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On the asymptotic behaviour of the solutions of the two inhomogeneous differential equations occurring in the theory of the relativistic Stark effect

M. L. BARTLETT
Department of Physics, University College London
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Abstract. Evaluation of the coefficients up to the second order is made in the asymptotic expansion of the generalized hypergeometric function which arises in the problem of solving the Dirac equation for the electron of a hydrogen atom in an external electric field. The method used is a calculation of the residues in the Barnes integral for the function, and in doing this calculation a derivation of the coefficients is given, so showing how the method can be used for ${}_pF_p$ generalized hypergeometric functions in general.

1. Introduction

A calculation of the static polarizability, or equivalently the Stark energy shifts, of a ground-state hydrogen atom in an external constant and uniform electric field can be performed by Dalgarno's method (Dalgarno 1963). That is, α is required, where

$$\alpha = e^2 \sum_{n\neq 0}{}' \frac{\langle 0|z|n\rangle\langle n|z|0\rangle}{E_n - E_0}.$$

Because questions of convergence are central to the relativistic calculation, the method is here outlined to show how these arise if the above expression is used as the starting point.

If we define $|\chi\rangle$ as a solution of

$$(H-E_0)|\chi\rangle = z|0\rangle \tag{1}$$

where the H, $|n\rangle$ and E_n are the Dirac Hamiltonian, states and energies of the electron in the hydrogen atom, then it follows that

$$\sum_{n\neq 0}{}' \frac{\langle 0|z|n\rangle\langle n|z|0\rangle}{E_n - E_0} = \sum_{n\neq 0}{}' \frac{\langle 0|z|n\rangle\langle n|H-E_0|\chi\rangle}{E_n - E_0}$$

$$= \sum_{n\neq 0}{}' \langle 0|z|n\rangle\langle n|\chi\rangle = \langle 0|z|\chi\rangle$$

and so

$$\alpha = e^2\langle 0|z|\chi\rangle.$$

Alternatively, if we identify the α from the second-order Stark energy shift, the state $|\chi\rangle$ is the first-order correction to the ground-state wave function in a perturbation expansion in the perturbing electric field, and the same conditions on $|\chi\rangle$ are required as the above leads to. That is, $|\chi\rangle$ must be in the Hilbert space for the operator H. It is further required that the $|\chi\rangle$ gives in the non-relativistic limit the non-relativistic polarizability.

A reduction and separation of the equation (1) (Bartlett 1968) is fairly complex. If $|\chi\rangle$ is written

$$|\chi\rangle = Gq_+ + Fq_- + \bar{G}\bar{q}_+ + \bar{F}\bar{q}_-$$

where $q_\pm$ and $\bar{q}_\pm$ are spherical spinors, and $\bar{q}_\pm$ has angular momentum $j = \frac{1}{2}$, and $q_\pm$ has $j = \frac{3}{2}$, then the 'barred' part of the solution is relatively simple, and there are no convergence problems. The other parts of the solutions have a different character, if F and G

are written

$$F = \frac{1}{(m\alpha)^{1/2}} \frac{2^{\tau-\frac{3}{2}}\gamma}{(1+\gamma)^{1/2}\{\Gamma(1+2\gamma)\}^{1/2}3} x^{\tau-1} e^{-x}\left(\Psi - \frac{2-\gamma}{\gamma}\Phi\right)$$

$$G = -\frac{1}{(m\alpha)^{1/2}} \frac{\gamma}{\alpha}\left\{\frac{1+\gamma}{\Gamma(2\gamma+1)}\right\}^{1/2} \frac{2^{\tau-\frac{3}{2}}}{3} x^{\tau-1} e^{-x}\left(\Psi + \frac{2-\gamma}{\gamma}\Phi\right)$$

so defining Ψ and Φ. Then these Ψ and Φ satisfy the equations

$$x\frac{d^2\Phi}{dx^2} + (1+2\tau-x)\frac{d\Phi}{dx} - (\tau+1-\gamma)\Phi = x^{\gamma+1-\tau} \tag{2}$$

$$x\frac{d^2\Psi}{dx^2} + (1+2\tau-x)\frac{d\Psi}{dx} - (\tau-\gamma)\Psi = x^{\gamma+2-\tau} - \left\{2(1+\gamma) - \frac{3}{\gamma}\right\} x^{\gamma+1-\tau} \tag{3}$$

where $\gamma = (1-\alpha^2)^{1/2}$, $\tau = (4-\alpha^2)^{1/2}$; here α is the fine structure constant.

