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Computer Physics Communications 90 (1995) 244–250

Computer Physics
Communications

The relativistic multi-channel variable phase method for solving asymptotic equations in electron–atom and electron–ion scattering

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Received 18 June 1995

Abstract

The multi-channel variable phase method has been generalized to the relativistic case. The problem of solving a system of coupled radial Dirac equations without exchange has been reduced to the problem of direct outward integration of a non-linear differential equation satisfied by the reaction matrix $K(r)$. The method is suitable for solving relativistic asymptotic equations occurring in the electron–atom and electron–ion scattering theory. A matching procedure for the relativistic R -matrix method and the relativistic multi-channel variable phase approach has been described.

PACS: 34.80.-i; 34.10.+x; 03.80.+r; 11.80.-m

The last two decades have seen a rapid growth of interest in the relativistic description of electron–atom and electron–ion scattering processes [1]. So far the main effort has been directed towards developing relativistic methods suitable for solving the problem in an inner region, where a projectile and target electrons are treated as indistinguishable particles, e.g. the relativistic R -matrix method [2–4]. The outer region has attracted much less attention and in applications usually non-relativistic approximations have been used [5]. Although for neutral and low-charged targets such an approach does not introduce substantial errors, the situation is clearly unsatisfactory since an ultimate goal of the theory should be a fully relativistic description of the scattering process. The first steps towards changing this situation were undertaken by Johnson and co-workers and Chang [6], who formulated a relativistic version of the multi-channel quantum defect theory, and very recently by Young and Norrington [7], who developed relativistic forms of the Burke–Schey and Gailitis asymptotic expansions. A purpose of this paper is to present a relativistic generalization of another method of solving the scattering problem in the outer region – the multi-channel variable phase method. The non-relativistic multi-channel variable phase method has been independently formulated by several authors [8] and applied in various branches of atomic collision physics (e.g. Refs. [9–13]). A comprehensive description of the method may be found in monographs [14] and reviews [15]. To the best of our knowledge, the only attempt to generalize the method to the relativistic case was an early work of Kynch [16]. A deficiency of Kynch’s formulation, destined for nuclear or elementary particle physics rather than for atomic physics, was a restriction to a case with all scattering channels open. In electron scattering calculations one always deals with several weakly closed

channels which must be considered simultaneously with open channels. Below we present a general formulation of the relativistic multi-channel variable phase method in a form suitable for applications in electronic collision calculations. We describe also a procedure of matching the method with the relativistic *R*-matrix approach.

We assume that the inner and outer regions of the three-dimensional configuration space are separated by a spherical shell of radius *a* centred at the target nucleus and that there are *N*_o open and *N*_c closed channels which we wish to include in calculations in the outer region. In this region, characterized by a condition $r \geq a$, the radial relativistic close-coupling equations [17,7] may be written in a matrix form,

$$\frac{d}{dr}P(r) + \frac{\mathcal{K}}{r}P(r) = \frac{1}{c\hbar} [E + mc^2I - V(r)] Q(r), \tag{1}$$

$$-\frac{d}{dr}Q(r) + \frac{\mathcal{K}}{r}Q(r) = \frac{1}{c\hbar} [E - mc^2I - V(r)] P(r), \tag{2}$$

and should be solved subject to initial conditions

$$P(a) = P_0, \quad Q(a) = Q_0. \tag{3}$$

All matrices occurring in Eqs. (1)–(3) are square matrices with *N*_o + *N*_c rows and the same number of columns. *P*(*r*) and *Q*(*r*) are matrices representing the motion of the scattered electron and correspond to large (*P*) and small (*Q*) components of the electron radial wave function, \mathcal{K} is a diagonal matrix representing combined angular momentum and parity quantum numbers $\kappa_i = (2j_i + 1)(l_i - j_i)$ of the electron

$$[\mathcal{K}]_{ii} = \kappa_i, \tag{4}$$

I is a unit matrix and *E* is a diagonal matrix representing channel energies

$$[E]_{ii} = E_i. \tag{5}$$

(The channel *i* is open if $E_i > mc^2$ and closed if $E_i < mc^2$). Finally, the potential matrix *V*_{*C*}(*r*) is defined as

$$V_C(r) = -\frac{Ze^2}{r}I + V(r), \tag{6}$$

where *Ze* is a residual charge of the target and *V*(*r*) is a symmetric matrix with elements

$$[V(r)]_{ij} = \sum_{n=1}^{n_{max}} a_{ij}^{(n)} r^{-n-1}. \tag{7}$$

Rather than solving Eqs. (1) and (2) directly [17], we seek the solutions *P*(*r*) and *Q*(*r*) in the form

$$P(r) = N^{-1} [J_P(r)A(r) - Y_P(r)B(r)], \tag{8}$$

$$Q(r) = \left(\frac{\hbar}{2mc}\right) N [J_Q(r)A(r) - Y_Q(r)B(r)], \tag{9}$$

where *N* is a diagonal matrix whose elements, both for open and closed channels, are

$$[N]_{ii} = \left(\frac{2mc}{\hbar}\right)^{1/2} \left(\left|\frac{E_i - mc^2}{E_i + mc^2}\right|\right)^{1/4}, \tag{10}$$

