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A method for the numerical evaluation of the oscillatory integrals associated with the cuspoid catastrophes: application to Pearcey's integral and its derivatives

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Abstract. A numerical method for the evaluation of the cuspoid canonical integrals and their derivatives is described. The method exploits Cauchy's theorem and Jordan's lemma to write the infinite integration path along different contours in the complex plane. The method is straightforward to implement on a computer and in many cases results of high accuracy can be obtained using standard quadrature techniques. Application is made to Pearcey's integral P(x, y) and its two partial derivatives and the method is shown to have some significant advantages over other techniques that have been applied to this problem. Tables of P(x, y), $\partial P(x, y)/\partial x$, $\partial P(x, y)/\partial y$ and the real zeros of P(x, y) are presented for the grid $-8.0 \le x \le 8.0$ and $0 \le y \le 8.0$.

1. Introduction

This paper is concerned with the numerical evaluation of the integral

$$C_n(a) = \int_{-\infty}^{\infty} \exp(if_n(a; u)) \, du \qquad a = (a_1, a_2, \dots, a_{n-2})$$
(1)

and its (n-2) partial derivatives

$$\partial C_n(\boldsymbol{a})/\partial a_1, \, \partial C_n(\boldsymbol{a})/\partial a_2, \, \dots, \, \partial C_n(\boldsymbol{a})/\partial a_{n-2}$$
 (2)

where $f_n(\boldsymbol{a}; \boldsymbol{u})$ is the polynomial

$$f_n(\boldsymbol{a}\,;\,\boldsymbol{u}) = \boldsymbol{u}^n + \sum_{k=1}^{n-2} a_k \boldsymbol{u}^k \tag{3}$$

with u and a_k real, and n is a positive integer restricted to $n \ge 3$. In catastrophe theory (Thom 1975, Poston and Stewart 1978) the polynomial (3) is the canonical form for the cuspoid catastrophes, with n-2 the co-dimension of the singularity. It is therefore appropriate to call (1) the cuspoid canonical integral.

The (n-1) integrals (1) and (2) also arise in connection with one-dimensional oscillating integrals whose exponents possess many nearly coincident stationary phase or saddle points. When such an integral is evaluated by *uniform* asymptotic techniques, the result can be expressed in terms of the canonical integral (1) and its derivatives (2) (Bleistein 1967, Rice 1968, Ursell 1972, Berry 1976, Connor 1974, 1976). A key step in the theoretical treatment of many short-wavelength phenomena, such as collisions of atoms, molecules and heavy nuclear ions, the propagation of water, electromagnetic

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and acoustic waves, as well as scattering from surfaces, is the uniform asymptotic evaluation of oscillating integrals with many coalescing saddle points. Thus it is necessary to develop methods for the numerical evaluation of the integrals (1) and (2) if these short-wavelength theories are to be applied in practice.

For n = 3, the integral (1) is the well characterised regular Airy integral (Airy 1838, Miller 1971), or fold canonical integral in the language of catastrophe theory. There have been many numerical applications of the uniform Airy asymptotic approximation to physical problems following on from the initial researches of Chester *et al* (1957).

When n = 4, equation (1) becomes the cusp canonical integral or Pearcey's integral (Pearcey 1946), which we shall henceforth write in the form

$$P(x, y) = \int_{-\infty}^{\infty} \exp[i(u^4 + xu^2 + yu)] \, du.$$
(4)

Pearcey's integral occurs in the short-wavelength description of many physical phenomena, and a guide to the relevant literature is given by Connor and Farrelly (1981b)—see in addition the recent papers by Taborek and Goodstein (1980a, b), Wright (1980), Da Silveira (1981), Berry and Upstill (1980) and Stewart (1981) as well as the books by Schulman (1981) and Gilmore (1981).

However, only one numerical application of the uniform Pearcey asymptotic approximation has been made to date (Connor and Farrelly 1981b). There have been no numerical applications of uniform asymptotic techniques when $n \ge 5$ that we are aware of.

