potentials, closed form expressions for off-shell T matrix elements for arbitrary ℓ are not available in the literature. For the case $\ell = 0$ analytic expressions are available only for a few very special potentials like the exponential and Hulthen potential. Even for separable nonlocal potentials, for which the formal expressions for T matrix elements are relatively simple, expressions in closed form are available only for a very few special cases. Partly as a result of the frustrations encountered in calculating T matrices from potentials, attention is now being paid[64] to avoiding a potential formalism and fitting directly the T matrix elements as experimentally, since it is T and not V which is measured.

In this chapter we have derived in closed form expressions for T matrices (half-off-shell and off-shell) for the class of separable nonlocal potentials defined by Eq.(140). Equation (217) gives the expression for half-off-shell T matrix elements, whereas Eq. (224) gives the expression for the completely off-shell T matrix elements. In both equations the only unknowns are the matrix elements of $\mathbb{C}$, which can be determined in the manner discussed in Chapter II. However, Eq. (224) uses a special form of C; that is, the matrix elements of $\mathbb{L}$ which are given by Eq. (221).

CHAPTER V

APPLICATIONS

In Chapter II we derived equations for the phase shifts for a class of separable potentials. However, from the general expression for the phase shift for a many-term potential it is not clear how one can obtain exact algebraic expressions for the scattering length and effective range. If the potential is simple in form, then the proper matrices can be easily inverted and expressions for the scattering length and effective range can be found without much difficulty. For adjusting potential parameters to fit phase shift data, availability of such expressions makes the fitting much easier to handle.

As an application, we take the case of a well-known, two-term, separable potential, Mongan's potential (Case IV).[21] This potential has been widely used in nuclear calculations and certain drawbacks to the use of this potential have been pointed out. We begin our discussion of this potential by reproducing the known results and commenting on

these drawbacks. Next we find a two-term separable potential, but with only three adjustable parameters, which fits the $^1S_0$ n-p phase shift data reasonably well and is free from the shortcomings pointed out for the Mongan-potential.

1. Scattering Length and Effective Range

From the formula for the phase shift produced by a two-term potential it is possible to obtain explicit expressions for the scattering length and effective range in terms of the parameters of that potential. The scattering length and effective range are very sensitive functions of the potential parameters. For this reason, numerical approaches to the calculation of the scattering length and effective range can be misleading, and the exact expression should be used when possible.

The Mongan (Case IV) potential is of the form of Eq. (53) and is

$$g(r|r') = \frac{\hbar^2}{2m} [\lambda_1 e^{-\alpha_1(r+r')} + \lambda_2 e^{-\alpha_2(r+r')}] \qquad (225)$$

We found a reasonable fit to the $1S_0$ n-p phase shift data with the following set of parameters:

$$\lambda_1 = 3454.8 \text{ fm}^{-3} = 143264 \text{ MeV fm}^{-1}$$

$$\lambda_2 = -28.293 \text{ fm}^{-3} = -1173.25 \text{ MeV fm}^{-1}$$

$$\alpha_1 = 6.157 \text{ fm}^{-1}$$

$$\alpha_2 = 1.786 \text{ fm}^{-1} \quad .$$

In obtaining these values, he used a scattering length of -23.687 fm and an effective range of 2.729 fm. Recalculation of the values of these two parameters for the Mongan potential by Serduke and Afnan[65] has led to the revised numbers a = -23.862 fm and r = 2.323 fm.

As the analytic expressions for the scattering length and effective range for the potential of Eq. (225) we get

$$a = \frac{A}{C} \tag{226}$$

$$r = \frac{2}{A}\left(\frac{BC}{A} - D\right) \tag{227}$$

where

$$A = 2\alpha_1\,\alpha_2(\alpha_1+\alpha_2)\,[2(\alpha_1+\alpha_2)(\lambda_1\,\alpha_2^4+\lambda_2\,\alpha_1^4)+\lambda_1\lambda_2(\alpha_1-\alpha_2)^2\,] \tag{228}$$

$$B = 2(\alpha_1+\alpha_2)\,[4\alpha_1\,\alpha_2(\alpha_1+\alpha_2)(\lambda_1\,\alpha_2^2+\lambda_2\alpha_1^2)-\lambda_1\,\lambda_2(\alpha_1-\alpha_2)^2\,] \tag{229}$$

$$C = 2\alpha_1^2\alpha_2^2(\alpha_1+\alpha_2)^2[2\alpha_1^3\alpha_2^3+\lambda_1\,\alpha_2^3+\lambda_2\alpha_1^3]+\lambda_1\,\lambda_2\alpha_1^2\alpha_2^2(\alpha_1-\alpha_2)^2 \tag{230}$$