A(*r*) and *B*(*r*) are two unknown auxiliary matrices while *J*_{*P*}(*r*), *Y*_{*P*}(*r*), *J*_{*Q*}(*r*) and *Y*_{*Q*}(*r*) are diagonal basis matrices with elements

$$[J_P(r)]_{ii} = \begin{cases} 2 \operatorname{Re} \left[(\kappa_i - i\xi_i)^{1/2} (2ik_i r)^{-1/2} F_{\gamma_i-1/2}(i/2 - \eta_i, k_i r) \right] & \text{for open channels,} \\ \frac{\Gamma(\gamma_i - \eta_i + 1) (2k_i r)^{-1/2}}{\Gamma(2\gamma_i + 1) 2(\kappa_i + \xi_i)} \left[-(\gamma_i + \eta_i) M_{\eta_i+1/2, \gamma_i}(2k_i r) \right. \\ \left. + (\kappa_i + \xi_i) M_{\eta_i-1/2, \gamma_i}(2k_i r) \right] & \text{for closed channels,} \end{cases} \quad (11)$$

$$[Y_P(r)]_{ii} = \begin{cases} -2 \operatorname{Re} \left[(\kappa_i - i\xi_i)^{1/2} (2ik_i r)^{-1/2} G_{\gamma_i-1/2}(i/2 - \eta_i, k_i r) \right] & \text{for open channels,} \\ -(2k_i r)^{-1/2} \left[W_{\eta_i+1/2, \gamma_i}(2k_i r) + (\kappa_i + \xi_i) W_{\eta_i-1/2, \gamma_i}(2k_i r) \right] & \text{for closed channels,} \end{cases} \quad (12)$$

$$[J_Q(r)]_{ii} = \begin{cases} -2 \operatorname{Im} \left[(\kappa_i - i\xi_i)^{1/2} (2ik_i r)^{-1/2} F_{\gamma_i-1/2}(i/2 - \eta_i, k_i r) \right] & \text{for open channels,} \\ \frac{\Gamma(\gamma_i - \eta_i + 1) (2k_i r)^{-1/2}}{\Gamma(2\gamma_i + 1) 2(\kappa_i + \xi_i)} \left[(\gamma_i + \eta_i) M_{\eta_i+1/2, \gamma_i}(2k_i r) \right. \\ \left. + (\kappa_i + \xi_i) M_{\eta_i-1/2, \gamma_i}(2k_i r) \right] & \text{for closed channels,} \end{cases} \quad (13)$$

$$[Y_Q(r)]_{ii} = \begin{cases} 2 \operatorname{Im} \left[(\kappa_i - i\xi_i)^{1/2} (2ik_i r)^{-1/2} G_{\gamma_i-1/2}(i/2 - \eta_i, k_i r) \right] & \text{for open channels,} \\ (2k_i r)^{-1/2} \left[W_{\eta_i+1/2, \gamma_i}(2k_i r) - (\kappa_i + \xi_i) W_{\eta_i-1/2, \gamma_i}(2k_i r) \right] & \text{for closed channels.} \end{cases} \quad (14)$$

Here

$$\gamma_i = (\kappa_i^2 - (\alpha Z)^2)^{1/2}, \quad \xi_i = \alpha Z \frac{mc}{\hbar k_i}, \quad \eta_i = \alpha Z \frac{E_i}{c\hbar k_i}, \quad (15)$$

