Theory of axially symmetric cusped focusing: numerical evaluation of a Bessoid integral by an adaptive contour algorithm

2000 J. Phys. A: Math. Gen. 33 4797

(http://iopscience.iop.org/0305-4470/33/26/306)

J. Phys. A: Math. Gen. **33** (2000) 4797–4808. Printed in the UK PII: S0305-4470(00)11707-X

Theory of axially symmetric cusped focusing: numerical evaluation of a Bessoid integral by an adaptive contour algorithm

N P Kirk†, J N L Connor‡, P R Curtis‡‖ and C A Hobbs§

† Department of Mathematical Sciences, University of Liverpool, Liverpool L69 3BX, UK
‡ Department of Chemistry, University of Manchester, Manchester M13 9PL, UK
§ School of Computing and Mathematical Sciences, Oxford Brookes University, Gipsy Lane, Headington, Oxford OX3 0BP, UK

Received 8 February 2000

Abstract. A numerical procedure for the evaluation of the Bessoid canonical integral $J(x, y)$ is described. $J(x, y)$ is defined, for x and y real, by

$$J(x, y) = \int_0^\infty J_0(yt)\, t \exp[\mathrm{i}(t^4 + xt^2)]\, \mathrm{d}t$$

where $J_0(\cdot)$ is a Bessel function of order zero. $J(x, y)$ plays an important role in the description of cusped focusing when there is axial symmetry present. It arises in the diffraction theory of aberrations, in the design of optical instruments and of highly directional microwave antennas and in the theory of image formation for high-resolution electron microscopes. The numerical procedure replaces the integration path along the real t axis with a more convenient contour in the complex t plane, thereby rendering the oscillatory integrand more amenable to numerical quadrature. The computations use a modified version of the CUSPINT computer code (Kirk *et al* 2000 *Comput. Phys. Commun.* at press), which evaluates the cuspoid canonical integrals and their first-order partial derivatives. Plots and tables of $J(x, y)$ and its zeros are presented for the grid $-8.0 \leqslant x \leqslant 8.0$ and $-8.0 \leqslant y \leqslant 8.0$. Some useful series expansions of $J(x, y)$ are also derived.

1. Introduction

The *Pearcey function* [1, 2], $P(x, y)$, plays an important role in the uniform asymptotic theory of cusped focusing (see [3, 4] for many relevant references). $P(x, y)$ has the conditionally convergent integral representation

$$P(x, y) = \int_{-\infty}^{\infty} \exp\left[\mathrm{i}\left(t^4 + xt^2 + yt\right)\right] \mathrm{d}t \tag{1.1}$$

when x and y are real. It is an example of a *cuspoid integral* [3, 4].

In applications of the uniform asymptotic theory, it is necessary to compute $P(x, y)$ and its partial derivatives [3, 4]. Reference [5] described a contour-integral method in which the integration path along the real t axis of equation (1.1) is replaced by a more convenient contour in the complex t plane. This contour-integral method allowed the first practical application of the uniform Pearcey approximation, which was to the theory of cusped rainbows in $\mathrm{He}^+ + \mathrm{Ne}$ elastic scattering [6]. More recently, we have described a computer code [4] that is a modern implementation in FORTRAN 90 of the contour-integral method. This code has the novel

‖ Present address: Itex (Jersey) Ltd, 48–50 The Esplanade, St Helier, Jersey JE1 3UN, Channel Islands.

feature that the algorithm implements an *adaptive contour procedure*, choosing contours in the complex plane that avoid the violent oscillatory and exponential natures of the integrand and modifying its choice as necessary [4].

When *axial symmetry* is present, cusped focusing is characterized by a different (conditionally convergent) canonical integral [7–12], which we write as

$$J(x, y) = \int_0^\infty J_0(yt)\, t \exp\big[\mathrm{i}\big(t^4 + xt^2\big)\big]\, \mathrm{d}t \tag{1.2}$$

where x and y are real and $J_0(\cdot)$ denotes the Bessel function of order zero [13]. We will call (1.2) a *Bessoid integral*, or more precisely a Bessoid integral of type J, of order zero and of degree four. Here J denotes the type of Bessel function in the integrand, zero is its order and four is the degree of the polynomial in the exponent.

The purpose of this paper is to show how a modified version of our adaptive contour algorithm [4] can be used for the numerical evaluation of $J(x, y)$. In section 2, we first derive some useful properties of $J(x, y)$. Our numerical method is described in section 3, and results for $J(x, y)$ and its zeros are reported in section 4. Section 5 contains our concluding remarks.

An integral similar to (1.2) occurred in early work by Picht [7] on the diffraction theory of aberrations, with the difference that the upper limit of infinity was replaced by a small number (see also [8], p 153). In addition, the integral (1.2) with an upper limit of unity arises in the theory of primary spherical aberrations for three-dimensional scalar lightwaves [9, p 357]. Numerical values for $\pi J(x, y)$ were obtained by Pearcey and Hill using an early digital computer, with the results reported in an unpublished monograph [10]. Their study was motivated by the design of optical instruments and of highly directional microwave antennas. In a letter to one of us (JNLC), dated 27 September 1982, Pearcey suggested applying the contour-integral method [5] to $J(x, y)$ in order to check the earlier computations he and Hill had made (see section 4). Some preliminary calculations were indeed performed in 1982, but the results not published.

