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Asymptotic expansions for parabolic cylinder functions of large order and argument

D S F CROTHERS

Department of Applied Mathematics and Theoretical Physics, The Queen's University of Belfast, Belfast BT7 1NN, UK

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Abstract. Using the method of steepest descent, an exact and practicable asymptotic expansion for the parabolic cylinder function $D_p(z)$ is derived in the case when $|z|^2$ and $|p|$ are both large and of the same order. Limitations and defects in the existing literature on the subject are reviewed. Two-term approximations of considerable importance in the phase-integral analysis of four-transition-point problems are obtained. Several examples required in the analysis of double underdense-potential-barrier problems are given, including reliable estimates for $D_{-1-i\gamma}(2\,e^{\frac{1}{4}\pi i}\,T_0\sqrt{\gamma})$ and $D_{i\gamma}(2\,e^{\frac{1}{4}\pi i}\,T_0\sqrt{\gamma})$ in terms of simple trigonometric and logarithmic functions, under the conditions $T_0 > 0$ and $\gamma \gtrsim 1$. It is pointed out that such potential barrier problems are associated with perturbed symmetric resonance, strong rotational coupling and curve-crossing in atom–atom collision theory. New model transition probabilities are presented.

1. Introduction

Quantal differential cross sections for atom–atom collisions often exhibit strong Stueckelberg oscillations (cf Smith *et al* 1970), due to the nonadiabatic effects associated with the double passage through a pseudocrossing of the principal potential energy curves. Similar effects are also associated with the occurrence of perturbed symmetric resonance or indeed strong rotational coupling. The results of Stueckelberg (1932), which were derived by application of Zwaan–Stueckelberg phase-integral techniques to the four-transition-point underdense-potential-barrier problem, are known to be incorrect in the limit of symmetric resonance (Bates 1962). An alternative technique, the details of which will be presented in another paper, involves the use of comparison equations. The principal results, one of which gives the correct symmetric resonance limit, have already been reported (Crothers 1971) and depend critically on the appropriate asymptotic expansions of the parabolic cylinder function $D_p(z)$. Unfortunately the expansions in the standard encyclopaedia (cf Magnus *et al* 1966 and Miller 1965) are generally, though not exclusively, restricted to $|z| \gg \max(1, |p|)$. The purpose of and motivation for this paper is to obtain expansions for complex p and z, where $|z|^2$ and $|p|$ are both large and of the same order of magnitude. Having reviewed the existing literature, we shall use the method of steepest descent and thus generalize the work of Plancherel and Rotach (1929) on the Hermite polynomials.

2. Review of literature

As already indicated, the existing literature on the asymptotic expansions of $D_p(z)$, for complex p and z with $|z|^2$ and $|p|$ both large and of the same order, has its limitations and is at best confusing. Perhaps the least confusing is the work of Olver (1959). Kazarinoff (1961) has described Olver's work as being the definitive one on the asymptotic behaviour of Weber parabolic cylinder functions of large order, being based on a minimal set of complete uniform asymptotic expansions. This may be disputed. Olver first expresses each $D_p(z)$ as a linear combination of two contiguous functions. He then calculates the dominant contributions to each using the well known Langer method (1932, 1935). In principle this procedure is suspect because the individual subdominant contributions are ignored. Although in many cases the procedure may be shown *a posteriori* to give correct results, there are nevertheless many cases where it does not. Particularly confusing are erroneously predicted signs of the overall subdominant contribution: ambiguity in signs should of course only occur precisely on a Stokes line in the presence of a dominant contribution, as a result of the Stokes phenomenon (Dingle 1957, 1958). Indeed Olver himself admits that when the required result is totally subdominant, his procedure leads to a nugatory, that is worthless, result. Again, particularly crucial to the theory of avoided adiabatic or pseudocrossings in atom–atom collisions is the case $\arg(z) = \pm\frac{3}{4}\pi$ which Olver's formulae can not and do not cover.

