The scattering theory in the two states approximation

1984 J. Phys. A: Math. Gen. 17 609

(http://iopscience.iop.org/0305-4470/17/3/022)

J. Phys. A: Math. Gen. **17** (1984) 609–618. Printed in Great Britain

The scattering theory in the two states approximation

Cao xuan Chuan

Institute of Physics, University of Constantine, BP 260, Constantine, Algeria

Received 22 November 1982, in final form 4 May 1983

Abstract. The theory of coupled differential equations is applied to the problem of scattering in the two states approximation. It will be shown that the methodology can be substantially improved by introducing the 'three parameters approach' in the general non-resonance case and the 'two parameters approach' in the non-exact resonance case. The S matrix can be constructed from these results and satisfies the unitary and symmetry requirements as expected. Huck's model and triplet nucleon–nucleon scattering are taken as illustrative examples.

1. Introduction

Mathematically the multistate problem is formulated by a finite system of coupled differential equations:

$$[\Delta + k_\lambda^2 + U_{\lambda\lambda}]\psi_\lambda = \sum_{\mu \neq \lambda} U_{\lambda\mu}\psi_\mu \qquad \lambda, \mu = 0, 1, \ldots n \tag{1}$$

where as usual Δ is the Laplace operator; k_λ^2, $U_{\lambda\lambda}$ are respectively the energy and interaction potential corresponding to channel λ; and $U_{\lambda\mu}$ is the coupling term ($\lambda \neq \mu$). For an overview of this problem see for example Burke and Seaton (1971) and Hohlfing *et al* (1980). For the specific problem of two states approximation in which (1) is reduced to a system of two coupled differential equations (Huck 1957) which we shall write in the form:

$$[\Delta + k_0^2 + U_{00}]\psi_0 = U_{01}\psi_1 \qquad [\Delta + k_1^2 + U_{11}]\psi_1 = U_{10}\psi_0. \tag{2}$$

The difficulties which must be overcome are closely related to the magnitude of the coupling terms $U_{01}(r)$, $U_{10}(r)$. For simplicity we shall assume that $U_{10} = U_{01}$.

For the weak coupling case (i.e. $U_{10} \ll k_\lambda^2, U_{\lambda\lambda}$) this problem can be dealt with a number of excellent methods of approximation such as perturbation, the Born or DWB approximation, the iteration as well as the short wave length (JWKB) approaches etc which, if properly used, yield the solutions in a relatively simple manner without excessive lack of mathematical rigor in their derivation.

Things become quite different when we come to the strong coupling case (i.e. $U_{10} \geqslant k_\lambda^2, U_{\lambda\lambda}$) and the above methods are more difficult to accept from both the mathematical and the practical point of view due to the slow rate of convergence or divergence of the solutions.

This problem may however be examined from another point of view based on the so-called 'three parameters approach' in which one considers the two proper phase shift of the equations together with a mixing parameter (Mott and Massey 1965).

0305-4470/84/030609+10$02.25

However, in order to evaluate these parameters, one has to appeal to the conventional variational techniques of calculation, relying mostly on an appropriate choice of the trial functions and on the subsequent evaluation of the constants needed in the description of these functions.

Starting from the results obtained previously concerning the theory of coupled differential equations, (Cao 1981, 1982; hereafter referred to as I and II respectively) and from which the present work can be seen as a logical consequence, we present a new approach to this problem which, we believe, can make the situation much simpler because it allows a direct determination of these parameters.

We begin by recalling a number of most important aspects of the theory in the first paragraph namely the separation of the equations at first order. For the details we refer to II and to references therein.

Next will be the case of two coupled equations which will be separated according to a scheme to be developed allowing, therefore, a separate determination of the proper phase shift. The partial cross-section can then be induced in terms of these phase shifts and the mixing parameter.

The non-resonance case will be discussed and a modified 'three parameters approach' will be described in § 3 while the case of non-exact resonance is taken up in the next section where it is shown that the role of the mixing parameter becomes redundant and only the two proper phase shifts are needed to evaluate the partial elastic and inelastic cross-sections. The S matrix for this case is then constructed with its unitarity and symmetry property verified.

In the extreme case of exact resonance, these results yield complete agreement with already well known facts justifying, so to speak, the well founded character of their derivation.

Throughout the text, illustrative examples will be discussed serving either as a test or as suggestions for further use of the method.

