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Evaluation of Appell functions in relativistic Coulomb–Dirac form factors

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Abstract. The continuum–continuum transition matrix elements of the scalar and vector potentials of a pure Coulomb field with exact Dirac wavefunctions can be expressed in terms of generalised hypergeometric functions of two variables denoted as Appell functions. The domain of physical interest for the variables exceeds the convergence region of the original double sum. A method for analytical continuation of the Appell functions is given together with a recipe for their fast calculation.

1. Introduction

In atomic physics the Coulomb force plays the dominant role. A useful feature of this force is that the wavefunctions with a central pure Coulomb potential can be given analytically, at least for a one-electron problem, for bound states as well as for continuum states needed in collision theory. This holds true for the non-relativistic Schrödinger equation (see textbooks on quantum mechanics, e.g., Schiff (1968)) and also for the relativistic Dirac equation (Bethe and Salpeter 1957, Rose 1971). Matrix elements of a Coulomb field operator with these wavefunctions can be reduced by some angular momentum manipulations and integration over angles to one-dimensional radial integrals over products of radial wavefunctions with spherical Bessel functions (Jamnik and Zupancic 1957, Amundsen and Kocbach 1975, Amundsen 1978, Jakubassa-Amundsen 1982). Here we are interested in continuum–continuum transition matrix elements for relativistic Dirac wavefunctions. The corresponding non-relativistic case was extensively treated by Baur and Trautmann (1974, 1976).

In both relativistic and non-relativistic cases, the interesting radial integrals can be written as a finite sum over generalised hypergeometric functions denoted as Appell functions (Appell and Kampé de Feriet 1926, Almström and Olsson 1967, Wright *et al* 1977). The aim of this paper is threefold: first, in § 2, we express the relativistic Coulomb integrals by a sum over Appell functions. The derivation differs somewhat from the non-relativistic case because of non-integers replacing the non-relativistic principal quantum numbers. Second, in § 3, we derive for the group of four Appell functions, involved in the evaluation of the Coulomb integrals, a system of linear coupled differential equations which are of Fuchsian type (Walter 1976). The analysis of the solutions gives us the analytic continuation of the Appell functions needed for the interval of physical parameters. Finally, in § 4, we give the recipe for a fast calculation of the Appell functions and also of the Coulomb integrals for relativistic continuum–continuum transitions.

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2. Form factors with relativistic continuum functions

It can be shown (Amundsen and Aashamar (1981), for further references see Trautmann *et al* (1983) and Becker *et al* (1986)) that the coupling matrix elements of the Liénard-Wiechert potentials of a classically moving point charge of a projectile nucleus with Dirac wavefunctions centred at the target nucleus involve radial integrals (the form factors) of the type

$$F_l^{(1)}(s)=\int_0^\infty \mathrm{d}r\, r^2 j_l(sr)(g_i g_f+f_i f_f) \tag{1a}$$

$$F_l^{(2)}(s)=\int_0^\infty \mathrm{d}r\, r^2 j_l(sr) f_f g_i \tag{1b}$$

$$F_l^{(3)}(s)=\int_0^\infty \mathrm{d}r\, r^2 j_l(sr) f_i g_f. \tag{1c}$$

Here, g and f are radial functions of the larger and smaller components of the Dirac spinor for two states with index f and i, respectively; j_l is the spherical Bessel function of the first kind. The parameter s ranges from the minimum momentum transfer $q=|E_f-E_i|/v$ to infinity in first-order perturbation theory. E_f and E_i are the energies of the states f and i, respectively, and v is the relative velocity of the projectile and target.

For coupled-state calculations the lower bound of s is zero. It should be noted that for the final results an integration over s is necessary. Therefore a fast recipe is needed to calculate the form factors.

If at least one of the states labelled i or f is a bound state, integrals (1) yield finite sums over hypergeometric functions (Amundsen 1978). We are interested in couplings between continuum states. Then the radial wavefunctions can be represented in natural units ($\hbar=c=m=1$) by (Rose 1971)

$$\begin{aligned} g&=N(|E|\pm 1)^{1/2} r^{\gamma-1}\,\mathrm{Re}(\mathrm{e}^{-\mathrm{i}pr}\,\mathrm{e}^{\mathrm{i}\delta}(\gamma+\mathrm{i}\eta)\,{}_1F_1(1+\gamma+\mathrm{i}\eta, 2\gamma+1, 2\mathrm{i}pr))\\ f&=\mp N(|E|\mp 1)^{1/2} r^{\gamma-1}\,\mathrm{Im}(\mathrm{e}^{-\mathrm{i}pr}\,\mathrm{e}^{\mathrm{i}\delta}(\gamma+\mathrm{i}\eta)\,{}_1F_1(1+\gamma+\mathrm{i}\eta, 2\gamma+1, 2\mathrm{i}pr)). \end{aligned} \tag{2}$$

The upper signs hold for the positive continuum ($E>1$) and the lower signs for the negative continuum ($E<-1$). Further

$$\begin{aligned} &\gamma=[\kappa^2-(Z_\mathrm{T}\alpha)^2]^{1/2} \qquad p=(E^2-1)^{1/2} \qquad \eta=Z_\mathrm{T}\alpha E/p\\ &\mathrm{e}^{2\mathrm{i}\delta}=(-\kappa+\mathrm{i}\eta/E)/(\gamma+\mathrm{i}\eta) \qquad N=\mathrm{e}^{\pi\eta/2}|\Gamma(\gamma+\mathrm{i}\eta)|2^\gamma p^{\gamma-1/2}/(\pi^{1/2}\Gamma(2\gamma+1)) \end{aligned} \tag{3}$$

where α is the fine structure constant and Z_T is the charge number of the target nucleus. The quantum number κ is related to the quantum numbers of the total momentum j and the angular momentum l of the large component as follows: for $\kappa>0$, $j=\kappa-\frac{1}{2}$, $l=\kappa$ and for $\kappa<0$, $j=-\kappa-\frac{1}{2}$, $l=-\kappa-1$. In equations (2) ${}_1F_1$ is the confluent hypergeometric function.

