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LETTER TO THE EDITOR

On the analysis of diffraction catastrophes

H Trinkaus and F Drepper
Institut für Festkörperforschung der Kernforschungsanlage Jülich, 5170 Jülich, Germany

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Abstract. The most important diffraction catastrophes (caustics) occurring in two-dimensional diffraction are analysed: the fold (elementary caustic), the cusp, the hyperbolic and the elliptic umbilic catastrophe. Special emphasis is given to the inverse problem: what information can be obtained from an observed diffraction catastrophe pattern? We show that the critical lines (rainbow lines) in the object plane and the behaviour of the phase function in their neighbourhood can be determined approximately from the characteristic vectors and the intensities of the main peaks in the pattern of these diffraction catastrophes.

A common phenomenon in ray theory is the divergence of the density of classical trajectories in certain directions leading to infinite intensities. In light and electron optics such divergences are well known as caustics. Wave theory does not give infinite intensities, but it yields especially large intensities at caustics if the wavelength is very small. Therefore it is most important to study the asymptotic behaviour of wave fields near caustics for the limiting case of very small wavelengths (semiclassical theory).

The various possible forms which caustics take can be classified according to the catastrophe theory of Thom (1972). Therefore we call the related characteristic wave fields diffraction catastrophes. An extensive classification of such catastrophes has been given by Arnol'd (1972, 1973) (see also Duistermaat 1974).

Recently Connor (1976) has applied the ideas of catastrophe theory to semiclassical collision theory. Berry (1976) has presented a number of beautiful examples of diffraction catastrophes from smooth phase objects like undulated reflecting surfaces. In fact caustics, originally observed in optics, occur in various fields of wave and particle scattering: in atomic and molecular collisions (see Connor 1976), especially in atomic scattering from surfaces (see Berry 1975), as well as in diffuse scattering of neutrons and x-rays from displacement fields of dislocation loops in crystals (Trinkaus 1971, 1977).

Diffraction catastrophes are especially useful in analysing diffracting objects: first because of the high intensity near caustics and secondly because of the (nearly local) relationship between the critical points of the object (rainbow lines) and the points of the caustic. In this letter we will discuss the information which diffraction catastrophes can give about diffracting objects. For simplicity we will consider only two-dimensional phase functions generated by pure phase objects like displacement fields of reflecting surfaces.

For the problem of relating such phase functions to the properties of three-dimensional scattering potentials we refer to a recent paper of Drepper (1977). Moreover we will confine ourselves to the most important diffraction catastrophes occurring in scattering from two-dimensional objects, these are the fold (elementary caustic), the cusp, the hyperbolic and the elliptic umbilic catastrophe. For the following considerations we assume that the wave amplitude is given by (see Berry 1975)

$$A(\boldsymbol{\kappa}) = \frac{k}{2\pi} \int \mathrm{d}^2\boldsymbol{x}\, \mathrm{e}^{\mathrm{i}k(\boldsymbol{\kappa}.\boldsymbol{x}+\phi(\boldsymbol{x}))}. \tag{1}$$

Here k is the wavenumber, $\boldsymbol{\kappa}$ is the direction of observation and $\boldsymbol{x}$ is a point in the scattering plane or an impact parameter (see Drepper 1977). Our problem is to determine $\phi(\boldsymbol{x})$ from the pattern of the intensity $|A(\boldsymbol{\kappa})|^2$.

In the short-wavelength limit (large K) A is determined by the neighbourhood of stationary phase points $\boldsymbol{x}^s$

$$\kappa_i + \phi_{|i}(\boldsymbol{x}^s) = 0, \tag{2}$$

where $|i$ denotes differentiation with respect to the coordinate i. This defines a local mapping, $\boldsymbol{x} \rightarrow \boldsymbol{\kappa}$ of the real space into the reciprocal space. If the contributing points $\boldsymbol{x}^s$ are 'isolated', that is many wavelengths apart from each other, one has

$$|A(\boldsymbol{\kappa})|^2 \rightarrow \sum_s 1/D(x^s(\boldsymbol{\kappa})) \tag{3}$$

where $D = \det(\phi_{|ij})$ is the Hessian $H(\phi)$ that is the Jacobian of the mapping from $\boldsymbol{x}$ to $\boldsymbol{\partial}\phi$ and via (2) from $\boldsymbol{x}$ to $\boldsymbol{\kappa}$. According to (2) and (3), $|A(\boldsymbol{\kappa})|^2$ is given by the density of the classical trajectories and measures the density distribution of $\boldsymbol{\partial}\phi$. For more than one dimension this is not sufficient to determine $\phi(\boldsymbol{x})$.