2. Formulation

With the usual partial wave expansion, the wavefunction in (2) takes the form

$$\psi_i = \frac{1}{k_i r} \sum_l{}' (2l+1) v_{il}(r) P_l(\cos\theta) \qquad i = 0, 1 \tag{3}$$

where the functions $v_{il}(r)$ must satisfy the following equations with appropriate asymptotic conditions

$$\begin{aligned} &[\mathrm{d}^2/\mathrm{d}r^2 + k_0^2 - l(l+1)r^2 - U_{00}]v_{0l} = U_{01} v_{il} \\ &[\mathrm{d}^2/\mathrm{d}r^2 + k_1^2 - l(l+1)/r^2 - U_{11}]v_{il} = U_{10} v_{0l} \end{aligned} \tag{4}$$

for $r \to \infty$

$$\begin{aligned} &\psi_0 \simeq \exp(\mathrm{i}k_0 z) + f_{00}(\theta, \varphi) \exp(\mathrm{i}k_0 r)/r \\ &\psi_1 \simeq f_{10}(\theta, \varphi) \exp(\mathrm{i}k_1 r)/r. \end{aligned} \tag{5}$$

The phase shift corresponding to channels 0 and 1 may in principle, be evaluated by use of the Schwinger type of integral equations but here, however, because of the presence of the coupling terms, the exact analytical expression for the wavefunction appearing in the integrand is not generally known.

For the weak coupling case these functions may indeed always be approximated in considering the coupling term as a perturbation but, as this approach certainly becomes more and more unsafe for the strong coupling case, one has to introduce the so-called 'three parameters approach' which involves two proper phase shifts δ_{0l}^a, δ_{1l}^a and a mixing parameter χ_l whose evaluation presents a difficult problem. We refer to Mott and Massey (1965) where the question is clearly presented, see also Rubinow (1955).

In this paper, we shall start from the results obtained in the separation of the equations to show that simplifications to this problem is, in principle, possible with a direct determination of these three parameters. For convenience we first make a distinction between three cases which will be considered separately:

(a) The non-resonance case where $k_0 \neq k_1$, $U_{00} \neq U_{11}$

(b) The non-exact resonance case with $k_0 = k_1$, $U_{00} \neq U_{11}$

(c) The exact resonance case $k_0 = k_1$, $U_{00} = U_{11}$.

Of these three, the third one is well known already because in (2) the equations may always be separated so that the result obtained for it will merely serve as a test for those derived in the first and second cases.

3. The modified three parameters approach

We continue to keep the notations used in I and II i.e.

$$P = \mathrm{d}^2/\mathrm{d}r^2; \qquad f_i = k_i^2 - l(l+1)/r^2 - U_{ii}; \qquad B(r) = U_{10} = U_{01}. \tag{6}$$

It is seen immediately that a complete separation of the equations in (4) without changing the order of the equations is not possible except perhaps for some very special cases. However, it is also shown in II that a complete separation of the equations at some given order of approximation is generally possible for certain classes of coupling functions. More precisely, by use of a special transformation V to be defined later, the non-diagonal term, after transformation, can be expressed by a serial form:

$$\sum_{m=0}^{\infty} A_m[P, \Gamma^m] \tag{7}$$

where [ ] means the commutator bracket and

$$\Gamma = \gamma - \gamma_0, \qquad \gamma = B/(f_1 - f_0), \qquad \gamma_0 = n/\alpha$$

(see equations (14)–(18) of II); n, α are adjustable parameters introduced to ensure a rapid convergence of the expansion (7). The connection between these quantities is found to be

$$\alpha^2 = \tfrac{1}{2}[2n + (4n+1)^2/32n(2n+1)] \pm \tfrac{1}{2}\{[2n + (4n+1)^2/32n(2n+1)]^2 - 4n^2\}^{1/2}. \tag{8}$$

Therefore, once the value of n is appropriately chosen, α is automatically defined and the second coefficient in (7) is zero (i.e. $A_1(n, \alpha) \equiv 0$). We are then left with the series

$$A_0 + \sum_{m=2}^{\alpha} A_m[P, \Gamma^m].$$

Moreover, the choice of n may always be made such that the following condition is fulfilled

$$\Gamma \ll R = 1/4\alpha + \gamma_0, \tag{9}$$

R being the radius of convergence and, with some restrictions, the neglect of terms of second- and higher-order terms in (7) is justified at the first order of approximation. At the cost of some more complicated algebra, the same procedure may be repeated again if a higher order of approximation is needed.

