

CHAPTER VII

SINGULARITIES IN NEMATICS

Introduction

In an ideal homogeneously aligned nematic the director will everywhere be oriented in the same direction (viz., parallel to the direction in which the plates are rubbed). Therefore between two crossed polaroids one should get two extinction positions at which the specimen is uniformly dark. However, this never happens in actual practice. Generally one finds that instead of complete extinction there is an optical pattern consisting of dark points with bright and dark brushes running away from them. (Friedel 1922). In these regions the director orientation changes considerably from that imposed by the walls. When the crossed polarisers are rotated the brushes also rotate. One generally finds two types of points. For some the rotation of brushes is in the same direction as the rotation of the polarisers. These are called positive singularities. For others the rotation of the brushes is in the opposite direction and these are called negative singularities. The

strength of a singularity is defined as one fourth the number of bright (or dark) brushes starting from it. These defects are known as disclinations (Frank 1958) and are generally due to line singularities present in the medium with the singular line running normal to the plates. Singularities exhibit some interesting properties. For instance the sum of the strengths of all singularities in a specimen tends to zero. Also like singularities repel and unlike singularities attract one another. Two distinct singularities can coalesce to form a new singularity. Frank (1958) worked out the director orientation in the vicinity of singularities with the assumption that all elastic constants are equal. However he remarked in his paper "... non-equality of K_{11} and K_{33} should not make drastic changes but only changes of curvature in patterns of the same topology. This would be observed as a non-uniform rotation of extinction arms with uniform rotation of polarizer and analyser". Nehring and Saupe (1972) worked out the exact differential equation governing the director orientation in schlieren textures without resorting to the single constant approximation. However, for working out the structure of the optical patterns, the force and energy of interaction between singularities, etc. they used the single constant approximation.

In ordinary nematics the elastic constants are

in general unequal, but of the same order of magnitude. However it is known that if the nematic is preceded by a smectic phase there is a critical divergence of the bend and twist elastic constants which therefore can attain very high values. The single constant approximation then fails completely. For the planar configuration that we shall be discussing here only the splay and bend constants are of relevance in discussing the director field. A quantity which is convenient for characterising the elastic anisotropy is $\epsilon = (K_{33} - K_{11}) / (K_{33} + K_{11})$ which is usually very much less than unity. However as the smectic phase is approached $\epsilon \rightarrow 1$. In this chapter calculations on the energy, interaction energy and director orientation for $+1$, -1 , $+\frac{1}{2}$ and $-\frac{1}{2}$ singularities having schlieren texture have been reported for OBOOA which is a typical nematic exhibiting a smectic phase at lower temperatures.

Theory

In the schlieren texture the director is assumed to be confined to the xy plane making an angle φ with respect to x. Thus

$$\vec{n} = (\cos \varphi, \sin \varphi, 0) \quad (1)$$

where φ is a function of x and y . Since the defects have rotational symmetry about the normal to the plates plane polar coordinates r, ψ are more convenient. In polar coordinates the director can be written as

$$n_x = \cos(\varphi - \psi), \quad n_\psi = \sin(\varphi - \psi), \quad n_z = 0 \quad (2)$$

where φ is now a function of r and ψ .

The equations (23a) of Chapter I yield for plane polars the following differential equation for φ

$$\begin{aligned} K[\varphi_{,rr} + \frac{1}{r} \varphi_{,r} + \frac{1}{r^2} \varphi_{,\psi\psi}] + cK[\{\varphi_{,rr} - \frac{1}{r} \varphi_{,r}(1 - 2\varphi_{,\psi}) \\ - \frac{1}{r^2} \varphi_{,\psi\psi}\} \cos(2\varphi - 2\psi) + \{\frac{2}{r} \varphi_{,r\psi} - \varphi_{,r}^2 \\ - \frac{1}{r^2} \varphi_{,\psi} (2 - \varphi_{,\psi})\} \sin(2\varphi - 2\psi)] = 0 \end{aligned} \quad (3)$$