$\alpha = e^2/(c\hbar)$ is the Sommerfeld fine-structure constant and k_i is a channel wave number defined as

$$k_i = \frac{1}{c\hbar} (|E_i^2 - (mc^2)^2|)^{1/2}. \quad (16)$$

The definitions (15) and (16) hold in the cases of open and closed channels. The functions $M_{\kappa, \mu}(x)$ and $W_{\kappa, \mu}(x)$ are the Whittaker functions [18] while $F_\lambda(\eta, \rho)$ and $G_\lambda(\eta, \rho)$ are the regular and irregular Coulomb functions, respectively, as defined by Thompson and Barnett [19]. All these functions may be accurately computed using the COULCC program developed by these authors [20]. Normalization of the elements of $J_P(r)$, $Y_P(r)$, $J_Q(r)$ and $Y_Q(r)$ ensures that the Wronskian relation

$$J_P(r)Y_Q(r) - Y_P(r)J_Q(r) = 1 \quad (17)$$

is satisfied. In the $Z = 0$ case, i.e. when electrons are scattered by neutral targets, the matrix elements of the basis matrices simplify and may be expressed in terms of the Riccati–Bessel functions:

$$[J_P(r)]_{ii} = \begin{cases} \hat{j}_l(k_i r) & \text{for open channels,} \\ \hat{i}_l(k_i r) & \text{for closed channels,} \end{cases} \quad (18)$$

$$[Y_P(r)]_{ii} = \begin{cases} \hat{y}_l(k_i r) & \text{for open channels,} \\ -2\pi^{-1} \hat{k}_l(k_i r) & \text{for closed channels,} \end{cases} \quad (19)$$

$$[J_Q(r)]_{ii} = \begin{cases} \pm \hat{j}_{l, \mp 1}(k_i r) & \text{for open channels,} \\ \hat{i}_{l, \mp 1}(k_i r) & \text{for closed channels,} \end{cases} \quad (20)$$

$$[Y_Q(r)]_{ii} = \begin{cases} \pm \hat{y}_{l_i \mp 1}(k_i r) & \text{for open channels,} \\ 2\pi^{-1} \hat{k}_{l_i \mp 1}(k_i r) & \text{for closed channels.} \end{cases} \quad (21)$$

In Eqs. (20) and (21) the upper sign should be chosen for $\kappa_i > 0$ and the lower one for $\kappa_i < 0$. Since various definitions of the Riccati–Bessel functions may be found, we emphasize that the functions used in this paper are related to the Bessel functions [18] in the following way:

$$\hat{j}_l(x) = \left(\frac{1}{2}\pi x\right)^{1/2} J_{l+1/2}(x), \quad \hat{y}_l(x) = \left(\frac{1}{2}\pi x\right)^{1/2} Y_{l+1/2}(x), \quad (22)$$

$$\hat{i}_l(x) = \left(\frac{1}{2}\pi x\right)^{1/2} I_{l-1/2}(x), \quad \hat{k}_l(x) = \left(\frac{1}{2}\pi x\right)^{1/2} K_{l+1/2}(x). \quad (23)$$

Substituting Eqs. (8) and (9) into Eqs. (1) and (2) we get two first-order coupled differential equations satisfied by the matrices $A(r)$ and $B(r)$,

$$\begin{aligned} \frac{d}{dr}A(r) = & -\frac{2m}{\hbar^2}Y_P(r)N^{-1}V(r)N^{-1}[J_P(r)A(r) - Y_P(r)B(r)] \\ & -\frac{1}{2mc^2}Y_Q(r)NV(r)N[J_Q(r)A(r) - Y_Q(r)B(r)], \end{aligned} \quad (24)$$

$$\begin{aligned} \frac{d}{dr}B(r) = & -\frac{2m}{\hbar^2}J_P(r)N^{-1}V(r)N^{-1}[J_P(r)A(r) - Y_P(r)B(r)] \\ & -\frac{1}{2mc^2}J_Q(r)NV(r)N[J_Q(r)A(r) - Y_Q(r)B(r)], \end{aligned} \quad (25)$$

which should be integrated outward with initial conditions

$$A(a) \equiv A_0 = NY_Q(a)P(a) - \left(\frac{2mc}{\hbar}\right)N^{-1}Y_P(a)Q(a), \quad (26)$$

$$B(a) \equiv B_0 = NJ_Q(a)P(a) - \left(\frac{2mc}{\hbar}\right)N^{-1}J_P(a)Q(a). \quad (27)$$

Physically important is an $N_o \times N_o$ reaction submatrix K_{oo} ,

$$K_{oo} = [B(\infty)A^{-1}(\infty)]_{oo}, \quad (28)$$

describing open input and open output channels. $N_o \times N_o$ scattering (S_{oo}) and transition (T_{oo}) matrices are given in terms of the open-open reaction submatrix, K_{oo} , by the familiar formula

$$S_{oo} = I + T_{oo} = \frac{I + iK_{oo}}{I - iK_{oo}}. \quad (29)$$

An advantage of the relativistic variable phase method lies in that to get K_{oo} we need not solve the system of equations (24) and (25). Rather, we introduce an r -dependent matrix $K(r)$ related to the auxiliary matrices $A(r)$ and $B(r)$ in the following way:

$$K(r) = B(r)A^{-1}(r). \quad (30)$$

The matrix $K(r_0)$ has a simple interpretation – it is a reaction matrix for the problem with a truncated potential matrix

$$V(r, r_0) = \begin{cases} V(r) & \text{for } r < r_0, \\ 0 & \text{for } r > r_0. \end{cases} \quad (31)$$