With these preliminaries, we can now study the scattering problem with two separated equations by using the transformation

$$V(a, A) = T(A)T(a) \tag{10}$$

where T has already been defined in II and the quantity A, in the first order of approximation considered here, is equal to the quantity A_0 given by relation (17) of II. It can be seen from (10) that V must have the form

$$V = \begin{pmatrix} c & d \\ -d & c \end{pmatrix}$$

with

$$c = 2(a + A_0),\ d = 2(1 - aA_0).$$

The separated equations of system (4) are now:

$$\begin{aligned} &\{d^2/dr^2 + \tfrac{1}{2}(k_0^2 + k_1^2 + U_{00} + U_{11}) - l(l+1)/r^2 + \tfrac{1}{2}[(\Delta k^2 - AU)^2 + 4U_{10}^2]^{1/2}\} w_{0l} = 0 \\ &\{d^2/dr^2 + \tfrac{1}{2}(k_0^2 + k_1^2 + U_{00} + U_{11}) - l(l+1)/r^2 - \tfrac{1}{2}[(\Delta k^2 - \Delta U)^2 + 4U_{10}^2]^{1/2}\} w_{1l} = 0 \end{aligned} \tag{11}$$

where $\Delta k^2 = k_0^2 - k_1^2$ amd $\Delta U = U_{11} - U_{00}$.

The functions v_{0l}, v_{1l} in (4) may then be recovered by the inverse transformation V^{-1}. In matrix notation

$$\begin{aligned} &v = \begin{pmatrix} v_{0l} \\ v_{1l} \end{pmatrix} \qquad w = \begin{pmatrix} w_{0l} \\ w_{1l} \end{pmatrix} \\ &v = T^{-1}(a)\,T^{-1}(A_0)\,W. \end{aligned} \tag{12}$$

From (11) the proper phase shift may be derived in the usual way by noting that a large distance, U_{00}, U_{11}, U_{10} are generally expected to become negligible compared to the centrifugal term so that the asymptotic form of (11) will be:

$$\begin{aligned} &[d^2/dr^2 + k_0^2 - l(l+1)/r^2] w_{0l}^{\infty} = 0 \\ &[d^2/dr^2 + k_1^2 - l(l+1)/r^2] w_{1l}^{\infty} = 0. \end{aligned} \tag{13}$$

With the phase shift δ_{0l}^a, δ_{1l}^a the asymptotic forms of w_{il} are

$$\begin{aligned} w_{0l} &\simeq \frac{1}{k_0} A_{0l}^a \sin(k_0 r - \tfrac{1}{2} l\pi + \delta_{0l}^a) \\ w_{1l} &\simeq \frac{1}{k_1} A_{1l}^a \sin(k_1 r - \tfrac{1}{2} l\pi + \delta_{1l}^a) \end{aligned} \tag{14}$$

and the Schwinger form of the uncoupled integral equations determining the proper

phase shift will be

$$\sin \delta_{il}^{a} = -k_i \int_0^{\infty} r j_l(k_i r)\, w_{il}(r) K_i^{a}(r)\, \mathrm{d}r \tag{15}$$

in which $j_l(k_i r)$ is the spherical Bessel function and

$$K_i^{a}(r) = \tfrac{1}{2}(U_{00} + U_{11}) \pm [(\Delta k^2 - \Delta U)^2 + 4U_{10}^2]^{1/2} \qquad i = {}^{0}_{1}.$$

In terms of δ_{0l}^{a}, δ_{1l}^{a} one may choose two sets of solutions G_{0l}^{0}, G_{1l}^{0} corresponding to δ_{0l}^{a} and G_{1l}^{1} G_{0l}^{1} to δ_{1l}^{a} together with a mixing parameter χ_l. Defining

$$\exp(2\mathrm{i}\delta_l) = \begin{pmatrix} \exp(2\mathrm{i}\delta_{0l}^{a}) & 0 \\ 0 & \exp(2\mathrm{i}\delta_{1l}^{a}) \end{pmatrix}$$

the S matrix will be $S = U \exp(2\mathrm{i}\delta_l) U^{+}$ where the transformation matrix U can be expressed in terms of

$$U = \begin{pmatrix} \cos\varepsilon & \sin\varepsilon \\ -\sin\varepsilon & \cos\varepsilon \end{pmatrix} \qquad \left(\frac{k_1}{k_0}\right)^{1/2} \tan\varepsilon = \chi_l.$$