The index l of the Bessel function in the form factor $F_l^{(\nu)}$ in (1) is not free to vary but is restricted by angular momentum conservation. It yields:

$$\text{for } \nu=1 \qquad |l_i-l_f|\leqslant l\leqslant l_i+l_f \qquad \text{and} \qquad |l-j_i|\leqslant j_f\leqslant l+j_i \tag{4a}$$

$$\begin{aligned} &\text{for } \nu=2 \qquad |l_i-l'_f|\leqslant l\leqslant l_i+l'_f \qquad \text{and} \qquad |L-j_i|\leqslant j_f\leqslant L+j_i\\ &\qquad\qquad \text{with } |l-1|\leqslant L\leqslant l+1 \end{aligned} \tag{4b}$$

$$\text{for } \nu=3 \qquad |l_i'-l_f|\leqslant l\leqslant l_i'+l_f \qquad \text{and} \qquad |L-j_i|\leqslant j_f\leqslant L+j_i$$
$$\text{with } |l-1|\leqslant L\leqslant l+1 \tag{4c}$$

where l_i' and l_f' are the quantum numbers of the angular momentum of the small components. From (4) it may be deduced that the maximum index is

$$l_{\max}=|\kappa_i|+|\kappa_f|. \tag{5}$$

In the following we restrict ourselves to the case that E_i and E_f are both positive. The other cases differ only in the signs of E_i, η_i or E_f, η_f and possibly in a total minus sign.

Inserting (2) into (1) we obtain

$$F_l^{(1)}(s)=\tfrac{1}{2}N_iN_f\{[(E_f+1)(E_i+1)]^{1/2}\,\mathrm{Re}(I_{fi}^{(1)}(s)+I_{fi}^{(2)}(s))$$
$$-[(E_f-1)(E_i-1)]^{1/2}\,\mathrm{Re}(I_{fi}^{(1)}(s)-I_{fi}^{(2)}(s))\} \tag{6a}$$
$$F_l^{(2)}(s)=-\tfrac{1}{2}N_iN_f[(E_i+1)(E_f-1)]^{1/2}\,\mathrm{Im}(I_{fi}^{(1)}(s)+I_{fi}^{(2)}(s)) \tag{6b}$$
$$F_l^{(3)}(s)=-\tfrac{1}{2}N_iN_f[(E_i-1)(E_f+1)]^{1/2}\,\mathrm{Im}(I_{fi}^{(1)}(s)-I_{fi}^{(2)}(s)) \tag{6c}$$

where we have put

$$I_{fi}^{(1)}(s)=Z_fZ_i\int_0^\infty \mathrm{d}r\,r^{\gamma_f+\gamma_i}j_l(sr)\exp[-\mathrm{i}(p_f+p_i)r]\,{}_1F_1(1+\gamma_f+\mathrm{i}\eta_f,2\gamma_f+1,2\mathrm{i}p_fr)$$
$$\times\,{}_1F_1(1+\gamma_i+\mathrm{i}\eta_i,2\gamma_i+1,2\mathrm{i}p_ir) \tag{7a}$$
$$I_{fi}^{(2)}(s)=Z_fZ_i^*\int_0^\infty \mathrm{d}r\,r^{\gamma_f+\gamma_i}j_l(sr)\exp[-\mathrm{i}(p_f-p_i)r]\,{}_1F_1(1+\gamma_f+\mathrm{i}\eta_f,2\gamma_f+1,2\mathrm{i}p_fr)$$
$$\times[{}_1F_1(1+\gamma_i+\mathrm{i}\eta_i,2\gamma_i+1,2\mathrm{i}p_ir)]^* \tag{7b}$$

with the abbreviation $Z=\mathrm{e}^{\mathrm{i}\delta}(\gamma+\mathrm{i}\eta)$. For the further treatment of the integrals in (7) we enhance the convergence of the integrals at the upper limit by replacing $\exp[-\mathrm{i}(p_f\pm p_i)r]$ by $\exp\{-[\varepsilon+\mathrm{i}(p_f\pm p_i)]r\}$ with $\varepsilon>0$. In our final results we have to take the limit $\varepsilon\to 0$. A similar procedure was used by Baur and Trautmann (1974) in the non-relativistic case. The uniform convergence of the integrand with ε to the one without ε guarantees the correctness of the final results. Since $\gamma_f+\gamma_i>0$, there are no problems at the lower integration limit. But, in contrast to the non-relativistic case, $\gamma_f+\gamma_i$ is non-integer. On the other hand, precisely this fact gives us the possibility to write

$$I_{fi}^{(1)}(s)=Z_fZ_i\lim_{\varepsilon\to+0}\{\exp[2\pi\mathrm{i}(\gamma_f+\gamma_i)]-1\}^{-1}\int_C \mathrm{d}z\,z^{\gamma_f+\gamma_i}j_l(sz)\exp\{-[\varepsilon+\mathrm{i}(p_f+p_i)]z\}$$
$$\times\,{}_1F_1(1+\gamma_f+\mathrm{i}\eta_f,2\gamma_f+1,2\mathrm{i}p_fz)\,{}_1F_1(1+\gamma_i+\mathrm{i}\eta_i,2\gamma_i+1,2\mathrm{i}p_iz). \tag{8}$$

Here, C is a path in the complex z plane which follows the real axis from $z=+\infty+\mathrm{i}\delta$ to zero, encircles the origin anticlockwise and returns back along the real axis to $z=+\infty-\mathrm{i}\delta$.