More recently, $J(x, y)$ has played an important role in the theory of image formation for high-resolution electron microscopes [11, 12], in which $2J(x, y)$ represents the radial part of the (undamped) impulse–response function at normalized defocus x. In [12], Janssen applies the arguments of Paris [14] to obtain asymptotic results for a generalization of $J(x, y)$ (see section 5).

2. Properties of $J(x, y)$

This section derives some useful properties of $J(x, y)$. We also examine in more detail the special case $y = 0$.

2.1. Symmetry

Since $J_0(z) = J_0(-z)$ [13, p 2], it follows from the integral representation (1.2) that $J(x, y)$ is even in y, that is

$$J(x, y) = J(x, -y). \tag{2.1}$$

2.2. The Maclaurin series expansion

Next we derive a convergent series representation for $J(x, y)$. Consider first the contour $0 \to R \to R\exp(\mathrm{i}\pi/8) \to 0$ with $R > 0$. Since $J_0(z)$ is an entire function of z [13, p 1], the integrand of equation (1.2) contains no singularities and an integral taken around this contour is zero by the Cauchy theorem. Furthermore, since [15, p 108, item (9.2.1)]

$$J_0(z) \underset{|z|\to\infty}{\sim} \left(\frac{2}{\pi z}\right)^{1/2} \cos\big(z - \tfrac{1}{4}\pi\big) + \exp(\operatorname{Im} z)\mathrm{O}\left(\frac{1}{|z|}\right) \qquad |\arg z| < \pi \quad (2.2)$$

the contribution from the arc $R \to R\exp(\mathrm{i}\pi/8)$ tends to zero as $R \to \infty$ by an application of the Jordan lemma. We can therefore write

$$J(x, y) = \int_0^{\infty \exp(\mathrm{i}\pi/8)} J_0(yt)\, t \exp\big[\mathrm{i}\big(t^4 + xt^2\big)\big]\, \mathrm{d}t \qquad (2.3)$$

which is an absolutely convergent integral representation.

Next we substitute the Maclaurin series for $J_0(z)$ [15, p 104, item (9.1.12)] that is

$$J_0(z) = \sum_{k=0}^{\infty} \big(-\tfrac{1}{4}\big)^k \frac{z^{2k}}{(k!)^2} \qquad (2.4)$$

into equation (2.3) and interchange the summation and integration signs (which is justified by the dominated convergence theorem of Lebesgue [16]), to obtain

$$J(x, y) = \sum_{k=0}^{\infty} \frac{(-1)^k}{2^{2k}} \frac{y^{2k}}{(k!)^2} \int_0^{\infty \exp(\mathrm{i}\pi/8)} t^{2k+1} \exp\big[\mathrm{i}\big(t^4 + xt^2\big)\big]\, \mathrm{d}t. \qquad (2.5)$$

To proceed further, we must evaluate the integrals in the series (2.5). Defining

$$I_k(x) = \int_0^{\infty \exp(\mathrm{i}\pi/8)} t^{2k+1} \exp\big[\mathrm{i}\big(t^4 + xt^2\big)\big]\, \mathrm{d}t \qquad k = 0, 1, 2, \ldots \qquad (2.6)$$

and making the substitution $t = u\exp(\mathrm{i}\pi/8)$, yields

$$I_k(x) = \exp[\mathrm{i}(k+1)\pi/4] \int_0^{\infty} u^{2k+1} \exp\big[-u^4 + \exp(\mathrm{i}3\pi/4)xu^2\big]\, \mathrm{d}u \qquad k = 0, 1, 2, \ldots. \qquad (2.7)$$

Next we expand the term $\exp\big[\exp(\mathrm{i}3\pi/4)xu^2\big]$ in a Maclaurin series, interchange the summation and integration signs [16], and use the result

$$\int_0^{\infty} u^n \exp\big(-u^4\big)\, \mathrm{d}u = \tfrac{1}{4}\Gamma\big(\tfrac{1}{4}(n+1)\big) \qquad n = 0, 1, 2, \ldots$$

to obtain

$$I_k(x) = \exp[\mathrm{i}(k+1)\pi/4]\tfrac{1}{4} \sum_{\ell=0}^{\infty} \frac{\exp\,(\mathrm{i}3\ell\pi/4)}{\ell!} \Gamma\,\big(\tfrac{1}{2}(k+\ell+1)\big)\, x^{\ell} \qquad k = 0, 1, 2, \ldots \qquad (2.8)$$

where $\Gamma(\cdot)$ is the gamma function. Substituting equation (2.8) into (2.5) yields, after simplification,

$$J(x, y) = \tfrac{1}{4} \sum_{k=0}^{\infty} \sum_{\ell=0}^{\infty} \frac{\exp[\mathrm{i}\pi(3\ell - 3k + 1)/4]}{2^{2k}(k!)^2 \ell!} \Gamma\,\big(\tfrac{1}{2}(k+\ell+1)\big)\, x^{\ell} y^{2k}. \qquad (2.9)$$

Equation (2.9) is an absolutely convergent double-series representation for $J(x, y)$.