On solving these equations by the series method, the generalized hypergeometric function ${}_2F_2(x)$ is obtained for the particular integral, and the confluent hypergeometric function ${}_1F_1(x)$ for one of the complementary functions; these are given in § 5. To form the required combination of these functions in the physical problem above, the asymptotic behaviour at large x of these functions is required. However, only that for the confluent hypergeometric function is at present tabulated.

In this paper a procedure is developed to extract explicitly the lower-order coefficients in the asymptotic expansion of generalized hypergeometric functions of the form ${}_nF_n(x)$ with real x. It is based on Barnes's methods (Barnes 1907), but for these restricted functions required in the polarizability calculations the derivation is given as completely as is necessary to extract the coefficients.

The general procedure is as follows: a function $S(s)$ is defined such that the contour integral

$$\int_{\kappa+\nu+\lambda} S(s)x^s \, ds = K_pF_p(x)$$

with K a known constant. The function $S(s)$ has two series of poles, and the contour $\kappa+\nu+\lambda$, defined and illustrated in § 3, can be split into distinct parts κ, ν, λ. The total contour enclosing one series of poles yields the hypergeometric function, one of the parts containing the second series of poles giving the asymptotic series. The function $S(s)$ is defined as the analytic continuation of a function $T(s)$, which is a sum of terms $T_t(s)$, each a product of gamma functions. The asymptotic equalities of the gamma function are known, and via these the properties and poles of $S(s)$ are deduced; in particular, the residues at the poles give the expansion coefficients $f_r(s_r)$ in the asymptotic expansion.

For the particular functions involved as the solution to the radial equations ten coefficients—first- and second-order for five different functions—are evaluated.

2. The asymptotic behaviour of $T_t(s)$

The function $T_t(s)$ is defined by

$$T_t(s) = \frac{\Gamma(t-s)}{\Gamma(t+1)} \prod_{r=1}^{p} \frac{\Gamma(\alpha_r+t)}{\Gamma(\rho_r+t)}$$

for all s, with $\alpha_r\, \rho_r \neq 0, -1, -2, \ldots$, and $t = 0, 1, 2, \ldots$. An expansion asymptotic in the variable t is required for this function. To obtain this the asymptotic equality is needed for the gamma function, for which it is convenient to go back to Barnes's original papers on the gamma function (Barnes 1899). From there the equality is obtained:

$$\Gamma(z+\alpha) = (2\pi)^{1/2} e^{-z} z^{z+\alpha-\frac{1}{2}} \exp\left\{\sum_{r=1}^{n} \frac{(-1)^{r-1}}{r(r+1)} \frac{B_{r+1}(\alpha)+B_{r+1}}{z^r} + \frac{J_n(z,\alpha)}{z^n}\right\}$$

for $|\arg z| < \pi$, and n arbitrary, and where $B_r(x)$ and B_r are the Bernoulli polynomials and numbers respectively. $J_n(z, \alpha)$ is some function (note not Bessel) such that $|J_n(z, \alpha)| \to 0$ as $|z| \to \infty$. This is implied by later use of $J_n(z)$.