Since in general, more than one stationary phase point can occur for a given $\boldsymbol{\kappa}$ the inverse mapping to (2), that is from $\boldsymbol{\kappa}$ to $\boldsymbol{x}$, is not unique. The caustic given by

$$D(\boldsymbol{x}(\boldsymbol{\kappa})) = 0 \tag{4}$$

defines the bifurcation set for which at least two stationary phase points coalesce. In the $\boldsymbol{x}$ plane $D(\boldsymbol{x}) = 0$ will be called the rainbow line. For such points (3) becomes infinite and the ordinary method of stationary phases breaks down.

To analyse the behaviour of $A(\boldsymbol{\kappa})$ in the vicinity of the caustic we will use orthogonal coordinate systems, (x, y) and (u, v), locally adapted to the caustic such that one coordinate, say x and u respectively, in the $\boldsymbol{x}$ and in the $\boldsymbol{\kappa}$ plane is parallel to the caustic, which means parallel to the non-vanishing eigenvector of $\phi_{|ij}$. Then $D = 0$ means $\phi_{xy} = \phi_{yy} = 0$. In the $\boldsymbol{\kappa}$ plane we take $v = \kappa_y + \phi_{|y}$ to be zero at the caustic.

By differentiating (2) and (4) we get:

(i) the relation between the differentials of the rainbow line and the caustic

$$\mathrm{d}u = -\phi_{xx}\, \mathrm{d}x, \tag{5}$$

(ii) the slope of the rainbow line

$$y' = -\phi_{xyy}/\phi_{yyy}, \tag{6}$$

(iii) the curvature of the caustic

$$\frac{\mathrm{d}^2 v}{\mathrm{d}u^2} = \left(\phi_{xxy} - \frac{\phi_{xyy}^2}{\phi_{yyy}}\right)\phi_{xx}^{-2}. \tag{7}$$

The most elementary caustic can be classified as a fold catastrophe. It is a smooth caustic for which two stationary points coalesce. These points must be well separated from other eventually contributing points to guarantee 'structural stability' of the fold catastrophe. The wave field in the neighbourhood of the caustic is described by an Airy function. Perpendicular to the caustic we have

$$I=|A|^2\approx\frac{2\pi}{|\phi_{xx}|}\left|\frac{4k}{\phi^2_{yyy}}\right|^{1/3}\left|Ai\left[\left(\frac{2k^2}{\phi_{yyy}}\right)^{1/3}v\right]\right|^2. \tag{8}$$

The structural stability of the fold manifests itself in an invariant ratio $I_1/I_0\approx 0{\cdot}612$ of the first side-ridge intensity to the maximum intensity.

From the distance between the first side-ridge and the main ridge

$$\Delta v=v_1-v_0\approx-2{\cdot}2(\phi_{yyy}/2)^{1/3}k^{-2/3} \tag{9}$$

one gets ϕ_{yyy}. From the maximum intensity one can also determine ϕ_{xx}. But for this the measured intensity has to be put on an absolute scale. One possibility to achieve this will be shown below. However, even with the use of the caustic curvature (7), the rainbow line in the (x, y) plane cannot be reconstructed with the aid of (5) and (6) since for that purpose ϕ_{xyy} is needed, which cannot be determined separately from (7). We will see how the cusp catastrophe can help to some extent.

The caustic forms a cusp, $v\sim u^{3/2}$, with infinite curvature (7) if $\phi_{yyy}=0$ in the related point of the (x, y) plane. Since in most cases $\det(\phi_{|ij})=0=\phi_{yyy}$ has solutions, the cusp is a common phenomenon for two-dimensional diffraction. For a cusp point the rainbow line is perpendicular to the caustic according to (6) $(y'\to\infty)$ and its curvature becomes

$$\mathscr{K}\to\frac{2\phi_{xyy}}{\phi_{xx}}-\frac{\phi_{yyyy}}{\phi_{xyy}}. \tag{10}$$

A possible distortion of the cusp can be resolved by the shear transformation

$$x=\bar{x},\qquad y=\bar{y}-\frac{1}{2}\frac{\phi_{xxy}}{\phi_{xyy}}\bar{x}. \tag{11}$$

