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CATASTROPHES AND SEMICLASSICAL MECHANICS

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Catastrophe theory, in particular Thom's celebrated theorem[1] classifying the singularities of gradient maps, is central to the understanding of the relation between wave theories (such as quantum mechanics or electromagnetism) and ray or trajectory theories (such as classical mechanics or geometrical optics). The ray theories are approximations valid in the limiting case when the wavelength λ, and Planck's constant $\hbar$ in the quantum case, are small in comparison with other quantities in the problem which have the same physical dimensions. The limit $\lambda \rightarrow 0$ is a complicated one, because solutions of the wave equations are highly nonanalytic functions of λ at $\lambda=0$, and, moreover, the nature of the nonanalyticity can change suddenly as parameters in the wave function (positions, angles, etc.) are varied[2],[3].

Every wave field corresponds not to a single trajectory but to a family of trajectories. For example, a quantum scattering cross-section $\sigma(\theta)$, describing the intensity of particles scattered through angle θ by a centre of force, corresponds classically(fig. 1) to that family of trajectories which before being scattered are all moving in the same direction with the same energy (i. e. the family is characterised by its linear momentum vector). The most important features of a family of trajectories - its 'skeleton' one might say, are its singularities

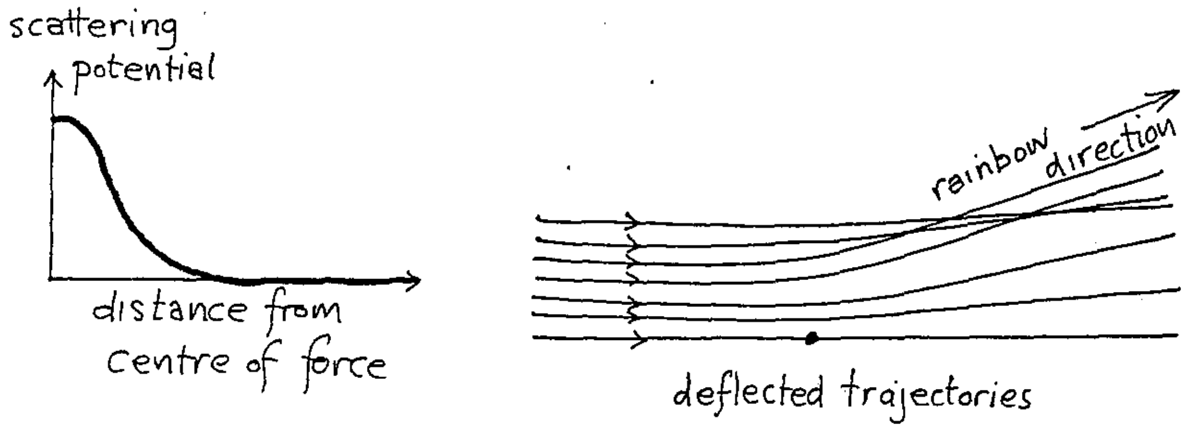

Figure 1 Scattering by a centre of force

where the density of rays is infinite. These singular regions, which are generalised foci, are called caustics. (An example is the 'rainbow angle' on fig. 1). They are singularities of the mapping from initial ray position to the position or direction of observation, and this

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mapping is moreover a gradient map, since by Hamilton's principle the rays minimise the action function (in Optics this is Fermat's principle of least time). Therefore Thom's theorem applies directly and classifies the forms of caustics, which dominate the observed images and cross-sections. This is easily demonstrated by shining a laser beam through irregular but smooth refracting surfaces, such as water 'droplet lenses' on glass, or corrugated glass of the type used in bathrooms(3). On a screen beyond the refracting surface can be clearly seen (fig. 2) fold lines and cusps, which are two-dimensional sections of umbilics, swallowtails, etc., which 'unfold' as parameters of the surface are varied (e.g. as a droplet lens evaporates).