Applying this asymptotic equality to $T_t(s)$ now gives

$$T_t(s) = t^{\delta-s-1} \exp\left\{\sum_{r=1}^{n} \frac{a_r}{t^r} + \frac{J_n(t)}{t^n}\right\}$$

with

$$\delta = \sum_{m=1}^{p} \alpha_m - \sum_{m=1}^{p} \rho_m$$

and

$$a_r = \frac{(-1)^{r-1}}{r(r+1)} \sum_{m=1}^{p} \{B_{r+1}(\alpha_m) - B_{r+1}(\rho_m) + B_{r+1}(-s) - B_{r+1}(1)\}.$$

Now using the exponential expansion

$$\exp\left(\frac{a}{t^n}\right) = 1 + \frac{a}{t^n} + \frac{a^2}{2!t^{2n}} + \ldots$$

then

$$\begin{aligned}\exp\left\{\sum_{r=1}^{n} \frac{a_r}{t^r} + \frac{J_n(t)}{t^n}\right\} &= \left(1 + \frac{a_1}{t} + \frac{a_1^2}{2!t^2} + \frac{a_1^3}{3!t^3} + \ldots\right) \\ &\times \left(1 + \frac{a_2}{t^2} + \frac{a_2^2}{2!t^{2\times 2}} + \frac{a_2^3}{3!t^{3\times 2}} + \ldots\right) \\ &\vdots \\ &\times \left(1 + \frac{a_n}{t^n} + \frac{a_n^2}{2!t^{2n}} + \frac{a_n^3}{3!t^{3n}} + \ldots\right) \\ &\times \left(1 + \frac{J_n'}{t^n} + \frac{J_n'^2}{2!t^{2n}} + \frac{J_n'^3}{3!t^{3n}} + \ldots\right).\end{aligned}$$

Hence, by multiplying out and collecting the same powers of t,

$$T_t(s) = t^{\delta-1-s}\left\{\sum_{r=0}^{n} \frac{f_r(s)}{t^r} + \frac{J_n'(t, s)}{t^n}\right\}$$

where this new $J_n'(t, s)$ has absorbed the terms arising from powers of t greater than t^n, and, from the process of collecting like terms, $f_r(s)$ is given by

$$f_r(s) = \sum_{p,q,u,\ldots w} \frac{a_r^p a_{r-1}^q a_{r-2}^u \ldots a_1^w}{p!q!u!\ldots w!} \tag{4}$$

where the sum is over all combinations of the r numbers $p, q, u, \ldots w$ such that

$$rp + (r-1)q + (r-2)u + \ldots + w = r$$

and

$$0 \leqslant p, q, u, \ldots w \leqslant r.$$

This expansion for $T_t(s)$ is valid at all s, and defines $J_n'(t, s)$ at all s. Now, the only poles of $T_t(s)$ arise from $\Gamma(t-s)$ and are at $s = t, t+1, t+2, \ldots$. So $J_n'(t, s)$ has its only poles at $s = t, t+1, t+2, \ldots$.

3. The Barnes integral

A function $T(s)$ is now defined by

$$T(s) = \sum_{t=0}^{\infty} T_t(s).$$

From the above asymptotic expansion for $T_t(s)$, for large t

$$T_t(s) \sim t^{\delta-s-1}$$

so $T(s)$ can be defined by this series for $\mathrm{Re}(s-\delta) > 0$, and in this region $T(s)$ can be written

$$T(s) = T_0(s) + \sum_{r=0}^{n} \left\{ \sum_{t=1}^{\infty} \frac{f_r(s)}{t^{r+1-\delta+s}} \right\} + \sum_{t=1}^{\infty} \frac{J_n'(t,s)}{t^{n+1-\delta+s}}.$$

Now, a function $S(s)$ is defined at all s by

$$S(s) = T_0(s) + \sum_{r=0}^{n} f_r(s)\zeta(r+1-\delta+s) + \sum_{t=1}^{\infty} \frac{J_n'(t,s)}{t^{n+1-\delta+s}}. \tag{5}$$