In the vicinity of the cusp, the phase $\phi(x, y)$ can be separated approximately in the two variables by the quadratic transformation $x=\xi-\phi_{xyy}\eta^2/(2\phi_{xx})$, $\bar{y}=\eta$ so that the two-dimensional integral (1) factors into two one-dimensional integrals. The method of stationary phases can be applied only to one of them. The other one is characteristic for the cusp catastrophe and was discussed in detail by Pearcey (1946). The structural stability of the cusp catastrophe manifests itself in an invariant ratio $I_{1,2}/I_0\approx 0{\cdot}68$ of the intensity of the two first side peaks to the maximum intensity.

The main information about $\phi(x, y)$ which can be obtained from the diffraction pattern near a cusp can be extracted from the maximum intensity and two characteristic vectors $\boldsymbol{\kappa}_1$ and $\boldsymbol{\kappa}_2$ pointing from the main peak (0) to the nearest side peaks (1) and (2) as shown in figure 1(*a*). The maximum intensity is

$$|A_0|^2\approx 2\pi 0{\cdot}86\left|\frac{k}{\phi^2_{xx}a}\right|^{1/2} \tag{12}$$

and the coordinates of the peaks are

$$\begin{aligned} u_0&=-0{\cdot}9\phi_{xx}|a|^{1/2}\,\mathrm{sgn}(a)/\phi_{xyy}k^{-1/2}, && v_0=0;\\ u_{1,2}&=1{\cdot}8u_0+\frac{1}{2}\frac{\phi_{xxy}}{\phi_{xyy}}v_{1,2}, && v_{1,2}\approx\pm|a|^{1/4}k^{-3/4} \end{aligned} \tag{13}$$