and

$$D = 8\alpha_1^3\alpha_2^3(\alpha_1^2+\alpha_2^2)(\alpha_1+\alpha_2)^2+2\lambda_1\,\alpha_2^3(\alpha_1+\alpha_2)^2\;(2\alpha_1^2-\alpha_2^2)$$

$$+2\lambda_2\alpha_1^3(\alpha_1+\alpha_2)^2\;(2\alpha_2^2-\alpha_1^2)\;-\lambda_1\,\lambda_2(\alpha_1-\alpha_2)^2\;(\alpha_1^2+\alpha_2^2+4\alpha_1\,\alpha_2) \tag{231}$$

Substituting into Eq. (226) and (227) the values of the Mongan potential parameters we obtain a = - 23.874 fm and r = 2.323 fm. Thus our expressions substantiate the revised values published by Serduke and Afnan.

2. An Alternate $^1S_0$ n-p Potential.

The solutions presented in Chapter II facilitate the inverse process of determining from the class of analytic forms under discussion the parameters of a particular potential appropriate to a given set of phase shifts. Since Mongan proposed the potential of Eq. (225) more accurate values of the $^1S_0$ n-p scattering length and effective range have become available. The accepted values are now[66]

$$a = - 23.715 \pm 0.015 \text{ fm}$$

$$r = 2.73 \pm 0.03 \text{ fm}.$$

Our expressions for these parameters have shown that the calculations of Serduke and Afnan are essentially correct with respect to the Mongan Case IV potential, which is thus no longer in agreement with the newly accepted values of a and r. In addition, it has been pointed out by Arnold and MacKellar[43] that there may be other difficulties associated with the use of the Mongan Case IV potential, in that it has a spurious state at 19.6 BeV.

We consider now an alternate potential of a different analytic form, namely

$$g(r,r') = \frac{\hbar^2}{2m}[\lambda_1 + \lambda_2 (r,r')^2 \,] e^{-\alpha(r+r')}. \qquad (232)$$

This potential is a special case of the type presented in Eq. (44). The phase shift is given by

$$\tan \delta = - N/M \qquad (233)$$

where

$$N = \lambda_1 32\alpha^6 k(\alpha^2+k^2)^5 + \lambda_2 128\alpha^6 k(\alpha^2+k^2)(3\alpha^2-k^2)^2$$

$$+\lambda_1 \lambda_2 8\alpha k (21\alpha^8 - 4\alpha^6 k^2 - 42\alpha^4 k^4 - 20\alpha^2 k^6 - 3k^8) \qquad (234)$$

and

$$M = 32\alpha^6(\alpha^2+k^2)^7 + \lambda_1 16\alpha^5 (\alpha^4-k^4)(\alpha^2+k^2)^4$$

$$+ \lambda_2 8\alpha(\alpha^2+k^2)(33\alpha^{10} - 215\alpha^8 k^2 - 30\alpha^6 k^4 - 54\alpha^4 k^6 - 19\alpha^2 k^8 - 3k^{10})$$

$$+2\lambda_1 \lambda_2 (17\alpha^{10} - 135\alpha^8 k^2 - 182\alpha^6 k^4 - 14\alpha^4 k^6 + 21\alpha^2 k^8 + 5k^{10}). \qquad (235)$$

In pursuing a fit with the potential of Eq. (232) our objectives were to use a simpler potential (note that the potential of Eq. (232) has only three adjustable parameters as compared to four for the Mongan potential) and to obtain a potential for which the Fredholm determinant would be

greater than zero for all energies (no spurious states), while normalizing to the new values of the scattering length and effective range. With these considerations in mind, we were able to find a reasonable fit to the $^1S_0$ n-p phase shifts of MacGregor et al.[67] The potential parameters we found which best fulfilled the criteria used were

$$\lambda_1 = 3.91 \text{ fm}^{-3} = 162.2 \text{ MeV fm}^{-1}$$

$$\lambda_2 = -41.06 \text{ fm}^{-7} = -1702.8 \text{ MeV fm}^{-5}$$

$$\alpha = 2.286 \text{ fm}^{-1} \quad .$$

In all calculations in this chapter we have used $\hbar^2/2m = 1/41.47 \text{ MeV}^{-1}\text{fm}^{-2}$. Figure 1 compares our calculated values of the phase shifts with the experimental values. The values of the scattering length and effective range for this potential are

$$a = -23.711 \text{ fm}$$

$$r = 2.718 \text{ fm}.$$

In order to provide a comparison of this potential with the Mongan potential, we have plotted the Fredholm determinant $\Delta(k)$ in Fig. 2. The insert in Fig. 2 is the Fredholm determinant for the Mongan potential. Figure 3 provides a plot of the zero energy wave functions for the potential of Eq. (232), using the parameters listed above. Since there is no spurious state, the wave function does not exhibit the extra node which occurs for the Mongan wave function, plotted on the same figure for comparison.