Then for $\mathrm{Re}(s-\delta) > 0$, $T(s) = S(s)$, where $\zeta(z)$ is the Riemann zeta function. It can be seen directly that $S(s)$ has poles at $s = 0, 1, 2, \ldots$. Now, if we consider the regions outside these values of s, then $T_0(s)$ has no poles and neither has $J_n'(t, s)$. Further, $|J_n'(t, s)| \to 0$ as $t \to \infty$, so

$$\sum_{t=1}^{\infty} \left\{ \frac{J_n'(t,s)}{t^{n+1-\delta+s}} \right\}$$

has no poles for $\mathrm{Re}(n+s-\delta) > 0$. In this region $\zeta(r+1-\delta+s)$ has poles at $s = \delta-r$, $r = 0, 1, 2, \ldots n$. But n is arbitrary; therefore the only poles of $S(s)$ outside $s = 0, 1, 2, \ldots$ are the series of poles at $s = -r$, $r = 0, 1, 2, \ldots$.

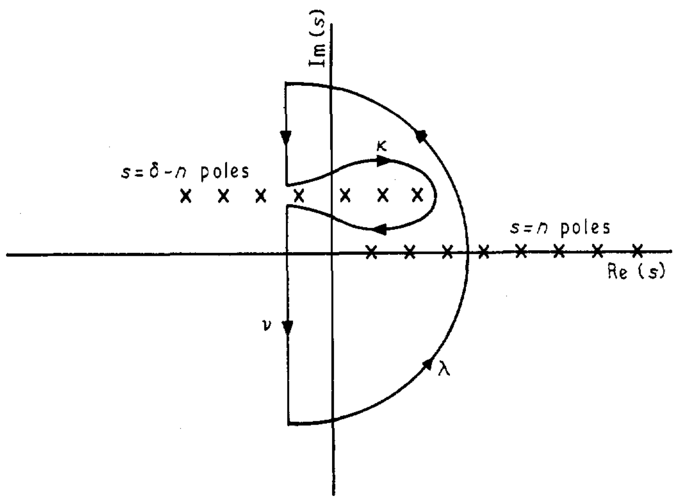

Figure 1.

These are shown in the diagram, where the contours ν, κ, λ are defined such that κ encloses $k+1$ of the $s = \delta-n$ poles, ν is parallel to the imaginary axis, and λ is an arc of a circle which does not pass through any of the $s = n$ poles and terminates on the ν contour.

The integrals $\Lambda_{\nu,\kappa,\lambda}(x)$ are now considered where $\Lambda_{\nu+\lambda+\kappa}(x) = \Lambda_\nu(x) + \Lambda_\lambda(x) + \Lambda_\kappa(x)$, and the $\Lambda_{\nu,\lambda,\kappa}(x)$ are defined by

$$\Lambda_{\kappa,\lambda,\nu}(x) = -\frac{1}{2\pi \mathrm{i}} \int_{\kappa,\lambda,\nu} S(s)x^s \,\mathrm{d}s.$$

If the limit is taken as the radius of the contour $\lambda \to \infty$, then $\Lambda_{\nu+\lambda+\kappa}(x)$ encloses all the $s = n$ poles and

$$\Lambda_{\nu+\lambda+\kappa}(x) = \sum_{n=0}^{\infty}\sum_{t=0}^{\infty}\prod_{r=1}^{p}\frac{\Gamma(\alpha_r+n)}{\Gamma(\rho_r+n)}\frac{x^{n+t}}{\Gamma(n+1)}\frac{(-1)^t}{\Gamma(t+1)}$$
$$= \Gamma\begin{pmatrix}(\alpha)\\(\rho)\end{pmatrix} e^{-x}{}_pF_p\begin{pmatrix}(\alpha)\\(\rho)\end{pmatrix}x\Big)$$

where

$$\Gamma\begin{pmatrix}(\alpha)\\(\rho)\end{pmatrix} = \prod_{r=1}^{p}\frac{\Gamma(\alpha_r)}{\Gamma(\rho_r)}.$$

If $\mathrm{Re}(\delta) < 0$, then, as is done above, the definition of $T(s)$ can be used to calculate the residues from the residues of the gamma function, as then in the region of these poles $T(s) = S(s)$. If $\mathrm{Re}(s) > 0$, then the residues at the poles which are excluded from this region can be calculated via the residues of $J_n'(t, s)$, and the result is the same.