The expansion of the Bessel function (Watson 1966)

$$j_l(x)=\frac{1}{2x}\sum_{n=0}^{l}\frac{(l+n)!}{n!(l-n)!}\frac{1}{(2x)^n}[\exp(\mathrm{i}x)i^{n-l-1}+\exp(-\mathrm{i}x)i^{l+1-n}] \tag{9}$$

inserted in (8) leaves us with a sum over integrals of the type

$$I_n=\lim_{\varepsilon\to+0}\{\exp[2\pi\mathrm{i}(\gamma_f+\gamma_i)]-1\}^{-1}\int_C \mathrm{d}z\,z^{\gamma_f+\gamma_i-n-1}\exp[-(\varepsilon+\mathrm{i}q)z]$$
$$\times\,{}_1F_1(1+\gamma_f+\mathrm{i}\eta_f,2\gamma_f+1,2\mathrm{i}p_fz)\,{}_1F_1(1+\gamma_i+\mathrm{i}\eta_i,2\gamma_i+1,2\mathrm{i}p_iz) \tag{10}$$

with $q=p_f+p_i\mp s$.

Using for ${}_1F_1$ the integral representation of the confluent hypergeometric functions (Abramowitz and Stegun 1972)

$$ {}_1F_1(a, b, x) = \frac{\Gamma(b)}{\Gamma(a)\Gamma(b-a)} \int_0^1 e^{xu} u^{a-1} (1-u)^{b-a-1}\, du \tag{11} $$

with the condition $\operatorname{Re} b > \operatorname{Re} a > 0$, which is fulfilled in our case, changing the order of integrations, and identifying the contour integral as proportional to a Γ function for non-integer arguments (Erdélyi 1953)

$$ \Gamma(\alpha) = \xi^{\alpha} (e^{2\pi i\alpha} - 1)^{-1} \int_C z^{\alpha-1} e^{-z\xi}\, dz \tag{12} $$

for $\alpha \neq 0, \pm 1, \pm 2, \ldots$ and $-\pi/2 < \arg \xi < \pi/2$, which is also fulfilled for $\varepsilon > 0$, we are left with the following expression for I_n:

$$ \begin{aligned} I_n = \lim_{\varepsilon\to+0} & \frac{\Gamma(\gamma_f+\gamma_i-n)}{(\varepsilon+iq)^{\gamma_f+\gamma_i-n}} \frac{\Gamma(2\gamma_f+1)\Gamma(2\gamma_i+1)}{\Gamma(\gamma_f-i\eta_f)\Gamma(\gamma_i-i\eta_i)\Gamma(1+\gamma_f+i\eta_f)\Gamma(1+\gamma_i+i\eta_i)} \\ & \times \int_0^1 \int_0^1 u^{\gamma_i+i\eta_i}(1-u)^{\gamma_i-i\eta_i-1} v^{\gamma_f+i\eta_f}(1-v)^{\gamma_f-i\eta_f-1} \\ & \times (1-u\bar{x}-v\bar{y})^{-(\gamma_i+\gamma_f-n)}\, du\, dv \end{aligned} \tag{13} $$

with $\bar{x} = i2p_i/(\varepsilon+iq)$ and $\bar{y} = i2p_f/(\varepsilon+iq)$.

Finally, the double integral together with a part of the factor is an integral representation of Euler's type for a generalisation of the hypergeometric functions, in our case one of the Appell functions (Appell and Kampé de Feriet 1926):

$$ I_n = \lim_{\varepsilon\to+0} \frac{\Gamma(\gamma_f+\gamma_i-n)}{(\varepsilon+iq)^{\gamma_f+\gamma_i-n}} F_2(\gamma_f+\gamma_i-n, \gamma_i+1+i\eta_i, \gamma_f+1+i\eta_f, 2\gamma_i+1, 2\gamma_f+1; \bar{x}, \bar{y}). \tag{14} $$

In fact, the identity of the contour integral in (10) with the right-hand side of (14) is a special case of a more general formula given already by Erdélyi (1936).

Defining the following abbreviations:

$$ \begin{aligned} F_2^{(1)} &= F_2(\alpha, \beta, \beta', \gamma, \gamma'; x, y) \\ F_2^{(2)} &= F_2(\alpha, \beta+1, \beta', \gamma, \gamma'; x, y) \\ F_2^{(3)} &= F_2(\alpha, \beta, \beta'+1, \gamma, \gamma'; x, y) \\ F_2^{(4)} &= F_2(\alpha, \beta+1, \beta'+1, \gamma, \gamma'; x, y) \end{aligned} \tag{15} $$

where

$$ x = \frac{2p_i}{p_i+p_f+s+i\varepsilon} \qquad y = \frac{2p_f}{p_i+p_f+s+i\varepsilon} $$

$$ \alpha = \gamma_f+\gamma_i-n \qquad \beta = \gamma_i - i\eta_i \qquad \beta' = \gamma_f - i\eta_f \qquad \gamma = 2\gamma_i+1 \qquad \gamma' = 2\gamma_f+1 $$

we may write, using (14) and (9) in (8) and in the analogous expression for $I_{fi}^{(2)}$,

$$ \begin{aligned} I_{fi}^{(1)}(s) = {} & Z_f Z_i [2s(p_i+p_f+s)^{\gamma_i+\gamma_i}]^{-1} \sum_{n=0}^{l} \frac{(l+n)!}{n!(l-n)!} \Gamma(\gamma_f+\gamma_i-n) \left(\frac{s+p_i+p_f}{2s}\right)^n \\ & \times [i^{\gamma_i+\gamma_f-l-1} F_2^{(1)} + i^{l+1-\gamma_i-\gamma_f} (F_2^{(4)})^*] \end{aligned} \tag{16a} $$

$$I_{fi}^{(2)}(s)=Z_fZ_i^*[2s(p_i+p_f+s)^{\gamma_f+\gamma_i}]^{-1}\sum_{n=0}^{l}\frac{(l+n)!}{n!(l-n)!}\Gamma(\gamma_f+\gamma_i-n)\left(\frac{s+p_i+p_f}{2s}\right)^n$$
$$\times[\mathrm{i}^{\gamma_i+\gamma_f-l-1}F_2^{(2)}+\mathrm{i}^{l+1-\gamma_i-\gamma_f}(F_2^{(3)})^*]. \tag{16b}$$