Finally, we have plotted as Fig. 4 the nonlocal potential of Eq. (232) for the case r'=r. In order to provide a depth parameter in MeV, the potential has been divided by α.

3. Summary

In this chapter we have employed the solutions derived in Chapter II to obtain pertinent results for two different separable potentials, one being the well-known Mongan potential (Case IV) and the other being a potential which has not previously been reported in the literature. Since Mongan's potential has been widely used in nuclear calculations, our purpose in applying the present method to obtain exact results for this potential was twofold. First, we wanted to reproduce the two-nucleon data which are available from numerical calculations, thus verifying in this special case the correctness of the exact expressions derived in Chapter II. Second, we wanted to compare these calculations with the results obtained using the new potential. By also fitting the data with a second potential, we were able to demonstrate the utility of both the class of potentials discussed in this dissertation and the method presented for obtaining exact solutions for potentials of this class.

CHAPTER VI

CONCLUSION

In considering the use of a nonlocal potential for the description of the nucleon-nucleon interaction, several important points must be emphasized. There is no a priori reason to assume that the interaction between two nucleons can be expressed in terms of a local nucleon-nucleon interaction. In fact,in the attempt to compress the description of this very complex interaction into the form of a standard two-body Schrödinger equation one would, until evidence could be produced to the contrary, expect the potential to be of the most general form, i.e., nonlocal. In the case of the many body problem of a nucleon interacting with a nucleus, it has been demonstrated by Feshbach[8] that the more general nonlocal interaction is required for its description. In this case, the evidence for the necessity that the potential be nonlocal has been provided by the demonstrations, particularly by Perey and Buck[9] and Mulligan,[2] that nonlocality can lead to the dependence of the depth of the optical potential upon the energy of the incident particle required for

fitting the experimental data. Although there has been much success with the description of nucleon-nucleon data in terms of local potential models, evidence is now beginning to surface strongly suggesting that the use of a nonlocal interaction is required if a description of all of the experimental data is to be had in terms of a potential model. The work of Arnold and Seyler[46] is the first really strong evidence that a nonlocal potential may be required for fitting experimental data in the case of the nucleon-nucleon interaction.

Replacing the more commonly used local interaction by a nonlocal one in the description of the nucleon-nucleon problem should not be looked upon as resulting in a further complication of an already very complex calculational problem. For example, Kermode[68] has shown that a precise fit to the experimental $^1S_0$ neutron-proton phase shifts with a local potential requires fourteen terms. Although a precision fit using a nonlocal potential has not yet been obtained, it is hoped that such a fit will require fewer terms. Also, as shown in the calculations of this dissertation, it is relatively easy to obtain exact expressions in closed form for wavefunctions, T matrices, phase shifts, etc. for a large number of separable nonlocal potentials. Exact analytic solutions for so wide a class of local potentials have not yet become available. Considering the complexity of the calculations which make use of wavefunctions and T

matrices to start with, it is important to keep expressions as simple as possible for these. Another point to be considered in the use of separable nonlocal potentials is the simplification of the three-body problem which takes place when T matrices using these potentials are introduced.

Figure 1

$^1S_0$ n-p phase shifts. For this figure the experimental phase shifts in the 0.1 to 10 MeV region have been calculated from the following accepted values:[66] scattering length = - 23.715 fm and effective range = 2.73 fm, using the formula $k \cot \delta = -\frac{1}{a} + \frac{1}{2} r k^2$. The values above 10 MeV are from MacGregor et al.,[67] who normalized their fits to a smaller value for the effective range. The experimental phase shifts are shown by the solid line. The phase shifts calculated using the potential of Eq. (232) and the parameter values quoted in the text are shown by the short broken lines. Phase shifts for the Mongan potential (Case IV) were calculated using the expression developed in this paper, and are indicated by the long broken lines.

