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LETTER TO THE EDITOR

Analytic singularities in dispersive wave phenomena based on topological singularities of dispersion relations

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Abstract. The connection between topological singularities of dispersion relations and analytic singularities with respect to frequency of spectral densities and wavefunctions in dispersive media due to time harmonic sources is demonstrated. The topological singularities are discussed within the framework of imperfect bifurcation theory, regarding the frequency as a distinguished bifurcation parameter and the wavenumbers as bifurcation variables, and using a recently obtained classification of topological singularities up to codimension four which is given in terms of a list of normal forms. To each normal form corresponds an analytic singularity, governed by characteristic exponents which are tabulated.

Dispersive wave phenomena are, in general, governed by a dispersion relation (Whitham 1974, Lighthill 1979)

$$B(\omega, k)=0, \tag{1}$$

where ω is the frequency, $k=(k_1, \ldots, k_n)$ are wavenumbers and B is a smooth function of ω and k which will be called the 'dispersion function'. There are two types of integrals associated with B, namely

$$u(\omega)=\int \mathrm{d}k\, \delta[B(\omega, k)]|\partial B(\omega, k)/\partial \omega| \tag{2a}$$

and

$$u(\xi, \omega)=\int \mathrm{d}k\, \mathrm{e}^{-\mathrm{i}k\cdot\xi}/B(\omega-\mathrm{i}0, k), \tag{2b}$$

where δ in $(2a)$ is Dirac's delta function. The integral $(2a)$ occurs in crystal vibrations with $u(\omega)$ being the crystal's spectral density. If (1) yields a unique solution $\omega=\hat{\omega}(k)$, $(2a)$ reduces to $u(\omega)=\int \mathrm{d}k\, \delta[\omega-\hat{\omega}(k)]$ which is of standard form (Wannier 1959), but the representation $(2a)$ is more general than the latter expression. The function $u(\xi, \omega)$ given by $(2b)$ is, apart from a factor $\exp(\mathrm{i}\omega t)$, the response at the space point $\xi=(\xi_1, \ldots, \xi_n)$ in a dispersive medium due to an oscillating point source of frequency ω at the origin. Equation $(2b)$ can be written (Lighthill 1979) as a surface integral,

$$u(\xi, \omega)=-2\pi\mathrm{i}\int_{S_\omega^-} \mathrm{d}S\, \mathrm{e}^{-\mathrm{i}k\cdot\xi}/|\nabla_k B(\omega, k)|, \tag{3}$$

where S_ω^- is that part of the surface $B(\omega, k)=0$ in k space on which $(\xi\cdot\nabla_k B)\partial B/\partial\omega<0$. A similar expression holds for $(2a)$.

The purpose of this paper is to demonstrate the connection between the analytic singularities with respect to ω of the integrals $(2a, b)$ and the generic topological singularities of the underlying dispersion function B. We do this by deriving a canonical expression for an integral of the form $(2a, b)$ from the canonical form for its integrands in the neighbourhood of a large class of topological singularities, as classified by Dangelmayr (1982). The behaviour of the integrals with respect to frequency is governed by characteristic exponents, which we also find.

We say that B has a topological singularity at (ω_0, k_0) if $B(\omega_0, k_0)=0$ and $|\nabla_k B(\omega_0, k_0)|=0$. It is important to note that the topological singularities originate in equations, and consequently cannot be described generically as singularities of smooth functions in the sense of elementary catastrophe theory (Poston and Stewart 1978), as is commonly done for non-dispersive waves (Berry 1976, 1982, Dangelmayr and Güttinger 1982). The point is that $\partial B(\omega_0, k_0)/\partial\omega$ can be zero, giving rise to multivalued and non-smooth behaviour of ω as a function of k. To classify singularities of dispersion relations one has to use a framework which is rather different from catastrophe theory, namely, the theory of imperfect bifurcations in the sense of Golubitsky and Schaeffer (1979). The idea is to consider (1) as a bifurcation equation for the wavenumbers k ('bifurcation variables') and to regard the frequency ω as a distinguished bifurcation parameter. For fixed ω, equation (1) defines a manifold S_ω of codimension one in k space. Suppose that for some $\omega=\omega_0$, S_{ω_0} exhibits a singularity at k_0; in other words, the topological type of S_ω changes when ω passes through its critical value ω_0. The standard singularity-theoretic approach to studying the behaviour of the solutions of (1) in a neighbourhood of (ω_0, k_0) is to choose a coordinate system in which B takes a canonical (normal) form. Putting $\tilde\omega=\omega-\omega_0$, $\tilde k=k-k_0$ and $\tilde B(\tilde\omega, \tilde k)=B(\omega, k)$ so that $\tilde B(0,0)=0$, imperfect bifurcation theory allows for transformations of the form