where $K = \frac{1}{2}(K_{11} + K_{33})$. Experimental observations (see e.g., Nehring and Saupe 1972) indicate that the director orientation does not depend on r except in the vicinity of the singular point. We shall not consider ~~only~~ regions very close to the singularity. To seek solutions which are entirely independent of r one sets all derivatives with respect to r as well as the sum of all coefficients of the same power of r to

zero. Then equation (3) reduces to the following differential equation for φ

$$\varphi_{,\psi\psi} - \varepsilon [\varphi_{,\psi\psi} \cos(2\varphi - 2\psi) + \varphi_{,\psi} (2 - \varphi_{,\psi}) \sin(2\varphi - 2\psi)] = 0 \quad \dots(4)$$

If one equates K_{11} to K_{33} or equivalently puts $\varepsilon = 0$ one obtains

$$Q_{,\psi\psi} = 0$$

or

$$\varphi = s\psi + c = s \tan^{-1} \frac{y}{x} + c \quad (5)$$

where $s = \pm \frac{1}{2}$ integer and c is an arbitrary constant.

These solutions describe the familiar structures of the Oseen-Frank singularities. The properties of these singularities have been studied in detail by Frank (1958) and by Nehring and Saupe (1972).

When $\varepsilon \neq 0$ the only exact solutions are

$$\varphi = \psi, \quad \varphi = \psi + \frac{\pi}{2}, \quad \text{and} \quad \varphi = 2\psi + c$$

which correspond to $s = 1$ or 2 . Singularities of strength 2 are not very common and consequently they will not be discussed below.

For a general value of s equation (4) has to be solved at every value of ϵ . This has been done numerically by the orthogonal collocation method. For a given value of s when $\epsilon = 0$, $\varphi = s\psi + c$ with $\psi = 0$ and $\psi = 2\pi$ as the boundaries for the variable ψ , Similarly the boundary values for φ will be $\varphi_1 = c$ and $\varphi_2 = 2s\pi + c$. It is convenient to start with $\varphi = s\psi + c$ as the appropriate solutions and solve (4) exactly for φ with the boundary conditions: 0 , and $\varphi(\pi) = \varphi_2$ for a particular ϵ . The solution $\varphi \equiv \varphi(\psi)$ so obtained describes a singularity at $r = 0$ for that value of ϵ . Since this solution goes over into the neat solution (5) when $t \rightarrow 0$, s , which is defined in equation (5) shall be continued to be called the strength of the disclination even for $\epsilon \neq 0$. Once φ is known it is in principle possible to calculate the energy for that singularity by integrating over the sample Frank's expression for free energy density.

When more than one singularity is present in the sample the equilibrium equation is solved locally for each singularity to obtain the angles $\varphi_1, \varphi_2, \dots$ etc. corresponding to the different singularities. These solutions are now added to obtain the orientation

of the director ϕ at any point in the sample. This superposition principle is exactly valid when $\epsilon = 0$ since ϕ satisfies eqn. (5). However, (4) is a non-linear differential equation. Hence in general for any value of ϵ the superposition principle cannot hold. As the value of ϵ increases one can expect this superposed solution to be less and less accurate and to fail when ϵ attains its maximum value of 1. Thus the superposed solution is quite accurate for small values of ϵ and is only approximate at higher values of ϵ .

Results

Calculations have been made for a $50 \mu\text{m} \times 50 \mu\text{m}$ sample of unit thickness and with singularities of strengths $+s$ and $-s$ (both with $c = 0$) placed symmetrically about the centre on a line running through the centre parallel to one edge. The distance between the two singularities has been varied between $2.5 \mu\text{m}$ and $10.0 \mu\text{m}$. To avoid the singular points each singularity has been assumed to be surrounded by a core. When the energy calculations are made the free energy density is integrated over the whole of the sample except the cores surrounding the singularities. The data of

Cheung et al. (1973) on the elastic constant variation of CBOOA has been used.