The χ_l parameter can be obtained from the asymptotic conditions imposed on G_{il}^{0}, G_{il}^{1} after some simple algebra (see for example Mott and Massey 1965). Therefore, with δ_{0l}^{a}, δ_{1l}^{0} given by (15) and the above mixing parameter, it is then possible to obtain the partial elastic Q_l^{00} and inelastic Q_l^{01} cross-section of the process.

3.1. Example

Consider for instance model A of Huck (1957) in which the coupling function $B(r)$ is simply assumed to be a constant $C \neq 0$ and the function $f_i(r)$ set equal to the energy term k_i^2 (i.e. for the $l = 0$ case). We shall not consider for the moment the Huck's model B which is a system of coupled integro differential equations so that the above theorem cannot be applied in a straightforward manner and would require further modifications.

For the model A then and for $0 < r < a$, a being the range of the coupling term, the quantitity γ becomes a constant so that the theorem does apply (i.e. $T(A) = I$, I: unit matrix) and the separated equations are in Huck's notation

$$(\mathrm{d}^2/\mathrm{d}r^2 + m^2) w_0 = 0$$

$$(\mathrm{d}^2/\mathrm{d}r^2 + p^2) w_1 = 0$$

where we find

$$\begin{matrix} m^2 \\ p^2 \end{matrix} = \tfrac{1}{2}(k_0^2 + k_1^2) \pm \tfrac{1}{2}[(k_1^2 - k_0^2)^2 + 4C^2]^{1/2}.$$

Writing the regular solutions as $w_0 = \alpha \sin mr$, $w_1 = \beta \sin pr$, evaluating the original functions f_0 f_1 by the transformation

$$\begin{pmatrix} f_0 \\ f_1 \end{pmatrix} = \begin{pmatrix} 1-a & -(1+a) \\ 1+a & 1-a \end{pmatrix} \begin{pmatrix} w_0 \\ w_1 \end{pmatrix}$$

and noting finally the following identities

$$(1+a)/(1-a) = (1/C)(k_0^2 - m^2); \qquad (1-a)/(1+a) = -(1/C)(k_1^2 - p^2)$$

it can be seen that the exact solution given by Huck is completely recovered here. It can also be mentioned that the numerical aspects of this model A has been recently discussed from the point of view of variational calculations (Nesbet 1981) where rapid convergence to exact results has been obtained.

Furthermore, it is interesting to note that the model A can even be enlarged to the case $l \neq 0$, i.e. with

$$f_i(r) = k_i^2 - l(l+1)/r^2,$$

because for this case the theorem still remains valid. The separated equations are now

$$[\mathrm{d}^2/\mathrm{d}r^2 + m^2 - l(l+1)/r^2]w_{0l} = 0$$
$$[\mathrm{d}^2/\mathrm{d}r^2 + p^2 - l(l+1)/r^2]w_{1l} = 0$$

with the regular solutions $w_{0l} = \alpha j_l(mr)$; $w_{1l} = \beta j_l(pr)$, j_l being the usual spherical Bessel functions. Therefore, with the same procedure, exact solutions can also be obtained suggesting that it would perhaps be appropriate to have in the future a comparison between these exact solutions with those obtained from the variational approach extended to this enlarged case.

4. The two parameters approach

Along these lines one may further wonder whether more simplifications are possible at least for the second case of non-exact resonance ($k_0 = k_1$, $U_{00} \neq U_{11}$). This is indeed possible with the 'two parameters approach' where it will be seen that the role of the mixing parameter χ_l now becomes redundant.