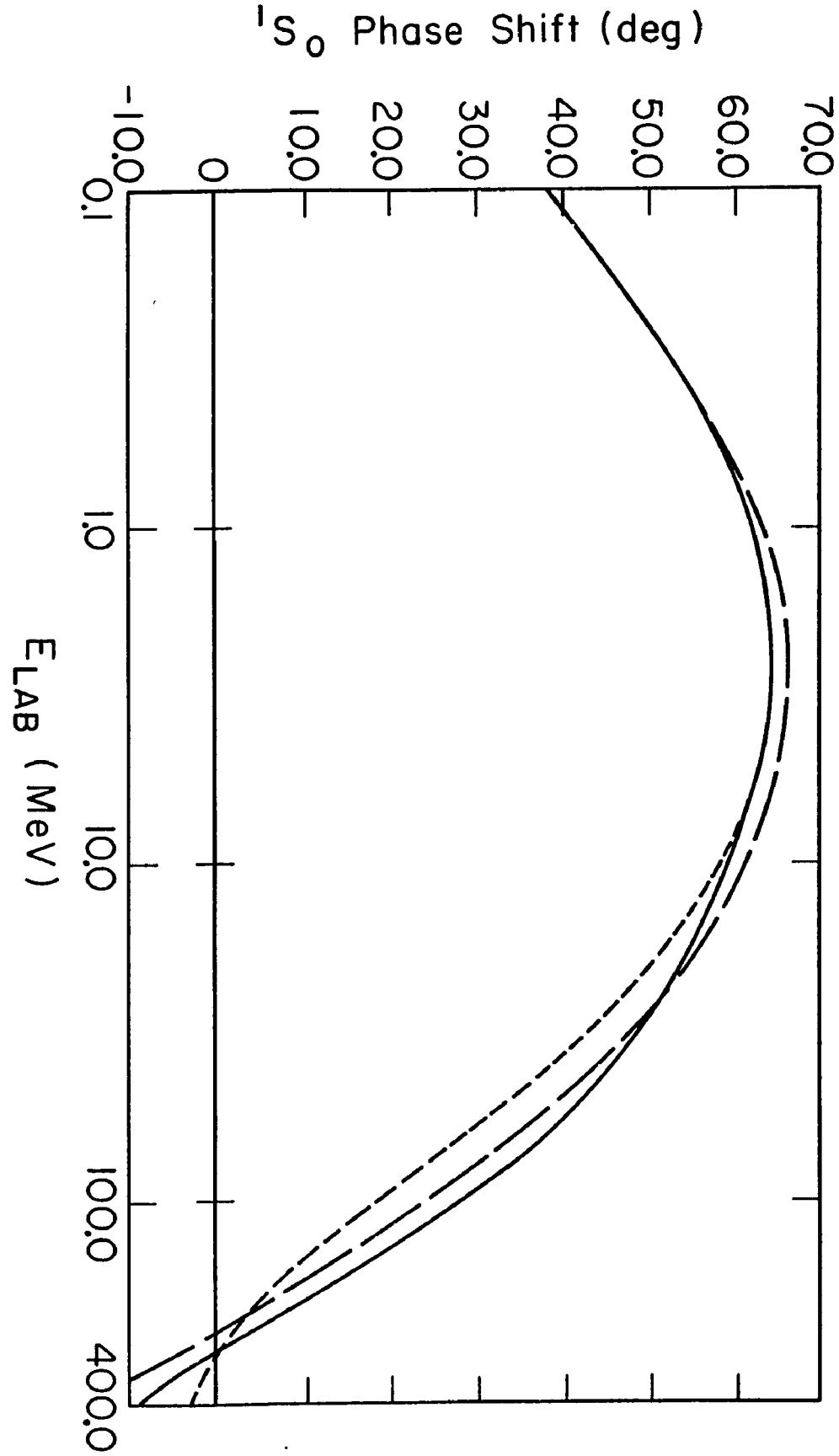

$^1S_0$ Phase Shift (deg)
-10.0
0
10.0
20.0
30.0
40.0
50.0
60.0
70.0
0.1
1.0
10.0
100.0
400.0
E_{LAB} (MeV)

Figure 2

The Fredholm determinant $\Delta(k)$ for the potential of Eq. (232) with the parameter values quoted in the text. The phase shifts shown in Fig. 1 by the short broken lines correspond to this potential. The insert is the Fredholm determinant for the Mongan potential (Case IV). The phase shifts for this potential are given in Fig. 1 by the long broken lines.