The arguments x and y are to be taken in the limit $\varepsilon\to+0$. The fact that the arguments x and y are the same in all F_2 functions is due to transformations of Euler type, valid for the Appell functions (Erdélyi 1953). The Euler-type transformations in turn originate from Kummer transformations for the ${}_1F_1$ functions. According to Kummer transformations, for instance, the integral (8) remains unchanged if one replaces in the integrand simultaneously p_i by $-p_i$ and $1+\mathrm{i}\eta_i$ by $-\mathrm{i}\eta_i$, or p_f by $-p_f$ and $1+\mathrm{i}\eta_f$ by $-\mathrm{i}\eta_f$, or both.

As mentioned before the lower bound for the numerical integration over s is zero in coupled-states calculations. Evidently $s\to0$ leads to numerical difficulties in (16), which were introduced by the expansion (9) into the otherwise well behaving integral (8). For very small s an expansion of $j_l(sr)$ in a power series of the argument is preferable. This leads to the formula

$$I_{fi}^{(1)}(s)=Z_fZ_i\frac{\sqrt{\pi}}{2}\left(\frac{s}{2}\right)^l[\mathrm{i}(p_f+p_i)]^{-\gamma_f-\gamma_i-l-1}\sum_{n=0}^{\infty}\frac{\Gamma(2n+1+l+\gamma_i+\gamma_f)}{n!\Gamma(l+\frac{1}{2}+n+1)}$$
$$\times\left(\frac{s}{2(p_f+p_i)}\right)^{2n}(F_2^{(4)}(\alpha=\gamma_i+\gamma_f+l+2n+1;\,x(s=0),\,y(s=0)))^* \tag{17}$$

and a similar expression for $I_{fi}^{(2)}(s)$ with Z_i replaced by Z_i^* and $(F_2^{(4)})^*$ replaced by $(F_2^{(3)})^*$. The arguments of the F_2 functions are the same as defined in (15) besides α; x and y are to be taken for $s=0$. The series (17) is convergent for $s<p_i+p_f$, whereas the series with $F_2^{(3)}$ only converges for $s<|p_f-p_i|$. This follows from the ratio test together with the reduction formula of Jaeger and Hulme (1935) for the $F_2^{(j)}$ functions (see the next section).

3. Evaluation of the Appell functions

The original defining power series for the F_2 functions (Appell and Kampé de Feriet 1926)

$$F_2(\alpha,\beta,\beta',\gamma,\gamma';x,y)=\sum_{m,n=0}^{\infty}\frac{(\alpha)_{m+n}(\beta)_n(\beta')_m}{(\gamma)_n(\gamma')_m n!\,m!}x^ny^m \tag{18}$$

is convergent only for $|x|+|y|<1$. We see from (15) that this is equivalent to $p_i+p_f<s$ $(s\geq0)$ for $\varepsilon\to+0$. Since we need also small values of $s<p_i+p_f$ we have to look for an analytical continuation.

In the notation of equations (15) and by showing the dependences on the parameter α and arguments x and y explicitly, the following reduction formula holds (Jaeger and Hulme (1935), with or without the limit $\varepsilon\to+0$):

$$F_2^{(i)}(\alpha+1;x,y)=\sum_j A_j^{(i)}F_2^{(j)}(\alpha;x,y). \tag{19}$$

This may be proved by using (18) or, better, with the aid of the double integral representation (Erdélyi 1953) already used to obtain equation (14) from (13).

The $A_j^{(i)}$ are

$$A_1^{(1)}=\frac{\alpha-\beta-\beta'}{\alpha} \qquad A_2^{(1)}=\frac{\beta}{\alpha} \qquad A_3^{(1)}=\frac{\beta'}{\alpha} \qquad A_4^{(1)}=0$$

$$A_1^{(2)}=\frac{\gamma-\beta-1}{(1-x)\alpha} \qquad A_2^{(2)}=\frac{\alpha-\beta'+\beta+1-\gamma}{(1-x)\alpha} \qquad A_3^{(2)}=0 \qquad A_4^{(2)}=\frac{\beta'}{(1-x)\alpha}$$

$$A_1^{(3)}=\frac{\gamma'-\beta'-1}{(1-y)\alpha} \qquad A_2^{(3)}=0 \qquad A_3^{(3)}=\frac{\alpha-\beta+\beta'+1-\gamma'}{(1-y)\alpha} \qquad A_4^{(3)}=\frac{\beta}{(1-y)\alpha}$$

$$A_1^{(4)}=0 \qquad A_2^{(4)}=\frac{\gamma'-\beta'-1}{(1-x-y)\alpha} \qquad A_3^{(4)}=\frac{\gamma-\beta-1}{(1-x-y)\alpha}$$

$$A_4^{(4)}=\frac{\alpha+\beta+\beta'-\gamma-\gamma'+2}{(1-x-y)\alpha}. \tag{20}$$

Furthermore, we may write

$$F_2^{(1)}=F_2(\alpha,\beta,\beta',\gamma,\gamma';x,y)$$
$$=\frac{\int_C \mathrm{d}z\, z^{\alpha-1}\exp[-(\varepsilon+\mathrm{i}q)z]\,{}_1F_1(\beta,\gamma,2\mathrm{i}p_i z)\,{}_1F_1(\beta',\gamma',2\mathrm{i}p_f z)}{\int_C \mathrm{d}z\, z^{\alpha-1}\exp[-(\varepsilon+\mathrm{i}q)z]} \tag{21}$$

with $q=p_f+p_i+s$ and x and y as given in (15). Similar expressions hold for $F_2^{(2)}$, $F_2^{(3)}$ and $F_2^{(4)}$. We note that this expression can also be used for positive integer values of $\alpha=1,2,3,\ldots$, if we replace the contour integral by $\int_0^\infty \mathrm{d}z\ldots$.