It is tempting (as was done in [10]) to derive (2.9) by substituting directly into equation (1.2) the Maclaurin series (2.4) and that for $\exp\big(\mathrm{i}xt^2\big)$, interchanging the summation and integration signs, and then using *for all n* the result

$$\int_0^{\infty} u^n \exp\big(\mathrm{i}u^4\big)\, \mathrm{d}u = \tfrac{1}{4}\Gamma\big(\tfrac{1}{4}(n+1)\big) \exp\,\big(\tfrac{1}{8}\mathrm{i}(n+1)\pi\big) \qquad n = 0, 1, 2. \qquad (2.10)$$

Although the answer obtained is correct, this simple 'derivation' makes two errors. (a) Interchanging the summation and integration signs produces divergent integrals when $k \geqslant 1$ in the series (2.4), and (b) the left-hand side of (2.10) is divergent for $n = 3, 4, 5, \ldots$. However, this 'derivation' can be made rigorous by the use of converging factors (see [17] for the case of $P(x, y)$).

2.3. Series expansion of $J(x, y)$ in Fresnel functions

In equation (2.5), we expanded the integral $I_k(x)$ (2.6) in the Maclaurin series (2.8), which resulted in the double series (2.9) for $J(x, y)$. An alternative is to express $I_k(x)$ in terms of the derivatives of a Fresnel function, thereby producing a single-series representation for $J(x, y)$.

We first define the Fresnel function (x real)

$$F(x) = \int_0^\infty \exp\bigl[\mathrm{i}\bigl(u^2 + xu\bigr)\bigr]\,\mathrm{d}u \tag{2.11}$$

or equivalently

$$F(x) = \int_0^{\infty\exp(\mathrm{i}\pi/4)} \exp\bigl[\mathrm{i}\bigl(u^2 + xu\bigr)\bigr]\,\mathrm{d}u. \tag{2.12}$$

Differentiating equation (2.12) under the integral sign, with respect to x, $k = 0, 1, 2, \ldots$ times (which is allowed [16]) and making the substitution $u = t^2$, leads to

$$\frac{\mathrm{d}^k F(x)}{\mathrm{d}x^k} = 2\mathrm{i}^k \int_0^{\infty\exp(\mathrm{i}\pi/8)} t^{2k+1} \exp\bigl[\mathrm{i}\bigl(t^4 + xt^2\bigr)\bigr]\,\mathrm{d}t \qquad k = 0, 1, 2, \ldots. \tag{2.13}$$

Note that differentiating equation (2.11) under the integral sign (as was done in [10]) leads to divergent integrals. Comparison of equations (2.6) and (2.13) shows that

$$I_k(x) = \frac{1}{2\mathrm{i}^k}\frac{\mathrm{d}^k F(x)}{\mathrm{d}x^k} \qquad k = 0, 1, 2, \ldots.$$

Substituting into equation (2.5) then yields the following single-series representation for $J(x, y)$:

$$J(x, y) = \tfrac{1}{2}\sum_{k=0}^{\infty} \frac{\mathrm{i}^k}{2^{2k}(k!)^2}\frac{\mathrm{d}^k F(x)}{\mathrm{d}x^k} y^{2k}. \tag{2.14}$$

$F(x)$ can also be expressed in terms of the standard cosine and sine Fresnel integrals. We have from [18] (p 91, items (7.4.38) and (7.4.39))

$$F(x) = \left(\tfrac{1}{2}\pi\right)^{1/2} \exp\left(-\mathrm{i}x^2/4\right)\left\{\frac{\exp(\mathrm{i}\pi/4)}{2^{1/2}} - \left[C\left(\frac{x}{(2\pi)^{1/2}}\right) + \mathrm{i}S\left(\frac{x}{(2\pi)^{1/2}}\right)\right]\right\} \tag{2.15}$$

where the definitions of $C(\cdot)$ and $S(\cdot)$ are those of [18] (p 87, items (7.3.1) and (7.3.2)), namely

$$C(x) = \int_0^x \cos\bigl(\pi t^2/2\bigr)\,\mathrm{d}t \qquad S(x) = \int_0^x \sin\bigl(\pi t^2/2\bigr)\,\mathrm{d}t.$$

The case $y = 0$. When $y = 0$, the series (2.14) reduces to a single term

$$J(x, 0) = \tfrac{1}{2}F(x). \tag{2.16}$$

In particular, when $x = 0$, using equation (2.15) gives

$$J(0, 0) = \tfrac{1}{4}\pi^{1/2}\exp(\mathrm{i}\pi/4).$$

This result also follows from equation (2.9) since $\Gamma\left(\frac{1}{2}\right) = \pi^{1/2}$ or from the integral (1.2) using $J_0(0) = 1$.

We can use known asymptotic approximations for $C(x)$ and $S(x)$ to derive simple formulae for $J(x, 0)$, which are valid for $x \to \pm\infty$. When $x \to \infty$, asymptotic approximations for $C(x)$ and $S(x)$ are [19, p 431, equation (15)]

$$C(x) \sim \frac{1}{2} + \frac{1}{\pi x}\sin\left(\tfrac{1}{2}\pi x^2\right)$$

and

$$S(x) \sim \frac{1}{2} - \frac{1}{\pi x} \cos\left(\tfrac{1}{2}\pi x^2\right).$$

Substituting these approximations into equations (2.15) and (2.16) shows that

$$J(x, 0) \sim \frac{\mathrm{i}}{2x} \qquad x \to \infty. \tag{2.17}$$

Thus $J(x, 0)$ damps to zero as $x \to \infty$.