Now, let us consider the separate parts of the integrals: first $\Lambda_\kappa(x)$. The residues at the poles enclosed by this integral are obtained from (5), it being noted that the residue of $\zeta(z)$ at $z = 1$ is 1. So

$$\Lambda_\kappa(x) = -\Lambda_{-\kappa}(x) = -x^\delta\left\{1+\sum_{r=1}^{k}\frac{f_r(s_r)}{x^r}\right\}$$

where $s_r = \delta - r$. For $\Lambda_\nu(x)$ we have

$$\Lambda_\nu(x) = -\frac{x^u}{2\pi i}\int_\nu S(s)x^{iv}\,dv$$

where $s = u+iv$, and so $u = \mathrm{Re}(\delta-\theta-k)$ with $0 < \theta < 1$. That is,

$$\Lambda_\nu(x) = J_k(x)x^{\delta-k}$$

where $|J_k(x)| \to 0$ as $x \to \infty$. And for $\Lambda_\lambda(x)$, from the asymptotic forms of the $\Gamma(z)$ and $\zeta(z)$ functions, then in the limit as the radius of the arc $\to \infty$

$$\Lambda_\lambda(x) = 0.$$

Adding all these contributions now gives the formula

$${}_pF_p\begin{pmatrix}(\alpha)\\(\rho)\end{pmatrix}x\Big) = \Gamma\begin{pmatrix}(\rho)\\(\alpha)\end{pmatrix} e^x x^\delta\left\{1+\sum_{r=1}^{k}\frac{f_r(s_r)}{x^r}+\frac{J_k(x)}{x^k}\right\} \tag{6}$$

where k is arbitrary.

4. The coefficients $f_r(s_r)$

The coefficients $f_r(s_r)$ are now examined more closely. The procedure is checked against the confluent hypergeometric coefficients, for these are found tabulated (Erdelyi *et al.* 1953). The rth coefficient is given by $f_r(s_r)$, where $s_r = \delta - r$ and $f_r(s)$ is given by (4); so, using the method of § 2,

$$f_0(s_0) = a_0{}^0 = 1$$
$$f_1(s_1) = a_1{}^1 = a_1$$
$$f_2(s_2) = \frac{a_2{}^1a_1{}^0}{1}+\frac{a_2{}^0a_1{}^2}{2} = a_2+\frac{a_1{}^2}{2}$$
$$a_r = \frac{(-1)^{r-1}}{r(r+1)}\{B_{r+1}(\alpha)-B_{r+1}(\rho)+B_{r+1}(-s_2)-B_{r+1}(1)\}.$$

So, if we note that

$$B_2(x) = x^2-x+\tfrac{1}{6}$$

and

$$B_3(x) = x^3 - \tfrac{3}{2}x^2 + \tfrac{1}{2}x$$

then, in particular, for the confluent hypergeometric function ${}_1F_1(\alpha, \rho, x)$, where now $p = 1$,

$$f_1(s_1) = (\rho-\alpha)(1-\alpha)$$

and

$$f_2(s_2) = \tfrac{1}{2}(1-\alpha)(2-\alpha)(\rho-\alpha)(\rho-\alpha+1).$$

These agree with the tabulated formulae.

Now, taking the

$${}_2F_2\begin{pmatrix}\alpha_1, & \alpha_2; & \\ \rho_1, & \rho_2; & x\end{pmatrix}$$

function, then by a similar process

$$f_1(s_1) = (\alpha_1{}^2+\alpha_2{}^2+\alpha_1\alpha_2+\rho_1\rho_2-\alpha_1\rho_1-\alpha_1\rho_2-\alpha_2\rho_1-\alpha_2\rho_2+\rho_1+\rho_2-\alpha_1-\alpha_2)$$

is obtained.