$$\tilde B(\tilde\omega, \tilde k)=T(x, \lambda)G(x, \lambda) \tag{4}$$

where $x=(x_1, \ldots, x_n)=x(\tilde k, \tilde\omega)$, $\lambda=\lambda(\tilde\omega)$, $\det(\partial x_i/\partial\tilde k_j)>0$, $\mathrm{d}\lambda/\mathrm{d}\tilde\omega>0$ and the function $T(x, \lambda)$ is non-zero. Observe that λ does not depend on $\tilde k$, which emphasises the role of the frequency as distinguished parameter, consistent with the integrals in (2) where the wavenumbers are integrated out. As in catastrophe theory, the class of transformations given by (4) induces equivalence classes (orbits) in the space of all functions $G(x, \lambda)$ or $\tilde B(\tilde\omega, \tilde k)$ vanishing at the origin. In the framework of imperfect bifurcation theory in the sense of Golubitsky and Schaeffer (1979), one associates with any function $G(x, \lambda)$ a codimension cod G and a universal unfolding $F(x, \lambda, \alpha)$ satisfying $F(x, \lambda, 0)=G(x, \lambda)$ where $\alpha=(\alpha_1, \ldots, \alpha_l)$ is a set of parameters and $l=\operatorname{cod} G$. The role of F is similar to the universal unfoldings of catastrophe theory and will not be exploited here further. For a presentation of imperfect bifurcation theory from a physical point of view see e.g. Stewart (1981). We call any (locally smooth) function $G(x, \lambda)$ satisfying $G(0,0)=0$ and $\nabla_x G(0,0)=0$ a singularity (which should not be confused with singularities in the catastrophe-theoretic sense). A classification of singularities up to codimension four has been obtained recently by Dangelmayr (1982) in terms of a list of normal forms. Putting $\hat x=(x_{s+1}, \ldots, x_n)$, $x=(\tilde x, \hat x)$, and defining the non-degenerate quadratic form,

$$Q_{p,q}(\hat x)=\sum_{i=1}^{p} x_{s+i}^2-\sum_{i=1}^{q} x_{s+p+i}^2 \qquad (s+p+q=n), \tag{5}$$

any normal form with codimension less than or equal to four can be written as

$$G(x, \lambda) = G_0(\tilde{x}, \lambda) + Q_{p,q}(\hat{x}), \tag{6}$$

where G_0 is the degenerate part of G and $s = 0, 1, 2$ is the corank of $G(x, 0)$ in the standard catastrophe-theoretic sense (Poston and Stewart 1978). The normal forms G_0, together with their unfolding terms, are listed in table 1, where $\tilde{x} = X$ or $\tilde{x} = (X, Y)$ according to $s = 1$ or $s = 2$, respectively. In table 1 we have used Arnold's (1974) notation for $G(x, 0)$, viewed as a singularity in the sense of catastrophe theory, to which we have added a second index to denote the difference between cod G and the (catastrophe-theoretic) codimension of $G(x, 0)$. Observe that table 1 contains some normal forms of the form $G_0 = \lambda \pm f(\tilde{x})$ with f being a standard Thom–Arnold singularity. In this case the catastrophe-theoretic codimension of f coincides with cod G_0, though in more degenerate cases these two types of codimension may be different (cf Dangelmayr 1982). The normal forms $D_{4,2}$, $A_{2,4}$ and $A_{3,3}$ have codimension five, but one unfolding term is associated with a modal parameter (indicated by the asterisk) so that their topological codimension (cf Golubitsky and Schaeffer 1979) is, in fact, four.