The deformation energy per unit thickness of the sample for a singularity is given by

$$F_T = F + F_0$$

where

$$F = \int_{-a/2}^{a/2} \int_{-a/2}^{a/2} W(x,y) dx dy, \quad (6)$$

a is the edge length, F_0 the core energy and W the Frank's free energy density. Estimation of F_0 requires a precise knowledge of core structure. Since the details of core structure are not known F_0 has been ignored though in principle F_0 should also be considered. Even the dependence of F_0 on ϵ as well as on the type of singularity has not been considered. When more than one singularity is present in the sample a similar expression holds for: the collection of singularities except that W is now calculated from the orientation obtained from the superposition principle and F_0 includes the core

energies of both the singularities. Ignoring the contribution from the core the interaction energy F_{INT} between the singularities s and $-s$ is defined as

$$F_{INT} = F(+s) + F(-s) - F(+s, -s) \quad .$$

Here $F(+s)$ is the value of F given by (6) when the sample contains only the $+s$ singularity at a distance $d/2$ from the centre. Similarly $F(-s)$ is the value of F given by (6) when only the $-s$ singularity is present in the sample at a distance $-d/2$ from the centre. But $F(+s, -s)$ is the value F when both singularities are present in their respective positions.

In Figure 1 F has been shown as a function of ϵ for $+1$, -1 , $+\frac{1}{2}$ and $-\frac{1}{2}$ singularities. It is found that the value of F varies very little whether the singularity is at the centre or at a distance $d/2$ from the centre. For $s = +1$ and for $s = -\frac{1}{2}$ F does not change much with ϵ . This is because the deformation in both cases is predominantly determined by splay (involving K_{11}) and since K_{11} does not change much with the temperature F does not change much. On the other hand the deformations for the singularities $s = -1$ and $s = +\frac{1}{2}$ involves a considerable amount of