On the other hand, when $x \to -\infty$, we can use the identities [18, p 88, item (7.3.17)]

$$C(-x) = -C(x) \qquad S(-x) = -S(x)$$

to obtain from equations (2.15) and (2.16) the asymptotic result

$$J(x, 0) \sim \tfrac{1}{2}\pi^{1/2} \exp\left[-\tfrac{1}{4}\mathrm{i}\left(x^2 - \pi\right)\right] + \frac{\mathrm{i}}{2x} \qquad x \to -\infty. \tag{2.18}$$

In this case, $J(x, 0)$ is oscillatory as $x \to -\infty$.

3. Numerics

Our numerical computations for $J(x, y)$ used a modified version of the CUSPINT computer code [4]. This code, written in FORTRAN 90, computes cuspoid integrals and their first-order partial derivatives, which are defined by

$$C_n(a_1, a_2, \ldots, a_{n-2}) = \int_{-\infty}^{\infty} \exp\left[\mathrm{i}\left(t^n + \sum_{j=1}^{n-2} a_j t^j\right)\right] \mathrm{d}t \tag{3.1}$$

and

$$\frac{\partial C_n(a_1, a_2, \ldots, a_{n-2})}{\partial a_k} = \mathrm{i} \int_{-\infty}^{\infty} t^k \exp\left[\mathrm{i}\left(t^n + \sum_{j=1}^{n-2} a_j t^j\right)\right] \mathrm{d}t \tag{3.2}$$

respectively, where the a_j are real, $n = 3, 4, 5, \ldots$, and $k = 1, 2, 3, \ldots, n-2$. CUSPINT first replaces the doubly infinite integral (3.1) or (3.2) by the sum of two infinite integrals on $[0, \infty)$. For the first infinite integral (which is the one relevant to $J(x, y)$), a quadrature is performed along the integration path

$$0 \to R_0 \to R_0 \exp(\mathrm{i}\pi/2n) \to M \exp(\mathrm{i}\pi/2n)$$

where R_0 and M are real, with $R_0 \leqslant M$. This path avoids (for suitable R_0 and M) the violent oscillatory and exponential natures of the integrand of (3.1) or (3.2) in the complex t plane [4]. CUSPINT chooses suitable initial values for R_0 and M and has the novel feature that it can change R_0 and M if this is necessary for a successful quadrature, i.e. CUSPINT implements an adaptive contour algorithm [4].

It is evident that a modified version of CUSPINT can be used to compute values of $J(x, y)$, provided we can evaluate $J_0(z)$ in the sector $0 \leqslant \arg z \leqslant \pi/8$. We accomplished this by means of the code BESJYH of Ardill and Moriarty (catalogue number ACYQ in the Computer Physics Communications Program Library) [20]. BESJYH is written in FORTRAN IV. We converted it to FORTRAN 90 so that it could be incorporated into CUSPINT. All the results in section 4 were obtained using the default accuracy/workload parameters described in [4]. Note that it is only necessary to compute $J(x, y)$ for $y \geqslant 0$ because of the symmetry relation (2.1).

4. Results

Figure 1 shows perspective and contour plots of $|J(x, y)|$. The grid used is $x = -8.0(0.2)8.0$ and $y = -8.0(0.2)8.0$. Thus each plot required 6561 evaluations of $J(x, y)$. The corresponding contour plot for $\arg J(x, y)/\mathrm{deg}$ is shown in figure 2. It is demonstrated in the appendix that the caustic associated with $J(x, y)$ is given by the equations

$$y = \pm(-2x/3)^{3/2} \qquad \text{and} \qquad y = 0 \qquad \text{for} \quad x \leqslant 0$$

which are also drawn on the contour plots in figures 1 and 2. Note that [10–12] did not include the half-line, $y = 0$ for $x \leqslant 0$, as part of the caustic.

Table 1 reports values of $J(x, y)$ on the grid $x = -8.0(2.0)8.0$ and $y = 0.0(2.0)8.0$; they can be compared with the corresponding values for $P(x, y)$ given in table 1 of [4] or in table 1 of [5].

It is evident from figures 1 and 2 that $J(x, y)$ exhibits a complicated interference structure inside the caustic branches given by $8x^3 + 27y^2 = 0$, which is quickly damped on passing outside these branches. Qualitatively, these plots are similar to those for $P(x, y)$ shown in figures 3–5 of [6]. This similarity can be understood as follows. The result (2.2) shows that $J_0(yt)$ has the asymptotic approximation

$$J_0(yt) \sim \left(\frac{2}{\pi yt}\right)^{1/2} \cos\left(yt - \tfrac{1}{4}\pi\right) \qquad yt \to \infty. \tag{4.1}$$

Substituting this approximation into equation (1.2) gives

$$J(x, y) \sim \left(\frac{2}{\pi y}\right)^{1/2} \int_0^\infty \cos\left(yt - \tfrac{1}{4}\pi\right) t^{1/2} \exp\left[\mathrm{i}\left(t^4 + xt^2\right)\right] \mathrm{d}t \qquad y \to \infty \tag{4.2}$$

