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1984 J. Phys. A: Math. Gen. 17 283

(http://iopscience.iop.org/0305-4470/17/2/016)

J. Phys. A: Math. Gen. 17 (1984) 283–310. Printed in Great Britain

The uniform asymptotic swallowtail approximation: practical methods for oscillating integrals with four coalescing saddle points

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Received 15 April 1983, in final form 8 August 1983

Abstract. Practical methods for the numerical implementation of the uniform swallowtail approximation have been developed. This approximation arises in the uniform asymptotic evaluation of oscillating integrals with four coalescing saddle points. A complex contour quadrature technique has been used to evaluate the swallowtail canonical integral $S(x, y, z)$ and its partial derivatives $\partial S/\partial x$, $\partial S/\partial y$, $\partial S/\partial z$. This method has the advantage that it is straightforward to implement on a computer and results of high accuracy are readily obtained. A comparison is made with other methods that have been reported in the literature for the evaluation of $S(x, y, z)$. Isometric plots of $|S(x, y, z)|$, $|\partial S/\partial x|$, $|\partial S/\partial y|$, $|\partial S/\partial z|$ are presented and some properties of the zeros of $S(0, y, z)$ that lie on the line $y=0$ are also discussed. Two methods for the evaluation of the mapping parameters (x, y, z) are described: an iterative method that is valid when (x, y, z) is not close to the swallowtail caustic and an algebraic method valid for (x, y, z) on the caustic and for $y=0$. Symbolic algebraic computer programs have been used to carry out the necessary algebraic manipulations. In practice both methods for determining (x, y, z) are complementary. An application of the uniform swallowtail approximation to the butterfly canonical integral has been made. The uniform asymptotic swallowtail approximation can now be regarded as a practical tool for the evaluation of oscillating integrals with four coalescing saddle points.

1. Introduction

An important step in many short wavelength scattering theories is the uniform asymptotic evaluation of oscillating integrals of the form

$$I(\boldsymbol{\alpha}) = \int_{-\infty}^{\infty} g(t) \exp[\mathrm{i} f(\boldsymbol{\alpha}; t)/\hbar] \, \mathrm{d}t, \qquad \hbar \to 0. \tag{1.1}$$

In (1.1), $g(t)$ and $f(\boldsymbol{\alpha}; t)$ are analytic functions of their arguments, and $\boldsymbol{\alpha} = (\alpha_1, \alpha_2, \ldots)$ is a set of real parameters. We shall also assume that $f(\boldsymbol{\alpha}; t)$ is real for real values of t. In addition $g(t)$ may depend on $\boldsymbol{\alpha}$ but this has not been indicated explicitly.

When asymptotic techniques are used to evaluate $I(\boldsymbol{\alpha})$, it is well known (Bleistein and Handelsman 1975) that the main contribution comes from regions around the

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0305-4470/84/020283 + 28$02.25

stationary phase or saddle points t_i of $f(\boldsymbol{\alpha}; t)$, which are defined by

$$\partial f(\boldsymbol{\alpha}; t)/\partial t = 0 \qquad \text{for } t = t_i(\boldsymbol{\alpha}), \qquad i = 1, 2, \ldots. \tag{1.2}$$

Equation (1.2) shows that the positions of the saddle points depend on $\boldsymbol{\alpha}$, and so can move close together or coalesce as $\boldsymbol{\alpha}$ varies. When this coalescence is allowed for in the uniform asymptotic integration, the result is expressed in terms of certain *canonical integrals* and their partial derivatives (Ludwig 1966, Bleistein 1967, Rice 1968, Ursell 1972, Connor 1974). Each canonical integral is characteristic of a given number of coalescing saddle points.

The present paper is concerned with the case of three real parameters and four (real or complex) saddle points. The canonical integral is then given by

$$S(x, y, z) = \int_{-\infty}^{\infty} \exp[\mathrm{i}(u^5 + xu^3 + yu^2 + zu)]\, \mathrm{d}u \tag{1.3}$$

with x, y and z real, and its partial derivatives are

$$\frac{\partial S(x, y, z)}{\partial x} = \mathrm{i} \int_{-\infty}^{\infty} u^3 \exp[\mathrm{i}(u^5 + xu^3 + yu^2 + zu)]\, \mathrm{d}u, \tag{1.4}$$

$$\frac{\partial S(x, y, z)}{\partial y} = \mathrm{i} \int_{-\infty}^{\infty} u^2 \exp[\mathrm{i}(u^5 + xu^3 + yu^2 + zu)]\, \mathrm{d}u, \tag{1.5}$$

$$\frac{\partial S(x, y, z)}{\partial z} = \mathrm{i} \int_{-\infty}^{\infty} u \exp[\mathrm{i}(u^5 + xu^3 + yu^2 + zu)]\, \mathrm{d}u. \tag{1.6}$$

The exponent in the integrands of (1.3)–(1.6) is the universal unfolding of the swallowtail catastrophe in elementary catastrophe theory (Thom 1975, Poston and Stewart 1978, Saunders 1980, Gilmore 1981) and we shall therefore call $S(x, y, z)$ the *swallowtail canonical integral.* Although we shall be using the language of elementary catastrophe theory throughout this paper, it is important to note that all the uniform asymptotic expansions for the integral (1.1) were originally obtained without the help of catastrophe theory (Ludwig 1966, Bleistein 1967, Rice 1968, Ursell 1972, Connor 1974).

The purpose of this paper is to describe methods that can be used in the numerical implementation of the uniform swallowtail approximation. In § 2, we present (to lowest order) the explicit expression for the uniform swallowtail approximation. This expression shows that there are three problems that must be overcome in practice before we can numerically apply the swallowtail approximation to any given problem. *Firstly,* we must evaluate $S(x, y, z)$, $\partial S/\partial x$, $\partial S/\partial y$ and $\partial S/\partial z$ accurately and efficiently for many values of (x, y, z). For example the isometric plots shown later in figures 3–5 require 175692 evaluations of these integrals. *Secondly,* we need techniques for expressing the arguments x, y and z of the swallowtail integral in terms of the exponent $f(\boldsymbol{\alpha}; t)$ of (1.1). *Thirdly,* the terms that multiply $S(x, y, z)$ and its partial derivatives must be calculated from the pre-exponential factor $g(t)$ in (1.1). We will see in § 2 that this third problem is the easiest one to solve.

In § 3, we show that a quadrature method recently developed by two of us (Connor and Curtis 1982) can be used for the accurate numerical evaluation of $S(x, y, z)$ and its partial derivatives. We present isometric plots of $|S(x, y, z)|$, $|\partial S/\partial x|$, $|\partial S/\partial y|$ and $|\partial S/\partial z|$ to illustrate some of the properties of these integrals. For $S(x, y, z)$ we also compare our results with those obtained by Pearcey and Hill (1963), Wright (1977), Dronov *et al* (1978) and Pope (1981). In addition we discuss some properties of the zeros of $S(0, y, z)$.

Section 4 considers the problem of obtaining the arguments of the swallowtail integral from $f(\boldsymbol{\alpha}; t)$. Two methods are described for solving this problem. The first method is an iterative scheme similar to that employed previously in our calculations for the uniform Pearcey approximation (Connor 1973, Connor and Farrelly 1981). The second method is more algebraic in nature and exploits results from the theory of equations and the theory of symmetric polynomials. We have used several symbolic algebraic computer programs to carry out the necessary algebraic manipulations. In order to illustrate the methods developed in this paper, we consider in § 5 the asymptotic evaluation of the butterfly canonical integral. Our conclusions are in § 6.

The swallowtail canonical integral (1.3) plays an important role in several short wavelength phenomena including the elastic, inelastic and reactive scattering of atoms and molecules (Connor 1974, 1976, Connor *et al* 1982, Dickinson and Richards 1982), collisional broadening in molecular orbital x-ray spectra (Fritsch and Wille 1978), heavy nuclear ion collisions (Da Silveira 1978, Crowley 1980), the asymptotic evaluation of path integrals (Levit and Smilansky 1977, Dangelmayr and Veit 1979, Schulman 1981), optical caustics (Lee 1983, Berry and Upstill 1980, Stewart 1981, Hannay 1982, 1983), the theory of inverse scattering (Dangelmayr and Güttinger 1982), the propagation of radio waves (Lukin and Palkin 1976, 1978, Dronov *et al* 1978, Arnold 1982), bound-continuum matrix elements (Krüger 1981), non-adiabatic transitions (Vartanyan 1980), synchro-Compton radiation of relativistic electrons (Leubner 1981a, b, 1982), as well as in general theories of high frequency scattering (Pearcey 1963, Kravtsov 1967, 1968, Maslov 1972, Maslov and Fedoriuk 1981, Guillemin and Sternberg 1977, Gorman *et al* 1981, Arnold 1978, Peslyak 1981), see also Barrett (1978). However, none of these works make any numerical applications of the uniform swallowtail approximation, the only exception being the very recent papers of Leubner (1981b, 1982). However in his applications the saddle points are always complex, so we necessarily have $t_1 = t_3^*$ and $t_2 = t_4^*$, and there are also additional symmetry restrictions on their positions which help simplify the numerical treatment. In contrast, the techniques we shall describe in this paper apply for any configuration of the saddle points, in particular for cases where there are two or four real saddle points. These cases give rise to the most interesting structure in $S(x, y, z)$ and its derivatives.

2. Uniform asymptotic expansion

In this section we give to lowest order the uniform asymptotic expansion for the integral (1.1) when $f(\boldsymbol{\alpha}; t)$ possesses four saddle points. From equation (3.8) of Connor (1976), we have for $\hbar \to 0$

$$I(\boldsymbol{\alpha}) \sim \exp(\mathrm{i}A/\hbar) \sum_{k=0}^{3} \hbar^{(k+1)/5} q_k U_k(\hbar^{-2/5}x, \hbar^{-3/5}y, \hbar^{-4/5}z) \tag{2.1}$$

where $U_k(x, y, z)$ denotes the integral

$$U_k(x, y, z) = \int_{-\infty}^{\infty} u^k \exp[\mathrm{i}(u^5 + xu^3 + yu^2 + zu)]\, \mathrm{d}u, \qquad k = 0, 1, 2, 3. \tag{2.2}$$

It is evident that $U_k(x, y, z)$ for $k=0$, 1, 2, 3 are proportional to the swallowtail integral (1.3) and its partial derivatives (1.4)–(1.6).

The parameters x, y, z and A in (2.1) are obtained from the *nonlinear* set of equations

$$f(\boldsymbol{\alpha}; t_i) = u_i^5 + xu_i^3 + yu_i^2 + zu_i + A, \qquad i = 1, 2, 3, 4, \tag{2.3}$$

where the u_i for $i = 1$, 2, 3, 4 are the roots of the quartic equation

$$5u^4 + 3xu^2 + 2yu + z = 0. \tag{2.4}$$

We also assume that the t_i and $f(\boldsymbol{\alpha}; t_i)$ on the left-hand side (LHS) of (2.3) are known.

The saddle points t_i and u_i are labelled so that

$$f(\boldsymbol{\alpha}; t) = u^5 + xu^3 + yu^2 + zu + A \tag{2.5}$$

defines a local one-to-one uniformly analytic change of variables from t to $u = u(\boldsymbol{\alpha}; t)$. The new parameters x, y, z and A are functions of $\boldsymbol{\alpha}$ but not of t. It is important to note that the local change of variables (2.5) is exact and not a truncated Taylor expansion. The correct labelling of the $\{u_i\}$ can usually be done by inspection, for example by examining the paths of the $\{t_i(\boldsymbol{\alpha})\}$ in the complex t plane as $\boldsymbol{\alpha}$ varies. Sometimes it is also useful to inspect the Taylor expansion of $f(\boldsymbol{\alpha}; t)$ to fifth order since then the complex t and u planes become identical up to a scale transformation.