In fact, equation (21) is even correct for $\alpha=0,-1,-2,\ldots$. Then $F_2^{(j)}(\alpha;x,y)$ are polynomials in x and y which follows directly from the double sum due to the property of the Pochhammer symbol

$$(-M)_{M+1}=0 \qquad \text{for } M=0,1,2,\ldots.$$

We take the derivative of F_2 with respect to q or equivalently with respect to s. From (21) we obtain

$$\frac{\mathrm{d}F_2(\alpha)}{\mathrm{d}q}=\frac{\mathrm{d}F_2(\alpha)}{\mathrm{d}s}=\frac{\mathrm{i}\alpha}{\varepsilon+\mathrm{i}q}(F_2(\alpha)-F_2(\alpha+1)). \tag{22}$$

In parentheses we have indicated the dependence of F_2 on the parameter α. The other parameters do not change. Combining (19) with (20) and (22), introducing a column vector $\boldsymbol{F}_2$ with the components $F_2^{(1)}$, $F_2^{(2)}$, $F_2^{(3)}$, $F_2^{(4)}$ and carrying out the limit $\varepsilon\to+0$, we get a system of coupled differential equations for the $F_2^{(i)}$ which we may write in matrix form as (Becker *et al* 1986)

$$\frac{\mathrm{d}\boldsymbol{F}_2}{\mathrm{d}q}=\frac{\mathrm{d}\boldsymbol{F}_2}{\mathrm{d}s}=\sum_{k=1}^{4}\frac{1}{s-s_k}\boldsymbol{R}_k\boldsymbol{F}_2=\sum_{k=1}^{4}\frac{1}{q-q_k}\boldsymbol{R}_k\boldsymbol{F}_2. \tag{23}$$

This system is of Fuchsian type (Walter 1976). The four poles q_k lie on the real axis. We have

$$q_1=+\mathrm{i}0 \qquad q_2=2p_i-\mathrm{i}0 \qquad q_3=2p_f-\mathrm{i}0 \qquad q_4=2(p_i+p_f)-\mathrm{i}0. \tag{24}$$

The addition of $\pm\mathrm{i}0$ is the remainder of the limiting process $\varepsilon\to+0$ and gives the prescription how to treat the vicinity of the poles if necessary. Although an extension of the methods presented here to complex q values is possible, we are primarily interested in real q values because of the physical application given in § 2. As long as $\varepsilon > 0$, though small, a pole can be passed, e.g., at $q_4 = 2(p_i + p_f) - i\varepsilon$ from $q = \mathrm{Re}(q_4) - \delta$ to $q = \mathrm{Re}(q_4) + \delta$, on the real axis without any numerical or conceptual difficulties. In the limit $\varepsilon \to +0$ also the limit of this regular behaviour has to be taken.

The four matrices $\boldsymbol{R}_i$ are easily constructed. We only write down the non-vanishing matrix elements:

$$
\begin{array}{llll}
\boldsymbol{R}_1: & R_{1,11} = \beta + \beta' \quad R_{1,12} = -\beta & R_{1,13} = -\beta' & R_{1,22} = R_{1,33} = R_{1,44} = \alpha \\
\boldsymbol{R}_2: & R_{2,21} = 1 + \beta - \gamma & R_{2,22} = \gamma + \beta' - \beta - \alpha - 1 & R_{2,24} = -\beta' \\
\boldsymbol{R}_3: & R_{3,31} = 1 + \beta' - \gamma' & R_{3,33} = \gamma' + \beta - \beta' - \alpha - 1 & R_{3,34} = -\beta \\
\boldsymbol{R}_4: & R_{4,42} = 1 + \beta' - \gamma' & R_{4,43} = 1 + \beta - \gamma & R_{4,44} = \gamma + \gamma' - 2 - \alpha - \beta - \beta'.
\end{array}
\tag{25}
$$

The aim is now to obtain a fundamental system for the differential equation (23), i.e. a set of four independent solutions for all q or s values needed for the physical problem mentioned in § 2. The F_2 functions are a special solution and, therefore, a linear combination of the fundamental solutions.

As the general theory shows, the fundamental solutions can be written about each pole q_k as a series of the form

$$\boldsymbol{F} = (q - q_k)^{\lambda} \sum_{j=0}^{\infty} (q - q_k)^j \boldsymbol{C}_j. \tag{26}$$

In our case the $\boldsymbol{C}_j$ are constant column vectors as demonstrated below and only in the worst case, for $p_i = p_f$, of the structure $\boldsymbol{C}_j = \boldsymbol{a}_j \ln(q - q_k) + \boldsymbol{b}_j$. The series (26) are absolutely convergent in the region (Walter 1976)

$$|q - q_k| < \min_{j \neq k} |q_j - q_k|. \tag{27}$$

To be definite, let us assume that $p_f > p_i > 0$. Then we obtain the situation depicted in figure 1.