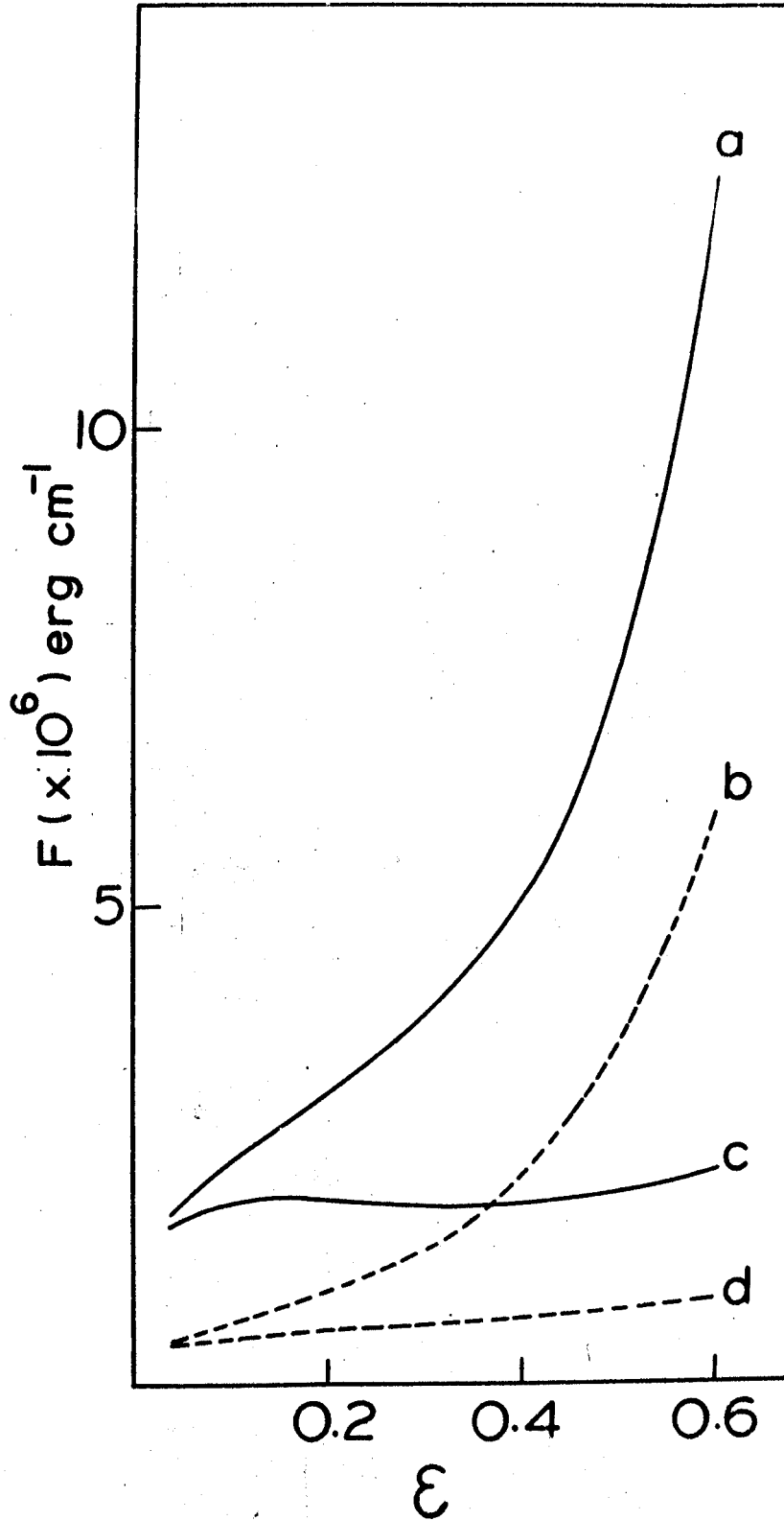


Figure 1: Deformation energies of (a) -1 (b) $\frac{1}{2}$ (c) 1 and (d) $-\frac{1}{2}$ singularities as functions of $\epsilon = (K_{33} - K_{11}) / (K_{33} + K_{11})$.

bend (involving K_{33} which changes quite fast with the temperature) even when $\epsilon = 0$. Consequently in these two cases F shows a large increase when ϵ is increased.

In figure 2 F_{INT} for unlike pairs $(+1, -1)$ and $(+\frac{1}{2}, -\frac{1}{2})$ of singularities has been plotted as a function of ϵ for three distances d between the singularities ($d = 2.5 \mu\text{m}$, $5 \mu\text{m}$ and $10 \mu\text{m}$). It is seen that at any distance the interaction energy increases with ϵ .

In figure 3 F_{INT} for the two pairs has been plotted as a function of the distance d separating them for a given value of ϵ . The interaction energy decreases as the distance separating the singularities is increased. This fact is also clear from figure 2 where it is found that in general at any value of ϵ

$$F_{INT}(d = 2.5 \mu\text{m}) > F_{INT}(d = 5 \mu\text{m}) > F_{INT}(d = 10 \mu\text{m}).$$

Since F_{INT} increases with ϵ it is clear that unlike singularities tend to come closer together as the smectic transition is approached.