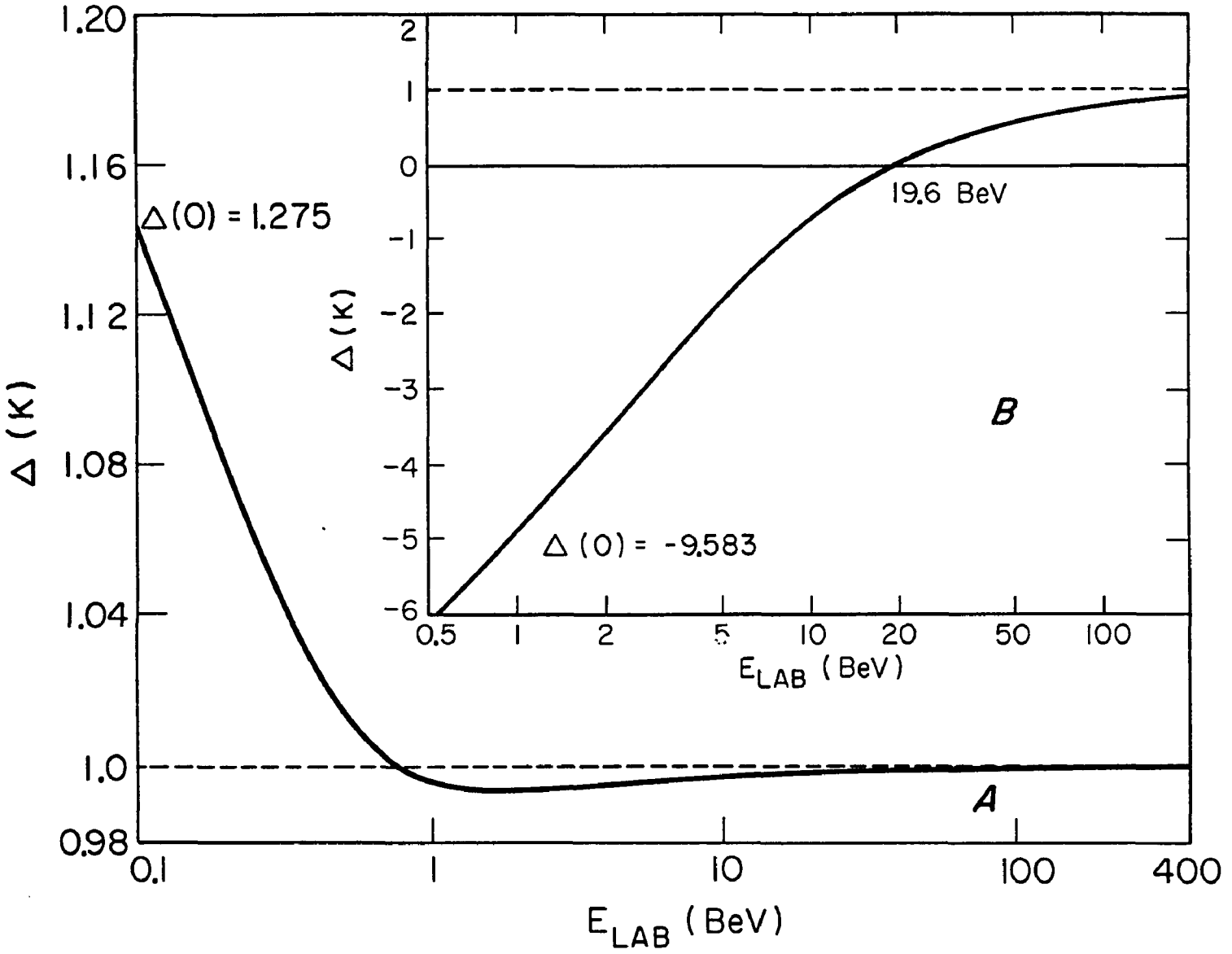

1.20
1.16
1.12
1.08
1.04
1.0
0.98
Δ (K)
Δ(0) = 1.275
0.1
1
10
100
400
E_LAB (BeV)
A
2
1
0
-1
-2
-3
-4
-5
-6
Δ (K)
19.6 BeV
B
Δ (0) = -9.583
0.5
1
2
5
10
20
50
100
E_LAB (BeV)

Figure 3

Zero energy wave functions for the potential of Eq. (232) (solid line) and for the Mongan potential (Case IV) (broken line).