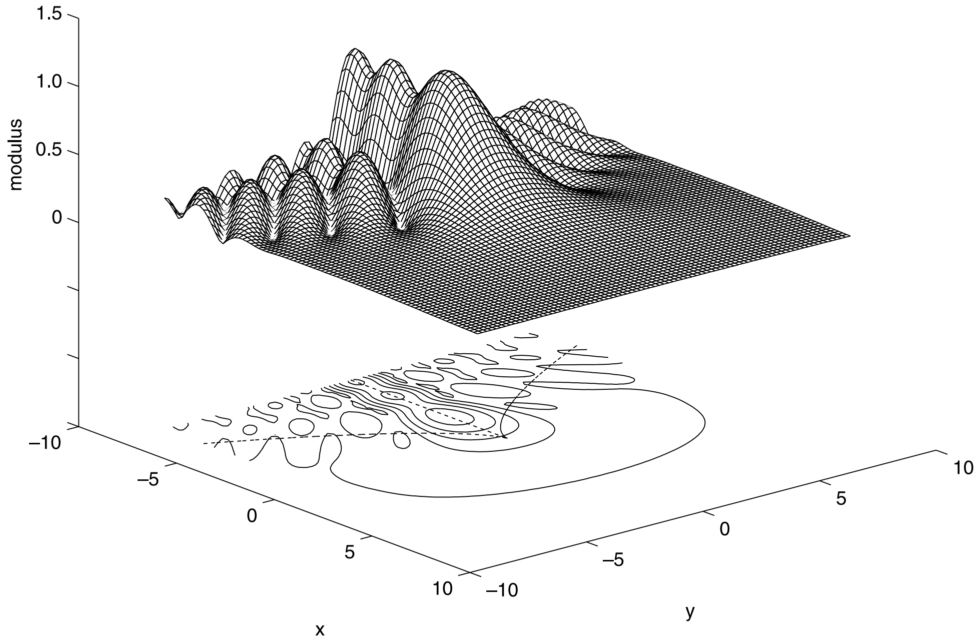

Figure 1. Perspective and contour plots of $|J(x, y)|$ on the grid $x = -8.0(0.2)8.0$ and $y = -8.0(0.2)8.0$. The branches of the caustic are indicated by broken curves.

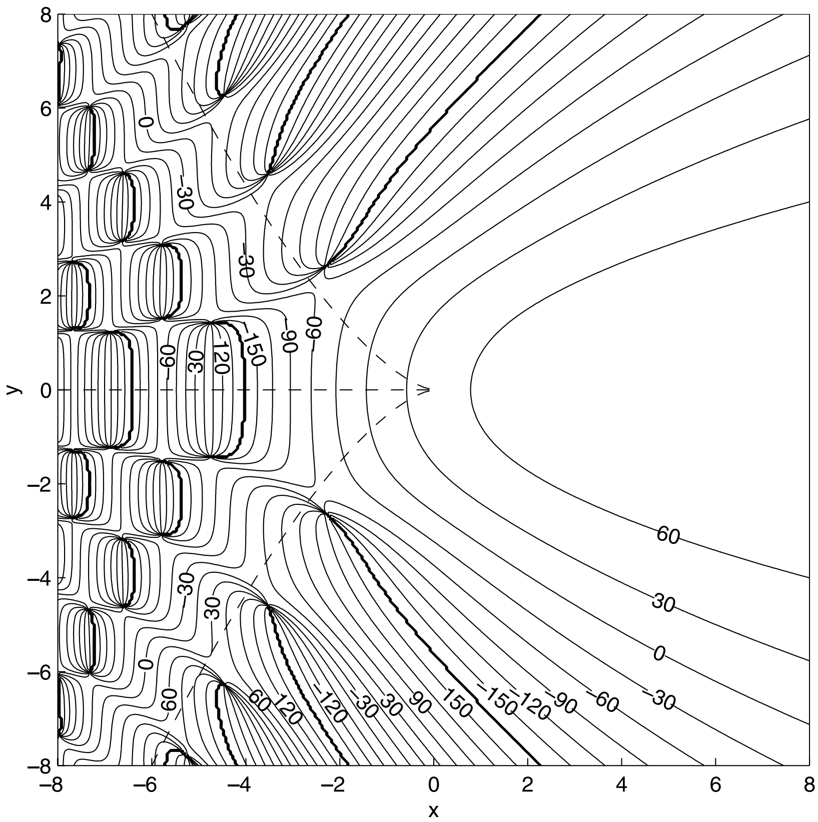

Figure 2. Contour plot of arg $J(x, y)$/deg on the grid $x = -8.0(0.2)8.0$ and $y = -8.0(0.2)8.0$. The contours are $-180(30)180$. The thick full curves mark the phase discontinuities where arg $J(x, y)$/deg jumps in value from -180 to 180. The branches of the caustic are indicated by broken curves.

which is similar to the following integral representation for $P(x, y)$:

$$P(x, y) = 2\int_0^{\infty} \cos(yt)\exp\left[\mathrm{i}\left(t^4 + xt^2\right)\right] \mathrm{d}t.$$

However, the right-hand side of the result (4.2) is only a gross approximation to $J(x, y)$ because use of (4.1) implies that the contribution from the neighbourhood of $t = 0$ has not been properly taken into account.

It should also be noted that the position of the largest maximum of $|J(x, y)|$ is different from that of $|P(x, y)|$. For the Bessoid integral, the largest maximum occurs at $x = -3.0511$, $y = 0$ where $|J(x, y)| = 1.0375$, whereas for the Pearcey function, it occurs at $x = -2.1986$, $y = 0$ where $|P(x, y)| = 2.6351$.