In fact, starting from (2) and with the usual Green's function technique, it is easy to see that the transformed wavefunctions ϕ_0, ϕ_1 are of the form

$$\begin{aligned} \phi_0 &= (k_0 r)^{-1} \sum A_{0l}^b w_{0l}^b P_l(\cos\theta) \\ \phi_1 &= (k_1 r)^{-1} \sum A_{1r}^b w_{1l}^b P_l(\cos\theta) \end{aligned} \tag{17}$$

with

$$A_{il}^b = C_i(2l+1)\exp(\mathrm{i}\delta_{il}^b), \qquad i = 0, 1$$

C_0, C_1 are arbitrary constants. More explicitly we may write

$$\phi_0 = C_0\{\exp(\mathrm{i}k_0 z) + [\exp(\mathrm{i}k_0 r)/r]\sum (2l+1)[\exp(2\mathrm{i}\delta_{0l}^b) - 1]P_l(\cos\theta)\}$$
$$\phi_1 = C_1\{\exp(\mathrm{i}k_0 z) + [\exp(\mathrm{i}k_0 r)/r]\sum (2l+1)[\exp(2\mathrm{i}\delta_{1l}^b) - 1]P_l(\cos\theta)\}.$$

Remembering (12) and the boundary conditions (5) for w_{0l}, w_{1l} and ψ_0, ψ_1 it can be shown that C_0, C_1 must satisfy the relations:

$$\begin{aligned} C_0 &= c/(c^2+d^2) = \tfrac{1}{2}(a + A_0)/(1 + a^2 + A_0^2 + a^2 A_0^2) \\ C_1 &= -d/(c^2+d^2) = -\tfrac{1}{2}(1 - aA_0)//(1 + a^2 + A_0^2 + a^2 A_0^2) \end{aligned} \tag{18}$$

and it can be verified that with the inverse transformation $Y = V^{-1}\phi$ the asymptotic form (5) is automatically recovered. Therefore by identification we have:

$$\begin{aligned} f_{00} &= 1/(c^2+d^2)\sum (2l+1)\{c^2[\exp(2\mathrm{i}\delta_{0l}^b) - 1] + d^2[\exp(2\mathrm{i}\delta_{1l}^b) - 1]\}P_l(\cos\theta) \\ f_{01} &= [dc/(c^2+d^2)]\sum (2l+1)\{\exp(2\mathrm{i}\delta_{0l}^b) - \exp(2\mathrm{i}\delta_{1l}^b)\}P_l(\cos\theta) \end{aligned} \tag{19}$$

which lead straightly to the elastic and inelastic partial cross-sections

$$Q_l^{00} = [\pi(2l+1)/k_0^2(c^2+d^2)^2][4c^4 \sin^2 \delta_{0l}^b + 4d^4 \sin^2 \delta_{1l}^b - 4d^2c^2 \sin^2(\delta_{0l}^b - \delta_{1l}^b) + 2d^2c^2(2 - \cos 2\delta_{0l}^b - \cos 2\delta_{1l}^b)]$$
$$Q_l^{01} = [\pi(2l+1)/k_0^2(c^2+d^2)^2]4d^2c^2 \sin^2(\delta_{0l}^b - \delta_{1l}^b) \tag{20}$$

where the phase shift δ_{0l}^b, δ_{1l}^b are given by

$$\sin \delta_{il}^b = -k_i \int_0^\infty r j_l(k_i r) w_i(r) K_i^b(r)\, \mathrm{d}r$$
$$K_i^b(r) = \tfrac{1}{2}\{U_{00} + U_{11} \pm [(\Delta U)^2 + 4U_{01}^2]^{1/2}\} \qquad i = {}^0_1. \tag{21}$$

4.1. Construction of the S matrix

If in (17) we replace C_0, C_1 respectively by $-C_1$, C_0 and after performing the V^{-1} transformation $Y = V^{-1}\phi$, we obtain the following asymptotic form of Y

$$y_0 = f_{10} \exp(\mathrm{i}k_0 r)/r \qquad y_1 = \exp(\mathrm{i}k_0 z) + f_{11} \exp(\mathrm{i}k_0 r)/r \tag{22}$$

which enables us to derive the expressions for f_{10}, f_{11}

$$f_{10} = [dc/(c^2+d^2)] \sum (2l+1)[\exp(2\mathrm{i}\delta_{0l}^b) - \exp(2\mathrm{i}\delta_{1l}^b)]P_l(\cos\theta)$$
$$f_{11} = [1/(c^2+d^2)] \sum (2l+1)\{d^2(\exp(2\mathrm{i}\delta_{0l}^b) - 1) + c^2(\exp(2\mathrm{i}\delta_{1l}^b) - 1)\}P_l(\cos\theta) \tag{23}$$