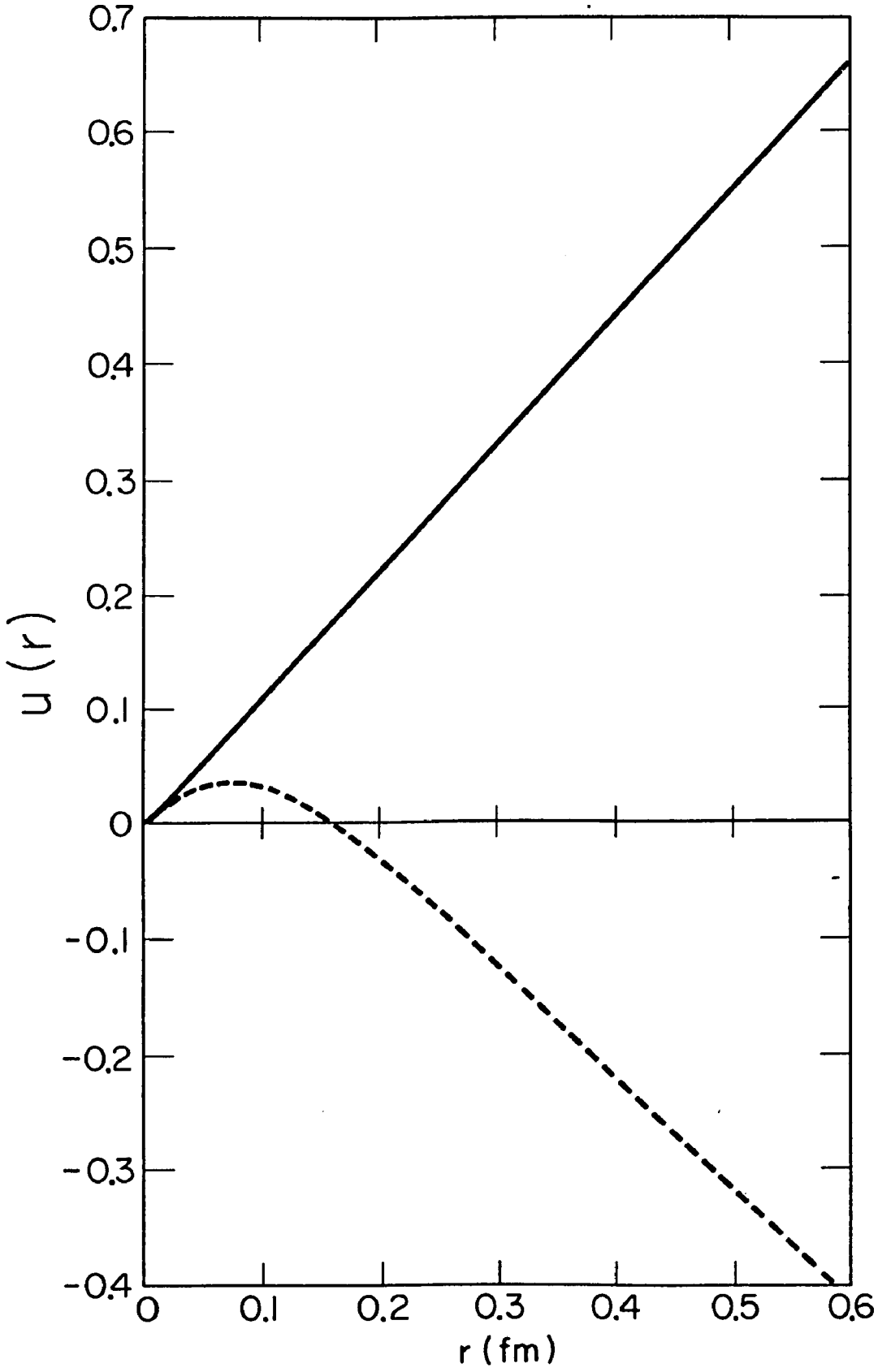
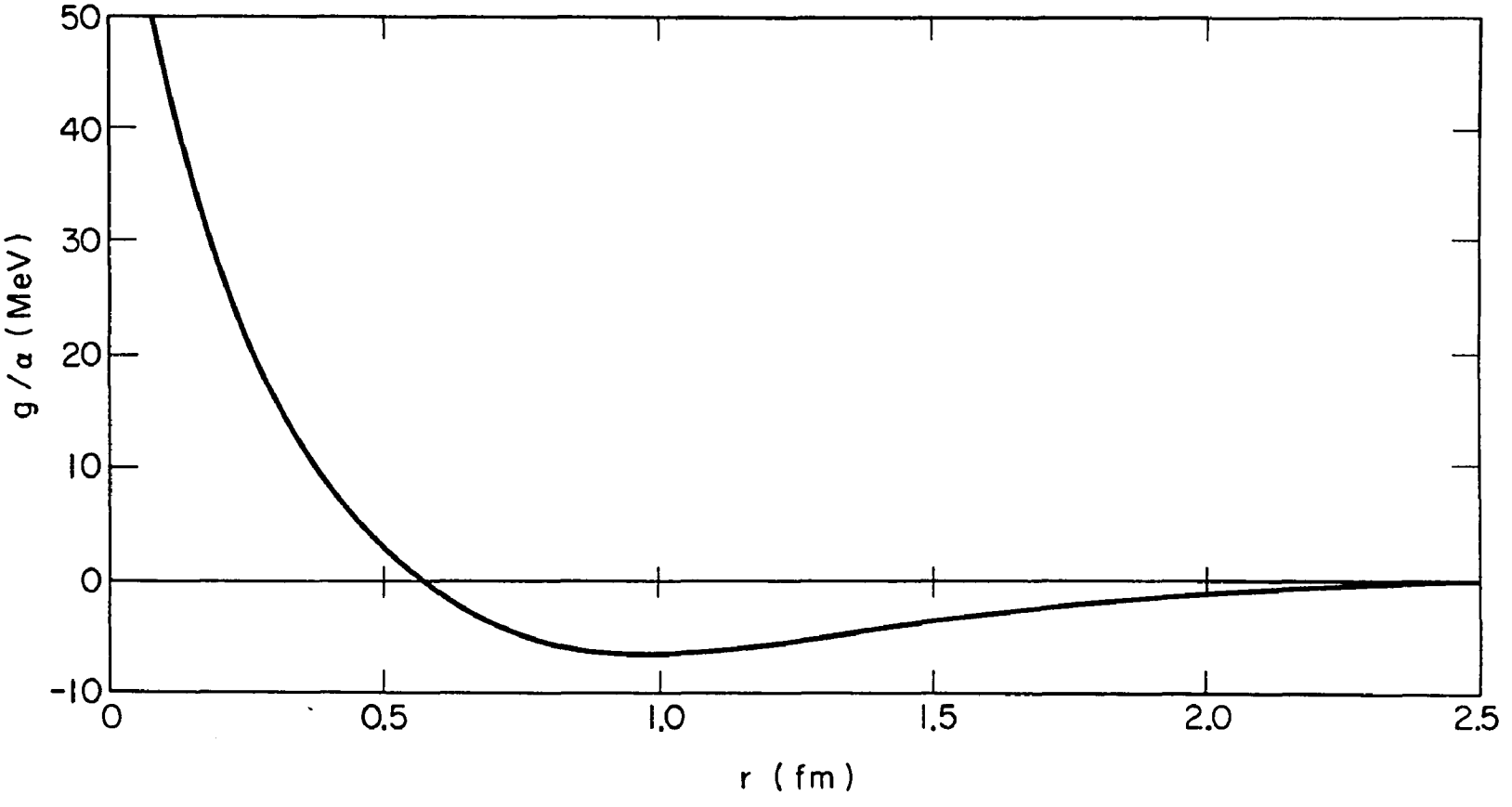