The final set of unknowns in (2.1) that we must determine is q_k for $k = 0$, 1, 2, 3. These quantities are obtained from the *linear* equations (Connor 1976)

$$g(t_i)\left(\frac{20u_i^3 + 6xu_i + 2y}{\partial^2 f(\boldsymbol{\alpha}; t)/\partial t^2|_{t=t_i}}\right)^{1/2} = q_0 + q_1 u_i + q_2 u_i^2 + q_3 u_i^3, \qquad i = 1, 2, 3, 4. \tag{2.6}$$

Since the LHS of (2.6) is assumed to be known, we can readily solve these four linear equations to obtain the q_k. The only point of numerical difficulty occurs when two or more saddle points have coalesced. In this situation the LHS of (2.6) becomes numerically indeterminate, being of the form $(0/0)^{1/2}$. The simplest way to avoid this difficulty is to return to the original integral (1.1) and Taylor expand $f(\boldsymbol{\alpha}; t)$ and $g(t)$ about the point of coalescence of the saddle points, thereby obtaining a *transitional* approximation to $I(\boldsymbol{\alpha})$ (Connor 1976). This transitional approximation is numerically satisfactory for values of t very close to, or at, the point of coalescence. The transitional approximation does not destroy the uniform nature of the expansion (2.1) but rather is contained within it as a special case. Since the determination of the q_k is in principle straightforward, we do not consider this problem any further. It should also be remembered that the derivation of the uniform expansion (2.1) assumes that $g(t)$ does not possess any zeros or other singularities close to the saddle points.

Finally we note that essentially the same expansion (2.1) applies to a class of multidimensional integrals of the form (see § 5 of Connor 1974)

$$I(\boldsymbol{\alpha}) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty} g(t_1, t_2, \ldots, t_n) \exp[\mathrm{i}f(\boldsymbol{\alpha}; t_1, t_2, \ldots, t_n)/\hbar]\, \mathrm{d}t_1\, \mathrm{d}t_2 \ldots \mathrm{d}t_n$$

$$\equiv \int_{-\infty}^{\infty} g(\boldsymbol{t}) \exp[\mathrm{i}f(\boldsymbol{\alpha}; \boldsymbol{t})/\hbar]\, \mathrm{d}\boldsymbol{t}. \tag{2.7}$$

Suppose that $f(\boldsymbol{\alpha}; \boldsymbol{t})$ has four saddle points which coalesce at $\boldsymbol{t}^{(0)}$ for $\boldsymbol{\alpha} = \boldsymbol{\alpha}_0$ and assume that the corank of $f(\boldsymbol{\alpha}_0; \boldsymbol{t}^{(0)})$ is 1, i.e. the rank of the Hessian matrix $[\partial^2 f(\boldsymbol{\alpha}_0; \boldsymbol{t}^{(0)})/\partial t_i\, \partial t_j]$ is $n-1$. Then for $(\boldsymbol{\alpha}, \boldsymbol{t})$ close to $(\boldsymbol{\alpha}_0, \boldsymbol{t}^{(0)})$, we can make the exact local change of variables defined by

$$f(\boldsymbol{\alpha}; \boldsymbol{t}) = u_1^5 + xu_1^3 + yu_1^2 + zu_1 + A + Q(u_2, u_3, \ldots, u_n) \tag{2.8}$$

where $Q(u_2, u_3, \ldots, u_n)$ is a Morse function in the remaining $n-1$ variables. These variables can now be removed by integration and the problem reduces to a one-dimensional integral of the type (1.1) (for more details see Connor (1974, 1976)).

3. Calculation of $S(x, y, z)$ and its partial derivatives

In this section, we describe an efficient method for the numerical evaluation of $S(x, y, z)$, $\partial S/\partial x$, $\partial S/\partial y$ and $\partial S/\partial z$, and discuss the results we have obtained.

3.1. Numerical calculations

We have recently described a quadrature method for the evaluation of the oscillating integrals associated with the cuspoid catastrophes (Connor and Curtis 1982). It is this method we have applied to $S(x, y, z)$ and its partial derivatives.

We explain our implementation of the method for $S(x, y, z)$, the treatment for $\partial S/\partial x$, $\partial S/\partial y$, $\partial S/\partial z$ being similar. First we write $S(x, y, z)$ as the sum of the following two integrals:

$$S(x, y, z) = \int_0^\infty \exp[\mathrm{i}(u^5 + xu^3 + yu^2 + zu)]\,\mathrm{d}u + \int_0^\infty \exp[\mathrm{i}(-u^5 - xu^3 + yu^2 - zu)]\,\mathrm{d}u. \tag{3.1}$$

Next we exploit Cauchy's theorem and Jordan's lemma to write (3.1) in the form

$$S(x, y, z) = \int_{\Gamma_+} \exp[\mathrm{i}(u^5 + xu^3 + yu^2 + zu)]\,\mathrm{d}u + \int_{\Gamma_-} \exp[\mathrm{i}(-u^5 - xu^3 + yu^2 - zu)]\,\mathrm{d}u \tag{3.2}$$

where the integration contours Γ_+ and Γ_- are shown in figure 1. The contour Γ_+, for example, proceeds from the origin to a point R on the real u axis, then along an arc of a circle to the point $R\exp(\mathrm{i}\pi/10)$ and finally out to $\infty\exp(\mathrm{i}\pi/10)$.

By choosing R sufficiently large, the infinite integrals along $\Gamma_\pm$ from $R\exp(\pm\mathrm{i}\pi/10)$ to $\infty\exp(\pm\mathrm{i}\pi/10)$ can be made negligibly small. We accomplished this by choosing R to be the largest real root of (Connor and Curtis 1982)

$$r^5 + x\sin(3\pi/10)r^3 + y\sin(2\pi/10)r^2 + z\sin(\pi/10)r - 100 = 0. \tag{3.3}$$

This choice ensures that the modulus of the integrands of the infinite integrals are less than e^{-100}.

In a previous application of this quadrature method to Pearcey's integral (Connor and Curtis 1982), we used 16-point gaussian integration to evaluate the remaining two finite integrals. For the present application, we again employed gaussian integration for the integration from $(R, 0)$ to $R\exp(\pm\mathrm{i}\pi/10)$, but for the integral from $(0, 0)$ to $(R, 0)$ we used an adaptive integrator, which is especially suited for oscillating non-singular integrands and which has recently become available in the Numerical Algorithms Group Library (1981a).

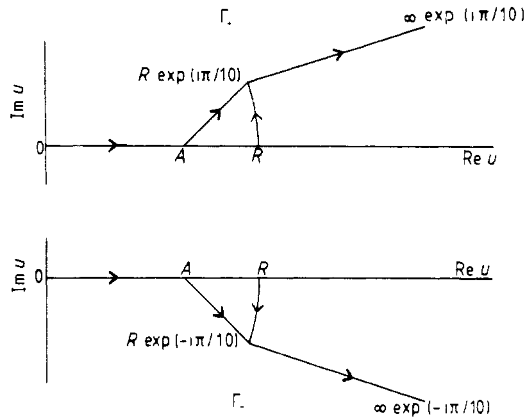

Figure 1. Integration contours in the complex u plane for the numerical evaluation of the swallowtail canonical integral and its partial derivatives.

In addition, it was found that the efficiency of the integration method could be improved by a 'corner cutting' technique (Connor and Curtis 1982). In this the integration along the arc from $(R, 0)$ to $R\exp(\pm i\pi/10)$ is replaced by an integration along a straight line from $(A, 0)$ to $R\exp(\pm i\pi/10)$ where $0<A<R$. Empirically the choice $A=(1.5+R)/2$ was found to be satisfactory. This alternative corner cutting contour is also shown in figure 1.

By means of the techniques just described, we were able to calculate $S(x, y, z)$, $\partial S/\partial x$, $\partial S/\partial y$ and $\partial S/\partial z$ to at least seven figure accuracy over the grid $-10<x<10$, $0\leqslant y<10$ and $-10<z<10$. Note that we need only carry out calculations for $y\geqslant 0$, because of the relation

$$S(x, -y, z)=S^*(x, y, z). \tag{3.4}$$

We checked the accuracy of our computations in three ways.

(a) For small x, y and z, we numerically summed the exact series representation for $S(x, y, z)$ (Connor 1974, Connor *et al* 1983), which is given by

$$\begin{aligned} S(x, y, z)=\tfrac{1}{5}\sum_{l=0}^{\infty}\sum_{m=0}^{\infty}\sum_{n=0}^{\infty}\frac{z^l}{l!}\frac{y^m}{m!}\frac{x^n}{n!}\Gamma[(1+l+2m+3n)/5] \\ \times\{\exp[i(1+6l+7m+8n)\pi/10] \\ +(-1)^m\exp[-i(1+6l+7m+8n)\pi/10]\}. \end{aligned} \tag{3.5}$$

The series representation (3.5) converges for all x, y and z and on differentiation, the series representations for $\partial S/\partial x$, $\partial S/\partial y$ and $\partial S/\partial z$ are obtained. We always obtained agreement to at least seven significant figures between the results from the quadrature method and the series representation.

(b) In another paper (Connor *et al* 1983), we have developed a differential equation method for the numerical evaluation of $S(x, y, z)$, $\partial S/\partial x$, $\partial S/\partial y$ and $\partial S/\partial z$. This method integrates a set of coupled ordinary differential equations satisfied by $S(x, y, z)$. The method is numerically stable for values of (x, y, z) inside the tail of the swallowtail caustic (see figure 2), but eventually becomes numerically unstable outside this region. In the region of numerical stability, the differential equation and quadrature methods always agreed to at least five significant figures.

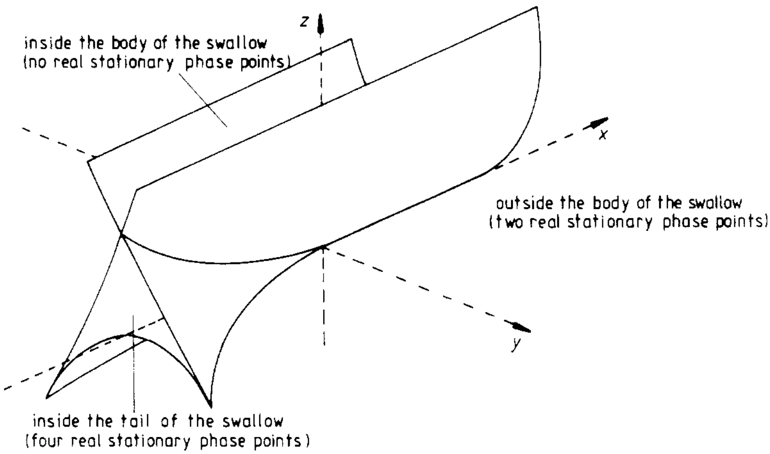

Figure 2. The caustic for the swallowtail catastrophe.

(c) For the integral

$$F(z) = (2\pi)^{-1} \int_{-\infty}^{\infty} \exp[\mathrm{i}(t^5/5 + zt)]\,\mathrm{d}t \tag{3.6}$$

Krüger (1981) has given the asymptotic trapezoid formula

$$F(z) \sim h \sum_{k=0}^{N} \phi[h(k+\tfrac{1}{2})] \tag{3.7}$$

where h is the step length and

$$\phi(t) = \pi^{-1} \exp(-\alpha^5/5 - z\alpha - \alpha t^4 + 2\alpha^3 t^2) \cos[t^5/5 - 2\alpha^2 t^3 + (\alpha^4 + z)t] \tag{3.8}$$

with $\alpha > 0$. We used values of $\alpha = 1$, $h = 0.1$ and N up to 40, obtaining agreement to at least eight significant figures with our quadrature method when $-17.0 < z < 17.0$. Note that $S(0, 0, z)$ and $F(z)$ are related by

$$S(0, 0, z) = (2\pi/5^{1/5})F(z/5^{1/5}). \tag{3.9}$$

Finally we remark that $S(x, y, z)$ can be expressed in terms of Airy–Hardy integrals of order five (Watson 1966) for the special case $x = 5\alpha$, $y = 0$ and $z = 5\alpha^2$.