where the symmetric character between (19) and (23) becomes quite transparent. If we now define

$$\exp(2\mathrm{i}\delta_l^b) = \begin{pmatrix} \exp(2\mathrm{i}\delta_{0l}^b) & 0 \\ 0 & \exp(2\mathrm{i}\delta_{1l}^b) \end{pmatrix}$$

and consider the transformation

$$S = V \exp(2\mathrm{i}\delta_l^b)\, V^+; \qquad S = \begin{pmatrix} S_{00} & S_{01} \\ S_{10} & S_{11} \end{pmatrix}$$

we obtain

$$S_{00} = c^2 \exp(2\mathrm{i}\delta_{0l}^b) + d^2 \exp(2\mathrm{i}\delta_{1l}^b)$$
$$S_{10} = S_{01} = dc[\exp(2\mathrm{i}\delta_{0l}^b) - \exp(2\mathrm{i}\delta_{1l}^b)] \tag{24}$$
$$S_{11} = d^2 \exp(2\mathrm{i}\delta_{0l}^b) + c^2 \exp(2\mathrm{i}\delta_{1l}^b).$$

From (19) and (23), (24) it is now easy to verify the following relations

$$Q_l^{ii} = \frac{\pi}{k_0^2}|1 - S_{ii}|^2 \qquad Q_l^{ik} = \frac{\pi}{k_0^2}|S_{ik}|^2 \qquad i, k = 0, 1$$

which merely express the unitarity property of the S matrix.

4.2. Example

To illustrate this non-exact resonance case we shall for instance briefly outline the triplet nucleon–nucleon coupling case (in fact both the three and the two parameters approach are equally valid here but the second one is preferred for simplicity). The

two coupled equations will be (see e.g. Newton 1966) where we have adopted the notation:

$$[d^2/dr^2+k^2-j(j+1)/r^2-U_c+2[(j-1)/(2j+1)]U_t]v_0=\{6[j(j+1)]^{1/2}/(2j+1)\}U_t v_1$$
$$[d^2/dr^2+k^2-(j+1)(j+2)/r^2-U_c+2[(j+2)/(2j+1)]U_t]v_1 \qquad (25)$$
$$=6[j(j+1)]^{1/2}/(2j+1)U_t v_0$$

U_c, U_t are respectively the nuclear interaction corresponding to the central and tensor part. For this case the quantity γ is no more constant so that the method described in II must be called for. In first-order approximation and under transformation V defined above, the separated equations are

$$[d^2/dr^2+k^2-[j(j+1)+1]/r^2-(U_c+U_t)\pm D_i]w_i(r)=0 \qquad i=0,1$$
$$D_i=[1/(2j+1)]\{3[2j(j+1)+3]U_t^2-6(2j+1)^2/r^2\,U_t+(2j+1)^4/r^4\}^{1/2}. \qquad (26)$$

As it is expected that U_c and U_t decrease rapidly as r increases, their asymptotic form will be

$$[d^2/dr^2+k^2-j(j-1)/r^2]w_0=0$$
$$[d^2/dr^2+k^2-(j+1)(j+2)/r^2]w_1=0.$$

For the phase shift we have

$$\sin\delta_i^b=-\tfrac{1}{2}k\int_0^\infty r\bar{j}_i(k_ir)K_i^b(r)w_i(r)\,dr \qquad i=0,1$$

where for notation convenience $\bar{j}_i(k_ir)$ now denotes the spherical Bessel functions

$$\bar{j}_i(k_ir)=\begin{cases}\bar{j}_{(j-1)}(k_ir) & i=0\\ \bar{j}_{(j+1)}(k_ir) & i=1\end{cases}$$

and

$$K_i^b(r)=1/r^2+U_c+U_t\mp D_i(r).$$

These phase shift can thus be evaluated directly from the uncoupled integral equations. Here we have voluntarily ignored the spin orbit term for simplicity but its inclusion does not bring any substantial modifications in the general line of approach.

However, it must be kept in mind that condition (9) must always be satisfied and can be discussed in noting that the quantity $\gamma(r)$ depends only on the product r^2U_t

$$\gamma(r)=[j(j+1)]^{1/2}/\{\tfrac{1}{3}[(2j+1)^2/r^2U_t]-1\}.$$

We must therefore have $\gamma\ll R$, R being the radius of convergence defined in terms of the parameter n the choice of it relying of course on the assumed analytical form of U_t.