Any topological singularity of the dispersion function B at (ω_0, k_0) gives rise to an analytic singularity of the integrals (2) at ω_0. In a neighbourhood of (ω_0, k_0) the dispersion function can be transformed into a normal form $G(x, \lambda)$ (equation (4)) with G_0 being one of the normal forms of table 1. More degenerate singularities (codimension $\geqslant 1$) may occur in B due to a dependence of B on additional parameters (e.g. pressure, temperature, external fields in the case of crystal vibrations and spatial position or parameters characterising the medium in the case of dispersive waves). The dominant singular behaviour of $u(\omega)$ resp $u(\xi, \omega)$ near $\omega = \omega_0$ is then governed by canonical integrals,

$$I_1(\lambda) \equiv \int \mathrm{d}x |\partial G(x, \lambda)/\partial\lambda| \delta(G(x, \lambda)) \tag{7a}$$

resp

$$I_2(\xi, \lambda) \equiv \int_{S_\lambda} \mathrm{d}S \, \mathrm{e}^{-\mathrm{i}x\cdot\xi}/|\nabla_x G(x, \lambda)|, \tag{7b}$$

Table 1. Normal forms G_0 up to topological codimension four. Here, $\varepsilon = \pm 1$ and $r = p + q = n - s$.

Type	G_0	Restriction	Unfoldings	cod G	ρ_1	ρ_2
$A_{1,m-1}$	λ^m	$1 \leqslant m \leqslant 5$	$\lambda^j\ (1 \leqslant j \leqslant m-2)$	$m-1$	$\frac{1}{2}mr - 1$	$m(\frac{1}{2}r - 1)$
$A_{m-1,0}$	$\varepsilon\lambda + X^m$	$3 \leqslant m \leqslant 6$	$X^j\ (1 \leqslant j \leqslant m-2)$	$m-2$	$\frac{1}{m} + \frac{r}{2} - 1$	$\frac{1}{m} + \frac{r}{2} - 1$
$A_{m-1,1}$	$X^m + \varepsilon X\lambda$	$3 \leqslant m \leqslant 5$	$1, \lambda, X^j\ (2 \leqslant j \leqslant m-2)$	$m-1$	$\frac{mr+2}{2(m-1)} - 1$	$\frac{rm}{2(m-1)} - 1$
$A_{2,2}$	$X^3 + \varepsilon\lambda^2$	—	$1, X, X\lambda$	3	$r - \frac{1}{3}$	$r - \frac{4}{3}$
$D_{m+1,0}$	$\lambda + \varepsilon X^m + XY^2$	$m = 3, 4$	$Y, X^j (1 \leqslant j \leqslant m-1)$	m	$\frac{1}{2}(r - 1 + 1/m)$	$\frac{1}{2}(r - 1 + 1/m)$
$D_{4,2}$	$X^3 + \varepsilon XY^2 + cX\lambda + Y\lambda$	$c^2 + \varepsilon \neq 0$	$1, X, Y^2, \lambda; X\lambda$	5*	$\frac{3}{4}r$	$\frac{3}{4}r - \frac{1}{2}$
$A_{2,4}$	$X^3 + 2cX^2\lambda + \varepsilon X\lambda^2$	$c^2 \neq \varepsilon$	$1, X, \lambda, X^2; X^2\lambda$	5*	$\frac{3}{2}r$	$\frac{3}{2}r - 2$
$A_{3,3}$	$X^4 + 2cX^2\lambda + \varepsilon\lambda^2$	$c^2 \neq \varepsilon$	$1, X. \lambda, X\lambda; X^2\lambda$	5*	$r - 1$	$r - \frac{3}{2}$

where S_λ^- is defined analogously to S_ω^-. (The function $T(x, \lambda)$ and the determinant of the transformation $k \to x$ have been ignored in equations (7), because their effect on the dominant analytic singularity of u near ω_0 is just multiplication of (7) by a positive constant.) The behaviour of I_1 and I_2 near $\lambda = 0$ is characterised by exponents ρ_1 and ρ_2, respectively, i.e.

$$I_i \sim |\lambda|^{\rho_i} \qquad \text{as } \lambda \to 0, \quad i = 1, 2. \tag{8}$$

The values of ρ_1 and ρ_2 for each normal form are given in table 1 (obtained from simple scaling arguments). Accurate expressions for I_1 for the non-modal singularities of table 1 are presented below. Finally, we give results for I_2 but confine ourselves to $n = 1$ and to the non-modal singularities of table 1.