Although Buchholz (1969) considers the closely related $M_{\mathscr{H},\mu/2}(z)$ using the saddle point method, the analysis is limited to real values of $z/\mathscr{H}$. Buchholz also points out that the asymptotic forms, given by Taylor (1939), are *only an order of magnitude approximation*. Taylor's results are indeed unsatisfactory, as may be gleaned from his reliance on *ad hoc* arguments: for instance, on his page 43 his C_2 coefficient is set equal to zero in order to avoid, *a posteriori*, absurd results. In any case Taylor fails to realize, indeed compounds, the ambiguities in the results of Schwid (1935) and so never obtains an accurate subdominant term, basically because like Olver he uses Langer's approach. Taylor's errors are themselves compounded in the Bateman Manuscript Project (1954a), in which it is stated in chapter 6 on page 281 that Taylor introduces the auxiliary variable

$$\xi = \mathrm{i}\left\{\tfrac{1}{2}x^{1/2}(x-4K)^{1/2} - K\ln\left(\frac{\{x^{1/2}+(x-4K)^{1/2}\}^2}{4K}\right)\right\}$$

where the arguments of x, K and $(x-4K)$ are all zero when these quantities are positive. This is ambiguous, since if $x = z^2$ as is required for the analytic function $D_p(z)$, then $x \in R^+$, no matter whether $\arg(z) = 2n\pi$ or $(2n+1)\pi$. As already mentioned a precursor of Taylor's work was that of Schwid (1935), who gave some consideration to $D_p(z)$, though using a definition inconsistent with modern usage. On his page 351, Schwid presents his principal results in theorem I and table II. This table contains entirely ambiguous phases, which on principle cannot be resolved within his treatment; for instance, to get the correct result for certain $D_p(z)$ with $\arg(z) = \frac{1}{4}\pi$, then in the final row of the table (-1) must be taken as $e^{3\pi i}$, $e^{\pi i}$, $e^{3\pi i}$, and $e^{-\pi i}$ in the first, second, third and fourth columns respectively. Clearly then, the Bateman Manuscript Project (1954b), in its chapter 8 on parabolic cylinder functions, is incorrect in § 8.4, where it is claimed that the behaviour of $D_p(z)$, as $|p| \to +\infty$ and for arbitrary values of z which satisfy $|z| < |p|^{1/2}$, has been *completely* discussed by Schwid.

In the introduction we referred to Magnus *et al* (1966). In fact they merely refer to Schwid and to Miller (1965), who in turn merely refers to Darwin (1949), whose work gives only the *dominant* term for $D_{-\frac{1}{2}-ia}(x\,e^{-\frac{1}{4}\pi i})$ for $x^2-4a \gg 0$. Jorna (1964a, b) has also derived some rather unwieldy results for $W_{k,m}(z)$, from which Green-type expansions for parabolic cylinder functions may be deduced, which are essentially equivalent to those derived by Olver and Darwin.

In any case, apart from the above defects and limitations, there is the question of elegance and efficiency. A glance at the papers of Langer, Schwid, Taylor and Olver reveals somewhat involved procedures. By contrast, the method, which we shall present below, although well known in principle, resolves the detailed analytical difficulties in a simple topological manner and at the same time takes care of the algebraic detail in an exact and natural combinatorial manner. Most important of all, the method resolves all phases without ambiguity.

3. Exact asymptotic expansions for $D_p(z)$

We may take as our definition for the parabolic cylinder function:

$$D_p(z) \equiv \frac{\Gamma(1+p)}{2\pi i}\, e^{-\frac{1}{4}z^2} \int e^{zs-\frac{1}{2}s^2}\, s^{-1-p}\, ds. \tag{1}$$

We assume p is not an integer. The principal branch of s^{-p} is assumed and the contour is indicated in figure 1. Evidently $D_p(z)$ has no singularities in the finite complex z

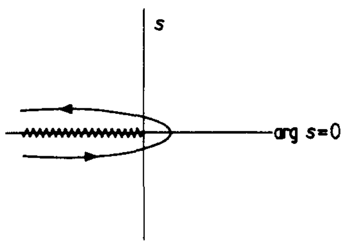

Figure 1. Contour and branch for the chosen representation of $D_p(z)$, given in equation (1).

plane, but has an essential singularity at ∞. It is easily verified by expanding $\exp(zs)$ that:

$$D_p(z) = 2^{p/2}\, e^{-\frac{1}{4}z^2}\left\{\frac{\sqrt{\pi}}{\Gamma((1-p)/2)}\,{}_1F_1\left(\frac{-p}{2};\frac{1}{2};\frac{z^2}{2}\right) - \frac{\sqrt{(2\pi)}z}{\Gamma(-p/2)}\,{}_1F_1\left(\frac{1-p}{2};\frac{3}{2};\frac{z^2}{2}\right)\right\} \tag{2}$$

so that $D_p(z)$ is closely related to the confluent hypergeometric function. Indeed in the limit as p becomes a positive integer $D_p(z)$ represents the familiar harmonic oscillator wavefunctions, the bracketed terms in (2) being then the Hermite polynomials.