In order to make numerical applications of the powerful uniform asymptotic methods mentioned above for n > 3, it is clearly necessary to be able to evaluate the integrals (1) and (2) efficiently and accurately for a wide range of values of their arguments. The purpose of the present paper is to describe a numerical method we have developed for the calculation of the integrals (1) and (2). In many cases the method is simple and straightforward, and is easily programmed on a computer. It exploits the fact that the integrands of (1) and (2) are analytic functions of u in the finite complex u plane. A combination of Cauchy's theorem and Jordan's lemma then allows the most convenient integration path in the complex u plane to be chosen for the numerical quadrature. We describe our integration method in § 2. Although the method in principle works for any n, in practice the most important cases are for values of n which are not too large (e.g. n = 4, 5, 6). In § 3 we apply the method to Pearcey's integral and its two derivatives and show that our method has some significant advantages over other numerical techniques that have been applied to P(x, y). Our conclusions are in § 4.

2. The contour integral method

The main numerical problem associated with the cuspoid canonical integral (1) and its derivatives (2) is the behaviour of the integrand at the end-points of the range of integration. This is one of infinitely rapid oscillations, making a direct numerical quadrature impossible.

To resolve this problem, we choose a different contour in the complex u plane along which to perform the numerical integration by exploiting the fact that the integrand of (1) is an analytic function of u in the finite complex u plane. Our method is a modification of one described earlier by Connor and Farrelly (1981a).

First we write (1) in the form

$$C_n(\boldsymbol{a}) = \int_0^\infty \exp(\mathrm{i}f_n(\boldsymbol{a}\,;\,\boldsymbol{u}))\,\mathrm{d}\boldsymbol{u} + \int_0^\infty \exp(\mathrm{i}f_n(\boldsymbol{a}\,;\,-\boldsymbol{u}))\,\mathrm{d}\boldsymbol{u}. \tag{5}$$

When n is odd we shall have to consider each integral in equation (5) separately; for n even this will not be necessary.

One method which has been used for the numerical quadrature of integrals of the type (5) (Connor and Farrelly 1981a) replaces the contour from 0 to ∞ by a ray from 0 to $\infty \exp(\pm i\pi/2n)$ together with a contour from $\infty \exp(\pm i\pi/2n)$ to ∞ where the plus sign is taken, except for *n* odd in the second integral of equation (5), when the minus sign is taken. An application of Jordan's lemma shows that the contribution from the arc $\infty \exp(\pm i\pi/2n)$ to ∞ vanishes. Along the ray 0 to $\infty \exp(\pm i\pi/2n)$, the appropriate integrands of equation (5) eventually diminish rapidly like $\exp(-u^n)$.

To illustrate the advantages of this method as well as its main difficulty, we use Pearcey's integral as an example and write equation (5) in the form

$$P(x, y) = \int_0^\infty 2\cos(yu) \exp[i(u^4 + xu^2)] \, du.$$
 (6)

Figure 1 shows the real and imaginary parts of the integrand of equation (6) in the complex u plane for x = 3, y = 2. The oscillatory nature of the integrand along the Re u axis can be clearly seen. Along the ray 0 to $\infty \exp(\frac{1}{8}i\pi)$, on the other hand, the integrand rapidly diminishes with no violent oscillations along the way. It is thus straightforward to obtain an accurate value for P(x = 3, y = 2) to, say, seven or eight significant figures along this contour using standard numerical quadrature techniques.

Figure 2 shows the same plots as in figure 1 but for the case x = -3, y = 2. There are now large oscillations along the path 0 to $\infty \exp(\frac{1}{8}i\pi)$. These oscillations arise from the term $\exp(ixu^2)$ in equation (6) which, for negative x, can become very large before the term $\exp(iu^4)$ is eventually dominant. Although a numerical quadrature can obtain accurate values for P(x = -3, y = 2) for the situation shown in figure 2, this method eventually fails as x becomes more negative (Connor and Farrelly 1981a).