3.2. Results

In tables 1 and 2, we report numerical values of $S(x, y, z)$, $\partial S/\partial x$, $\partial S/\partial y$ and $\partial S/\partial z$ for x, y, z in the range $-8.0 \leqslant x \leqslant 4.0$, $0 \leqslant y \leqslant 8.0$ and $-4.0 \leqslant z \leqslant 8.0$. Note that $S(x, 0, z)$, $\partial S(x, 0, z)/\partial x$ and $\partial S(x, 0, z)/\partial z$ are purely real whereas $\partial S/\partial y$ for $y = 0$ is purely imaginary. The values in tables 1 and 2 are not suitable for interpolation purposes, rather they are given so that readers can check the accuracy of their own computer programs when using the present quadrature technique or some other numerical method.

Figures 3–5 show isometric plots of $|S(x, y, z)|$, $|\partial S/\partial x|$, $|\partial S/\partial y|$ and $|\partial S/\partial z|$ for $x = 4$, 0, -6 respectively. These figures, together with those for the y and z sections shown in Connor *et al* (1983), illustrate in a systematic manner the main properties

Table 1. Values of the swallowtail canonical integral $S(x, y, z)$ and its derivative $\partial S/\partial x$. Note that these values are not suitable for interpolation purposes.

x	y	z	Re $S(x, y, z)$	Im $S(x, y, z)$	Re $\partial S/\partial x$	Im $\partial S/\partial x$
−8.0	0.0	−4.0	−0.127 926	0.0	−3.953 975	0.0
−8.0	0.0	0.0	0.834 808	0.0	5.137 042	0.0
−8.0	0.0	4.0	1.399 509	0.0	−4.122 258	0.0
−8.0	0.0	8.0	−1.242 289	0.0	0.022 815	0.0
−8.0	4.0	−4.0	0.335 222	0.140 466	−2.173 409	−3.352 497
−8.0	4.0	0.0	0.445 859	−0.100 687	1.025 633	0.683 959
−8.0	4.0	4.0	1.028 569	0.448 795	2.378 969	−1.470 893
−8.0	4.0	8.0	0.103 103	−0.960 347	−1.490 439	4.543 323
−8.0	8.0	−4.0	0.272 153	−0.918 526	−0.882 258	−1.432 001
−8.0	8.0	0.0	1.252 635	0.597 791	4.711 406	0.129 286
−8.0	8.0	4.0	0.342 893	−0.942 189	0.133 977	2.727 696
−8.0	8.0	8.0	0.249 568	−0.378 296	2.439 104	−2.714 808
−4.0	0.0	−4.0	0.499 340	0.0	−2.692 013	0.0
−4.0	0.0	0.0	1.292 366	0.0	−2.668 336	0.0
−4.0	0.0	4.0	1.762 313	0.0	−2.139 382	0.0
−4.0	0.0	8.0	0.283 634	0.0	1.076 655	0.0
−4.0	4.0	−4.0	−0.269 035	−0.774 994	−1.310 667	−1.907 003
−4.0	4.0	0.0	0.871 603	0.795 804	−2.105 000	1.009 805
−4.0	4.0	4.0	0.287 285	−0.050 953	−0.041 723	1.888 670
−4.0	4.0	8.0	−0.443 670	−0.387 741	0.710 333	1.500 717
−4.0	8.0	−4.0	0.863 798	0.381 639	1.895 486	0.091 227
−4.0	8.0	0.0	0.674 440	0.405 010	−0.386 186	−2.009 470
−4.0	8.0	4.0	0.441 549	−0.070 475	−1.930 586	0.514 006
−4.0	8.0	8.0	0.043 569	−0.349 045	0.254 491	1.928 173
0.0	0.0	−4.0	−0.650 212	0.0	0.758 251	0.0
0.0	0.0	0.0	1.746 461	0.0	−0.442 899	0.0
0.0	0.0	4.0	−0.018 329	0.0	0.103 036	0.0
0.0	0.0	8.0	−0.000 200	0.0	−0.005 828	0.0
0.0	4.0	−4.0	0.934 004	0.207 328	0.808 996	−0.230 302
0.0	4.0	0.0	0.246 876	0.945 782	0.464 762	0.659 704
0.0	4.0	4.0	0.648 861	−0.768 462	−0.536 053	0.049 610
0.0	4.0	8.0	−0.145 050	0.133 417	0.132 543	−0.111 015
0.0	8.0	−4.0	0.268 911	0.178 526	−0.011 252	1.224 533
0.0	8.0	0.0	0.088 816	0.374 295	−0.252 956	1.129 520
0.0	8.0	4.0	0.300 086	−0.093 529	−0.745 858	0.766 520
0.0	8.0	8.0	0.318 946	−1.137 172	−1.019 773	−0.353 428
4.0	0.0	−4.0	0.977 637	0.0	0.088 131	0.0
4.0	0.0	0.0	0.969 252	0.0	−0.077 223	0.0
4.0	0.0	4.0	0.145 824	0.0	0.015 940	0.0
4.0	0.0	8.0	0.006 031	0.0	0.003 855	0.0
4.0	4.0	−4.0	0.178 618	0.323 542	0.125 541	0.276 008
4.0	4.0	0.0	1.167 437	0.327 591	−0.083 282	−0.148 715
4.0	4.0	4.0	0.188 905	−0.247 068	0.004 864	0.052 835
4.0	4.0	8.0	−0.019 771	−0.018 961	0.009 778	−0.007 565
4.0	8.0	−4.0	0.923 594	0.203 421	0.027 546	−0.538 384
4.0	8.0	0.0	0.145 392	0.856 692	0.343 326	0.280 580
4.0	8.0	4.0	0.868 786	−0.428 015	−0.253 788	−0.084 391
4.0	8.0	8.0	−0.210 106	−0.126 207	0.089 696	0.033 892

Table 2. Values of the derivatives of the swallowtail canonical integral $\partial S/\partial y$ and $\partial S/\partial z$. Note that these values are not suitable for interpolation purposes.

x	y	z	Re $\partial S/\partial y$	Im $\partial S/\partial y$	Re $\partial S/\partial z$	Im $\partial S/\partial z$
−8.0	0.0	−4.0	0.0	−1.541 981	−0.711 633	0.0
−8.0	0.0	0.0	0.0	0.275 967	1.263 724	0.0
−8.0	0.0	4.0	0.0	1.571 155	−1.076 744	0.0
−8.0	0.0	8.0	0.0	−2.640 845	−0.367 763	0.0
−8.0	4.0	−4.0	−1.182 796	0.848 992	−0.416 318	−0.659 324
−8.0	4.0	0.0	0.696 370	−2.161 289	0.447 043	0.155 905
−8.0	4.0	4.0	0.582 336	1.860 085	0.247 886	−0.290 777
−8.0	4.0	8.0	0.582 916	0.004 567	−0.166 810	0.928 174
−8.0	8.0	−4.0	2.371 367	−0.350 475	0.409 847	−0.342 089
−8.0	8.0	0.0	−0.147 618	1.183 267	0.829 056	0.555 834
−8.0	8.0	4.0	2.546 623	−0.363 666	0.933 649	0.410 654
−8.0	8.0	8.0	0.027 618	0.775 058	0.518 804	−0.836 967
−4.0	0.0	−4.0	0.0	0.986 215	−0.916 172	0.0
−4.0	0.0	0.0	0.0	0.839 926	−0.817 108	0.0
−4.0	0.0	4.0	0.0	1.966 182	−1.750 736	0.0
−4.0	0.0	8.0	0.0	1.118 637	1.210 015	0.0
−4.0	4.0	−4.0	1.257 383	−0.580 895	−0.046 769	−0.985 828
−4.0	4.0	0.0	0.090 366	−0.581 570	−1.043 621	0.591 813
−4.0	4.0	4.0	0.122 079	−0.857 428	0.059 691	0.393 398
−4.0	4.0	8.0	−0.293 065	−0.939 458	−0.029 873	0.607 063
−4.0	8.0	−4.0	−1.198 412	0.105 875	0.380 754	0.342 982
−4.0	8.0	0.0	0.189 405	0.965 747	−0.119 055	−0.531 297
−4.0	8.0	4.0	0.967 928	−0.249 592	−0.479 674	0.021 106
−4.0	8.0	8.0	−0.090 752	−0.968 101	−0.081 688	0.416 393
0.0	0.0	−4.0	0.0	−0.760 029	0.930 533	0.0
0.0	0.0	0.0	0.0	0.350 130	−0.521 521	0.0
0.0	0.0	4.0	0.0	−0.130 615	−0.077 957	0.0
0.0	0.0	8.0	0.0	0.007 450	0.004 685	0.0
0.0	4.0	−4.0	−0.653 688	0.434 653	0.622 351	0.132 002
0.0	4.0	0.0	−0.490 979	−0.638 989	0.351 794	0.492 871
0.0	4.0	4.0	0.589 899	0.042 989	−0.711 305	−0.230 270
0.0	4.0	8.0	−0.174 125	0.043 096	0.181 630	0.049 547
0.0	8.0	−4.0	−0.056 481	−0.757 639	−0.026 670	0.659 286
0.0	8.0	0.0	0.143 347	−0.794 665	−0.112 713	0.523 013
0.0	8.0	4.0	0.511 061	−0.533 516	−0.350 187	0.261 236
0.0	8.0	8.0	0.921 990	0.314 171	−0.947 274	−0.273 923
4.0	0.0	−4.0	0.0	0.266 933	0.486 345	0.0
4.0	0.0	0.0	0.0	0.015 740	−0.284 722	0.0
4.0	0.0	4.0	0.0	−0.047 945	−0.092 998	0.0
4.0	0.0	8.0	0.0	−0.005 048	−0.005 815	0.0
4.0	4.0	−4.0	−0.188 915	−0.252 703	0.228 719	0.584 494
4.0	4.0	0.0	0.029 348	0.211 804	−0.096 172	−0.365 880
4.0	4.0	4.0	0.040 790	−0.088 672	−0.173 936	0.059 412
4.0	4.0	8.0	−0.016 560	−0.004 665	0.006 384	0.021 492
4.0	8.0	−4.0	−0.071 676	0.511 466	0.013 028	−0.337 563
4.0	8.0	0.0	−0.381 472	−0.326 117	0.394 706	0.321 830
4.0	8.0	4.0	0.298 342	0.167 870	−0.401 209	−0.349 319
4.0	8.0	8.0	−0.084 492	−0.096 365	0.024 153	0.175 803

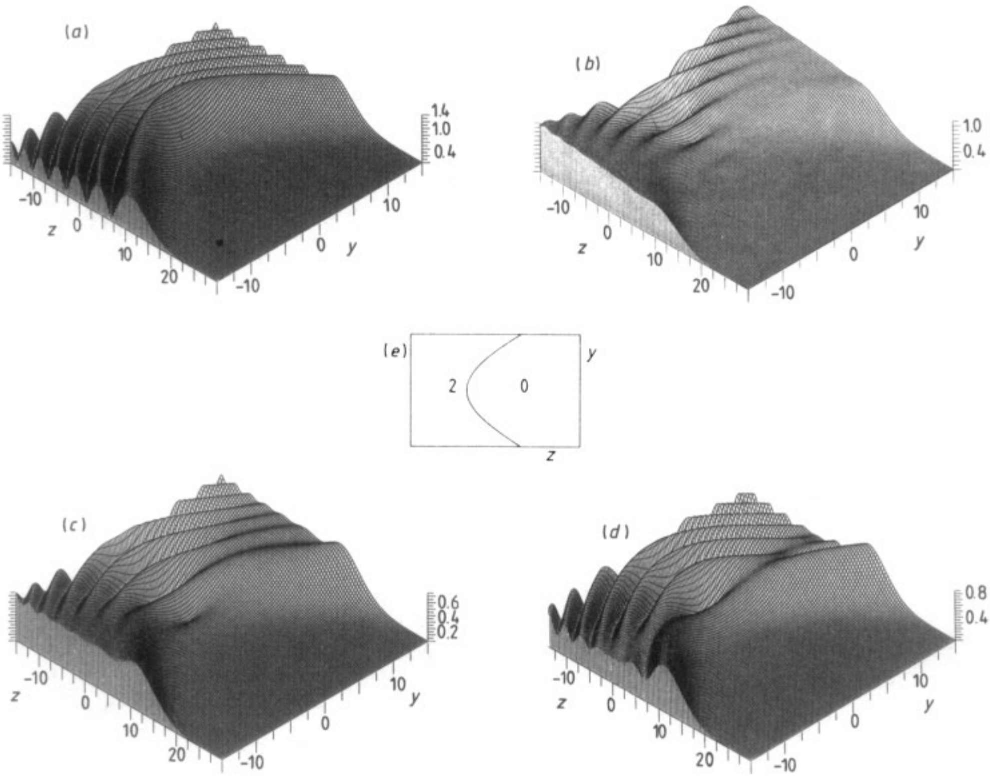

Figure 3. Isometric plots of (a) $|S(x, y, z)|$, (b) $|\partial S/\partial x|$, (c) $|\partial S/\partial y|$ and (d) $|\partial S/\partial z|$ for $x=4$. The numbers on the caustic section (e) are the number of real stationary phase points in different regions of (x, y, z) space.

of the modulus of $S(x, y, z)$ and its derivatives. We also show in figures 3–5 the appropriate x sections of the swallowtail caustic of figure 2.