After simple manipulations with Eqs. (24), (25) and (30) the matrix $K(r)$ may be shown to satisfy the equation

$$\begin{aligned} \frac{d}{dr}K(r) = & -\frac{2m}{\hbar^2} [J_P(r) - K(r)Y_P(r)] N^{-1}V(r)N^{-1} [J_P(r) - Y_P(r)K(r)] \\ & -\frac{1}{2mc^2} [J_Q(r) - K(r)Y_Q(r)] NV(r)N [J_Q(r) - Y_Q(r)K(r)], \end{aligned} \quad (32)$$

while Eq. (24) satisfied by the matrix $A(r)$ may be rewritten as

$$\begin{aligned} \frac{d}{dr}A(r) = & -\frac{2m}{\hbar^2} Y_P(r)N^{-1}V(r)N^{-1} [J_P(r) - Y_P(r)K(r)] A(r) \\ & -\frac{1}{2mc^2} Y_Q(r)NV(r)N [J_Q(r) - Y_Q(r)K(r)] A(r). \end{aligned} \quad (33)$$

An initial condition for outward integration of Eq. (32) is

$$K(a) \equiv K_0 = B_0 A_0^{-1}. \quad (34)$$

It is worth noting that although formally Eqs. (32) and (33) constitute the set of coupled equations, the former does not depend on $A(r)$ and this is a main virtue of the relativistic variable phase method. This corresponds to the well-known fact that for evaluation of the reaction matrix, normalization of a wave function is inessential. Thus, to get the open–open reaction submatrix K_{oo} for the problem (1)–(3) one solves Eq. (32) subject to the initial condition (34) and uses an obvious formula

$$K_{oo} = [K(\infty)]_{oo}. \quad (35)$$

The relativistic variable phase method seems to be especially suitable for solving electron–atom and electron–ion scattering problems in conjunction with the relativistic R -matrix method [2–4]. The initial condition for Eq. (32) may be rewritten using one of the following equivalent relations:

$$K_0 = [Y_P(a) - NRNY_Q(a)]^{-1} [J_P(a) - NRNJ_Q(a)], \quad (36)$$

$$K_0 = [J_P(a) - J_Q(a)NRN] [Y_P(a) - Y_Q(a)NRN]^{-1}, \quad (37)$$

if one uses the matrix R defined by Hamacher and Hinze [3] and

$$K_0 = [Y_P(a) - aN(b + \mathcal{R}^{-1})^{-1}NY_Q(a)]^{-1} [J_P(a) - aN(b + \mathcal{R}^{-1})^{-1}NJ_Q(a)], \quad (38)$$

$$K_0 = [J_P(a) - aJ_Q(a)N(b + \mathcal{R}^{-1})^{-1}N] [Y_P(a) - aY_Q(a)N(b + \mathcal{R}^{-1})^{-1}N]^{-1}, \quad (39)$$

if one uses the matrix \mathcal{R} defined by Szymtkowski and Hinze [?] (here b is the diagonal matrix of constants used to generate the R -matrix basis sets in different channels).

Johnson and Secrest [9] have pointed out that those elements of a non-relativistic basis matrix $J(r)$ which correspond to closed channels diverge exponentially for large r what causes numerical problems. The same problem arises for the relativistic basis matrices $J_P(r)$ and $J_Q(r)$. To avoid this disadvantage we shall follow a non-relativistic recipe due to Johnson and Secrest [9] (cf. also Refs. [12,13]) and replace the basis matrices $J_P(r)$, $J_Q(r)$, $Y_P(r)$ and $Y_Q(r)$ by matrices

$$\bar{J}_P(r) = J_P(r)C(r), \quad \bar{J}_Q(r) = J_Q(r)C(r), \quad (40)$$

$$\bar{Y}_P(r) = Y_P(r)C^{-1}(r), \quad \bar{Y}_Q(r) = Y_Q(r)C^{-1}(r), \quad (41)$$

and the auxiliary matrices $A(r)$ and $B(r)$ by matrices

$$\bar{A}(r) = C^{-1}(r)A(r), \quad \bar{B}(r) = C(r)B(r). \quad (42)$$

Here $C(r)$ is a diagonal matrix defined as

$$[C(r)]_{ii} = \begin{cases} 1 & \text{for open channels,} \\ \exp(-k_i r) & \text{for closed channels.} \end{cases} \quad (43)$$