The regions of convergence of the series (26), shown in figure 1 and denoted by the encircled numbers 1, 2, 3 and 4, are given by (24) and the criterion (27). The region 5 tending to infinity is due to the convergence criterion of the original expansion (18). In fact, $q = \infty$ is also a weak singularity of the differential equation (23) and an expansion similar to (26) (in $1/q$) with appropriate coefficients is equivalent to the

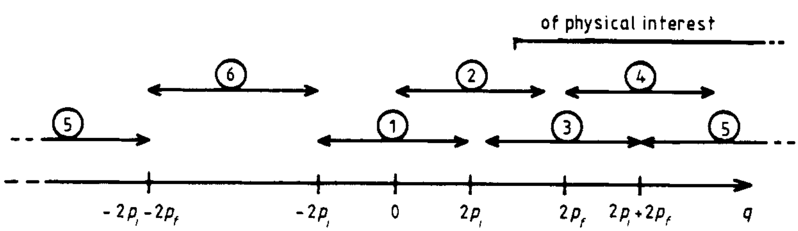

Figure 1. Convergence regions of the series (26) and of the original expansion (18). For further explanation see text.

double sum (18). We note that the region of physical interest, $0 \leq s < \infty$ or $p_i + p_f \leq q < \infty$, is completely covered by the regions 3, 4 and 5. Nevertheless, an extension to all q values might be of mathematical interest. We see that the region 6, $-2p_i - 2p_f \leq q \leq -2p_i$, has no series expansion of the types considered. We may obtain values of F_2 for such q values by using the Euler transformation (Erdélyi 1953)

$$F_2(\alpha, \beta, \beta', \gamma, \gamma'; x, y)$$
$$= (1-x-y)^{-\alpha} F_2\left(\alpha, \gamma-\beta, \gamma'-\beta', \gamma, \gamma'; \frac{x}{x+y-1}, \frac{y}{x+y-1}\right) \tag{28}$$

which transforms q to $q' = 2p_i + 2p_f - q$. Therefore, the arguments of the right-hand side of (28) are in the convergence regions of the double sum for $-2p_i - 2p_f \leq q \leq -2p_i$.

3.1. *The fundamental solutions of equation (23) for the non-degenerate case $p_i \neq p_f$*

Inserting the ansatz $\boldsymbol{F} = \Sigma_{j=0}^{\infty} (q-q_k)^{j+\lambda} \boldsymbol{C}_j$ into the equation $\mathrm{d}\boldsymbol{F}/\mathrm{d}q = \Sigma_{l=1}^{4} (q-q_l)^{-1} \boldsymbol{R}_l \boldsymbol{F}$ and multiplying by the product $\Pi_{i=1}^{4} (q-q_i)$ we obtain

$$\sum_{j=0}^{\infty} (q-q_k)^{j+\lambda} \left(\sum_{l=1}^{4} \boldsymbol{R}_l \prod_{i\neq l} (q-q_i) - (j+\lambda) \prod_{i\neq k} (q-q_i) \right) \boldsymbol{C}_j = 0 \qquad \text{for } k = 1, 2, 3, 4. \tag{29}$$

The equation which determines λ and $\boldsymbol{C}_0$ is obtained from the coefficients of the lowest power in $q - q_k$ as

$$(\boldsymbol{R}_k - \lambda \mathbf{1}) \boldsymbol{C}_0 = 0 \tag{30}$$

where $\mathbf{1}$ is the 4×4 unit matrix. The secular equation for λ is

$$\det|\boldsymbol{R}_k - \lambda \mathbf{1}| = 0. \tag{31}$$

For the higher indices we have the recursion relation

$$z_1 z_2 z_3 [\boldsymbol{R}_k - (\lambda + j)\mathbf{1}] \boldsymbol{C}_j + \left((z_1 z_2 + z_1 z_3 + z_2 z_3)[\boldsymbol{R}_k - (\lambda + j - 1)\mathbf{1}] + \sum_{\substack{i;i\neq l, i\neq m \\ l<m}} \boldsymbol{R}_{r_i} z_l z_m \right) \boldsymbol{C}_{j-1}$$
$$+ \left(\sum_i z_i [\boldsymbol{R}_k - (\lambda + j - 2)\mathbf{1}] + \sum_{\substack{i;i\neq l, i\neq m \\ l<m}} \boldsymbol{R}_{r_i} (z_l + z_m) \right) \boldsymbol{C}_{j-2}$$
$$+ \left(\sum_i \boldsymbol{R}_i - (\lambda + j - 3)\mathbf{1} \right) \boldsymbol{C}_{j-3} = 0 \tag{32}$$

for $j = 1, 2, 3, \ldots$, with $\boldsymbol{C}_{-1} = \boldsymbol{C}_{-2} = 0$, and where we have put

$$z_i = q_k - q_{r_i} \qquad r_i \neq k \qquad i = 1, 2, 3.$$

Obviously the recursion formula works well as long as $\lambda + j$ is no eigenvalue of $\boldsymbol{R}_k$ for $j \geq 1$.

In the following we give the eigenvalues and possible vectors $\boldsymbol{C}_0$ for all $\boldsymbol{R}_k$.

$k = 1$. The pole is $q_1 = 0$ ($s_1 = -p_i - p_f$).