The swallowtail caustic plays an important role in rationalising the structure in the isometric plots. It is obtained by eliminating real u from the equations

$$5u^4+3xu^2+2yu+z=0, \tag{3.10}$$

$$20u^3+6xu+2y=0. \tag{3.11}$$

Equation (3.10) with u real or complex also defines the number of real (and hence complex conjugate) stationary phase points in different regions of (x, y, z) space. The number of real stationary phase points is indicated in figure 2, which also defines the regions 'inside the body of the swallow', 'outside the body of the swallow' and 'inside the tail of the swallow'.

Equation (3.11) is the condition for two or more of these stationary phase points to be equal. Using the standard formula for the discriminant of a fourth-degree polynomial (Ferrar 1943, Shafee and Shafee 1978), we obtain

$$81x^4z-27x^3y^2-360x^2z^2+540xy^2z-135y^4+400z^3=0. \tag{3.12}$$

Equation (3.12) shows explicitly that the swallowtail caustic is symmetric about $y=0$. The caustic surface in figure 2 is defined by the condition that two or more *real* roots

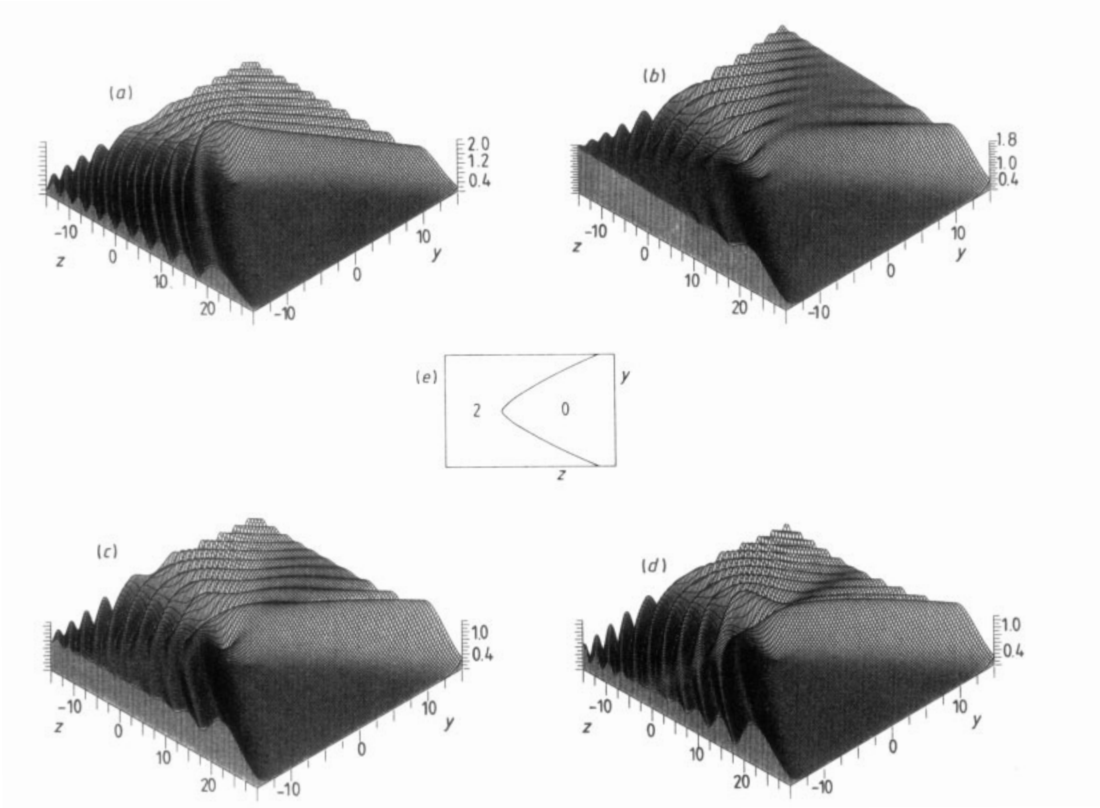

Figure 4. Same as figure 3 except for $x=0$.

of (3.10) are equal, whereas (3.12) also includes the possibility that two *complex* roots are equal. This possibility occurs on the line $y=0$, $x=2(5z)^{1/2}/3$, $z>0$ which is the 'complex whisker' mentioned by Poston and Stewart (1976) and Wright (1981). The line $y=0$, $x=-2(5z)^{1/2}/3$, $z>0$ on the other hand corresponds to the coalescence of two pairs of real roots and is the line of self-intersection of the caustic in figure 2.

The trends revealed in figures 3–5 are similar to those discussed in detail in Connor *et al* (1983). It should also be noticed that the folds in the integrals are damped out for a given x in the order $|S(x, y, z)| \to |\partial S/\partial z| \to |\partial S/\partial y| \to |\partial S/\partial x|$ as $|y|$ increases from $y=0$.

Another interesting property of $S(x, y, z)$ is its zeros which occur on lines in (x, y, z) space. We shall consider the zeros of $S(0, y, z)$ in more detail. Because the zeros of $S(0, y, z)$ cannot be seen in figure 4, we show in figure 6 an isometric plot of $\ln|S(0, y, z)|$ for $0 \leq y \leq 8.0$ and $-20.0 \leq z \leq 20.0$. The zeros of $S(0, y, z)$ can be clearly seen lying along the line $y=0$. Notice that the isometric plot shows no numerical irregularities even for values of $|S(0, 0, z)|$ as small as 10^{-8}. This demonstrates the high accuracy of our quadrature method.

In table 3 we report the positions of 12 zeros of $S(0, 0, z)$ that lie on either side of $z=0$. We calculated the zeros by a continuation method based on a secant iteration (Numerical Algorithms Group 1981b). This method allows the zeros to be calculated to an accuracy of about seven significant figures when used in conjunction with our quadrature method.

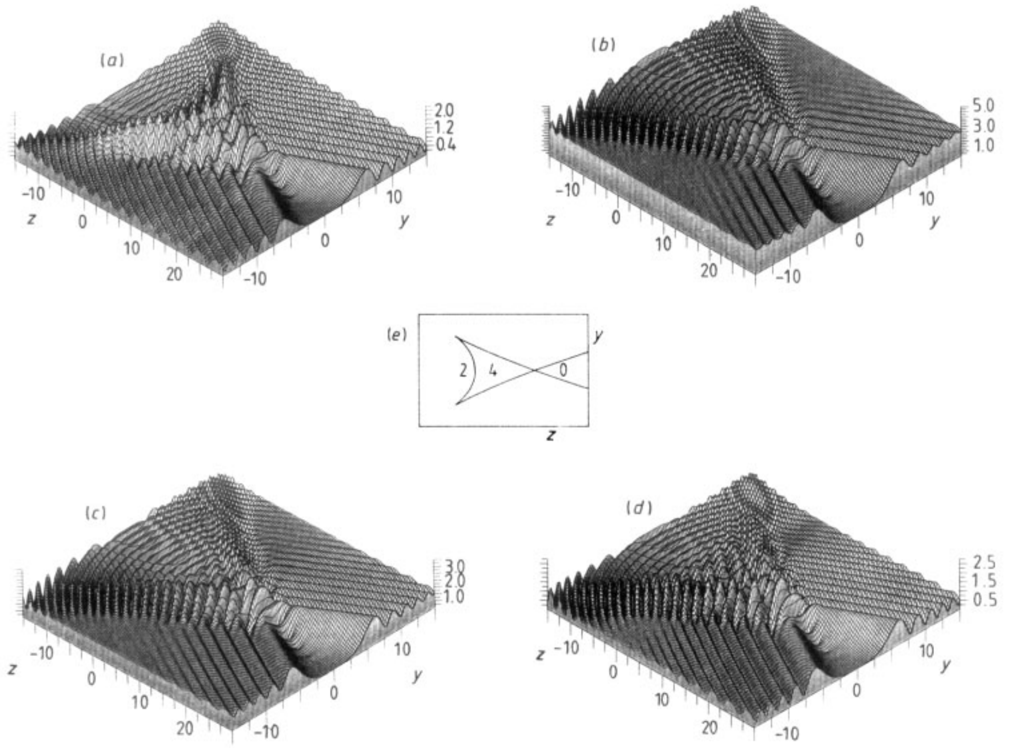

Figure 5. Same as figure 3 except for $x=-6$.

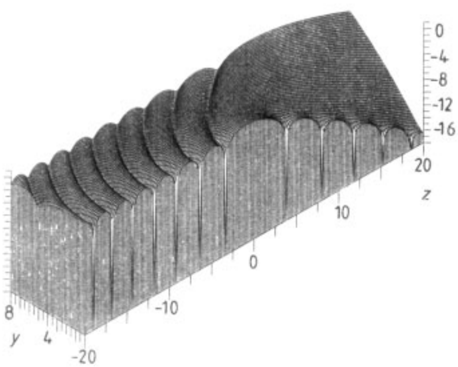

Figure 6. Isometric plot of $\ln|S(x, y, z)|$ for $x=0$, $0 \leqslant y \leqslant 8$, $-20 \leqslant z \leqslant 20$.

It is also interesting to compare the accurate zeros in table 3 with the results of the stationary phase (or saddle point) method. In the lit region where $z<0$, there are two real stationary phase points for $S(0, 0, z)$, as well as two complex conjugate ones. The real stationary phase points are situated at $u=\pm(-z/5)^{1/4}$. If we neglect the contribution from the complex ones, then the first-order stationary phase method gives (Pearcey and Hill 1963)

$$S(0, 0, z) \sim [(2\pi)^{1/2}/5^{1/8}(-z)^{3/8}] \cos[4(-\tfrac{1}{5}z)^{5/4} - \tfrac{1}{4}\pi], \qquad z<0, \tag{3.13}$$

Table 3. Zeros of $S(0, 0, z)$ for $-19.0 < z < 19.0$. The accurate numerical zeros have been found using the quadrature method of § 3.1. The asymptotic zeros have been calculated using the first-order stationary phase and saddle point methods and are given by (3.14) and (3.16) respectively.

Accurate	Asymptotic	Accurate	Asymptotic
−18.995 8	−18.988 3	−3.412 46	−3.274 09
−16.711 5	−16.702 3	3.800 13	3.733 86
−14.346 5	−14.335 0	8.044 26	8.019 30
−11.880 3	−11.865 0	11.784 1	11.769 5
−9.280 09	−9.257 81	15.247 1	15.237 0
−6.484 75	−6.448 70	18.523 5	18.515 8

and the zeros are therefore located at

$$z = -5[\tfrac{1}{4}\pi(n+\tfrac{3}{4})]^{4/5}, \qquad n = 0, 1, 2, \ldots. \tag{3.14}$$

On the dark side where $z > 0$, all the saddle points are complex, being located at $u_1 = (z/5)^{1/4}\exp(\mathrm{i}\frac{1}{4}\pi)$, $u_2 = (z/5)^{1/4}\exp(\mathrm{i}\frac{3}{4}\pi)$, $u_3 = u_1^*$ and $u_4 = u_2^*$. In the saddle point method, the only saddle points which contribute are u_1 and u_2 and we then find to first order (Pearcey and Hill 1963)

$$S(0,0,z) \sim \frac{(2\pi)^{1/2}}{5^{1/8}z^{3/8}}\exp\left[-2^{3/2}\left(\frac{z}{5}\right)^{5/4}\right]\cos\left[2^{3/2}\left(\frac{z}{5}\right)^{5/4} - \frac{\pi}{8}\right], \qquad z > 0. \tag{3.15}$$

From (3.15) the zeros on the dark side are located at

$$z = 5[2^{1/2}\tfrac{1}{4}\pi(m+\tfrac{5}{8})]^{4/5}, \qquad m = 0, 1, 2, \ldots. \tag{3.16}$$

In table 3, we compare the results from (3.14) and (3.16) with the accurate numerical results. On the bright side, the $n = 0$ zero from the first-order stationary phase method has an absolute error of 0.14 decreasing to only 0.0075 for $n = 6$. On the dark side, the corresponding errors for the first-order saddle point method are 0.066 for $m = 0$ and 0.0077 for $m = 4$.