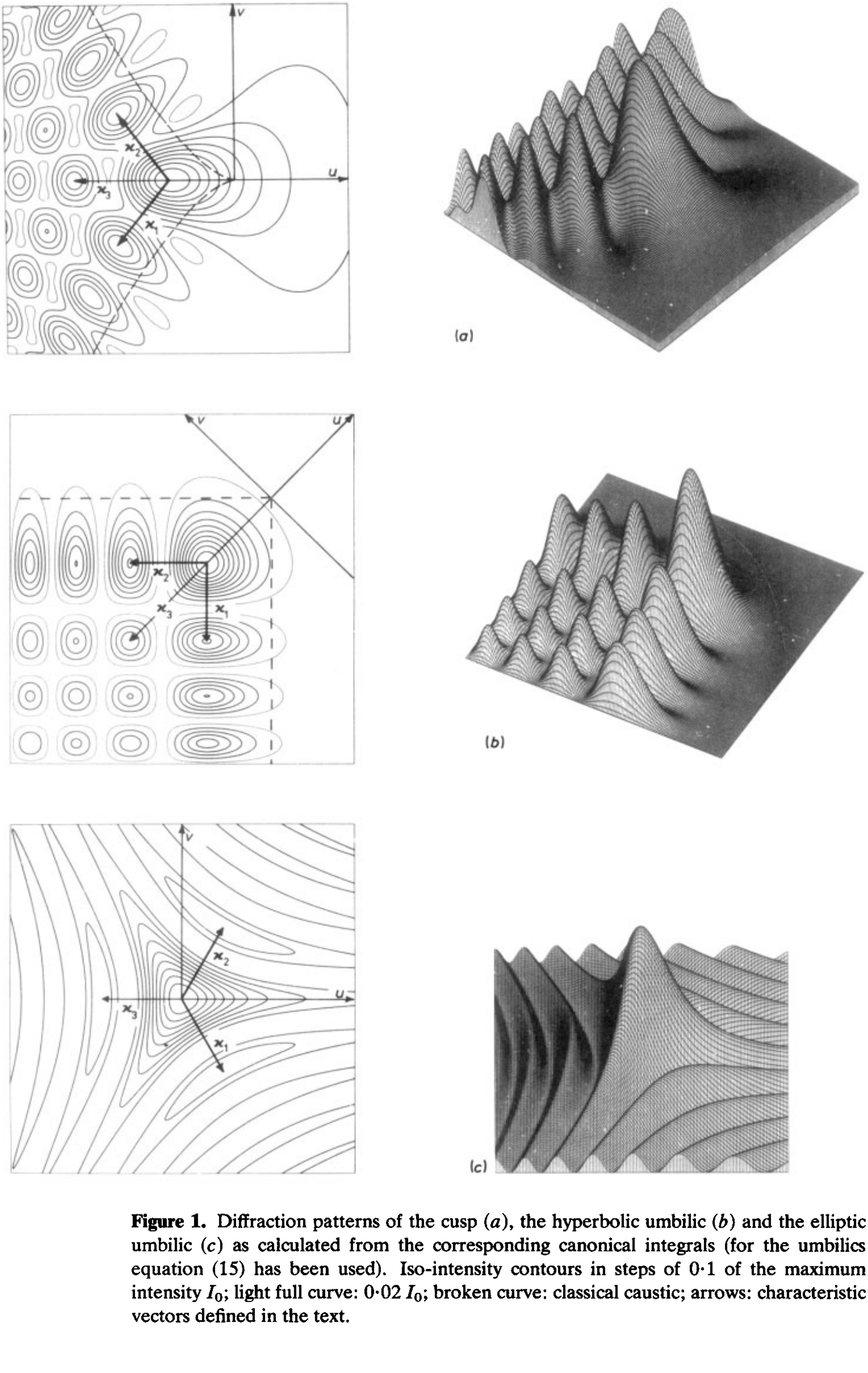

Figure 1. Diffraction patterns of the cusp (a), the hyperbolic umbilic (b) and the elliptic umbilic (c) as calculated from the corresponding canonical integrals (for the umbilics equation (15) has been used). Iso-intensity contours in steps of 0·1 of the maximum intensity I_0; light full curve: 0·02 I_0; broken curve: classical caustic; arrows: characteristic vectors defined in the text.

with $a=3\phi_{xyy}^2/\phi_{xx}-\phi_{yyyy}$. If the intensity is put on an absolute scale one can determine the derivatives ϕ_{xx}, ϕ_{xxy}, ϕ_{xyy} and ϕ_{yyy} (actually four possible sets) and thus also the curvature (10) of the rainbow line from (11) and (12). Hence we may note the most important result that the cusp pattern provides the direction ($y'\to\infty$) and the curvature (four possible values) of the rainbow line in the corresponding point of the (x, y) plane. If the caustic has several cusps (at least three) the topologically correct contour of the rainbow line can in general be found.

Various degeneracies of the cusp are possible. We discuss the most important one occurring for $\phi_{xx}\to 0$. In this case two additional cusps or an additional caustic approaches the first cusp forming elliptic or hyperbolic umbilics respectively (see Connor 1976, or Berry 1976). Thus, a threefold symmetry is often connected with an elliptic umbilic showing three cusps. Fully unfolded umbilics occur if the three conditions $\phi_{|ij}=0$ are fulfilled. This may happen accidentally or by symmetry. Thus, for a symmetry line with $\phi(-x, y)=-\phi(x, y)$ an umbilic will usually be found and a symmetry point with $\phi(-x, -y)=-\phi(x, y)$ (e.g. for a displacement field) is always connected with an umbilic.

The most important invariant governing the umbilics is the discriminant Δ of the cubic terms of the Taylor expansion of $\phi(x, y)$, that is the Hessian of D (see Gurevich 1964)

$$\Delta=H(D)=H(H(\phi))=\det[(\det\phi_{|ij})_{|kl}]. \tag{14}$$

For the elliptic umbilic $\Delta>0$ while for the hyperbolic one we have $\Delta<0$.

The 'natural' coordinate system of the umbilics has one axis parallel to the direction of one of the degenerating cusps, which is found as a real solution of $\phi_{|ijk}x_ix_jx_k=0$ (Gurevich 1964). In the fully unfolded case it is defined by the peak structure as shown in figures 1(*b*) and (*c*). In these coordinate systems we have

$$\phi_{yyy}=0 \qquad \text{and} \qquad -\Delta=(4\phi_{xxx}\phi_{xyy}-3\phi_{xxy}^2)\phi_{xyy}^2.$$