0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
-0.1
-0.2
-0.3
-0.4
U (r)
0
0.1
0.2
0.3
0.4
0.5
0.6
r (fm)

Figure 4

The nonlocal potential of Eq. (232) for the case $r'=r$. To provide a depth parameter in MeV, the potential has been divided by α.


50
40
30
20
10
0
-10
g / α (MeV)
0
0.5
1.0
1.5
2.0
2.5
r (fm)

APPENDIX

We want to derive expressions for the regular solution $U_\ell(r)$ and the irregular solution $\theta_\ell(r)$ in terms of the Jost solutions $f_\ell^{\pm}(k,r)$ and Jost functions $J_\ell^{\pm}(k)$.

Jost solutions are defined by the boundary conditions

$$\lim_{r\to\infty} f_\ell^{\pm}(k,r)\, e^{\mp ikr} = 1 , \tag{A-1}$$

and Jost functions by

$$J_\ell^{\pm}(k) = \lim_{r\to 0} W(f_\ell^{\pm}, u_\ell) \tag{A-2}$$

where $W(f_\ell^{\pm}, u_\ell)$ is the Wronskian of $f_\ell^{\pm}(k,r)$ and $u_\ell(r)$. Note that in the case of a nonlocal potential, the Wronskian will depend upon the point at which it is evaluated. This implies the necessity of the limiting process in the definition in Eq. (A-2). It can be shown that Eq. (A-2) is equivalent to the statement

$$J_\ell^{\pm}(k) = (2\ell+1) \lim_{r\to 0} r^\ell f_\ell^{\pm}(k,r) .$$

Thus in the case $\ell=0$, $J_0^{\pm}(k) = f_0^{\pm}(k,0)$.