3.3. Discussion

The isometric plots presented in figures 3–5 together with those in figures 2–4 of Connor *et al* (1983) require $24 \times 121 \times 121 = 351\,384$ evaluations of the integrals. It is therefore important to compare the efficiency and accuracy of the contour integral technique of § 3.1 with other methods that have been used in the literature. Calculations of $S(x, y, z)$ have been carried out by Pearcey and Hill (1963), Wright (1977), Dronov *et al* (1978) and Pope (1981). We are not aware of any previous computations for $\partial S/\partial x$, $\partial S/\partial y$ or $\partial S/\partial z$.

3.3.1. Differential equation methods. As mentioned in § 3.1(b), a completely different method solves a set of coupled ordinary differential equations satisfied by $S(x, y, z)$. This method was first used by Pearcey and Hill (1963) for the special case of $S(0, y, z)$ and has been generalised (and simplified) to cases where $x \neq 0$ by ourselves (Connor *et al* 1983). The advantage of this method is that $\partial S/\partial x$, $\partial S/\partial y$ and $\partial S/\partial z$ are obtained at the same time as $S(x, y, z)$ and values of the integrals at intermediate points (x', y', z') along the integration path are also readily obtained. The differential equation method is therefore a very efficient way of generating large grids of points such as are required for contour and isometric plots. The main disadvantage of this method is that it eventually becomes numerically unstable as we move out of the tail region of the swallowtail caustic.

3.3.2. Integration along complex contours. Another method used by Pearcey and Hill (1963) for $S(0, y, z)$ consists of integration along rays in the complex u plane. In terms of figure 1, the rays they used are $r\exp(\pm i\pi/10)$. The same integration paths have been used by Dronov *et al* (1978) for $S(x, y, z)$. The disadvantage of these paths (Pearcey and Hill 1963, Connor and Curtis 1982) is that for certain values of (x, y, z), the modulus of the integrand becomes very large before it becomes exponentially small as $r \to \infty$. In these cases, numerical accuracy is lost or it becomes impossible to obtain meaningful results. It was to avoid these problems that the alternative paths in figure 1 were introduced (Connor and Curtis 1982). In general, integration along suitably chosen contours in the complex u plane can produce results of high accuracy (e.g. seven or eight significant figures) and the method is straightforward to program on a computer.

3.3.3. Integration along real contours. The numerical methods of Wright (1977) and Pope (1981) involve integration along the real u axis. The method of Wright (1977) is similar to that originally used by Airy (1838) for his integral. When $S(x, y, z)$ has two or four real stationary phase points, Wright's method consists of a quadrature around the region of these stationary phase points. The remainder of the integral is then estimated by a three-term asymptotic expansion. In this way, an accuracy of about ± 0.005 was obtained for $S(x, y, z)$ by Wright. By including additional terms in the asymptotic series, more accurate results could be obtained.

By simply replacing the infinite limits in $S(x, y, x)$ with finite values, Pope (1981) was able to obtain an accuracy of about ± 0.01, and reported that a grid containing 4000 points took about 7.8 hours to calculate on a CDC 6400 computer. Evidently the simplicity of this method is offset by its computational inefficiency.

It is well known (Davis and Rabinowitz 1975, Rice 1975, Engels 1980, Phillips 1980) that the numerical integration of infinite integrals with oscillating integrands is a difficult problem and a number of recent papers discuss different real contour approaches to this problem (Guderley 1975, Pantis 1975, Blakemore *et al* 1976, Hillion and Nurdin 1977, Ting and Luke 1981, Fettis and Pexton 1982). In particular, Blakemore *et al* (1976) examined the performance of three basic integration methods when applied to eleven different test integrals. One of these methods (due to Pantis 1975) is similar to the method of Airy (1838) and Wright (1977). However Winterbon (1978) has pointed out that deforming the path of integration into the complex u plane is greatly superior to all the real u methods discussed by Blakemore *et al* (1976). We believe along with Pearcey and Hill (1963) and Dronov *et al* (1978) that a similar situation holds for the swallowtail canonical integral and its derivatives, and recommend exploiting complex contours of integration because they are easy to use and high accuracy is obtainable (see also Rice 1975 and Lugannani and Rice 1981). In principle the best integration contour would be the path of steepest descent through the relevant saddle points.

3.3.4. Asymptotic methods. When x, y or z become large, asymptotic techniques can be used for the evaluation of $S(x, y, z)$. In the region of the cuspoidal edges belonging to the caustic of figure 2, the uniform Pearcey approximation is the appropriate asymptotic method in use (Ursell 1972, Connor 1973, Connor and Farrelly 1981). On the fold lines, the simpler uniform Airy approximation can be employed (Chester *et al* 1957). This approximation was used by Wright (1977) inside the body of the swallow for (x, y, z) close to the 'complex whisker' where two complex saddle points have coalesced. Finally, when all the stationary phase or saddle points are well separated from one another, the appropriate asymptotic technique is the simple stationary phase or saddle point method. Asymptotic approximations cannot be used close to $(0, 0, 0)$, but in this region it is straightforward to sum numerically the exact series representation (3.5). This strategy has been adopted by Stamnes and Spjelkavik (1983) for Pearcey's integral.

When asymptotic methods are valid it should be noted that it is not necessary to invoke the uniform swallowtail approximation for the original oscillating integral (1.1). Rather $f(\boldsymbol{\alpha}; t)$ can be mapped directly onto the cusp, fold or Morse canonical polynomial forms as appropriate. From this point of view further discussion of asymptotic methods for the evaluation of $S(x, y, z)$ is beyond the scope of the present paper.

3.3.5. Other methods. Another possible method (Doyle 1982) for the numerical evaluation of $S(x, y, z)$ makes use of the projection identities derived by Berry and Wright (1980). Defining

$$\psi_C(c_1, c_2) = (2\pi)^{-1/2} \int_{-\infty}^{\infty} \exp[\mathrm{i}(\tfrac{1}{4}u^4 + \tfrac{1}{2}c_2u^2 + c_1u)]\, \mathrm{d}u \tag{3.17}$$

and

$$\psi_S(c_1, c_2, c_3) = (2\pi)^{-1/2} \int_{-\infty}^{\infty} \exp[\mathrm{i}(\tfrac{1}{5}u^5 + \tfrac{1}{3}c_3u^3 + \tfrac{1}{2}c_2u^2 + c_1u)]\, \mathrm{d}u \tag{3.18}$$

then Berry and Wright have shown that

$$|\psi_S(c_1, c_2, c_3)|^2 = 2^{3/5}\pi^{-1/2} \int_{-\infty}^{\infty} \psi_S(2^{4/5}[u^4 + c_3u^2 + c_2u + c_1], 0, 2^{2/5}[6u^2 + c_3])\, \mathrm{d}u \tag{3.19}$$

and

$$|\psi_S(c_1, c_2, c_3)|^2 = 2^{3/2}\pi^{-1/2}\, \mathrm{Re} \int_{-\infty}^{\infty} \mathrm{d}u\, (8u)^{-1/4} \exp[\mathrm{i}(\tfrac{2}{5}u^5 + \tfrac{2}{3}c_3u^3 + 2c_1u)]$$
$$\times \psi_C[2(8u)^{-1/4}c_2u, 4(8u)^{-1/2}(2u^3 + c_3u)]. \tag{3.20}$$

Since $\psi_C(x, y)$ and $\psi_S(x, y, z)$ are evidently closely related to $P(x, y)$ and $S(x, y, z)$ respectively, these identities would allow the calculation of $|S(x, y, z)|$ in terms of $S(x, 0, z)$ and $P(x, y)$. The disadvantage of this method is that the integrands of the identities (3.19) and (3.20) are considerably more complicated than is the integrand of the usual integral representation (1.3) for $S(x, y, z)$. In particular, in order to exploit the power of the complex contour integration method it would be necessary to analytically continue $S(x, 0, z)$ and $P(x, y)$ to complex values of x, y and z. This is a very difficult task compared with the analytic continuation of the integrand of (1.3). In addition the identities do not allow arg $S(x, y, z)$ to be calculated. This quantity is required for the uniform approximation (2.1).

3.3.6. Comparison of numerical results for $S(x, y, z)$. In §§ 3.3.1–5 we have compared different methods for the evaluation of $S(x, y, z)$. We now wish to compare the *numerical results* obtained by some of these methods with the results from the contour integral method of § 3.1.

The first calculations were by Pearcey and Hill (1963), who in an unpublished monograph reported contour plots for $|S(0, y, z)|$ and $\arg S(0, y, z)$ for $0 \leq y \leq 8$ and $-9 \leq z \leq 9$. Three numerical techniques were used to construct their contour plots: solution of differential equations, integration in the complex u plane along the rays $\arg u = \pm\pi/10$ of figure 1 and the use of asymptotic series. Our results for $S(0, y, z)$ agree with those of Pearcey and Hill (1963).

More extensive computations were reported by Wright (1977) for the integral (3.18). Note that $\psi_S(z, y, x)$ and $S(x, y, z)$ are related by

$$S(x, y, z) = [(2\pi)^{1/2}/5^{1/5}]\psi_S(5^{-1/5}z, (2/5^{2/5})y, (3/5^{3/5})x). \tag{3.21}$$

In the tail of the swallow and outside its body, the real u axis method outlined in § 3.3.3 was used, whereas inside the body (uniform) asymptotic techniques were employed (see § 3.3.4). Wright presented plots of $|\psi_S(c_1', c_2, c_3)|$ and $\arg \psi_S(c_1, c_2, c_3)$ for $c_3 = 6, 0, -4, -8$ with $0 \leq c_2 \leq 15$ and $-10 \leq c_1 \leq 20$. Because of their complexity, the contours were not labelled, rather shading techniques were used (see also figure 3.6 of Berry and Upstill (1980)). We can therefore only qualitatively compare our results with those of Wright, but when this is done, they are in agreement.

Dronov *et al* (1978) have shown contour plots of $|S(x, y, z)|$ and $\arg S(x, y, z)$ for $x = 1, 0, -1, -2, -3$ for $0 \leq y \leq 8$ and $-8 \leq z \leq 8$. Their plots, although not very detailed, are in agreement with our results. They used integration in the complex u plane along the rays $\arg u = \pm\pi/10$ of figure 1.

Finally we consider the numerical results of Pope (1981). Figure 13.10 of Gilmore (1981) shows an isometric plot for the modulus of the swallowtail canonical integral. According to pp 339–42 of Gilmore (1981), the plot illustrated is for the integral

$$I_G(b, c, d) = \left| \int_{-\infty}^{\infty} \exp[i(\tfrac{1}{5}u^5 + \tfrac{1}{3}bu^3 + \tfrac{1}{2}cu^2 + du)]\, du \right|^2 \tag{3.22}$$

for $b = 1$ and $-15 \leq c \leq 5$ and $-5 \leq d \leq 10$. We were unable to reproduce by our contour integral method the plot presented by Gilmore.