The problems discussed above can be avoided by choosing the integration contours shown in figure 3. In the following we shall only consider the case where n is even since the discussion for n odd is very similar. For even n, the contour proceeds from 0 to a point on the real axis R, then along the arc of a circle R to $R \exp(i\pi/2n)$ and finally along the ray $R \exp(i\pi/2n)$ to $\infty \exp(i\pi/2n)$. The contribution from $\infty \exp(i\pi/2n)$ to ∞ is again zero by Jordan's lemma. In this way, for a suitable choice of R, the violent oscillations that may occur along the direct ray from 0 to $R \exp(i\pi/2n)$ are avoided.

In order to see what factors govern the choice of R, let us consider the first integral in equation (5). Our choice of contour reduces the problem of calculating $C_n(a)$ to the numerical evaluation of the two finite integrals

$$\int_0^R \exp(\mathrm{i} f_n(\boldsymbol{a}\,;\,\boldsymbol{u}))\,\mathrm{d}\boldsymbol{u} \tag{7}$$

and

(* 1**0**)

-

$$\int_{R}^{R} \exp(if_n(\boldsymbol{a}\,;\,\boldsymbol{u}))\,\mathrm{d}\boldsymbol{u} \tag{8}$$



Figure 1. Plot of the integrand of equation (6) for x = 3, y = 2: (a) Re $(2 \cos(yu) \exp[i(u^4 + xu^2)])$ and (b) Im $(2 \cos(yu) \exp[i(u^4 + xu^2)])$.

as well as the infinite integral

$$\int_{R \exp(i\pi/2n)}^{\infty \exp(i\pi/2n)} \exp(if_n(\boldsymbol{a}\,;\,\boldsymbol{u})) \,\mathrm{d}\boldsymbol{u} \tag{9}$$

which can be written in the alternative form

$$\exp(i\pi/2n)\int_{\boldsymbol{R}}^{\infty}\exp\left(-r^{n}+\sum_{k=1}^{n-2}ia_{k}\exp(ik\pi/2n)r^{k}\right)\mathrm{d}r.$$
(10)

In the integral (10), if necessary we can always choose R sufficiently large that the modulus of (10) is arbitrarily small and hence negligible in the quadrature evaluation. This is because the factor $\exp(-r^n)$ for $r \gg 1$ dominates any terms of the kind $\exp(ia_k \exp(ik\pi/2n)r^k)$ with k < n.

More formally, suppose we require the modulus of the integrand of (10) to be less than or equal to, say, $\exp(-d)$ with d > 1. Then R is required to be the largest real root of the polynomial

$$r^{n} + \sum_{k=1}^{n-2} a_{k} \sin(k\pi/2n)r^{k} - d = 0.$$
(11)



Figure 2. The same as figure 1 except for x = -3, y = 2.

When solving numerically for this root it is helpful to have a bound on the location of the roots of the polynomial (11) in the complex r plane. We have found the following theorem of Datt and Govil (1978) to be useful in this regard. Let $A = \max\{d, |a_k| \sin(k\pi/2n)\}$ for k = 1, 2, ..., n-2; then the polynomial (11) has all its zeros in the ring-shaped region of the complex r plane given by

$$\frac{d}{2(1+A)^{n-1}(nA+1)} \le |r| \le 1 + \left(1 - \frac{1}{(1+A)^n}\right)A.$$
(12)

The above discussion has shown that we can always choose R so that the integral (10) is negligibly small. On the other hand, we do not want to choose R too large in case the oscillatory nature of the integrand of (7) makes it difficult (or even impossible) to obtain accurate values for this integral by numerical quadrature. Thus in practice a compromise value of R must often be used, one that facilitates the numerical evaluation of both (7) and (10). If the value of R does not make the integral (10) negligibly small then it is necessary to evaluate (10) by a numerical quadrature. As an alternative, the integral (10) could be expanded in an asymptotic series, with R chosen so that this series is a sufficiently accurate approximation to (10) (see Berry *et al* 1979). Having found a



Figure 3. Contours in the complex u plane used in the numerical evaluation of the canonical integrals (1) and (2): (a) contours used for n even in both integrals of equation (5) and for n odd in the first integral and (b) contours used for n odd in the second integral of equation (5).

suitable value of R for the integrals (7) and (10), the remaining integral (8) can also be evaluated by numerical quadrature.