The most convenient way of computing $I_1(\lambda)$ is to insert the Fourier integral representation of the delta function into (7a), leaving us with oscillatory integrals which can be easily evaluated for the non-modal singularities of table 1. The resulting Fourier inversion integral is then computed by making extensive use of Gelfand and Shilov's (1964) tables of Fourier transforms of generalised functions. In the case of the normal form $A_{1,0}$ the following expressions for I_1 are obtained:

$$(\pi^{p/2}/\Gamma(p/2))\theta(-\lambda)|\lambda|^{p/2-1} \qquad \text{for } q = 0, \tag{9a}$$

$$(\pi^{q/2}/\Gamma(q/2))\theta(\lambda)|\lambda|^{q/2-1} \qquad \text{for } p = 0, \tag{9b}$$

$$C + \pi^{n/2-1}\Gamma(1-n/2)[\theta(\lambda)\sin(q\pi/2) + \theta(-\lambda)\sin(p\pi/2)]|\lambda|^{n/2-1} \qquad \text{for } n \text{ odd and } p, q \geqslant 1, \tag{9c}$$

$$C + (\pi^{n/2}/\Gamma(n/2))[(-1)^{q/2}\theta(\lambda) + (-1)^{p/2}\theta(-\lambda)]|\lambda|^{n/2-1} \qquad \text{for } p, q \text{ both even and } \geqslant 2, \tag{9d}$$

$$C + (-1)^{(3p+q)/4}(\pi^{n/2-1}/\Gamma(n/2))[\ln|\lambda| - \psi(n/2)]|\lambda|^{n/2-1} \qquad \text{for } p, q \text{ both odd and } n = 2, 6, 10, \ldots, \tag{9e}$$

$$C + (-1)^{(p-1)/2}(\pi^{n/2-1}/\Gamma(n/2))[\psi(n/2) - \ln|\lambda|]|\lambda|^{n/2-1} \qquad \text{for } p, q \text{ both odd and } n = 4, 8, 12, \ldots. \tag{9f}$$

Here, Γ denotes the gamma function, ψ the psi function (Gradshteyn and Ryzhik 1980) and θ is the unit step function.

In (9c)–(9f), C is an arbitrary positive constant which appears in virtue of the unbounded support of the delta function, i.e. the Fourier inversion integral must be appropriately regularised. Expressions for I_1 for the normal forms $A_{1,m-1}$ with $m \geqslant 2$ are easily obtained from equations (9) by first replacing λ by λ^m and then multiplying the λ-dependent part of equations (9) by $m|\lambda|^{m-1}$.

For the normal forms $A_{m-1,0}$, $A_{m-1,1}$ and $D_{m+1,0}$ we obtain

$$I_1(\lambda) = C + \pi^{r/2-1}\Gamma(-\rho_1)A_0|\lambda|^{\rho_1}\phi(\lambda) \qquad (r = p + q) \tag{10}$$

where

$$\phi(\lambda) = \begin{cases} A_+\theta(\varepsilon\lambda) + A_-\theta(-\varepsilon\lambda) & \text{for } A_{m-1,0}, A_{m-1,1}, \\ A_+\theta(\lambda) + A_-\theta(-\lambda) & \text{for } D_{m+1,0}. \end{cases} \tag{11}$$

In equation (10), $\varepsilon = \pm 1$ (see table 1) and $C = 0$ if m is even and $p = 0$ or $q = 0$, otherwise C is arbitrary and positive as before. The amplitudes A_0, A_+, A_- are listed in table 2. The expression for I_1 for the normal form $A_{2,2}$ is obtained from the

Table 2. The amplitudes A_0, A_+, A_- (equations (10), (11)). Here, $r=p+q$ and $a_{m,\varepsilon}=\cos(\pi/4m)-\varepsilon\sin(\pi/4m)$.