Putting $t = e^{\pi i}zs$ and assuming $\arg(z) \in (-\frac{1}{2}\pi, +\frac{1}{2}\pi)$ we may rewrite (1) as

$$D_p(z) = \frac{-\Gamma(1+p)}{2\pi i}\, e^{-\frac{1}{4}z^2}\, z^p \int e^{-t-\frac{1}{2}(t^2/z^2)}\,(t\,e^{-i\pi})^{-1-p}\, dt \tag{3}$$

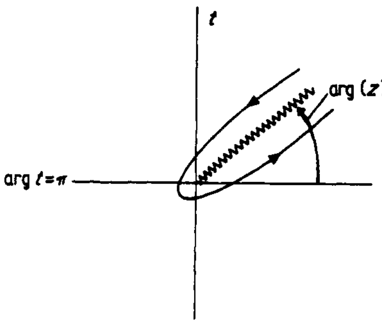

Figure 2. Contour and branch for the first transformed representation of $D_p(z)$, given in equation (3).

where the contour and the branch of t^{-p} are indicated in figure 2. Expanding $\exp(-\frac{1}{2}t^2/z^2)$ we obtain the usual asymptotic expansion

$$D_p(z) \simeq e^{-\frac{1}{4}z^2} z^p {}_2F_0\left(\frac{-p}{2}, \frac{1-p}{2};; \frac{-2}{z^2}\right) \tag{4}$$

the first term of which is a good approximation if $|z| \gg \max(1, |p|)$. Use of *exact* recurrence relations (cf Magnus *et al* 1966) yields the complete set of expansions covering all $\arg(z)$ and exhibiting the Stokes phenomenon. One consequence is that (4) is a good approximation within the extended region $|\arg(z)| < \frac{3}{4}\pi$, provided $\arg(z)$ is not too close to either of the anti-Stokes lines: $\arg(z) = \pm\frac{3}{4}\pi$. It may be noted that in obtaining (4), we have merely integrated term-by-term using Hankel's result for the reciprocal of the gamma function, that is by condensing the contour on to the upper and lower lips of the cut.

If $|z|$ is not very much greater than $|p|$, then expression (4) is poorly determined. Instead we put $v = z^{-1}s$ with $\arg(z) \in (-\pi, +\pi)$ so that

$$D_p(z) = \frac{\Gamma(1+p)}{2\pi i} e^{-\frac{1}{4}z^2} z \int \exp\{z^2(v - \tfrac{1}{2}v^2) - (1+p)\ln(zv)\}\, dv \tag{5}$$

where the contour and the branch of $\ln(v)$ are indicated in figure 3. We assume $|z|^2$ and $|p|$ are both large, so that the method of steepest descent may be applied. The two distinct

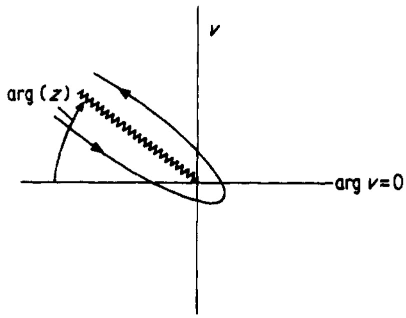

Figure 3. Contour and branch for the second transformed representation of $D_p(z)$, given in equation (5).

saddle points v_0, v_1 are given by

$$2zv_{\substack{0\\1}} = z \pm \{z^2 - 4(1+p)\}^{1/2} \tag{6}$$

provided $z^2 \neq 4(1+p)$ and where the square root branch is chosen so that

$$\arg(zv_j) \in (-\pi, +\pi).$$

The result is that

$$D_p(z) \simeq \frac{\Gamma(1+p)}{\mathrm{i}\sqrt{(2\pi)}} \mathrm{e}^{-\frac{1}{4}z^2} z \sum_{j=0}^{1} \frac{\exp(\mathrm{i}\alpha_j + f(v_j))}{|f''(v_j)|^{1/2}}$$
$$\times \left\{1 + \sum_{l=2}^{\infty} \frac{(2l-1)!!\exp(2\mathrm{i}l\alpha_j)}{v_j^{2l}|f''(v_j)|^l} \sum_{\{\lambda_n\}} \prod_{n=3}^{2l} \left(\frac{\{(1+p)/n\}^{\lambda_n}}{\lambda_n!}\right)\right\} \tag{7}$$