The method we have described above has a number of useful properties.

(a) The method is straightforward to implement on a computer and results of high accuracy can be obtained (e.g. seven or eight significant figures for P(x, y)—see § 3). In the simpler cases of n = 4 and 5 and for values of the parameters a which are not too large, the integrals (7)–(9) can be evaluated by standard quadrature routines that are available in most computer program libraries. In more difficult situations it may be necessary to use more specialised techniques. For example, the integral (7) may require methods that have been developed for oscillatory integrands (see the discussions of Davis and Rabinowitz (1975), Rice (1975) and Engels (1980)). When using a quadrature routine it is important to avoid any spurious numerical convergence to which oscillatory integrals are prone. In this situation it is helpful to make contour plots of the integral. If tabulated values alone are examined, it can be difficult to spot such errors, especially on a coarse grid.

(b) The method can be readily applied for different values of n, unlike some other techniques (such as differential equation methods) in which each n must be treated as a separate case.

(c) The method works equally well for the derivatives (2) of the canonical integral as for the canonical integral itself. This is important in applications since the uniform asymptotic techniques mentioned in § 1 require the evaluation of all (n-1) integrals (1) and (2). If only the canonical integral is evaluated, then one is restricted to less powerful *transitional* asymptotic approximations.

(d) Alternative contours to the one described above (namely $0 \rightarrow R \rightarrow R \exp(\pm i\pi/2n) \rightarrow \infty \exp(\pm i\pi/2n)$) can be used when convenient. One such alternative contour is shown in figure 3: instead of proceeding along the real u axis to R, it 'cuts the corner' by leaving the real axis at a point closer to the origin. An integration path that proceeds directly from 0 to $R \exp(\pm i\pi/2n)$ is the most suitable contour when the integrand is free of violent oscillations as in figure 1 for Pearcey's integral. Also, the path between R and $R \exp(\pm i\pi/2n)$ need not be an arc of a circle; other contours such as a straight line can be used. Finally, we note that it is not even necessary to integrate (9) along the ray arg $u = \pi/2n$ since the integrand actually converges in the sector $0 < \arg u < \pi/n$. Although the fastest decrease in the modulus of the integrand is obtained for arg $u = \pi/2n$, it may be convenient to use a different path lying in the sector $0 < \arg u < \pi/n$ in some situations.

(e) In our discussion so far we have always used the canonical form (3) for the cuspoid polynomial. However, in some applications it may be more suitable to use the form

$$a_n u^n + a_{n-1} u^{n-1} + \sum_{k=1}^{n-2} a_k u^k$$
(13)

in the definition of the canonical integral where a_{n-1} and a_n are real numbers. It is clear that our method, with obvious modifications, also applies to the non-canonical form (13).

(f) Our technique for dealing with an infinitely oscillating integrand by exploiting Cauchy's theorem and Jordan's lemma can also be applied to the two-dimensional canonical integrals for the elliptic and hyperbolic umbilic catastrophes since both these integrals can be reduced to one-dimensional integrals by means of suitable transformations (Poston and Stewart 1978, Berry *et al* 1979).

3. Application to Pearcey's integral and its derivatives

In this section we apply the method of § 2 to Pearcey's integral (4) and its two partial derivatives

$$\frac{\partial P(x, y)}{\partial x} = i \int_{-\infty}^{\infty} u^2 \exp[i(u^4 + xu^2 + yu)] du$$
(14)

and

$$\frac{\partial P(x, y)}{\partial y} = i \int_{-\infty}^{\infty} u \exp[i(u^4 + xu^2 + yu)] du.$$
(15)

It is only necessary to calculate P(x, y), $\partial P(x, y)/\partial x$ and $\partial P(x, y)/\partial y$ for $y \ge 0$ because of the relations

$$P(x, -y) = P(x, y) \tag{16}$$

$$\partial P(x, -y)/\partial x = \partial P(x, y)/\partial x$$
 (17)

$$\partial P(x, -y)/\partial y = -\partial P(x, y)/\partial y.$$
 (18)