Symmetrization with the aid of (10) and normalization lead to the normal forms $\xi^3\pm\xi\eta^2$. After a special transformation of the integration paths in the complex plane for the elliptic umbilic, a rotation of the coordinate system by 45° yields in the vicinity of the fully unfolded umbilics

$$\begin{gathered} A=2^{5/3}\pi\left|\frac{k^2}{\Delta}\right|^{1/6}\operatorname{Re}(\operatorname{Ai}(\mu+\nu)F(\mu-\nu)) \\ \mu=a\left|\frac{2}{\Delta}\right|^{1/3}\phi_{xyy}\left(u-\frac{1}{2}\frac{\phi_{xxy}}{\phi_{xyy}}v\right)k^{2/3}, \qquad \nu=b\frac{|\Delta|^{1/6}v}{2^{2/3}\phi_{xyy}}k^{2/3}; \end{gathered} \tag{15}$$

where F is either the regular or the irregular Airy function Ai or Bi, $a=+1$ and -1, $b=+1$ and $-\mathrm{i}$, for the hyperbolic and the elliptic umbilics respectively. The structural stability of the umbilics manifests itself in an invariant ratio $I_{1,2}/I_0=0{\cdot}612$ for the hyperbolic umbilic and 0·287 for the elliptic one.

The main information which the diffraction pattern of the umbilics can give is contained in the maximum intensity and in two characteristic vectors $\boldsymbol{\kappa}_1$ and $\boldsymbol{\kappa}_2$($\boldsymbol{\kappa}_1+\boldsymbol{\kappa}_2=\pm\boldsymbol{\kappa}_3$) as shown in figure 1(*b*) and (*c*). The maximum intensity is

$$|\Delta|^{1/3}|A_0/2\pi|^2\approx 0{\cdot}21k^{2/3} \qquad \text{and} \qquad \approx 0{\cdot}12k^{2/3} \tag{16}$$

and the coordinates of the peaks are given by

$$\mu = -1{\cdot}02 \qquad \nu = 0$$

$$\mu_{1,2} + 1{\cdot}02 = \pm\nu_{1,2} = -1{\cdot}115 \tag{17}$$

and

$$\mu_0 = \nu_0 = 0, \qquad \mu_{1,2} = \pm\nu_{1,2}/\surd 3 = 0{\cdot}885,$$

for the hyperbolic and elliptic umbilics respectively. We see that the complete set of the third derivatives of $\phi(x, y)$ can be determined from two characteristic vectors alone. Since both $|A_0|^2$ and the parallelogram $\boldsymbol{\kappa}_1 \times \boldsymbol{\kappa}_2$ are determined by Δ we may write

$$(\boldsymbol{\kappa}_1 \times \boldsymbol{\kappa}_2)^2 |A_0/2\pi|^2 = 2{\cdot}032k^{-2} \qquad \text{and} \qquad = 1{\cdot}04k^{-2} \tag{18}$$

for the hyperbolic and elliptic umbilics respectively. Therefore the maximum intensity can be used to put the intensity on an absolute scale.

If none of the symmetries mentioned above is present no fully unfolded umbilics will appear in general. However, sometimes they may be realized by adjusting an appropriate control parameter. We suggest this be done, if possible, in order to gauge the intensity. All other special points on a caustic (centres of other catastrophes), like swallow tails or parabolic umbilics, are more unlikely in the sense that more control parameters have to be adjusted (points in a higher-dimensional space).

Summarizing, we conclude that a rainbow line in the $\boldsymbol{x}$ plane and the field $\phi(\boldsymbol{x})$ in its neighbourhood can be reconstructed approximately from the properties of the diffraction pattern in the neighbourhood of the caustic.

References

Arnol'd V I 1972 *Funct. Anal. Appl.* **6** 254–72

—— 1973 *Funct. Anal. Appl.* **7** 230–1

Berry M V 1975 *J. Phys. A: Math. Gen.* **8** 566–84

—— 1976 *Adv. Phys.* **25** 1–26

Connor J N L 1976 *Molec. Phys.* **31** 33–55

Drepper F 1977 *J. Phys. C: Solid St. Phys.* submitted for publication

Duistermaat J J 1974 *Commun. Pure Appl. Math.* **27** 207–81

Gurevich G B 1964 *Foundation of the Theory of Algebraic Invariants* (Groningen: Noordhoff)

Pearcey T 1946 *Phil. Mag.* **37** 311–7

Thom R 1972 *Stabilité Structurelle et Morphogénèse* (Reading, Mass.: Benjamin) (1975 *Structural Stability and Morphogenesis* (Reading, Mass.: Benjamin))

Trinkaus H 1971 *Z. Angew. Phys.* **31** 229–35

—— 1977 *Phys. Stat. Solidi* b to be published