	A_0	m	A_+	A_-
$A_{m-1,0}$	$\frac{2}{m}\Gamma\left(\frac{1}{m}\right)$	even	$\sin\left(\frac{q\pi}{2}\right)$	$\sin\left[\left(\frac{1}{m}+p\right)\frac{\pi}{2}\right]$
		odd	$\cos\left(\frac{\pi}{2m}\right)\sin\left[\left(\frac{1}{m}+q\right)\frac{\pi}{2}\right]$	$\cos\left(\frac{\pi}{2m}\right)\sin\left[\left(\frac{1}{m}+p\right)\frac{\pi}{2}\right]$
$A_{m-1,1}$	$\frac{1}{m-1}\Gamma\left(\frac{r+2}{2(m-1)}\right)$	even	$\sin\left[\left(q-\frac{p}{2}\right)\frac{\pi}{2}\right]+\sin\left(\frac{mp+q+2}{m-1}\frac{\pi}{2}\right)$	A_+
		odd	$\sin\left[\left(p+\frac{2}{m-1}\right)\frac{\pi}{2}\right]+\sin\left(\frac{q\pi}{2}\right)$	$\sin\left(\frac{mp+q+2}{m-1}\frac{\pi}{2}\right)+\sin\left(\frac{p+mq}{m-1}\frac{\pi}{2}\right)$
$D_{m+1,0}$	$\left(\frac{2\pi}{m}\right)^{1/2}\Gamma\left(\frac{1}{2m}\right)$	even	$\sin\left[\left(2q+1+\frac{1-\varepsilon}{m}\right)\frac{\pi}{4}\right]$	$\sin\left[\left(2p+1+\frac{1+\varepsilon}{m}\right)\frac{\pi}{4}\right]$
		odd	$a_{m,\varepsilon}\sin\left[\left(2q+1+\frac{1}{m}\right)\frac{\pi}{4}\right]$	$a_{m,\varepsilon}\sin\left[\left(2p+1+\frac{1}{m}\right)\frac{\pi}{4}\right]$

expression for the normal form $A_{2,0}$ by first replacing λ by λ^2 and then multiplying the second term in (10) by $2|\lambda|$. Equation (10) is not valid for normal forms $A_{m-1,1}$ if ρ_1 (see table 1) is a non-negative integer. In the latter case, (10) must be replaced by

$$I_1(\lambda)=C+\begin{cases}A_0(\pi^{r/2-1}/2\rho_1!)\cos(q\pi/2)|\lambda|^{\rho_1} & (\rho_1\text{ odd})\\ A_0(\pi^{r/2-1}/\rho_1!)\sin(q\pi/2)[\ln|\lambda|-\psi(\rho_1+1)]\lambda^{\rho_1} & (\rho_1\text{ even})\end{cases} \tag{12}$$

for m even, and

$$I_1(\lambda)=C+aA_0\left(\frac{\pi^{r/2-1}}{\rho_1!}\right)\left[\sin\left(\frac{q\pi}{2}\right)-\sin\left(\frac{p+mq}{m-1}\frac{\pi}{2}\right)\right]\lambda^{\rho_1}\ln|\lambda|+O(\lambda^{\rho_1}) \tag{13}$$

for m odd. In equation (13), $a=\varepsilon$ ($a=-1$) if ρ_1 is even (odd).