In order to apply the techniques of § 2, we first set d = 100 so that the infinite integral (10) is negligibly small. Next we solved the polynomial equation (11) for its largest real root R and then evaluated the two finite integrals (7) and (8) by gaussian quadrature. In table 1, we report values of P(x, y), $\partial P(x, y)/\partial x$ and $\partial P(x, y)/\partial y$ for the grid x = -8.0 (2.0) 8.0 and y = 0.0 (2.0) 8.0. Using the error control parameter in the

Table 1. Values of Pearcey's integral P(x, y) and its two partial derivatives $\partial P(x, y)/\partial x$ and $\partial P(x, y)/\partial y$ for the grid x = -8.0(2.0)8.0 and y = 0.0(2.0)8.0.

x	у	$\operatorname{Re} P(x, y)$	$\operatorname{Im} P(x, y)$	Re $\partial P/\partial x$	Im $\partial P/\partial x$	Re ∂ <i>P</i> /∂y	Im ∂P/∂y
-8.0	0.0	-0.337 44	-0.876 36	1.692 77	-3.158 15	0.0	0.0
-6.0	0.0	0.159 28	-1.483 42	2.903 65	-1.149 39	0.0	0.0
-4.0	0.0	-0.647 56	-0.609 62	-0.163 43	-2.588 17	0.0	0.0
-2.0	0.0	2.385 66	-1.085 51	0.541 89	1.522 44	0.0	0.0
0.0	0.0	1.674 81	0,693 73	-0.566 07	0.234 47	0.0	0.0
2.0	0.0	0.924 03	0.729 01	-0.215 94	~0.069 98	0.0	0.0
4.0	0.0	0.646 98	0.593 70	-0.086 96	-0.057 63	0.0	0.0
6.0	0.0	0.520 85	0.500 05	-0.045 95	-0.037 60	0.0	0.0
8.0	0.0	0.447 92	0.437 62	-0.029 09	-0.025 92	0.0	0.0
-8.0	2.0	1.004 22	-0.114 80	-0.887 49	2.113 47	-1.175 31	-0.484 74
-6.0	2.0	0.965 27	0.464 13	-2.55501	1.265 98	-0.197 55	-0.396 87
-4.0	2.0	1.963 41	-0.734 19	0.598 63	2.278 23	0.719 24	0.127 63
-2.0	2.0	0.354 55	-0.051 84	0.116.05	-0.785 69	-1.186 12	0.915 10
0.0	2.0	1.124 75	-0.176.08	0.139 22	0.342 75	-0.599 81	-0.625 28
2.0	2.0	0.993 72	0.312.73	-0.14711	0.119.25	0.004 17	-0.395 59
4.0	2.0	0 740 10	0.413.32	-0.099.09	0.008.36	0.071.04	-0.185.21
6.0	2.0	0 587 73	0 403 53	-0.057.68	~0.012.00	0.058.42	-0.100.67
8.0	$\frac{2.0}{2.0}$	0 495 82	0.405 55	-0.036 57	-0.01373	0.043.89	-0.063.52