Another very interesting feature comes out when

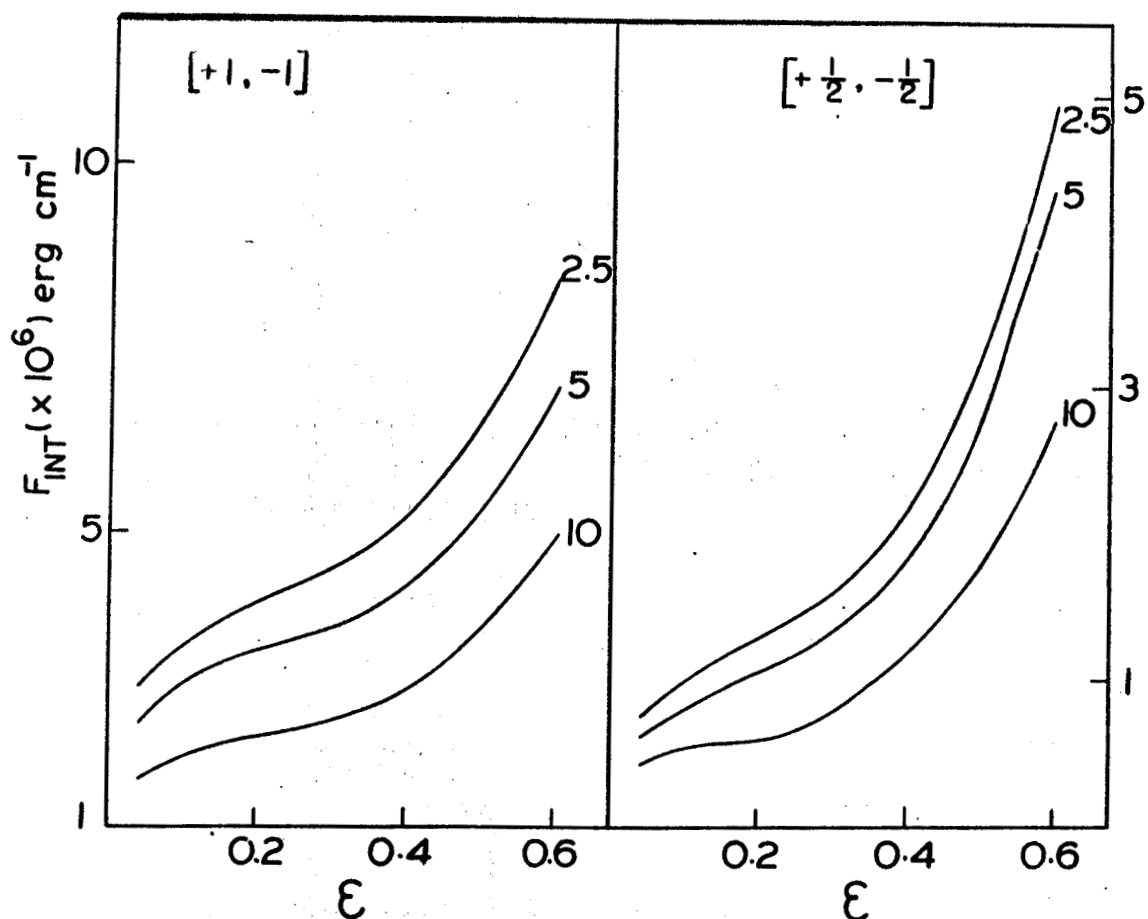


Figure 2: Interaction energy between 1 and -1 and that between $\frac{1}{2}$ and $-\frac{1}{2}$ singularities as function of ϵ . Distances between singularities 2.5 μm , 5 μm and 10 μm .