From (31), (25) and (15) we have $(\alpha-\lambda)^3(\beta+\beta'-\lambda)=0$, from which we obtain

$$\lambda_{1,2,3}=\alpha=\gamma_f+\gamma_i-n \qquad \lambda_4=\beta+\beta'=\gamma_f+\gamma_i-\mathrm{i}(\eta_f+\eta_i) \tag{33a}$$

and further from (30), if we write $C_{l,0}$ for C_0 corresponding to λ_l, we have the independent solutions

$$C_{1,0}=\begin{pmatrix}(\gamma_i-\mathrm{i}\eta_i)/[n-\mathrm{i}(\eta_f+\eta_i)]\\1\\0\\0\end{pmatrix} \qquad C_{2,0}=\begin{pmatrix}(\gamma_f-\mathrm{i}\eta_f)/[n-\mathrm{i}(\eta_f+\eta_i)]\\0\\1\\0\end{pmatrix}$$
$$C_{3,0}=\begin{pmatrix}0\\0\\0\\1\end{pmatrix} \qquad C_{4,0}=\begin{pmatrix}1\\0\\0\\0\end{pmatrix}. \tag{33b}$$

$k=2$. The pole is $q_2=2p_i$ ($s_2=p_i-p_f$). The eigenvalues are

$$\lambda_{1,2,3}=0 \qquad \lambda_4=\beta'+\gamma-\beta-\alpha-1=n-\mathrm{i}(\eta_f-\eta_i). \tag{34a}$$

A set of independent solutions to (30) is

$$C_{1,0}=\begin{pmatrix}0\\0\\1\\0\end{pmatrix} \qquad C_{2,0}=\begin{pmatrix}1\\(\gamma_i+\mathrm{i}\eta_i)/[n-\mathrm{i}(\eta_f-\eta_i)]\\0\\0\end{pmatrix}$$
$$C_{3,0}=\begin{pmatrix}0\\(\gamma_f-\mathrm{i}\eta_f)/[n-\mathrm{i}(\eta_f-\eta_i)]\\0\\1\end{pmatrix} \qquad C_{4,0}=\begin{pmatrix}0\\1\\0\\0\end{pmatrix}. \tag{34b}$$

$k=3$. The pole is $q_3=2p_f$ ($s_3=p_f-p_i$). The eigenvalues are

$$\lambda_{1,2,3}=0 \qquad \lambda_4=\beta+\gamma'-\beta'-\alpha-1=n+\mathrm{i}(\eta_f-\eta_i) \tag{35a}$$

and a set of independent solutions is

$$C_{1,0}=\begin{pmatrix}0\\1\\0\\0\end{pmatrix} \qquad C_{2,0}=\begin{pmatrix}1\\0\\(\gamma_f+\mathrm{i}\eta_f)/[n+\mathrm{i}(\eta_f-\eta_i)]\\0\end{pmatrix}$$
$$C_{3,0}=\begin{pmatrix}0\\0\\(\gamma_i-\mathrm{i}\eta_i)/[n+\mathrm{i}(\eta_f-\eta_i)]\\1\end{pmatrix} \qquad C_{4,0}=\begin{pmatrix}0\\0\\1\\0\end{pmatrix}. \tag{35b}$$

$k=4$. The pole is $q_4=2p_i+2p_f$ ($s_4=p_i+p_f$). The eigenvalues are

$$\lambda_{1,2,3}=0 \qquad \lambda_4=\gamma+\gamma'-2-\alpha-\beta-\beta'=n+\mathrm{i}(\eta_f+\eta_i) \tag{36a}$$

and a set of independent solutions is

$$C_{1,0}=\begin{pmatrix}1\\0\\0\\0\end{pmatrix}\qquad C_{2,0}=\begin{pmatrix}0\\1\\0\\(\gamma_f+\mathrm{i}\eta_f)/[n+\mathrm{i}(\eta_f+\eta_i)]\end{pmatrix}$$
$$C_{3,0}=\begin{pmatrix}0\\0\\1\\(\gamma_i+\mathrm{i}\eta_i)/[n+\mathrm{i}(\eta_f+\eta_i)]\end{pmatrix}\qquad C_{4,0}=\begin{pmatrix}0\\0\\0\\1\end{pmatrix}. \tag{36b}$$

In each case the higher expansion coefficients can be calculated from the recursion relation (32).

3.2. The fundamental solutions of equation (23) for the degenerate case $p_i = p_f$

If we have $p_i = p_f$ which means for E_i and $E_f > 0$ also $E_i = E_f$, we obtain $\eta_i = \eta_f$ from (3). Equations (34*a*) and (35*a*) show that $\lambda_{1,2,3}+n$ is an eigenvalue of $\boldsymbol{R}_2$ or $\boldsymbol{R}_3$, respectively. Therefore, the recursion relations (32) break down. We have to look for another set of independent solutions of (23) in the neighbourhood of the pole $q_2 = q_3 = 2p_i$. With the ansatz (26), but letting the coefficients $\boldsymbol{C}_j$ depend on q in the form $\boldsymbol{C}_j(t)$ with

$$q-2p=\exp(t) \qquad (p=p_i=p_f) \tag{37}$$

we have from (23) the new recursion relation

$$4p^2\{[\boldsymbol{R}_2+\boldsymbol{R}_3-(\lambda+j)\mathbf{1}]\boldsymbol{C}_j-\boldsymbol{C}'_j\}+2p(\boldsymbol{R}_1-\boldsymbol{R}_4)\boldsymbol{C}_{j-1}$$
$$+[-(\boldsymbol{R}_1+\boldsymbol{R}_2+\boldsymbol{R}_3+\boldsymbol{R}_4)+(\lambda+j-2)\mathbf{1}]\boldsymbol{C}_{j-2}+\boldsymbol{C}'_{j-2}=0 \tag{38}$$

for $j = 0, 1, 2, \ldots$, with $\boldsymbol{C}_{-1}=\boldsymbol{C}_{-2}=\boldsymbol{C}'_{-1}=\boldsymbol{C}'_{-2}=0$, where the prime means differentiation with respect to t.

First, we try to find solutions of the same kind as before, that is, we put $\boldsymbol{C}'_j = 0$ for $j \geqslant 0$. From the characteristic equation for λ and $\boldsymbol{C}_0$,

$$(\boldsymbol{R}_2+\boldsymbol{R}_3-\lambda\mathbf{1})\boldsymbol{C}_0=0 \tag{39}$$

we find $\lambda_{1,2}=0$ and $\lambda_{3,4}=n$.