-8.0	40	0.753.72	-0 239 33	-0.15757	0.019 79	1 772 46	0.584.28
-6.0	4.0	0.793.72	-0 843 73	1 956 37	-1 635 66	0 792 28	1 001 21
-4.0	4.0	0 143 60	0.043 / 5	-0 777 99	-1 379 35	-1 069 48	1.001.21
-2.0	4.0	0.080.86	0.902 44	-1 022 67	0.011.30	0.612.42	-0 414 20
2.0	4.0	-0.385.02	-0 545 14	0 574 02	-0 509 84	-0.611.87	0.419.59
2.0	4.0	0.505 72	-0.565.16	0.253.10	0.242 19	-0 448 40	-0 345 74
4.0	4.0	0.350 40	-0.132.66	-0.016.09	0.158.87	-0.006.43	-0 334 14
4.0 6.0	4.0	0.700.00	0.081 20	-0.050.79	0.066.57	0.011.27	-0.219.89
0.0	4.0	0.003 91	0.061 29	-0.03079	0.000 37	0.011 27	-0.219 89
0.0	4.0	-0.128.20	0.109.35	-0.042 04	-2 767 56	-1 123 22	0 240 77
-6.0	6.0	1 179 99	1 084 43	-0.120 00	2.707.30	-1.125 22	-0.120.70
-0.0	0.0 4 0	1.1/0.00	0.240.46	-0.728 55	2.166 22	-1.363 33	-1 222 26
-4.0	6.0	0.040 30	0.240 40	1 100 11	0.954 04	-0.04381	-0.167.05
-2.0	6.0	0.023 99	-0.33790	0.775.56	0.150 01	-0.731 38	-0.107 95
0.0	0.0	-0.233 37	0.392.03	-0.773 30	-0.208 13	-0 411 92	0.223 20
2.0	0.0	-0.470 83	-0.309 21	0.338 19	-0.308 44	-0.411 85	0.443 40
4.0	6.0	0.225 51	-0.668 10	0.251 58	0.100 91	-0.427 38	-0.108 80
0.0	6.0	0.515 90	-0.405 73	0.004 33	0.129 34	-0.201 30	-0.226 59
8.0	0.0	0.505 95	-0.192 54	-0.001 03	2 116 07	-0.07/37	-0.202.09
-8.0	8.0	1.009.30	0.223 83	-1.090 20	3.110 97	0.000 85	0.410 49
-0.0	8.0	-1.101 57	0.582 29	-1.1004/	-1.002 47	0.909 85	-0.72015
-4.0	8.0	-0.490 13	0.021 99	-0.419 /0	-1.190 11	0.4/4.30	0.797 09
-2.0	8.0	-0.180.03	0.409 13	-1.123 02	-0.30/24	0.73143	0.203 01
0.0	8.0	0.51018	-0.2009/	0.441 81	0.799 03	-0.349 29	-0.034 /3
2.0	8.0	-0.308 92	0.545 15	-0.555 55	-0.290 50	0.300 93	0.204 08
4.0	8.0	-0.50/03	-0.308 14	0.183 33	-0.332 49	-0.214 10	0.449 40
0.0	8.0	-0.090 57	-0.014 55	0.21947	-0.015 //	-0.302 03	0.074 05
8.0	8.0	0.229.86	-0.55241	0.110.29	0.0/181	-0.233 22	-0.033 30