However, according to Pope (1981), the results shown by Gilmore actually represent the integral

$$I_P(b, c, d) = \left| \int_{-\infty}^{\infty} \exp[i\pi(\tfrac{1}{5}u^5 + \tfrac{1}{3}bu^3 + \tfrac{1}{2}cu^2 + du)]\, du \right|^2 \tag{3.23}$$

for $b = 1$. We computed (3.23) by our contour integral method, but were still unable to reproduce Pope's results. We therefore believe that the results shown in figure 13.10 of Gilmore (1981) are wrong.

4. Calculation of x, y, z and A

In this section, we describe two methods for solving (2.3) and (2.4) for the unknowns x, y, z and A. The first method is an iterative numerical technique which is a generalisation of a procedure used earlier for the uniform Pearcey approximation

(Connor and Farrelly 1981). The second method adopts an algebraic approach, and uses results from the theory of equations and the theory of symmetric polynomials. In practice both methods are complementary. The iterative method is described in § 4.1 and the algebraic method in § 4.2. Some important practical points associated with both methods are discussed in § 4.3.

Throughout this section, it will be convenient to change variable, $u \to u/5^{1/5}$, in the mapping equation (2.3), as well as to redefine x, y, z according to $x \to x/5^{3/5}$, $y \to y/5^{2/5}$, $z \to z/5^{1/5}$. Equation (2.3) then becomes

$$f(\boldsymbol{\alpha}; t_i) = \tfrac{1}{5}u_i^5 + xu_i^3 + yu_i^2 + zu_i + A, \qquad i = 1, 2, 3, 4, \tag{4.1}$$

where the $u_i = u_i(x, y, z)$ are the roots of

$$u_i^4 + 3xu_i^2 + 2yu_i + z = 0, \qquad i = 1, 2, 3, 4. \tag{4.2}$$

We shall also use the abbreviation $f_i \equiv f(\boldsymbol{\alpha}; t_i)$.

4.1. Iterative method

First we simplify equation (4.1). Multiplying (4.2) by u_i shows that

$$u_i^5 = -3xu_i^3 - 2yu_i^2 - zu_i, \qquad i = 1, 2, 3, 4,$$

and equation (4.1) then becomes

$$f_i = \tfrac{2}{5}xu_i^3 + \tfrac{3}{5}yu_i^2 + \tfrac{4}{5}zu_i + A, \qquad i = 1, 2, 3, 4. \tag{4.3}$$

Next we form the following differences:

$$f_1 - f_2, \qquad f_3 + f_4 - f_1 - f_2, \qquad f_3 - f_4, \tag{4.4}$$

where the t_i are labelled so that the differences (4.4) are either purely real or purely imaginary (the stationary points t_i, $i = 1, 2, 3, 4$, like the f_i, are either real, or occur in complex conjugate pairs). Equation (4.3) can now be written as a matrix equation:

$$\begin{pmatrix} u_1^3 - u_2^3 & u_1^2 - u_2^2 & u_1 - u_2 \\ u_3^3 + u_4^3 - u_1^3 - u_2^3 & u_3^2 + u_4^2 - u_1^2 - u_2^2 & u_3 + u_4 - u_1 - u_2 \\ u_3^3 - u_4^3 & u_3^2 - u_4^2 & u_3 - u_4 \end{pmatrix} \begin{pmatrix} 2x \\ 3y \\ 4z \end{pmatrix} = 5 \begin{pmatrix} f_1 - f_2 \\ f_3 + f_4 - f_1 - f_2 \\ f_3 - f_4 \end{pmatrix}. \tag{4.5}$$

Since the t_i and u_i are labelled in a one-to-one manner

$$t_i \leftrightarrow u_i, \qquad i = 1, 2, 3, 4,$$

the differences in the 3×3 matrix are also either purely real or purely imaginary. This means that (4.5) can always be rewritten in a purely real form and we assume that this simplification has been done.

Equation (4.5) is now solved by iteration. Starting from an initial guess x_0, y_0, z_0, the $u_i(x_0, y_0, z_0)$ in the 3×3 matrix are calculated by solving (4.2). The linear equations (4.5) are then solved to yield improved values x_1, y_1, z_1. This process is repeated until convergence is obtained. The remaining variable A can then be obtained from (4.3).

The method just described is simple in principle, but in practice there can be difficulties, e.g. in the choice of the initial guess (x_0, y_0, z_0) and in the convergence of the method as (x, y, z) approaches the caustic set. Methods for dealing with these difficulties are discussed in § 4.3. Note that the method fails for values of (x, y, z) actually on the caustic, i.e. where two or more of the u_i are equal.

4.2. Algebraic method

The strategy of the second method is to eliminate the u_i from (4.3) using results from the theory of equations and the theory of symmetric polynomials (Uspensky 1948, Archbold 1970, Peregrine and Smith 1979, Connor and Farrelly 1981, Uzer and Child 1982).

First we define the elementary symmetric polynomials (Mostowski and Stark 1964, p 346)

$$\tau_1\{r_i\} = \sum_{i=1}^{4} r_i = r_1 + r_2 + r_3 + r_4, \tag{4.6}$$

$$\tau_2\{r_i\} = \sum_{j>i}^{4} \sum_{i=1}^{4} r_i r_j = r_1 r_2 + r_1 r_3 + r_1 r_4 + r_2 r_3 + r_2 r_4 + r_3 r_4, \tag{4.7}$$

$$\tau_3\{r_i\} = \sum_{k>j}^{4} \sum_{j>i}^{4} \sum_{i=1}^{4} r_i r_j r_k = r_1 r_2 r_3 + r_1 r_2 r_4 + r_1 r_3 r_4 + r_2 r_3 r_4, \tag{4.8}$$

$$\tau_4\{r_i\} = \sum_{l>k}^{4} \sum_{k>j}^{4} \sum_{j>i}^{4} \sum_{i=1}^{4} r_i r_j r_k r_l = r_1 r_2 r_3 r_4, \tag{4.9}$$

together with

$$s_n\{r_i\} = \sum_{i=1}^{4} r_i^n = r_1^n + r_2^n + r_3^n + r_4^n, \qquad n = 1, 2, 3, \ldots \tag{4.10}$$

(note that $s_1\{r_i\} = \tau_1\{r_i\}$). The quantity $s_n\{r_i\}$ is introduced to facilitate the use of Newton's formulae (Uspensky 1948, pp 260–2). Next we construct the quantities

$$\bar{f} = \tfrac{1}{4}\tau_1\{f_i\}, \tag{4.11}$$

$$\Sigma = \tfrac{1}{6}\tau_2\{f_i - \bar{f}\}, \tag{4.12}$$

$$\Xi = \tfrac{1}{4}\tau_3\{f_i - \bar{f}\}, \tag{4.13}$$

$$\Pi = \tau_4\{f_i - \bar{f}\}. \tag{4.14}$$

Since the f_i are assumed to be known, $\bar{f}$, Σ, Ξ, Π are also known quantities. Notice that $\bar{f}$, Σ, Ξ, Π are always real even if f_i is complex. The aim now is to express $\bar{f}$, Σ, Ξ, Π in terms of $s_n\{u_i\}$, and hence by Newton's formulae in terms of x, y, z. Equations (4.11)–(4.14) will then result in four simultaneous polynomial equations for x, y, z, A.

To achieve this aim, we use the identities

$$\tau_2\{f_i - \bar{f}\} = \tau_2\{f_i\} - 3\bar{f}\tau_1\{f_i\} + 6\bar{f}^2, \tag{4.15}$$

$$\tau_3\{f_i - \bar{f}\} = \tau_3\{f_i\} - 2\bar{f}\tau_2\{f_i\} + 3\bar{f}^2\tau_1\{f_i\} - 4\bar{f}^3, \tag{4.16}$$

$$\tau_4\{f_i - \bar{f}\} = \tau_4\{f_i\} - \bar{f}\tau_3\{f_i\} + \bar{f}^2\tau_2\{f_i\} - \bar{f}^3\tau_1\{f_i\} + \bar{f}^4, \tag{4.17}$$

together with (Mostowski and Stark 1964, p 358)

$$\tau_1\{f_i\} = s_1\{f_i\}, \tag{4.18}$$

$$\tau_2\{f_i\} = \tfrac{1}{2}[\tau_1^2\{f_i\} - s_2\{f_i\}], \tag{4.19}$$

$$\tau_3\{f_i\} = \tfrac{1}{3}[s_3\{f_i\} - \tau_1^3\{f_i\} + 3\tau_1\{f_i\}\tau_2\{f_i\}], \tag{4.20}$$

$$\tau_4\{f_i\} = \tfrac{1}{4}[\tau_1^4\{f_i\} - 4\tau_1^2\{f_i\}\tau_2\{f_i\} + 2\tau_2^2\{f_i\} + 4\tau_1\{f_i\}\tau_3\{f_i\} - s_4\{f_i\}]. \tag{4.21}$$

Equations (4.15)–(4.21) allow $\bar{f}$, Σ, Ξ, Π to be written in terms of $s_1\{f_i\}(=4\bar{f})$, $s_2\{f_i\}$, $s_3\{f_i\}$, $s_4\{f_i\}$.

The next step is to use (4.3) to express $s_n\{f_i\}$ in terms of $s_n\{u_i\}$. For example, for $s_1\{f_i\}$ and $s_2\{f_i\}$ we have from (4.3):

$$s_1\{f_i\} = \tfrac{2}{5}xs_3\{u_i\} + \tfrac{3}{5}ys_2\{u_i\} + \tfrac{4}{5}zs_1\{u_i\} + 4A, \tag{4.22}$$

$$\begin{aligned} s_2\{f_i\} = [&4x^2s_6\{u_i\} + 12xys_5\{u_i\} + (16xz + 9y^2)s_4\{u_i\} + (20xA + 24yz)s_3\{u_i\} \\ &+ (16z^2 + 30yA)s_2\{u_i\} + 40zAs_1\{u_i\} + 100A^2]/25. \end{aligned} \tag{4.23}$$

The final step is to express the $s_n\{u_i\}$, $n = 1, \ldots, 12$, in terms of x, y, z using Newton's formulae (Uspensky 1948, pp 260–2). From (4.2), we find $s_1\{u_i\} = 0$, $s_2\{u_i\} = -6x$, $s_3\{u_i\} = -6y$, $s_4\{u_i\} = 18x^2 - 4z$ and

$$s_{4+k} + 3xs_{2+k} + 2ys_{1+k} + zs_k = 0, \qquad k = 1, 2, 3, \ldots. \tag{4.24}$$

The steps described above are simple in principle but involve a very large amount of algebraic manipulation. To overcome this problem, the calculations have been carried out using both the REDUCE and SCHOONSHIP algebraic manipulation computer programs. As an additional check, the algebra has also been performed using the MACSYMA computer program. The results obtained are

$$\bar{f} = A - \tfrac{3}{2}xy, \tag{4.25}$$

$$\Sigma = \tfrac{1}{5}(\tfrac{18}{5}x^5 - 6x^3z - \tfrac{23}{4}x^2y^2 + \tfrac{8}{3}xz^2 + 3y^2z), \tag{4.26}$$

$$\Xi = \tfrac{1}{25}y(81x^6 - 153x^4z - 41x^3y^2 + 88x^2z^2 + 36xy^2z + \tfrac{27}{5}y^4 - 16z^3), \tag{4.27}$$

$$\begin{aligned} \Pi = \tfrac{1}{25}(&243x^7y^2 - 513x^5y^2z + \tfrac{249}{16}x^4y^4 + 16x^4z^3 + 344x^3y^2z^2 + \tfrac{27}{2}x^2y^4z \\ &- \tfrac{128}{5}x^2z^4 + \tfrac{162}{5}xy^6 - \tfrac{336}{5}xy^2z^3 - \tfrac{27}{5}y^4z^2 + \tfrac{256}{25}z^5). \end{aligned} \tag{4.28}$$

Equations (4.26), (4.27) and (4.28) represent three simultaneous polynomial equations for x, y, z. These can be solved in principle and the remaining variable A can then be obtained from (4.25). Note that in general (4.26)–(4.28) contain many solutions for x, y, z in addition to the particular solution we are interested in.