Since $f_\ell^{\pm}(k, r)$ are two linearly independent solutions of the integro-differential equation we can write

$$u_\ell(r) = a f_\ell^{+} + b f_\ell^{-} \tag{A-3}$$

and

$$\theta_\ell(r) = c f_\ell^{+} + d f_\ell^{-1} \tag{A-4}$$

where the constants a, b, c and d are to be determined. To find the values of a and b we make use of the fact[41] that for an integro-differential equation with a symmetric kernal the Wronskian of the two independent solutions satisfies the condition

$$W\big|_{r \to 0} \equiv W\big|_{r \to \infty} \tag{A-5}$$

Evaluating the Wronskian of f_ℓ^{+} and f_ℓ^{-} as $r \to \infty$ and making use of Eq. (A-5) we get

$$W(f_\ell^{+}, f_\ell^{-}) \xrightarrow[r \to 0]{} - 2ik \tag{A-6}$$

Using Eq. (A-3) we can write

$$W(f_\ell^{+}, u_\ell) = b\, W(f_\ell^{+}, f_\ell^{-}) \tag{A-7}$$

$$W(f_\ell^{-}, u_\ell) = a\, W(f_\ell^{-}, f_\ell^{+}) \tag{A-8}$$

If we substitute Eq. (A-6) into Eqs. (A-7) and (A-8) and use Eq. (A-2) we find that

$$a = \frac{J_\ell^-(k)}{2ik} \tag{A-9}$$

$$b = -\frac{J_\ell^+(k)}{2ik} \tag{A-10}$$

It then follows that

$$u_\ell(r) = \frac{1}{2ik}\left[J_\ell^-(k)\, f_\ell^+(k,r) - J_\ell^+(k)\, f_\ell^-(k,r)\right] \tag{A-11}$$

It is more complicated to obtain an expression for the (real) irregular solution $\theta_\ell(r)$ in terms of Jost solutions and Jost functions. For this purpose we can divide Eq. (A-7) into Eq. (A-8) or take the Wronskian of u_ℓ with u_ℓ as given by Eq. (A-3) to get

$$0 = aW(f_\ell^+, u_\ell) + bW(f_\ell^-, u_\ell)$$

or

$$\frac{a}{b} = -\frac{W(f_\ell^-, u_\ell)}{W(f_\ell^+, u_\ell)} = \text{const} \tag{A-12}$$

Similarly, taking the Wronskian of θ_ℓ with θ_ℓ as given by Eq. (A-4) we get

$$\frac{c}{d} = -\frac{W(f_\ell^-, \theta_\ell)}{W(f_\ell^+, \theta_\ell)} = \text{const}\,. \tag{A-13}$$

We now use the property of the solutions at infinity. We can show from the definitions of the asymptotic forms of $f_\ell^{\pm}$ and of u_ℓ and θ_ℓ given in Chapter III that

$$W(f_\ell^+, \theta_\ell)\, W(f_\ell^-, u_\ell) \xrightarrow[r \to \infty]{} -ik \tag{A-14}$$

and

$$W(f_\ell^-, \theta_\ell) \cdot W(f_\ell^+, u_\ell) \xrightarrow[r \to \infty]{} ik \tag{A-15}$$

From Eqs. (A-14) and (A-15) we can immediately conclude

$$\frac{W(f_\ell^+, \theta_\ell)}{W(f_\ell^-, \theta_\ell)} = -\frac{W(f_\ell^+, u_\ell)}{W(f_\ell^-, u_\ell)} \tag{A-16}$$

Noting that the ratios in Eqs. (A-12) and (A-13) are constants everywhere, it follows that Eq. (A-16) is true for all r. Thus from Eq. (A-16),

$$\frac{c}{d} = \frac{J_\ell^-(k)}{J_\ell^+(k)} \tag{A-17}$$

Also, from Eqs. (A-3) and (A-4) we can write

$$W(u_\ell, \theta_\ell) = bc\, W(f_\ell^-, f_\ell^+) + ad\, W(f_\ell^+, f_\ell^-)$$

$$= (bc - ad)\, W(f_\ell^-, f_\ell^+)$$

But at infinity $W(u_\ell, \theta_\ell) = 1$ and $W(f_\ell^-, f_\ell^+) = 2ik$.

Therefore $bc-ad = \frac{1}{2ik}$ (A-18)

Utilizing Eqs. (A-9), (A-10), (A-17) and (A-18) we see that

$$c = -\frac{1}{2J_\ell^+(k)}$$

$$d = -\frac{1}{2J_\ell^-(k)}$$

Hence from Eq. (A-4) we get

$$\theta_\ell(r) = -\tfrac{1}{2}\left[J_\ell^+(k)^{-1} f_\ell^+(k,r) + J_\ell^-(k)^{-1} f_\ell^-(k,r)\right] \quad \text{(A-19)}$$

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