5. The exact resonance case

It is well known that for the case $k_0=k_1$ $U_{00}=U_{11}$, system (4) can always be separated regardless of the analytical form of the coupling term U_{10}. The transformation needed here is X_1 (defined in I p 1071) and the transformed wavefunction as well as the two

proper phase shift are given by

$$\begin{aligned} &\phi = \tfrac{1}{2}(\psi_0 \pm \psi_1) \qquad i = {}^{0}_{1} \\ &\sin \delta_i^c = -k_0 \int_0^\infty r j_l(k_0 r) K_i^c(v) w_i(v)\, \mathrm{d}v \\ &K_i^c = U_{00} \pm U_{01}. \end{aligned} \tag{27}$$

For this special case the two approaches presented above are not needed but we rather use this case as a limiting one in order to test the validity of their derivation. Note first that in the case of exact resonance the quantity a which has been defined as a root of equation (5) in II† will be zero here. We may therefore choose $\alpha = 0$ so that the quantities A_0 defined in II and c, d in (18) above become

$$A_0 = -1 \qquad c = -2 \qquad d = 2.$$

Replacing them in (20) we then obtain the well known result (with $\delta_{il}^b \to \delta_i^c$)

$$\begin{aligned} Q_l^{00} &= (\pi/k_0^2)(2l+1)\{2\sin^2\delta_0^c + 2\sin^2\delta_1^c - \sin^2(\delta_0^c - \delta_1^c)\} \\ Q_l^{01} &= (\pi/k_0^2)(2l+1)\sin^2(\delta_{0l}^c - \delta_1^c). \end{aligned} \tag{28}$$

Likewise if we use the three parameters approach, noting that $\delta_{0l}^a \to \delta_0^c$, $\delta_{1l}^a \to \delta_1^c$ and taking $\chi_l \to 1$ (because the equations are separated now), it may be easily checked that (28) is recovered again. This is an interesting point because it shows that the two approaches described above on one hand do yield the same result which on the other hand, is in complete agreement with the exact one given for instance in Mott and Massey (1965).

6. Conclusion

The following remarks will close the present discussion.

(1) One may wonder whether the procedure used in the two parameters approach can also be extended to the case of non-resonance in order to replace the three parameters avoiding therefore the tedious calculation of the mixing parameter χ_l. Unfortunately we find that the answer turns out to be negative because the S matrix constructed from this method does not lead to the unitarity and symmetry requirements.

(2) For the case b (non-exact resonance) both the three and two parameters are in principle valid but the second one clearly is much simpler.

(3) The generalisation of this method to the case where the number of coupled equations is larger than 2 is possible but with more technical difficulties. For example in the case of three coupled equations, it can be shown that extension of the approach for the two equations case combined with the step by step diagonalisation technique can provide a new representation in which the equations become partially separated in such a manner that a direct determination of the phase shift is possible as above (to be published).

(4) The methods are described in the frame of first-order separation approximation. Although extension to higher order is possible at the cost of more complications, it may be noted that the first order is already flexible enough to be adapted to many

† Note a small error in the text of II where the quantity B in equation (5) must be replaced by C.

cases. This is because the validity condition of this approximation is based on adjustable parameters n and α (which in fact are reduced to one parameter because of (8)) to be chosen at our convenience.

Acknowledgment

For extremely warm hospitality, I wish to thank Professor Abdus Salam and the International Centre for Theoretical Physics Trieste where part of this paper has been written.

References

Burke P G and Seaton N J 1971 *Methods of Computational Physics* **10** 1971
Cao xuan Chuan 1981 *J. Phys. A: Math. Gen.* **14** 1069.
—— 1982 *J. Phys. A: Math. Gen.* **15** 2727
Hohlfing E N, Loeson J C, de Pristo A B and Rabitz N 1980 *J. Chem. Phys.* **72** I 464
Huck R J 957 *Proc. Phys. Soc.* A **70** 369
Nesbet R K 1981 *Phys. Rev. A* **24** 2975
Newton R G 1966 *Scattering Theory of Waves and Particles* (New York: McGraw Hill)
Mott N F and Massey H S W 1965 *Theory of Atomic Collisions* (Oxford: Clarendon)
Rubinow S I 1955 *Phys. Rev.* **98** 183