There are, however, practical difficulties in attempting a solution of (4.26), (4.27) and (4.28) for x, y, z. One approach would be to use the theory of resultants (Mostowski and Stark 1964, ch 10) to deduce from (4.26)–(4.28) a single polynomial equation in x, one in y and one in z, and then to solve these three single variable polynomial equations by a numerical procedure. The difficulty with this approach is that the degrees of the resulting x, y and z polynomials are so large that they would cause severe problems for numerical root finding procedures.

Another approach is to regard (4.26)–(4.28) as a set of nonlinear equations. If the RHS of (4.26), (4.27) and (4.28) are denoted by $\Sigma(x, y, z)$, $\Xi(x, y, z)$ and $\Pi(x, y, z)$ respectively then we could attempt to minimise the function

$$F(x, y, z) = (\Sigma(x, y, z) - \Sigma)^2 + (\Xi(x, y, z) - \Xi)^2 + (\Pi(x, y, z) - \Pi)^2. \tag{4.29}$$

The difficulty with this method is that $F(x, y, z)$ contains many stationary points which are not roots of $F(x, y, z) = 0$ and numerical procedures tend to find them unless the initial guess is very good. In this situation, (4.29) has no advantage over the iterative technique of § 4.1.

There is, however, one case where the algebraic method is very useful. This is when (x, y, z) actually lies on the caustic, i.e. when x, y, z satisfy the equations

$$u^4+3xu^2+2yu+z=0, \qquad 4u^3+6xu+2y=0. \tag{4.30}$$

For any x and y, these equations imply that z is constrained to a maximum of three possible (real) values. This is also evident from figure 2 or equation (3.12). Since it is assumed that we know which of the u_i, $i=1$, 2, 3, 4, have coalesced, the three possible values for z are actually reduced to one as explained in figure 5.7 of Gilmore (1981). The numerical procedure for determining (x, y, z) on the caustic then consists of finding the roots of

$$F(x, y, z(x, y))=0. \tag{4.31}$$

This is a much simpler problem than finding the roots of the unconstrained function (4.29).

There is also a particular case where the polynomial equations (4.26)–(4.28) can be considerably simplified. This is when $y=0$, and we then obtain

$$\Sigma=\tfrac{1}{5}(\tfrac{18}{5}x^5-6x^3z+\tfrac{8}{3}xz^2), \tag{4.32}$$

$$\Xi=0, \tag{4.33}$$

$$\Pi=\tfrac{1}{25}(16x^4z^3-\tfrac{128}{5}x^2z^4+\tfrac{256}{25}z^5). \tag{4.34}$$

Note that $y=0$ implies that $f(\boldsymbol{\alpha}, t)-A$ is locally an odd function and that the u_i satisfy

$$u_1=-u_3, \qquad u_2=-u_4. \tag{4.35}$$

It is now possible to use the theory of resultants (Mostowski and Stark 1964, ch 10) to reduce (4.32) and (4.34) to two single polynomial equations in x and z. We find

$$\begin{aligned}&2^8 3^4 5^{-13}x^{25}-2^8 3^3 5^{-10}\Sigma x^{20}+2^4 3^1 5^{-8}71^1\Sigma^2x^{15}-2^3 3^{-2}5^{-6}503^1\Sigma^3x^{10}+3^{-5}\Pi^2x^5\\&\qquad -3^{-3}\Sigma^2\Pi x^5+2^2 3^{-1}5^{-4}17^1\Sigma^4x^5-2^1 5^{-3}\Sigma^5=0\end{aligned} \tag{4.36}$$

and

$$\begin{aligned}&2^{44}3^{-4}5^{-20}z^{25}+2^{31}3^{-4}5^{-15}17^1 19^1\Pi z^{20}-2^{31}3^{-2}5^{-11}\Sigma^2z^{20}+2^{16}3^{-1}5^{-11}127^1 233^1\Pi^2z^{15}\\&\qquad -2^{17}5^{-6}37^1\Sigma^2\Pi z^{15}+2^{16}5^{-2}\Sigma^4z^{15}+2^8 3^4 5^{-7}7^1 149^1\Pi^3z^{10}\\&\qquad -2^{12}3^3 5^{-2}\Sigma^2\Pi^2z^{10}+2^5 3^5 5^{-3}31^1\Pi^4z^5-3^8\Pi^5=0.\end{aligned} \tag{4.37}$$

Equation (4.36) is a fifth-degree polynomial in x^5 and similarly (4.37) is a fifth-degree polynomial in z^5. These polynomials can readily be solved numerically, and yield a maximum of 25 real pairs for (x, z) (i.e. up to five real x values from (4.36) and up to five real z values from (4.37)). Substituting back into (4.32) and (4.34) reduces the number of acceptable pairs, and a final reduction to one pair is made from the fact that the u_i and f_i are in a known one-to-one correspondence

$$f_i \leftrightarrow u_i, \qquad i=1, 2, 3, 4. \tag{4.38}$$

4.3. *Practical considerations*

The iterative method is most useful for (x, y, z) not close to the caustic, whereas the algebraic method is applicable for (x, y, z) on the caustic and for $y=0$. In numerical applications of these methods, there are a number of practical considerations that must be kept in mind.

(a) In some problems, the $|f(\boldsymbol{\alpha}; t_i)|$ are numerically large, which results in large values for the parameters x, y, z. This tends to make the numerical procedures in the iterative method unstable. In this situation, it is useful to scale the mapping equation (4.1). If we write $u = av$, then (4.1) becomes

$$f(\boldsymbol{\alpha}; t_i)/a^5 = \tfrac{1}{5}v_i^5 + x'v_i^3 + y'v_i^2 + z'v_i + A', \qquad i = 1, 2, 3, 4, \tag{4.39}$$

with

$$x' = x/a^2, \qquad y' = y/a^3, \qquad z' = z/a^4, \qquad A' = A/a^5.$$

Any convenient value for a that results in relatively small values for x', y', z' can be used. In our iterative calculations we have chosen

$$a = [\max(|f_1 - f_2|, |f_3 + f_4 - f_1 - f_2|, |f_3 - f_4|)]^{1/5}.$$

(b) The speed and stability of the iterative method is dependent on a good choice for the initial values x_0, y_0, z_0. We used the following procedure to obtain these initial estimates.

The first step is to construct the polynomial

$$(t - t_1)(t - t_2)(t - t_3)(t - t_4). \tag{4.40}$$

This can be written in the alternative form

$$t^4 - \tau_1\{t_i\}t^3 + \tau_2\{t_i\}t^2 - \tau_3\{t_i\}t + \tau_4\{t_i\} \qquad \{4.41\}$$

and with the change of variable $t = s + \frac{1}{4}\tau_1\{t_i\}$ the expression (4.41) becomes

$$s^4 + (\tau_2 - \tfrac{3}{8}\tau_1^2)s^2 + (\tfrac{1}{2}\tau_1\tau_2 - \tau_3 - \tfrac{1}{8}\tau_1^3)s + \tau_4 - \tfrac{1}{4}\tau_1\tau_3 + \tfrac{1}{16}\tau_1^2\tau_2 - \tfrac{3}{256}\tau_1^4. \tag{4.42}$$

We then set

$$\begin{aligned} x_0 &= \tfrac{1}{3}(\tau_2 - \tfrac{3}{8}\tau_1^2), \qquad y_0 = \tfrac{1}{2}(\tfrac{1}{2}\tau_1\tau_2 - \tau_3 - \tfrac{1}{8}\tau_1^3), \\ z_0 &= \tau_4 - \tfrac{1}{4}\tau_1\tau_3 + \tfrac{1}{16}\tau_1^2\tau_2 - \tfrac{3}{256}\tau_1^4. \end{aligned} \tag{4.43}$$

This method for choosing x_0, y_0, z_0 corresponds to fitting a fourth-degree polynomial through the stationary phase points t_i, $i = 1, 2, 3, 4$. Furthermore if we define

$$h_i \equiv h(s_i) = \tfrac{1}{5}s_i^5 + x_0 s_i^3 + y_0 s_i^2 + z_0 s_i \tag{4.44}$$

where $s_i = t_i - \frac{1}{4}\tau_1\{t_i\}$, we can introduce as before the scaled parameters (from $s_i = br_i$)

$$x_0' = x_0/b^2, \qquad y_0' = y_0/b^3, \qquad z_0' = z_0/b^4.$$

A convenient choice for b is

$$b = [\max(|h_1 - h_2|, |h_3 + h_4 - h_1 - h_2|, |h_3 - h_4|)]^{1/5}. \tag{4.45}$$

(c) Another important practical point concerns the change in the vector $\boldsymbol{w} = (x, y, z)$ in each step of the iteration for equation (4.5). Suppose $\boldsymbol{w}_n = (x_n, y_n, z_n)$ and $\boldsymbol{w}_{n+1} = (x_{n+1}, y_{n+1}, z_{n+1})$ are the vectors for the nth and $(n+1)$th steps respectively. Then $\boldsymbol{w}_{n+1}$ and $\boldsymbol{w}_n$ are related by

$$\boldsymbol{w}_{n+1} = \boldsymbol{w}_n + \boldsymbol{w}_n^{\mathrm{N}} \tag{4.46}$$

where $\boldsymbol{w}_n^{\mathrm{N}}$ is the (Newton) correction vector. It may happen that the $u_i(\boldsymbol{w}_{n+1})$ on the

LHS of the matrix equation (4.5) have a different stationary phase point structure from the f_i on the RHS. This occurs if $\boldsymbol{w}_{n+1}$ has crossed the caustic in (x, y, z) space and causes the iterative method to fail. To allow for this possibility, we calculate a new vector $\boldsymbol{w}'_{n+1}$ from

$$\boldsymbol{w}'_{n+1} = \boldsymbol{w}_n + \boldsymbol{w}_n^{\mathrm{c}}$$

where the correction vector $\boldsymbol{w}_n^{\mathrm{c}}$ is given by

$$\boldsymbol{w}_n^{\mathrm{c}} = 2^{-m}\boldsymbol{w}_n^{\mathrm{N}}, \qquad m = 0, 1, 2, 3, 4,$$

and use the smallest value of m that retains the correct stationary phase point structure. If this is still unsuccessful we choose instead

$$\boldsymbol{w}_n^{\mathrm{c}} = -2^{-m}\boldsymbol{w}_n^{\mathrm{N}}, \qquad m = 1, 2, 3, 4.$$

If this also fails then we try directions perpendicular to $\boldsymbol{w}_n^{\mathrm{N}}$ for the correction vector. By choosing different correction vectors in this manner, it is generally possible to get the iterative method to converge for cases where the direct use of (4.46) leads to non-convergence. Note that we have not performed a theoretical analysis of the convergence of the iterative method, the convergence of the procedures we have described being an empirical result.

(d) The numerical procedures described in (c) for the iterative method are usually satisfactory except when the parameters x, y, z are very close to the caustic. In this situation two or more of the f_i have almost coalesced and it is better to use a numerical procedure which exploits this fact.

Suppose for example that f_1 and f_2 have almost coalesced. To obtain an initial guess, we define the quantities

$$f'_1 = \tfrac{1}{2}(f_1 + f_2), \qquad f'_2 = \tfrac{1}{2}(f_1 + f_2), \qquad f'_3 = f_3, \qquad f'_4 = f_4,$$

so that (x, y, z) for the f'_i lie on the caustic because f'_1 and f'_2 are equal. Next we construct Σ, Ξ, Π for the f'_i and solve the caustic equation (4.31) to obtain x, y, z (z is obtained from (4.30)). The initial values required for the solution of (4.31) can be obtained from (4.43) using the original t_i but with the initial z calculated from (4.30).

The x, y, z obtained from the caustic equation (4.31) are then used as an initial guess for the solution of the general equation (4.29), which is valid for (x, y, z) off the caustic. This method for obtaining x, y, z has been found to work well in practice. Note that it is only used for cases where the iterative method fails.

5. Asymptotic evaluation of the butterfly canonical integral

In this section, we consider the asymptotic evaluation of the butterfly canonical integral in order to illustrate the methods of §§ 3 and 4. The butterfly integral is defined by

$$B(a, b, c, d) = \int_{-\infty}^{\infty} \exp[\mathrm{i}(\tfrac{1}{6}t^6 + at^4 + bt^3 + ct^2 + dt)]\,\mathrm{d}t \qquad (5.1)$$

with a, b, c, d real. The exponent of the integrand of (5.1) is the universal unfolding of the butterfly catastrophe (Poston and Stewart 1978). Note that we have chosen its singularity to be $\frac{1}{6}t^6$.