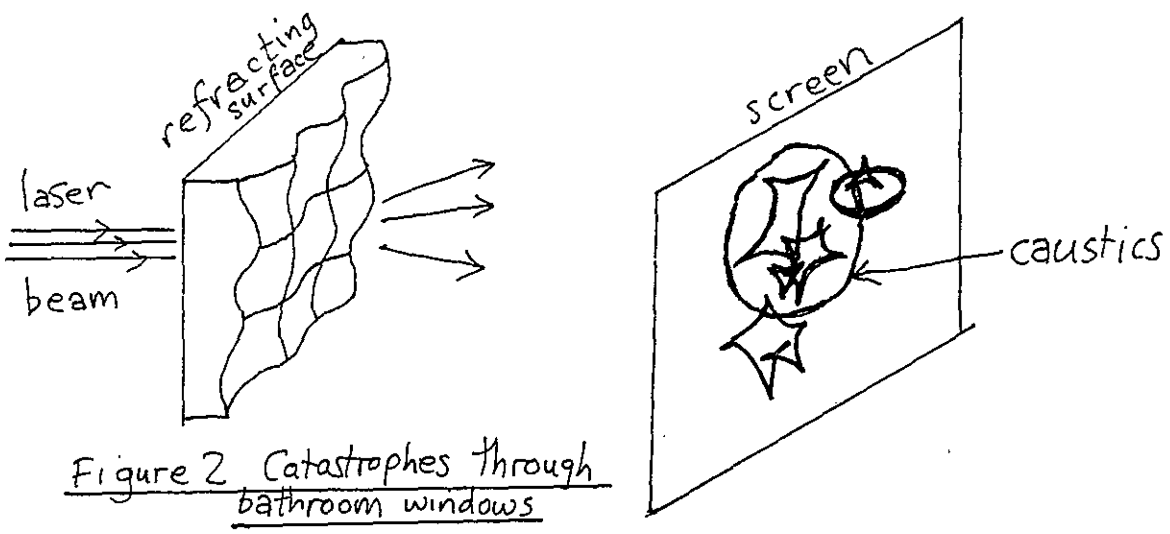

Figure 2 Catastrophes through bathroom windows

On a wave theory, intensities, cross-sections and other observables can never be infinite. On caustics of the ray pattern they rise to large values. How large? This question is answered by analyzing certain integral representations of the functions ("diffraction integrals") which are valid asymptotically as $\lambda \rightarrow 0$.(4),(5) The integrands are violently oscillating functions of both the integration variables, which turn out to be the "state variables" of catastrophe theory, and of the position and direction parameters, which are the "control variables". The integrands can be evaluated by a diffeomorphism changing the exponent into the "standard catastrophe" nearest the "control" point in question(5),(6). Thus the catastrophes define canonical integrals giving the wave pattern in regions where the ray pattern has caustics. The analysis shows that each catastrophe defines a singularity index, which is the inverse power of λ which gives the order of magnitude of the intensity I on the caustic. Thus at a fold(2),(3) (the rainbow - fig. 3a) $I \sim 0(\lambda^{-1/3})$ and at a cusp (fig. 3b) $I \sim 0(\lambda^{-\frac{1}{2}})$.(8),(9). In this way Thom's standard catastrophes form the classical bones on which is sewn the quantum flesh.

The theory can be used predictively, to find the wave pattern produced by a given system, as follows. A case of high symmetry is chosen, which can be solved analytically. The caustic is found to have singularities S of a higher dimension than would be expected. Breaking the symmetry unfolds S generically, in a manner found by simply inspecting the classification to find a higher dimensional caustic having S as a special section. This technique has proved useful in predicting the scattering pattern for atomic beams reflected by crystals.(3)