A striking property of figure 2 is the existence of zeros for $J(x, y)$ that lie within the rectangle $|x| \leqslant 8.0$ and $|y| \leqslant 8.0$. Their locations are given in table 2. It is also evident that the zeros fall into regular patterns. Similar behaviour is observed for the zeros of $P(x, y)$, and has been analysed in detail by Kaminski and Paris [21]. It would be interesting to adapt the analysis of [21] to the $J(x, y)$ case.

Table 1. Values of the Bessoid integral $J(x, y)$ for the grid $x = -8.0(2.0)8.0$ and $y = 0.0(2.0)8.0$.

x	y	Re $J(x, y)$	Im $J(x, y)$
−8.0	0.0	−0.782 47	−0.482 03
−6.0	0.0	−0.317 16	−0.911 85
−4.0	0.0	−0.897 28	−0.056 08
−2.0	0.0	0.807 85	−0.391 11
0.0	0.0	0.313 33	0.313 33
2.0	0.0	0.058 05	0.202 38
4.0	0.0	0.013 41	0.120 72
6.0	0.0	0.004 45	0.082 63
8.0	0.0	0.001 93	0.062 32
−8.0	2.0	0.325 82	0.086 60
−6.0	2.0	0.158 61	0.215 72
−4.0	2.0	0.185 55	−0.192 25
−2.0	2.0	0.220 44	−0.209 89
0.0	2.0	0.280 70	0.102 12
2.0	2.0	0.105 49	0.151 17
4.0	2.0	0.038 43	0.109 74
6.0	2.0	0.017 41	0.079 51
8.0	2.0	0.009 53	0.061 15
−8.0	4.0	−0.119 77	−0.108 15
−6.0	4.0	−0.126 29	−0.280 59
−4.0	4.0	0.117 44	−0.028 69
−2.0	4.0	−0.061 39	0.170 84
0.0	4.0	0.030 43	−0.133 47
2.0	4.0	0.136 89	−0.004 25
4.0	4.0	0.087 68	0.056 10
6.0	4.0	0.049 80	0.059 74
8.0	4.0	0.030 26	0.052 48
−8.0	6.0	0.028 22	−0.006 85
−6.0	6.0	0.312 46	0.094 71
−4.0	6.0	0.035 82	0.140 32
−2.0	6.0	0.077 19	−0.057 04
0.0	6.0	−0.101 02	0.046 26
2.0	6.0	0.000 95	−0.105 96
4.0	6.0	0.080 27	−0.042 78
6.0	6.0	0.072 56	0.007 00
8.0	6.0	0.052 99	0.025 05
−8.0	8.0	0.189 03	−0.060 47
−6.0	8.0	−0.169 49	0.136 30
−4.0	8.0	−0.096 71	−0.049 73
−2.0	8.0	−0.082 07	0.035 95
0.0	8.0	0.086 58	0.027 34
2.0	8.0	−0.084 96	0.024 92
4.0	8.0	−0.024 23	−0.076 23
6.0	8.0	0.038 87	−0.055 45
8.0	8.0	0.051 99	−0.021 48

Pearcey and Hill [10] computed values of $J_{\mathrm{PH}}(x, y) \equiv \pi J(x, y)$ using an early digital computer (see [22–24] for historical background). They evaluated $J_{\mathrm{PH}}(x, y)$ by summation of power-series expansions in x and y and from differential equations to which $J_{\mathrm{PH}}(x, y)$ is a solution, i.e. the numerical methods employed in [10] were completely different to ours. Pearcey and Hill reported contour plots for $|J_{\mathrm{PH}}(x, y)/\pi|$ and arg $J_{\mathrm{PH}}(x, y)$/deg on the grid

Table 2. Zeros of $J(x, y)$ for $x \geqslant -8.0$ and $0 \leqslant y \leqslant 8.0$. There is also a zero at $x \approx -8.012$ and $y \approx 6.072$. For each zero (x_z, y_z), there is a companion zero at $(x_z, -y_z)$.

x	y
Outside the caustic branches $8x^3 + 27y^2 = 0$	
−2.3219	2.6179
−3.5270	4.5952
−4.4512	6.2849
−5.2300	7.8182
Inside the caustic branches $8x^3 + 27y^2 = 0$	
−4.7565	1.4191
−5.7830	1.5267
−5.7881	3.0870
−6.6156	4.6046
−6.6368	3.1740
−6.8999	1.2130
−7.3281	6.0184
−7.3653	4.6730
−7.6762	1.3011
−7.6981	2.7084
−7.9639	7.3559

$-8.0 \leqslant x \leqslant 8.0$ and $0.0 \leqslant y \leqslant 8.0$. Our results in figure 2 for $\arg J(x, y)/\mathrm{deg}$ agree closely with those of [10]. However, for $|J(x, y)|$ (shown in figure 1), we only obtain agreement with [10] if the results in their contour plot for $|J_{\mathrm{PH}}(x, y)/\pi|$ are multiplied by $2/\pi$.

5. Concluding remarks

We have shown how $J(x, y)$ can be evaluated numerically using a modified version of the CUSPINT computer code. An essential requirement of our method is the ability to calculate $J_0(z)$ in the sector $0 \leqslant \arg z \leqslant \pi/8$. Provided this can be done, the method is straightforward to program on a computer and highly accurate results can be obtained.