where

$$f(v) \equiv z^2(v - \tfrac{1}{2}v^2) - (1+p)\ln(zv) \tag{8}$$

$$\alpha_j = \tfrac{1}{2}\pi - \tfrac{1}{2}\arg f''(v_j) \tag{9}$$

and where the innermost sum is over all distinct partitions of $2l$ given by non-negative integer solutions $\{\lambda_n\}$ such that

$$\sum_{n=3}^{2l} n\lambda_n = 2l. \tag{10}$$

The partitions for $2 \leqslant l \leqslant 6$ are given in the Appendix. The phases α_0, α_1 which give the directions of the lines of steepest descent are formally ambiguous by an additive factor of π and must be determined absolutely by reference to the prevailing global geometry. Very often a good approximation is to neglect the sum over l in (7). Then a convenient way of writing the result is

$$D_p(z) \approx \frac{-\mathrm{i}\exp\{(p+\frac{1}{2})\ln(p+1) - \frac{1}{2}(p+1) + \mathrm{i}\arg(z)\}}{\sqrt{2}|z^2 - 4(1+p)|^{1/4}}$$
$$\times \sum |z + \{z^2 - 4(1+p)\}^{1/2}|^{1/2} \exp[\mathrm{i}\alpha + \tfrac{1}{4}z\{z^2 - 4(1+p)\}^{1/2}]$$
$$\times \exp\left\{-(1+p)\ln\left(\frac{z + \{z^2 - 4(1+p)\}^{1/2}}{2}\right)\right\} \tag{11}$$

where

$$\alpha = \frac{\pi}{2} - \frac{1}{2}\arg\left(\frac{-z^2\{z^2 - 4(1+p)\}^{1/2}}{z + \{z^2 - 4(1+p)\}^{1/2}}\right) \tag{12}$$

where the sum in (11) is to be taken over the two sheets of $\{z^2 - 4(1+p)\}^{1/2}$ and where Stirling's formula has been applied to $\Gamma(1+p)$ so that the principal branches of both ln functions must be taken.

4. Particular two-term estimates

As an illustration we deduce unambiguously from (11) and (12) that

$$\sqrt{\gamma}D_{-1-\mathrm{i}\gamma}(2\,\mathrm{e}^{\frac{1}{4}\pi\mathrm{i}}\,T_0\sqrt{\gamma}) \approx \exp(\tfrac{1}{4}\pi\gamma + \mathrm{i}\gamma - \mathrm{i}\gamma\ln\gamma - \tfrac{1}{4}\pi\mathrm{i} - \mathrm{i}\theta)\sin g$$
$$- \exp(-\tfrac{3}{4}\pi\gamma - \tfrac{1}{4}\pi\mathrm{i} + \mathrm{i}\theta)\cos g \tag{13}$$

where

$$\theta = \frac{\gamma}{2} + \gamma \ln\left(\frac{\sqrt{(1+T_0^2)}+T_0}{\sqrt{\gamma}}\right) + \gamma T_0 \sqrt{(1+T_0^2)} \tag{14}$$

$$g = \tan^{-1}\{\sqrt{(1+T_0^2)} - T_0\}. \tag{15}$$

The prevailing geometry is shown in figure 4, in which both lines are extended to ∞ in both directions. Only principal values are taken in (13), (14) and (15). It may similarly

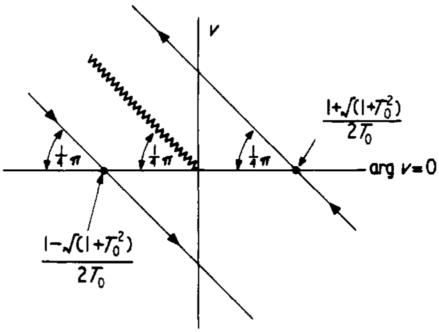

Figure 4. Contour of figure 3 specifically for $\arg(z) = \frac{1}{4}\pi$, but with contour deformed to facilitate evaluation by method of steepest descent. The indicated points are the saddle points specifically for the function $D_{-1-i\gamma}(2\,e^{\frac{1}{4}\pi i}\,T_0\sqrt{\gamma})$ of equation (13).