gaussian quadrature routine, our method readily supplies results accurate to seven or eight significant figures uniformly over the grid, although this degree of precision is not needed in most physical applications. It takes approximately 48 s of CPU time to calculate P(x, y), $\partial P/\partial x$ and $\partial P/\partial y$ to an accuracy of 10^{-8} for 512 values of (x, y) on a grid $-8 \le x \le 8$, $0 \le y \le 8$ using the CDC 7600 computer at the University of Manchester Regional Computer Centre.

Since there are no tables of P(x, y) or its derivatives in the literature to compare with, we have checked the accuracy of our results by carrying out two additional calculations. In the first of these, we integrated directly along the contour 0 to $\infty \exp(\frac{1}{8}i\pi)$ until the integrands became negligibly small (Connor and Farrelly 1981a). This method is accurate for positive values of x provided y is not too large, but fails as x becomes negative (see § 2). In the second method, we integrated a linear third-order differential equation satisfied by P(x, y) (Pearcey 1946, 1963) with appropriate initial conditions (see Connor and Farrelly 1981a). This method is accurate for negative values of x inside the caustic $8x^3 + 27y^2 = 0$, but becomes unstable for x outside the caustic at large y.

The reason for this (Pearcey 1963) is that there are three linearly independent solutions of the differential equation which may oscillate, exponentially increase or exponentially decrease when y is large and x is outside the caustic. In the step-by-step solution of the differential equation starting from (x, y = 0) errors increase exponentially, eventually limiting the accuracy to which P(x, y) can be calculated in this region. This instability is also evident in the sensitivity of the calculated values for P(x, y) and its derivatives to the accuracy of the initial conditions for the differential equation. For example, with the initial conditions accurate to ten significant figures and using a step size of h = 0.005, P(x = 10.0, y = 10.0) agrees to four figures with the value obtained from our quadrature method. But with the initial conditions accurate to only 8 significant figures there is a discrepancy of a factor of about 14 between the two calculations.

We always obtained agreement to at least seven significant figures between the results of our new method and the two previous methods in those regions of the (x, y) plane where the earlier methods exhibit no numerical instabilities. Note that our quadrature method is numerically stable over the grid of (x, y) values used in table 1.

Two other methods have also been employed for the calculation of P(x, y). Exact series representations can be obtained for P(x, y), $\partial P(x, y)/\partial x$ and $\partial P(x, y)/\partial y$ (Brillouin 1916, Pearcey 1963, Connor 1973, Maslin 1976, Connor and Farrelly 1981a, b) which in principle can be summed numerically for any values of x and y. In practice, however, this method is only useful for small values of x and y.

Wright (1977) has used a technique based on the stationary-phase method to compute P(x, y). In this method, a quadrature is performed around the region of the one or three real stationary-phase points that contribute to P(x, y). The tails of the integral are estimated by a three-term asymptotic expansion. This method is similar to one used originally by Airy (1838) for the evaluation of his integral (see Miller 1971). For the swallow-tail canonical integral, which has n = 5 in equation (1), it is necessary to perform a numerical quadrature over the contributing saddle points in the complex u plane when there are no real saddle points (see in addition Lugannani and Rice 1981).

In the method of Wright (1977) it is necessary to carry out a saddle-point analysis for each value of n. In contrast, a detailed understanding of the distribution of saddle points in the complex u plane is not usually required in our method, although when this information is available it can be used to advantage, since it provides knowledge similar to that illustrated in figures 1 and 2. However, in some situations, such as when there are no real saddle points, a numerical application of the steepest-descent method may be the only viable numerical technique (see Wright 1980).

For P(x, y), Wright (1977) used a three-term asymptotic expansion which gives an accuracy of about ± 0.001 . This is adequate for producing contour plots and for many other applications. By including more terms in the asymptotic expansion, higher accuracy could be obtained by this method. For P(x, y), Wright's method and the one presented here are similar in that both of them perform a quadrature for a finite interval of the Re u axis. In particular, Wright's method for determining the outermost real saddle point is analogous to our method for determining R in equation (11). Wright (1977) has also discussed the case n > 4. The main difference between the two methods is the technique used for estimating the remainder of the integral. Our method has the advantage of ease of application and that results correct to seven or eight significant figures are readily obtained; the only limit is the accuracy of the quadrature method employed.

In connection with the theory of wavefront dislocations, Berry *et al* (1979) and Wright (1980) have computed some of the real zeros of P(x, y) that lie within the rectangle $|x| \le 8.0$ and $0 \le y \le 8.0$. They use a different form for Pearcey's integral, namely

$$C(x, y) = (2\pi)^{-1/2} \int_{-\infty}^{\infty} \exp[i(\frac{1}{4}u^4 + \frac{1}{2}xu^2 + yu)] du.$$
(19)

This is related to P(x, y) by

$$C(x, y) = \pi^{-1/2} P(x, 2^{1/2} y).$$
⁽²⁰⁾

Table 2. Zeros of P(x, y) for $x \ge -8.0$ and $0 \le y \le 8.0$.

	This work	Berry et al (1979)							
x	у	x ^a	y ^b						
Outside the caustic $8x^3 + 27y^2 = 0$									
-1.743 60	2.352 18	-1.74	2.33						
-3.057 91	4.427 07	-3.07	4.43						
-4.035 51	6.161 85	-4.05	6.15						
-4.848 17	7.723 52	-4.86	7.71						
Inside the caustic $8x^3 + 27y^2 = 0$									
-4.378 04	0.527 68	-4.38	0.54						
-5.554 70	1.411 01	-5.56	1.41						
-5.523 21	2.360 94	-5.53	2.33						
-6.642 85	0.430 39	-6.64	0.42						
-6.446 24	3.063 89	-6.47	3.08						
-6.403 12	3.958 06	-6.39	3.96						
-7.196 29	4.565 37								
-7.147 18	5.422 06								
-7.499 06	1.216 05								
-7.486 29	2.029 22								
-7.857 23	5.966 69								
-7.804 56	6.795 38								

^a Estimated error ±0.05.