It is also clear that our method can be applied to generalizations of $J(x, y)$. One such generalization, studied by Janssen [12], is the integral

$$I'_\alpha(x, y) = 2\int_0^\infty J_\alpha(yt)t^{\alpha+1}\exp\left[\mathrm{i}\left(t^4 + xt^2\right)\right]\mathrm{d}t \qquad -1 < \alpha < \tfrac{5}{2}$$

where $J_\alpha(\cdot)$ is the Bessel function of order α. Note, for $\alpha = 0$, we have

$$I'_0(x, y) = 2J(x, y)$$

and for $\alpha = -\frac{1}{2}$, we obtain

$$I'_{-1/2}(x, y) = \left(\frac{2}{\pi y}\right)^{1/2} P(x, y)$$

upon using the identity [13, p 88, equation (6.7)]

$$J_{-1/2}(yt) = [2/(\pi yt)]^{1/2}\cos(yt).$$

We have extended our computer code so that it can also handle the cases $\alpha = 1$ and 2, as well as $\alpha = 0$.

Janssen studied the asymptotic behaviour of $I'_\alpha(x, y)$ using arguments of Paris [14]. In particular, asymptotic expansions were obtained for $x \to \pm\infty$ and $y > 0$ (equations (8) and (9) of [12]). It is interesting to note that putting $\alpha = 0$, then $y = 0$ in the first term of Janssen's expansions gives us the asymptotic approximations (2.17) and (2.18). Thus Janssen's results may be more generally valid than has been assumed in their derivation.

Acknowledgment

The support of this research by the UK Engineering and Physical Sciences Research Council is gratefully acknowledged.

Appendix

This appendix derives the caustic associated with $J(x, y)$. The Bessel function $J_0(yt)$ has the integral representation [13, p 57, equation (4.3)]

$$J_0(yt) = \frac{1}{\pi}\int_0^\pi \exp(\mathrm{i}yt\cos\theta)\,\mathrm{d}\theta.$$

It follows from equation (1.2) that $J(x, y)$ can be written as the double integral

$$J(x, y) = \frac{1}{\pi}\int_0^\pi \mathrm{d}\theta \int_0^\infty \mathrm{d}t\, t \exp[\mathrm{i}f(x, y; t, \theta)]$$

where

$$f(x, y; t, \theta) = t^4 + xt^2 + yt\cos\theta.$$

The caustic in (x, y) parameter space is obtained by eliminating real values of t and θ from the stationary phase equations

$$\frac{\partial f}{\partial t} = 0 \qquad \text{and} \qquad \frac{\partial f}{\partial \theta} = 0$$

together with the Hessian determinantal equation

$$\begin{vmatrix} \dfrac{\partial^2 f}{\partial t^2} & \dfrac{\partial^2 f}{\partial t\,\partial\theta} \\ \dfrac{\partial^2 f}{\partial\theta\,\partial t} & \dfrac{\partial^2 f}{\partial\theta^2} \end{vmatrix} = 0.$$

For $f(x, y; t, \theta)$, these three equations become

$$4t^3 + 2xt + y\cos\theta = 0 \tag{A.1}$$

$$-yt\sin\theta = 0 \tag{A.2}$$

$$-yt\cos\theta\left(12t^2 + 2x\right) - y^2\sin^2\theta = 0. \tag{A.3}$$

The solutions of equation (A.2) are $y = 0$ or $t = 0$ or $\theta = 0$ or $\theta = \pi$. We do not have to consider for θ other multiples of π because they lie outside the range of integration. We consider each solution separately.

The solution $y = 0$. Equation (A.3) is satisfied since the left-hand side is zero. Equation (A.1) becomes

$$2t\left(2t^2 + x\right) = 0$$

which has the solutions $t = 0$ or $t^2 = -x/2$ (since t is real, this implies $x \leqslant 0$). Thus $\{y = 0, x \leqslant 0\}$ is part of the caustic. Note that for $t = 0$, the left-hand side of equations (A.1)–(A.3) are all identically zero. Also, the stationary phase points for the $y = 0$ solution are not isolated, since the above equations place no restriction on the value of θ.

The solution $t = 0$. Equation (A.1) becomes

$$y\cos\theta = 0 \tag{A.1$'$}$$

with solutions $\theta = \pi/2$ or $y = 0$ and equation (A.3) becomes

$$-y^2\sin^2\theta = 0 \tag{A.3$'$}$$

with solutions $\theta = 0, \pi$ or $y = 0$.

Since we have already discussed the $y = 0$ case, we will assume that $y \neq 0$. Now for $\theta = \pi/2$, equation (A.1$'$) is satisfied, but equation (A.3$'$) gives $y = 0$, which contradicts our assumption on y, i.e $y \neq 0$ is not possible, rather we must have $y = 0$ when $t = 0$. Consideration of equations (A.1$'$) and (A.3$'$) for $\theta = 0$ and π leads to the same conclusion.

The solution $\theta = 0$. Equation (A.1) becomes

$$4t^3 + 2xt + y = 0 \tag{A.1$''$}$$

whilst equation (A.3) gives

$$-yt\left(12t^2 + 2x\right) = 0. \tag{A.3$''$}$$

The solutions of equation (A.3$''$) are $y = 0$ or $t = 0$ (both of which have already been discussed) or $12t^2 + 2x = 0$, i.e. $t = \pm(-x/6)^{1/2}$. If we take the positive square root and substitute it into equation (A.1$''$), we obtain for the caustic branch

$$y = -(-2x/3)^{3/2} \qquad x \leqslant 0.$$

Similarly, using the negative square root, equation (A.1$''$) gives for the caustic branch

$$y = +(-2x/3)^{3/2} \qquad x \leqslant 0.$$

The solution $\theta = \pi$. The analysis for this case is very similar to $\theta = 0$ and leads to the same equations for the two caustic branches.