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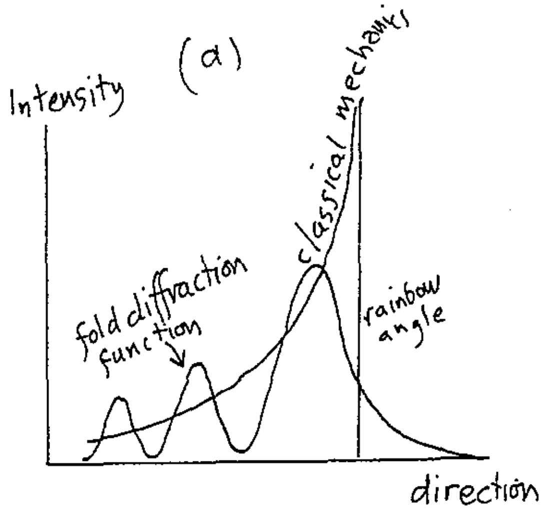

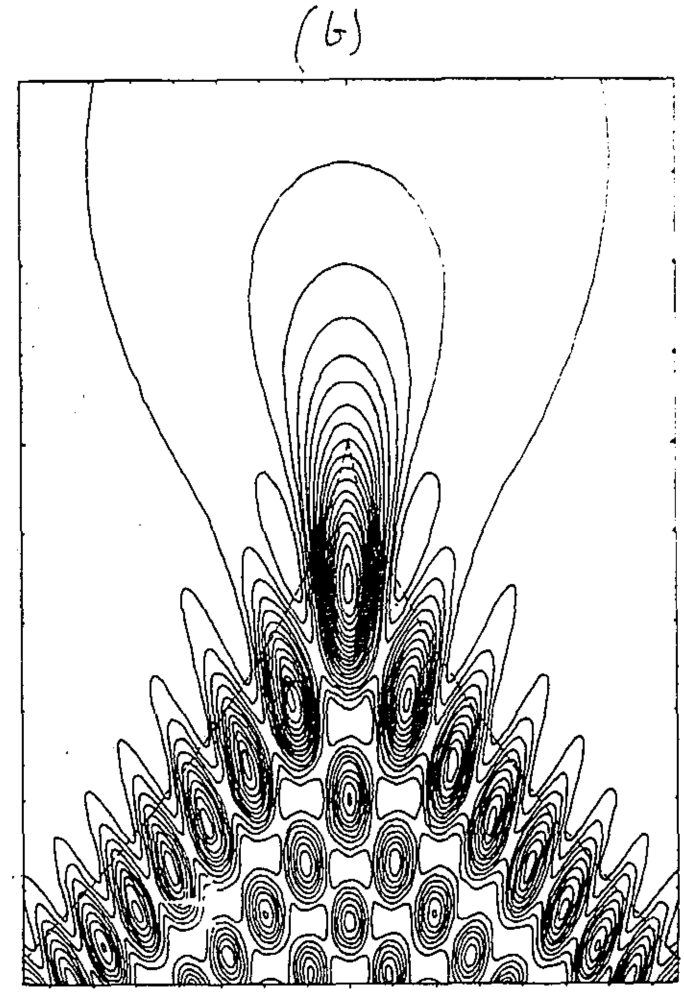

Figure 3
(a) Rainbow diffraction
(b) Cuspdiffraction (contours of intensity)

Finally, we point out that some caustics correspond to catastrophes of infinite order and so lie outside present classifications. Examples from potential scattering are as follows: (1) The glory [2], [9] is a point singularity in direction space, which can unfold in infinitely many ways into a closed cusped figure as the spherical symmetry of the centre of force is broken. For the glory, $I \sim O(\lambda^{-1})$. (2) Spiral scattering [2] is an infinite sequence of glories. (3) The forward diffraction peak [2], [9] is also a point in direction space whose singularity index depends on the way in which the tail of the scattering potential decays with distance (for the "Lennard-Jones" potential of atomic physics, $I \sim O(\lambda^{-2.8})$). The unfolding is produced in this case by destroying the tail by adding in a distribution of weak "scatterers at infinity". The point then unfolds into an infinite number of superposed cusped figures like those in figure 2.