^b Estimated error ± 0.07 .

Berry et al (1979) and Wright (1980) estimate the errors in their location of the zeros to be ± 0.05 for x and ± 0.07 for y. Using our new numerical technique for P(x, y), we have calculated all the real zeros that lie within the rectangle $|x| \le 8.0$ and $0 \le y \le 8.0$. The results are reported in table 2. It can be seen that our improved values for the zeros do indeed lie within the estimates of Berry et al (1979) and Wright (1980). We calculated the zeros by minimising |P(x, y)| using a Simplex method (Numerical Algorithms Group 1978). This procedure allows the zeros to be calculated with an accuracy of about eight significant figures when combined with our quadrature method.

4. Conclusions

In this paper, we have described a new method for the numerical evaluation of the oscillatory integrals (1) and (2) that are associated with the cuspoid catastrophes. Our method uses Cauchy's theorem and Jordan's lemma to deform the initial contour of integration into the complex u plane. In favourable cases this procedure results in two finite integrals which can be evaluated by standard quadrature routines and an infinite integral which can be made very small or negligible. The method is straightforward to program on a computer and results of high accuracy can be obtained. The same method can be applied to the integrals (1) and (2) for different values of n and alternative contours of integration can be used when this is convenient. Our method includes as a special case that of Connor and Farrelly (1981a). We applied our method to the calculation of P(x, y), $\partial P(x, y)/\partial x$, $\partial P(x, y)/\partial y$ and the zeros of P(x, y) for $-8.0 \le x \le 8.0$, $0 \le y \le 8.0$ and showed that it possessed some significant advantages over the other available techniques.

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References

Davis P J and Rabinowitz P 1975 Methods of Numerical Integration (New York: Academic) §2.10

Engels H 1980 Numerical Quadrature and Cubature (London: Academic) § 8.5

Gilmore R 1981 Catastrophe Theory for Scientists and Engineers (New York: Wiley) ch 13

Lugannani R and Rice S O 1981 J. Comput. Phys. 39 473-80

Maslin N M 1976 J. Atmos. Terr. Phys. 38 1251-63

Miller J C P 1971 The Airy Integral, Giving Tables of Solutions of the Differential Equation y" = xy (British Association for the Advancement of Science, Mathematical Tables, Part-volume B) (published for the Royal Society at the University Press, Cambridge)

Numerical Algorithms Group 1978 Fortran Library Manual, Mark 7 subroutine E04CCF

Pearcey T 1946 Phil. Mag. 37 311-7

----- 1963 in *The Effect of Aberrations upon the Optical Focus* by T Pearcey and G W Hill (Melbourne, Australia: Commonwealth Scientific and Industrial Research Organization) pp 1-40

Poston T and Stewart I 1978 Catastrophe Theory and its Applications (London: Pitman)

Rice S O 1968 Bell System Tech. J. 47 1970-2013

Stewart I 1981 Physica D 2 245-305

Schulman L S 1981 Techniques and Applications of Path Integration (New York: Wiley) ch 16

Taborek P and Goodstein D 1980a Phys. Rev. B 22 1550-63

------ 1980b Solid State Commun. 33 1191-4

Thom R 1975 Structural Stability and Morphogenesis. An Outline of a General Theory of Models (translated from the French edition, as updated by the author, by D H Fowler, with a Forward by C H Waddington) (Reading, Mass: Benjamin)

Ursell F 1972 Proc. Camb. Phil. Soc. 72 49-65

Wright F J 1977 PhD Thesis University of Bristol

----- 1980 J. Phys. A: Math. Gen. 13 2913-28