be shown that

$$D_{-i\gamma}(2\,e^{\frac{1}{4}\pi i}\,T_0\sqrt{\gamma}) \approx \exp(\tfrac{1}{4}\pi\gamma + i\gamma - i\gamma\ln\gamma - i\theta)\cos g + \exp(-\tfrac{3}{4}\pi\gamma + i\theta)\sin g. \tag{16}$$

Estimates (13) and (16) are valid for $T_0 > 0$ and of order unity, and $\gamma > 0$ and reasonably greater than unity. Their importance lies in the fact that they govern the theoretical description of perturbed symmetric resonance, and strong rotational coupling in atom–atom collisions. The corresponding results required for pseudocrossings are

$$D_{i\gamma}(2\,e^{\frac{1}{4}\pi i}\,T_0\sqrt{\gamma}) \approx \exp(\tfrac{1}{4}\pi\gamma - i\theta)\sin g + \exp(-\tfrac{3}{4}\pi\gamma + i\theta - i\gamma + i\gamma\ln\gamma)\cos g \tag{17}$$

and

$$\sqrt{\gamma}D_{-1+i\gamma}(2\,e^{\frac{1}{4}\pi i}\,T_0\sqrt{\gamma})$$

$$\approx \exp(\tfrac{1}{4}\pi\gamma - i\theta + \tfrac{1}{4}\pi i)\cos g - \exp(-\tfrac{3}{4}\pi\gamma + i\theta - i\gamma + i\gamma\ln\gamma + \tfrac{1}{4}\pi i)\sin g \tag{18}$$

which may be obtained from (11) and (12), as were (13) and (16). Other results are obtained from the above results simply by mapping the explicit i to $(-i)$, since, as may be seen from (2), $D_p(z)$ is a *real* function of two complex variables p and z.

In the impact parameter treatment of a two-state atom–atom collision the linear coefficients of the phase integrals may be subjected to a variation-of-parameters treatment to yield for instance the coupled equations (3) and (4) of Bates (1962). These equations may, in suitable form, be solved analytically using the method of steepest descent. The resulting comparison equations can then be solved exactly, yielding the new model transition probability

$$\mathscr{P} = \left(\frac{2\sqrt{\gamma}\,\mathrm{Re}[e^{-\frac{1}{4}\pi i}D_{-1-i\gamma}(2\,e^{\frac{1}{4}\pi i}\,T_0\sqrt{\gamma})\{D_{-i\gamma}(2\,e^{\frac{1}{4}\pi i}\,T_0\sqrt{\gamma})\}^*]}{\gamma|D_{-1-i\gamma}(2\,e^{\frac{1}{4}\pi i}\,T_0\sqrt{\gamma})|^2 + |D_{-i\gamma}(2\,e^{\frac{1}{4}\pi i}\,T_0\sqrt{\gamma})|^2}\right)^2 \tag{19}$$

$$\simeq \sin^2 x\,\mathrm{sech}^2\,y \tag{20}$$

where

$$x+\mathrm{i}y = \pm(\gamma-\gamma\ln\gamma-2\theta)+\mathrm{i}\pi\gamma \qquad (T_0 \gtrless 0) \tag{21}$$

$$= 4\gamma\int_{\pm|T_0|}^{\mathrm{i}} (1+T^2)^{1/2}\,\mathrm{d}T. \tag{22}$$

In the notation of Bates, the Stueckelberg variable T is $(\epsilon_p-\epsilon_q+V_{pp}-V_{qq})/2V_{pq}$, while the model parameters are given by

$$\left.\begin{aligned}\gamma &= \frac{1}{2v}V_{pq}\frac{\mathrm{d}Z}{\mathrm{d}T}\bigg|_{Z=\mathrm{Re}\,Z_c}\\ T_0 &= T|_{Z=0}\end{aligned}\right\} \tag{23}$$

where Z_c is the complex transition point also given by $T = \mathrm{i}$, the other three transition points being Z_c^*, $-Z_c^*$ and $-Z_c$. The general Zwaan–Stueckelberg interpretation of the model is that

$$x+\mathrm{i}y = \frac{1}{v}\int_0^{Z_c}\{4V_{pq}^2+(\epsilon_p-\epsilon_q+V_{pp}-V_{qq})^2\}^{1/2}\,\mathrm{d}Z \tag{24}$$

which in physical terms is a line integral representing the adiabatic action difference between the common turning point and the transition point. The significance and importance of the expansion (7) may be gauged by observing that in the case of perturbed symmetric resonance, the leading term in the weak-coupling expansion (4) yields a null transition probability $\mathscr{P}$, assuming that $T_0 \gtrsim \max(1/2\sqrt{\gamma}, \sqrt{\gamma}/2)$; moreover the higher-order terms possess no simple general physical interpretation.