The matrices \bar{A} and \bar{B} satisfy the following differential equations:

$$\begin{aligned} \frac{d}{dr}\bar{A}(r) = & D\bar{A}(r) - \frac{2m}{\hbar^2}\bar{Y}_P(r)N^{-1}V(r)N^{-1} [\bar{J}_P(r)\bar{A}(r) - \bar{Y}_P(r)\bar{B}(r)] \\ & - \frac{1}{2mc^2}\bar{Y}_Q(r)NV(r)N [\bar{J}_Q(r)\bar{A}(r) - \bar{Y}_Q(r)\bar{B}(r)], \end{aligned} \quad (44)$$

$$\begin{aligned} \frac{d}{dr}\bar{B}(r) = & -D\bar{B}(r) - \frac{2m}{\hbar^2}\bar{J}_P(r)N^{-1}V(r)N^{-1} [\bar{J}_P(r)\bar{A}(r) - \bar{Y}_P(r)\bar{B}(r)] \\ & - \frac{1}{2mc^2}\bar{J}_Q(r)NV(r)N [\bar{J}_Q(r)\bar{A}(r) - \bar{Y}_Q(r)\bar{B}(r)], \end{aligned} \quad (45)$$

with initial conditions (cf. Eqs. (26), (27) and (42))

$$\bar{A}(a) = C_0^{-1}A_0, \quad \bar{B}(a) = C_0B_0, \quad (46)$$

where

$$C_0 = C(a). \quad (47)$$

The diagonal matrix D is defined as

$$[D]_{ii} = \begin{cases} 0 & \text{for open channels,} \\ k_i & \text{for closed channels.} \end{cases} \quad (48)$$

Similarly, we may define a modified r -dependent reaction matrix $\bar{K}(r)$,

$$\bar{K}(r) = \bar{B}(r)\bar{A}^{-1}(r) = C(r)K(r)C(r). \quad (49)$$

Immediately, we have

$$\begin{aligned} \frac{d}{dr}\bar{K}(r) = & -[D\bar{K}(r) + \bar{K}(r)D] - \frac{2m}{\hbar^2} [\bar{J}_P(r) - \bar{K}(r)\bar{Y}_P(r)] N^{-1}V(r)N^{-1} [\bar{J}_P(r) - \bar{Y}_P(r)\bar{K}(r)] \\ & - \frac{1}{2mc^2} [\bar{J}_Q(r) - \bar{K}(r)\bar{Y}_Q(r)] NV(r)N [\bar{J}_Q(r) - \bar{Y}_Q(r)\bar{K}(r)], \end{aligned} \quad (50)$$

while Eq. (44) satisfied by the modified amplitude matrix $\bar{A}(r)$ may be rewritten as

$$\begin{aligned} \frac{d}{dr}\bar{A}(r) = & D\bar{A}(r) - \frac{2m}{\hbar^2}\bar{Y}_P(r)N^{-1}V(r)N^{-1} [\bar{J}_P(r) - \bar{Y}_P(r)\bar{K}(r)] \bar{A}(r) \\ & - \frac{1}{2mc^2}\bar{Y}_Q(r)NV(r)N [\bar{J}_Q(r) - \bar{Y}_Q(r)\bar{K}(r)] \bar{A}(r). \end{aligned} \quad (51)$$

An initial condition for Eq. (50) is (cf. Eqs. (46) and (49))

$$\bar{K}(a) = C_0K_0C_0. \quad (52)$$

The transformation (49) has that important feature that does not alter the open channel part of the reaction matrix, i.e.

$$\bar{K}_{00}(r) = K_{00}(r) \quad (53)$$

for arbitrary r , which implies

$$\bar{K}_{00} = K_{00}. \quad (54)$$

Summarising, $\bar{K}(r)$ carries the same physical information as $K(r)$ but is more suitable in numerical calculations.

In numerical applications one may be faced with another problem, namely elements of the matrix $\bar{K}(r)$ may have poles. To overcome this difficulty in a vicinity of a pole one may switch to numerical integration of an equation satisfied by the matrix $\bar{K}^{-1}(r)$ [12] which may be easily derived from Eq. (50) or use an alternative approach described by Croskery et al. [13].

The method will be used in electron–atom and electron–ion scattering calculations in conjunction with the relativistic R -matrix method [21].

Acknowledgments

I am grateful to Professor Jürgen Hinze for reading and commenting on the manuscript. This work was supported by the University of Gdańsk under grant no BW-5400-50064-5.

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