It is readily seen that for $\lambda_{3,4}=n$ solutions of the desired kind are obtained with, for instance,

$$C_{3,0}=\begin{pmatrix}0\\1\\0\\0\end{pmatrix}\qquad C_{4,0}=\begin{pmatrix}0\\0\\1\\0\end{pmatrix}. \tag{40}$$

The recursion relation with $\boldsymbol{C}'_j=0$ and $\lambda_{1,2}=0$ breaks down for $j=n$ if $n>0$. For $n=0$ no further linear independent column vectors, besides those given by (40), can be constructed.

Therefore, we have to consider the case $\boldsymbol{C}'_j \neq 0$ and have to distinguish between $n>0$ and $n=0$.

For $n>0$ we proceed as follows. We put $(\eta_i=\eta_f=\eta)$

$$C_{1,0}=\begin{pmatrix}1\\(\gamma_i+\mathrm{i}\eta)/n\\(\gamma_f+\mathrm{i}\eta)/n\\0\end{pmatrix}\qquad C_{2,0}=\begin{pmatrix}0\\(\gamma_f-\mathrm{i}\eta)/n\\(\gamma_i-\mathrm{i}\eta)/n\\1\end{pmatrix}\tag{41}$$

which both solve (39) for $\lambda=0$, and we use (38) with $C'_{k,j}=0$ $(k=1,2)$ up to $j=n-1$. We set

$$C_{k,j}=a_{k,j}t+b_{k,j}\tag{42}$$

for $j\geqslant n$ and have from (38)

$$(R_2+R_3-n\mathbf{1})(a_{k,n}t+b_{k,n})-a_{k,n}=d_k\tag{43}$$

where d_k is a known column vector dependent on the choice of $C_{k,0}$.

A solution of (43) is provided by the vector

$$C_{k,n}(t)=\begin{pmatrix}-d_{k,1}/n\\ [-d_{k,2}+(\gamma_i+\mathrm{i}\eta)d_{k,1}/n+(\gamma_f-\mathrm{i}\eta)d_{k,4}/n]t\\ [-d_{k,3}+(\gamma_f+\mathrm{i}\eta)d_{k,1}/n+(\gamma_i-\mathrm{i}\eta)d_{k,4}/n]t\\ -d_{k,4}/n\end{pmatrix}.\tag{44}$$

For $j>n$ the formula (38) provides no further problems.

For $n=0$ we start with

$$(R_2+R_3)C_0-C'_0=0\tag{45}$$

for which we find the two independent solutions

$$C_{1,0}=\begin{pmatrix}1\\-(\gamma_i+\mathrm{i}\eta)t\\-(\gamma_f+\mathrm{i}\eta)t\\0\end{pmatrix}\qquad C_{2,0}=\begin{pmatrix}0\\-(\gamma_f-\mathrm{i}\eta)t\\-(\gamma_i-\mathrm{i}\eta)t\\1\end{pmatrix}.\tag{46}$$

The higher coefficients are determined from (38) with (42). In the latter case we have two solutions with a logarithmic singularity at $q=2p$.

Two remarks may be added. Firstly, the degenerate case $p_i=p_f$ for $E_i=-E_f$ leads to $\eta_i=-\eta_f$ and, therefore, the pole $q=4p$ has to be treated separately (see (36*a*)). This can be done in the manner outlined above.

Secondly, functions of the type z^λ for non-integer or complex λ as well as $\ln z$ are multiple valued in the complex plane, even on the negative real axis. Thus, in using the expansions in the vicinity of a pole q_k and going from $q>q_k$ to $q<q_k$ it is necessary to fix the phase. We have the two possibilities $q-q_k=|q-q_k|\,\mathrm{e}^{\pm\mathrm{i}\pi}$ for $q<q_k$. The decision is made by (24), from which it follows that we must use $\mathrm{e}^{\mathrm{i}\pi}$ for q_2, q_3, q_4, and $\mathrm{e}^{-\mathrm{i}\pi}$ for q_1.

4. Numerical procedure for the calculation of the Appell functions

Since the four Appell functions F_2 defined in (15) solve the equations (23), they are expressible by the systems of fundamental solutions obtained in § 3. If we distinguish the independent solutions within the fundamental system by a superscript and use a subscript i to indicate the pole $q_i : \boldsymbol{F}_i^{(k)}$, then we have

$$\boldsymbol{F}_2 = \sum_{k=1}^{4} B_k^{(i)} \boldsymbol{F}_i^{(k)} \qquad \text{with } \boldsymbol{F}_i^{(k)} = (q - q_i)^{\lambda_k^{(i)}} \sum_{j=0}^{\infty} (q - q_i)^j \boldsymbol{C}_{k,j}^{(i)}. \tag{47}$$

$\boldsymbol{F}_i^{(k)}$ and $B_k^{(i)}$ are different for each pole q_i. We have $q - q_i = s - s_i$ with $s_i = q_i - p_i - p_f$.

A practicable procedure for calculating $\boldsymbol{F}_2$ for all s values arising in a numerical integration of the form factors (1) over s could be the use of the most appropriate expansion in the regions 2, 3, 4 and 5 of figure 1. Note that the regions 1 and 6 are not needed in the physical application. The determination of the coefficients $B_k^{(i)}$ is easily accomplished since the convergence domains overlap. Thus, beginning with the double sum (18) in the intersection of region 4 with 5 we obtain $B_k^{(4)}$. The continuation of $\boldsymbol{F}_2$ with (47) for $i = 4$ allows the determination of $B_k^{(3)}$, and so on.

Because of the many s values needed for an accurate evaluation of the scattering matrix elements, in practice it is faster to use the series only well within the convergence domains and to bridge the gaps by a fast numerical integration program for the coupled linear differential equations (23).

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