When we attempt to obtain a general formula for the $f_2(s_2)$ coefficient it soon becomes apparent that the algebra is formidable, but also that in particular functions with simple parameters, or simple relations between them, it is quick to use the formulae as given and calculate directly from these; and so collecting these formulae gives

$$f_2(s_2) = a_2 + \tfrac{1}{2}a_1{}^2$$

$$a_1 = \tfrac{1}{2}\sum_{n=1}^{2}\{B_2(\alpha_n) - B_2(\rho_n) + B_2(-s_2) - \tfrac{1}{6}\}$$

$$a_2 = -\tfrac{1}{6}\sum_{n=1}^{2}\{B_3(\alpha_n) - B_3(\rho_n) + B_3(-s_2)\}$$

$$s_2 = \alpha_1+\alpha_2-\rho_1-\rho_2-2.$$

5. Evaluation of the coefficients from the solutions Ψ, Φ

The asymptotic behaviour is required of the functions which form solutions to the equations

$$x\frac{d^2\Phi}{dx^2} + (1+2\tau-x)\frac{d\Phi}{dx} - (\tau+1-\gamma)\Phi = x^{\gamma+1-\tau} \tag{2}$$

$$x\frac{d^2\Psi}{dx^2} + (1+2\tau-x)\frac{d\Psi}{dx} - (\tau-\gamma)\Psi = x^{\gamma+2-\tau} - \left\{2(1+\gamma) - \frac{3}{\gamma}\right\}x^{\gamma+1-\tau}. \tag{3}$$

Solving the equation (2) by the series method gives the particular integral

$$\frac{x^{\gamma-\tau+2}}{(\gamma-\tau+2)(\gamma+\tau+2)}\,{}_2F_2\begin{pmatrix}1, & 3; & \\ \gamma-\tau+3, & \gamma+\tau+3; & x\end{pmatrix}.$$

The corresponding homogeneous equation is the confluent hypergeometric equation, and so the required complementary function is

$${}_1F_1(\tau-\gamma+1, 1+2\tau, x).$$

Similarly, the equation (3) has as a particular integral

$$\frac{x^{\gamma-\tau+3}}{(\gamma-\tau+3)(\gamma+\tau+3)}\,{}_2F_2\begin{pmatrix}1, & 3; & \\ \gamma-\tau+4, & \gamma+\tau+4; & x\end{pmatrix} - \left\{2(1+\gamma) - \frac{3}{\gamma}\right\}$$
$$\times\frac{x^{\gamma-\tau+2}}{(\gamma-\tau+2)(\gamma+\tau+2)}\,{}_2F_2\begin{pmatrix}1, & 2; & \\ \gamma-\tau+3, & \gamma+\tau+3; & x\end{pmatrix}$$

and the required complementary function

$$ {}_1F_1(\tau-\gamma,\, 1+2\tau,\, x). $$

For the five hypergeometric functions in these solutions the first- and second-order coefficients $f_1(s_1)$ and $f_2(s_2)$ as defined in (6) are evaluated by the method of § 4 and tabulated below.

Function	$f_1(s_1)$	$f_2(s_2)$
${}_1F_1(\tau-\gamma+1,\, 1+2\tau,\, x)$	-3	$3-3\gamma$
${}_1F_1(\tau-\gamma,\, 1+2\tau,\, x)$	$2\gamma-2$	$4\gamma^2-3\gamma-1$
${}_2F_2\left(\begin{matrix}1, & 3; & \\ \gamma-\tau+3, & \gamma+\tau+3; & \end{matrix}\, x\right)$	-3	$3-3\gamma$
${}_2F_2\left(\begin{matrix}1, & 3; & \\ \gamma-\tau+4, & \gamma+\tau+4; & \end{matrix}\, x\right)$	$2\gamma-2$	$4\gamma^2-3\gamma-1$
${}_2F_2\left(\begin{matrix}1, & 2; & \\ \gamma-\tau+3, & \gamma+\tau+3; & \end{matrix}\, x\right)$	$2\gamma-2$	$4\gamma^2-3\gamma-1$

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