Turning to I_2 and putting $n=1$, the integral in (7b) reduces to

$$I_2(\xi,\lambda)=\sum_j[\theta(-\xi G_{0\lambda}G_{0X})\exp(-iX_j\xi)/G_{0X}]_j, \tag{14}$$

where G_0 is one of the singularities of table 1 with corank $G_0\leqslant 1$ and $G_{0\lambda}$ (G_{0X}) is the derivative of G_0 with respect to λ (X). The index j after the second bracket in (14) denotes that $G_{0\lambda}$ and G_{0X} have to be evaluated at the jth solution $X_j(\lambda)$ of the equation $G_0(X,\lambda)=0$ and the sum is taken over all $X_j(\lambda)$. The expressions for $I_2(\xi,\lambda)$ for the normal forms $A_{1,m-1}$, $A_{m-1,0}$ and $A_{2,2}$ are:

$A_{1,m-1}$:

$$\tfrac{1}{2}[\theta(\xi\lambda)\exp(-i\xi|\lambda|^{m/2})-\theta(-\xi\lambda)\exp(i\xi|\lambda|^{m/2})]|\lambda|^{-m/2} \qquad (m\text{ even}, \varepsilon=-1), \tag{15a}$$

$$0 \qquad (m\text{ even}, \varepsilon=1), \tag{15b}$$

$$\tfrac{1}{2}\varepsilon[\theta(-\varepsilon\xi)\exp(-i\xi|\lambda|^{m/2})-\theta(\varepsilon\xi)\exp(i\xi|\lambda|^{m/2})]\theta(-\varepsilon\lambda)|\lambda|^{-m/2} \qquad (m\text{ odd}); \tag{15c}$$

$A_{m-1,0}$:

$$m^{-1}[\theta(-\varepsilon\xi)\exp(-\mathrm{i}\xi|\lambda|^{1/m})-\theta(\varepsilon\xi)\exp(\mathrm{i}\xi|\lambda|^{1/m})]\theta(-\varepsilon\lambda)|\lambda|^{(m-1)/m} \qquad (m \text{ even}), \tag{16a}$$

$$m^{-1}\theta(-\varepsilon\xi)\exp(\mathrm{i}\varepsilon\xi|\lambda|^{1/m})|\lambda|^{(m-1)/m} \qquad (m \text{ odd}); \tag{16b}$$

$A_{2,2}$:

$$\tfrac{1}{3}\theta(-\varepsilon\xi\lambda)\exp(\mathrm{i}\varepsilon\xi|\lambda|^{2/3})|\lambda|^{-4/3}. \tag{17}$$

The evaluation of I_2 for $A_{m-1,1}$ is more subtle than for the other normal forms, because the equation $G_0(X, \lambda)=0$ has always $X=0$ as a solution and $G_{0\lambda}(0, \lambda)=0$, so that the step function in (14) is not properly defined. To avoid this difficulty, we consider the (perturbed) equation

$$X^m+\varepsilon X\lambda+\alpha=0, \qquad \alpha\in\mathbb{R} \tag{18}$$

and define sgn $G_{0\lambda}^{\pm}(0, \lambda)$ to be the sign of that solution of equation (18) which goes into the trivial solution $X=0$ for $\alpha\to\pm 0$. Looking at the bifurcation diagrams associated with (18) (see Golubitsky and Schaeffer 1979), one infers immediately that

$$\operatorname{sgn} G_{0\lambda}^{\pm}(0, \lambda)=-\varepsilon \operatorname{sgn}(\pm\lambda). \tag{19}$$

Now define $I_2^{\pm}(\xi, \lambda)$ by equation (14) with $G_{0\lambda}(0, \lambda)$ replaced by sgn $G_{0\lambda}^{\pm}(0, \lambda)$ (since only the sign of the argument of a θ function is relevant) to obtain

$$I_2^{\pm}(\xi, \lambda)=\varepsilon\theta(\pm\xi)\lambda^{-1}+(1/m)[\theta(\varepsilon\xi)\exp(\mathrm{i}\xi|\lambda|^{1/(m-1)})$$
$$+\theta(-\varepsilon\xi)\exp(-\mathrm{i}\xi|\lambda|^{1/(m-1)})]\theta(-\varepsilon\lambda)|\lambda|^{-1} \qquad (m \text{ odd}), \tag{20a}$$

$$I_2^{\pm}(\xi, \lambda)=\varepsilon\theta(\pm\xi)\lambda^{-1}+(\varepsilon/m)\theta(-\varepsilon\xi)\lambda^{-1}\exp(\mathrm{i}\varepsilon\xi\lambda^{1/(m-1)}) \qquad (m \text{ even}). \tag{20b}$$

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