For pseudocrossings T_0 is negative and the formula (20) differs from the usual Stueckelberg expression

$$\mathscr{P} \simeq 4\,\mathrm{e}^{-2y}(1-\mathrm{e}^{-2y})\sin^2 x. \tag{25}$$

For large y they are, however, asymptotically equivalent. For smaller y then, if we can nevertheless assume that $|T_0| \gtrsim \max(1/2\sqrt{\gamma}, \sqrt{\gamma}/2)$, expression (19) yields another new model transition probability

$$\mathscr{P} \simeq 4\,\mathrm{e}^{-2y}(1-\mathrm{e}^{-2y})\sin^2\left\{x+\frac{\pi}{4}+\frac{y}{\pi}\ln\left(\frac{y}{\pi\mathrm{e}}\right)-\arg\Gamma\left(1+\frac{\mathrm{i}y}{\pi}\right)\right\} \tag{26}$$

which has the advantage that it not only agrees with (20) and (25) as y becomes large, but also gives the correct weak-coupling result as y becomes small (Bates and Crothers 1970). The derivation of (26) is not straightforward and for instance requires use of the exact recurrence relation:

$$D_{\mathrm{i}\gamma}(\mathrm{e}^{\frac{1}{4}\pi\mathrm{i}}\,2T_0\sqrt{\gamma}) = \mathrm{e}^{-\pi\gamma}D_{\mathrm{i}\gamma}(\mathrm{e}^{-\frac{3}{4}\pi\mathrm{i}}\,2T_0\sqrt{\gamma})+\frac{\mathrm{i}\sqrt{(2\pi)}}{\Gamma(-\mathrm{i}\gamma)}\mathrm{e}^{-\frac{1}{2}\pi\gamma}D_{-1-\mathrm{i}\gamma}(\mathrm{e}^{\frac{3}{4}\pi\mathrm{i}}\,2T_0\sqrt{\gamma}). \tag{27}$$

Since the dominant term of $D_{-1-\mathrm{i}\gamma}$ in (27) is always the overall dominant contribution, whether for weak or strong coupling, we can improve the accuracy of its coefficient by retaining $\Gamma(-\mathrm{i}\gamma)$ explicitly. However, we must then neglect the individual subdominant contributions to both $D_{\mathrm{i}\gamma}$ and $D_{-1-\mathrm{i}\gamma}$ on the right hand side of (27), and in the manner of Olver, if we are to obtain the correct strong coupling limit. Thus we actually assume that

$$D_{\mathrm{i}\gamma}(\mathrm{e}^{\frac{1}{4}\pi\mathrm{i}}\,2T_0\sqrt{\gamma}) \simeq \frac{\Gamma(1+\mathrm{i}\gamma)}{\sqrt{(2\pi\gamma)}}\exp(-\tfrac{1}{4}\pi\gamma+\mathrm{i}\theta-\tfrac{1}{4}\pi\mathrm{i})\cos g+\exp(\tfrac{1}{4}\pi\gamma-\mathrm{i}\theta)\sin g \tag{28}$$

where for consistency we have also left the $\Gamma(1+p)$ of expression (7) unexpanded. It should be noted that expression (28) should not be taken too literally in so far as the inherent fundamental solutions change their algebraic character as strong coupling ($\gamma \gtrsim 1$) gives way to weak coupling ($\gamma < 1$). However, the procedure does yield a uniform analytic expression for the all important Stokes constant (Crothers 1971 and references therein).

Acknowledgments

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Appendix. Partitions required to evaluate (7)

$2l$	$\pi = 3^{\lambda_3}, 4^{\lambda_4}, 5^{\lambda_5}, \ldots, (2l)^{\lambda_{2l}}$
4	4
6	6
	3^2
8	8
	3, 5
	4^2
10	10
	3, 7
	4, 6
	5^2
	$3^2, 4$
12	12
	3, 9
	4, 8
	5, 7
	6^2
	4^3
	3^4
	$3^2, 6$
	3, 4, 5.

Notation is similar to that of table 24.2 given by Goldberg *et al* (1965).

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