In summary, upon combining the above results, we find the equations for the branches of the caustic associated with $J(x, y)$ are

$$y = \pm(-2x/3)^{3/2} \qquad \text{and} \qquad y = 0 \qquad \text{for} \quad x \leqslant 0$$

which is the result quoted in section 4.

References

[1] Brillouin L 1916 Sur une méthode de calcul approchée de certaines intégrales dite méthode de col *Ann. Sci. École Norm. Sup. (Paris)* **33** 17–69

[2] Pearcey T 1946 The structure of an electromagnetic field in the neighbourhood of a cusp of a caustic *Phil. Mag.* **37** 311–7

[3] Connor J N L 1990 Practical methods for the uniform asymptotic evaluation of oscillatory integrals with several coalescing saddle points *Asymptotic and Computational Analysis, Conf. in Honor of Frank W J Olver's 65th Birthday* ed R Wong (New York: Dekker) pp 137–73

[4] Kirk N P, Connor J N L and Hobbs C A 2000 An adaptive contour code for the numerical evaluation of the oscillatory cuspoid canonical integrals and their derivatives *Comput. Phys. Commun.* at press

[5] Connor J N L and Curtis P R 1982 A method for the numerical evaluation of the oscillatory integrals associated with the cuspoid catastrophes: application to Pearcey's integral and its derivatives *J. Phys. A: Math. Gen.* **15** 1179–90

[6] Connor J N L and Farrelly D 1981 Theory of cusped rainbows in elastic scattering: uniform semiclassical calculations using Pearcey's integral *J. Chem. Phys.* **75** 2831–46

[7] Picht J 1925 1. Über den Schwingungsvorgang der einem beliebigen (astigmatischen) Strahlenbündel entspricht *Ann. Phys., Lpz.* **77** 685–782

[8] J Picht 1931 *Optische Abbildung Einführung in die Wellen- und Beugungstheorie Optischer Systeme* (Braunschweig: Vieweg)

[9] J J Stamnes 1986 *Waves in Focal Regions: Propagation, Diffraction and Focusing of Light, Sound and Water Waves* (Bristol: Hilger)

[10] Pearcey T and Hill G W 1963 Spherical aberrations of second order *The Effect of Aberrations upon the Optical Focus* (Melbourne: Commonwealth Scientific and Industrial Research Organization) pp 71–95

[11] Coene W and Jansen A J E M 1992 Image delocalisation and high resolution transmission electron microscopic imaging with a field emission gun *Scanning Microsc. Suppl.* **6** 379–403

[12] Janssen A J E M 1992 On the asymptotics of some Pearcey-type integrals *J. Phys. A: Math. Gen.* **25** L823–31

[13] Bowman F 1958 *Introduction to Bessel Functions* (New York: Dover)

[14] Paris R B 1991 The asymptotic behaviour of Pearcey's integral for complex variables *Proc. R. Soc.* A **432** 391–426

[15] Olver F W J 1984 Bessel functions of integer order *Pocketbook of Mathematical Functions* ed M Danos and J Rafelski (Thun: Harri Deutsch) (abridged edition of 1964 *Handbook of Mathematical Functions* ed M Abramowitz and I A Stegun (Washington, DC: US Govt Printing Office))

[16] Olver F W J 1997 *Asymptotics and Special Functions* (Wellesley, MA: Peters) p 54

[17] Connor J N L 1973 Semiclassical theory of molecular collisions: three nearly coincident classical trajectories *Mol. Phys.* **26** 1217–31

[18] Gautschi W 1984 Error function and Fresnel integrals *Pocketbook of Mathematical Functions* ed M Danos and J Rafelski (Thun: Harri Deutsch) (abridged edition of 1964 *Handbook of Mathematical Functions* ed M Abramowitz and I A Stegun (Washington, DC: US Govt Printing Office))

[19] Born M and Wolf E 1989 *Principles of Optics. Electromagnetic Theory of Propagation, Interference and Diffraction of Light* with contributions by A B Bhatia, P C Clemmow, D Gabor, A R Stokes, A M Taylor, P A Wayman and W L Wilcock, 6th corrected edn (Oxford: Pergamon)

[20] Ardill R W B and Moriarty K J M 1979 Accurate Bessel functions $J_n(z)$, $Y_n(z)$, $H_n^{(1)}(z)$ and $H_n^{(2)}(z)$ of integer order and complex argument *Comput. Phys. Commun.* **17** 321–36
Ardill R W B and Moriarty K J M 1986 *Comput. Phys. Commun.* **39** 303 (erratum)

[21] Kaminski D and Paris R B 1999 On the zeros of the Pearcey integral *J. Comput. Appl. Math.* **107** 31–52

[22] Beard M and Pearcey T 1984 The genesis of an early stored-program computer: CSIRAC *Ann. Hist. Comput.* **6** 106–15

[23] Pearcey T 1988 *A History of Australian Computing* (Caulfield East, Victoria: Chisholm Institute of Technology)

[24] Bennett J M, Broomham R, Murton P M, Pearcey T and Rutledge R W 1994 *Computing in Australia* (Sydney, NSW: Hale and Iremonger)