The stationary phase points for the butterfly can be written

$$\partial f(\boldsymbol{\alpha}; t)/\partial t = (t-t_1)(t-t_2)(t-t_3)(t-t_4)(t-t_5) = 0.$$

If t_1 is chosen sufficiently far removed from t_2, t_3, t_4, t_5, we can locally map $f(\boldsymbol{\alpha}; t)$ onto the swallowtail canonical form in the neighbourhood of t_2, t_3, t_4, t_5.

In order to test the numerical techniques used to solve the mapping equation (4.1) for the parameters x, y, z, A, we have set $t_1 = R_1$ and $|t_i| < R_2$, $i = 2, 3, 4, 5$ (note that the second condition includes complex values of t_i). For (R_1, R_2) we have used the combinations $(-10, 1)$, $(-20, 1)$, $(-5, 1)$, $(-8, 1)$. For each combination of (R_1, R_2) we then randomly selected 100 sets of $\{t_i, i = 2, 3, 4, 5\}$. The numerical procedures described in §§ 4.1–4.3 were found to work in a satisfactory manner for all 500 sets of butterfly input data.

Table 4 compares accurate values of $B(a, b, c, d)$ with the results from the uniform swallowtail approximation for t_2, t_3, t_4, t_5 together with the stationary phase method for t_1. Six sets of $\{a, b, c, d\}$ have been used; they give rise to one, three and five real stationary phase points. The exact values for $B(a, b, c, d)$ were calculated by our quadrature method (Connor and Curtis 1982). Table 2 shows that the exact and uniform swallowtail results are in excellent agreement for both the real and imaginary parts of $B(a, b, c, d)$. The error in the uniform swallowtail approximation is about 0.004% or better.

Since the same quadrature technique has been used to evaluate $B(a, b, c, d)$ as well as $S(x, y, z)$ and its partial derivatives, it might be thought that in practice it is always simpler to evaluate the butterfly integral directly rather than use the uniform asymptotic approximation (2.1). However, as the parameters $\{a, b, c, d\}$ become large, the numerical evaluation of $B(a, b, c, d)$ is computationally much more demanding than is the evaluation of the uniform approximation (2.1) (see also Leubner (1981b, 1982) for another example). For the parameters in table 4, the uniform swallowtail approximation can be computed at least five times faster than can $B(a, b, c, d)$. Note that it is not necessary to evaluate $S(x, y, z)$, $\partial S/\partial x$, $\partial S/\partial y$, $\partial S/\partial z$ separately because the same contour of integration is used in each integral. Rather if we define in the uniform expansion (2.1)

$$G(u) = \sum_{k=0}^{3} \hbar^{(k+1)/5} q_k u^k,$$

then it is only necessary to evaluate a single integral, namely

$$\int_{-\infty}^{\infty} G(u) \exp[\mathrm{i}(u^5 + \hbar^{-2/5} x u^3 + \hbar^{-3/5} y u^2 + \hbar^{-4/5} z u)]\, \mathrm{d}u. \tag{5.2}$$

In addition in some applications, an analytic formula for the exponent $f(\boldsymbol{\alpha}; t)$ of (1.1) is not available, rather $f(\boldsymbol{\alpha}; t)$ has to be computed numerically. This is the case, for example, in the semiclassical theory of inelastic and reactive molecular collisions. In these applications, the computation of $f(\boldsymbol{\alpha}; t)$ is often a formidable problem in its own right and it is an important advantage of the uniform swallowtail approximation that it requires only a knowledge of $g(t)$, $f(\boldsymbol{\alpha}; t)$ and $\partial^2 f(\boldsymbol{\alpha}; t)/\partial t^2$ at the four saddle points t_i.

We also report in table 4 the results of evaluating $B(a, b, c, d)$ by three other approximate methods. The first of these is the transitional swallowtail approximation, which is valid when t_2, t_3, t_4, t_5 are close together (see § 2). The expression for the

Table 4. Comparison of exact and approximate results for the butterfly canonical integral $B(a, b, c, d)$.

Butterfly parameters	Number of real stationary phase points	Exact value	Uniform swallowtail approximation†	Transitional swallowtail approximation†	Double uniform Airy approximation†	Primitive approximation†
$a=-2.989$, $b=8.569$	5	Re 0.527 01	0.526 99	0.4955	1.53	8.27
$c=-10.248$, $d=5.748$		Im 1.720 31	1.720 36	1.7257	4.98	22.71
$a=-3.985$, $b=12.129$	5	Re 1.282 99	1.282 98	1.3063	2.35	3.28
$c=-14.302$, $d=7.017$		Im 1.901 49	1.901 50	1.8669	3.66	5.06
$a=-3.792$, $b=13.055$	3	Re 0.809 74	0.809 76	0.8308	1.45	2.21
$c=-20.957$, $d=16.634$		Im −1.280 64	−1.280 63	−1.2939	−1.12	−0.77
$a=-3.705$, $b=12.642$	3	Re −0.123 44	−0.123 44	−0.1876	−0.20	−0.81
$c=-16.591$, $d=5.529$		Im −0.658 26	−0.658 27	−0.7325	−0.74	−0.96
$a=-4.298$, $b=16.377$	1	Re −0.770 62	−0.770 63	−0.7809	−1.46	−3.38
$c=-27.898$, $d=24.146$		Im 0.632 32	0.632 31	0.6245	0.56	0.97
$a=-4.033$, $b=13.447$	1	Re −0.487 07	−0.487 06	−0.4631	0.44	0.70
$c=-19.261$, $d=14.043$		Im −1.444 26	−1.444 26	−1.4706	−1.88	−5.91

† Includes stationary phase contribution from t_1.

transitional swallowtail approximation is obtained by first Taylor expanding $f(\boldsymbol{\alpha}; t)$ to fifth order

$$f(\boldsymbol{\alpha}; t) = \sum_{n=0}^{5} \frac{f^{(n)}(\boldsymbol{\alpha}; t_0)}{n!}(t-t_0)^n \tag{5.3}$$

where

$$f^{(n)}(\boldsymbol{\alpha}; t_0) = \partial^n f(\boldsymbol{\alpha}; t)/\partial t^n|_{t=t_0}.$$

The quantity t_0 is chosen so that

$$f^{(4)}(\boldsymbol{\alpha}; t_0) = 0.$$

Using equation (5.3), the integral (1.1) becomes

$$I(\boldsymbol{\alpha}) \approx \int_{-\infty}^{\infty} g(t) \exp\left[\mathrm{i}\left(\sum_{n=0}^{5} \frac{f^{(n)}(\boldsymbol{\alpha}; t_0)}{n!}(t-t_0)^n \right) \Big/ \hbar \right] \mathrm{d}t. \tag{5.4}$$

Next we make the additional approximation of replacing $g(t)$ by $g(t_0)$ in (5.4). With the change of variable when $f^{(5)}(\boldsymbol{\alpha}; t_0) > 0$

$$t - t_0 = [5!\hbar/f^{(5)}(\boldsymbol{\alpha}; t_0)]^{1/5} u$$

we finally obtain the following expression for $I(\boldsymbol{\alpha})$:

$$I(\boldsymbol{\alpha}) \approx g(t_0) \exp[\mathrm{i}f(\boldsymbol{\alpha}; t_0)/\hbar](5!\hbar/f^{(5)})^{1/5} S\left[\left(\frac{5!\hbar}{f^{(5)}}\right)^{3/5} \frac{f^{(3)}}{\hbar 3!}, \left(\frac{5!\hbar}{f^{(5)}}\right)^{2/5} \frac{f^{(2)}}{\hbar 2!}, \left(\frac{5!\hbar}{f^{(5)}}\right)^{1/5} \frac{f^{(1)}}{\hbar} \right] \tag{5.5}$$

where $f^{(n)} = f^{(n)}(\boldsymbol{\alpha}; t_0)$. Equation (5.5) is simple to apply provided that the $f^{(n)}(\boldsymbol{\alpha}; t_0)$ can be readily calculated (as is the case for $B(a, b, c, d)$). For the parameters in table 4, the stationary phase points t_2, t_3, t_4, t_5 are close together and the results of the transitional swallowtail approximation are in reasonable agreement with the exact values, although the agreement is not as good as that for the uniform swallowtail approximation.

Table 4 also shows the results for two further approximate methods. In the double uniform Airy approximation, the contribution from t_2, t_3 is evaluated by the uniform Airy formula as is the contribution from t_4, t_5, whereas the primitive approximation applies the stationary phase or saddle point method to each of the t_i. Explicit formulae for these methods can be found in Connor and Marcus (1971) for example. The double uniform Airy and primitive approximations both have large errors in comparison with the exact results, in particular the errors for the primitive approximation are larger than those for the double uniform Airy approximation. These large errors are expected because the proximity of t_2, t_3, t_4, t_5 means that the conditions for the validity of the double uniform Airy and primitive approximations are not satisfied.

We have also evaluated $B(a, b, c, d)$ for a further 150 sets of (a, b, c, d), with the restriction that t_1 is always well separated from the four remaining stationary phase points. The results are similar to those in table 4. This extensive set of calculations provides a consistency check on the accuracy of our exact computations for $B(a, b, c, d)$ and illustrates the practicality of the methods described in §§ 3 and 4 for the uniform swallowtail approximation.

6. Summary and conclusions

This paper has described practical methods for the numerical implementation of the uniform swallowtail approximation. There are two main problems that must be overcome: (a) methods are required for the computation of $S(x, y, z)$, $\partial S/\partial x$, $\partial S/\partial y$, $\partial S/\partial z$ and (b) it is necessary to evaluate x, y, z, A from the input function $f(\boldsymbol{\alpha}; t)$.

We have shown that integration along complex contours is an efficient and reliable method for the numerical evaluation of $S(x, y, z)$ and its partial derivatives and results of high accuracy are readily obtained. The method is straightforward to program on a computer. The numerical values given in tables 1–3 can be used by readers to check the accuracy of their own computer programs using either the complex contour quadrature technique or some other method. The isometric plots shown in figures 3–6 together with those in Connor *et al* (1983) systematically illustrate the main properties of $|S(x, y, z)|$, $|\partial S/\partial x|$, $|\partial S/\partial y|$, $|\partial S/\partial z|$.

We have also described two methods for the evaluation of the parameters x, y, z, A. The first of these is an iterative technique and is valid when (x, y, z) is not close to the swallowtail caustic. The second method is an algebraic technique and is most useful when (x, y, z) lies on the caustic and for the case $y = 0$. Thus in practice both methods are complementary. We used symbolic algebraic computer programs to carry out the necessary algebraic manipulations. As an example of the use of the uniform swallowtail approximation, we evaluated the butterfly canonical integral $B(a, b, c, d)$ for a large number of values of (a, b, c, d). Like the uniform Pearcey approximation (Connor and Farrelly 1981), the uniform swallowtail approximation can now be considered a practical tool for the asymptotic evaluation of oscillating integrals.

Acknowledgments

We thank Professor R Gilmore (Drexel University, Philadelphia) for helpful correspondence. Support of this research by the States of Jersey Education Committee, the Science and Engineering Research Council (UK) and the National Science Foundation, USA (grants CHE80-11412 and PHY82-00805) is gratefully acknowledged. Some of the numerical and algebraic calculations were carried out using the CDC 7600 computer of the University of Manchester Regional Computer Centre and the AS 7000 computer at Daresbury Laboratory. We also acknowledge the use of the MACSYMA algebraic manipulation program, which is maintained by the MIT Mathlab group and is supported in part by the US Energy Research and Development Administration (contract number E(11-1)-3070) and NASA (grant NSG 1323). JNLC thanks Professor R A Marcus for his hospitality at the AA Noyes Laboratory of Chemical Physics, California Institute of Technology, Pasadena, California, USA, where this paper was completed and NATO for a Senior Scientist award. We also thank the referees for their comments.

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