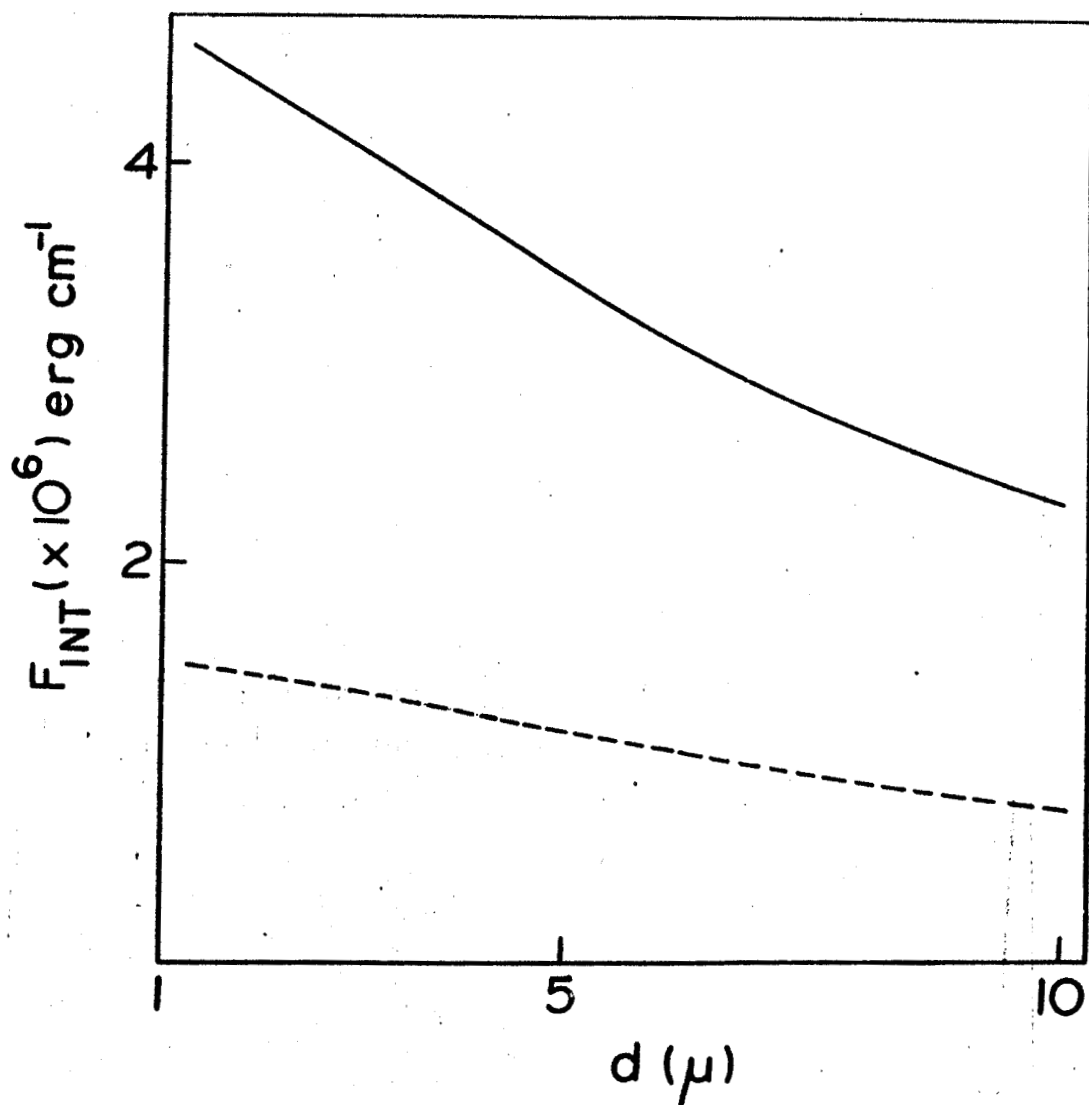


Figure 3: Interaction energy between 1 and -1 (full line) and that between $\frac{1}{2}$ and $-\frac{1}{2}$ (dashed line) as function of d the distance between singularities. $\epsilon = 0.2424$.

one compares F_{INT} for the integral and half integral singularities. In figure 4 the ratio

$$\Delta = \frac{F_{INT} (+1, -1)}{F_{INT} (+\frac{1}{2}, -\frac{1}{2})}$$

has been plotted against ϵ for a given value of d . It is seen that as ϵ increases Δ decreases'. This shows not only that F_{INT} for the two pairs of singularities does not change at the same rate with ϵ but also that as the smectic transition is approached the singularities of half strength have a greater chance of coming closer and annihilating each other than the singularities of integral strength.

The question can be raised as to whether the deformation at any point in the sample due to the singularities changes suddenly or gradually when ϵ is changed. The calculations show that the director orientation changes quite monotonically with ϵ . Figure 5 gives the changes in director orientation at a few representative points confirming that the schlieren texture will change only gradually when temperature is varied.

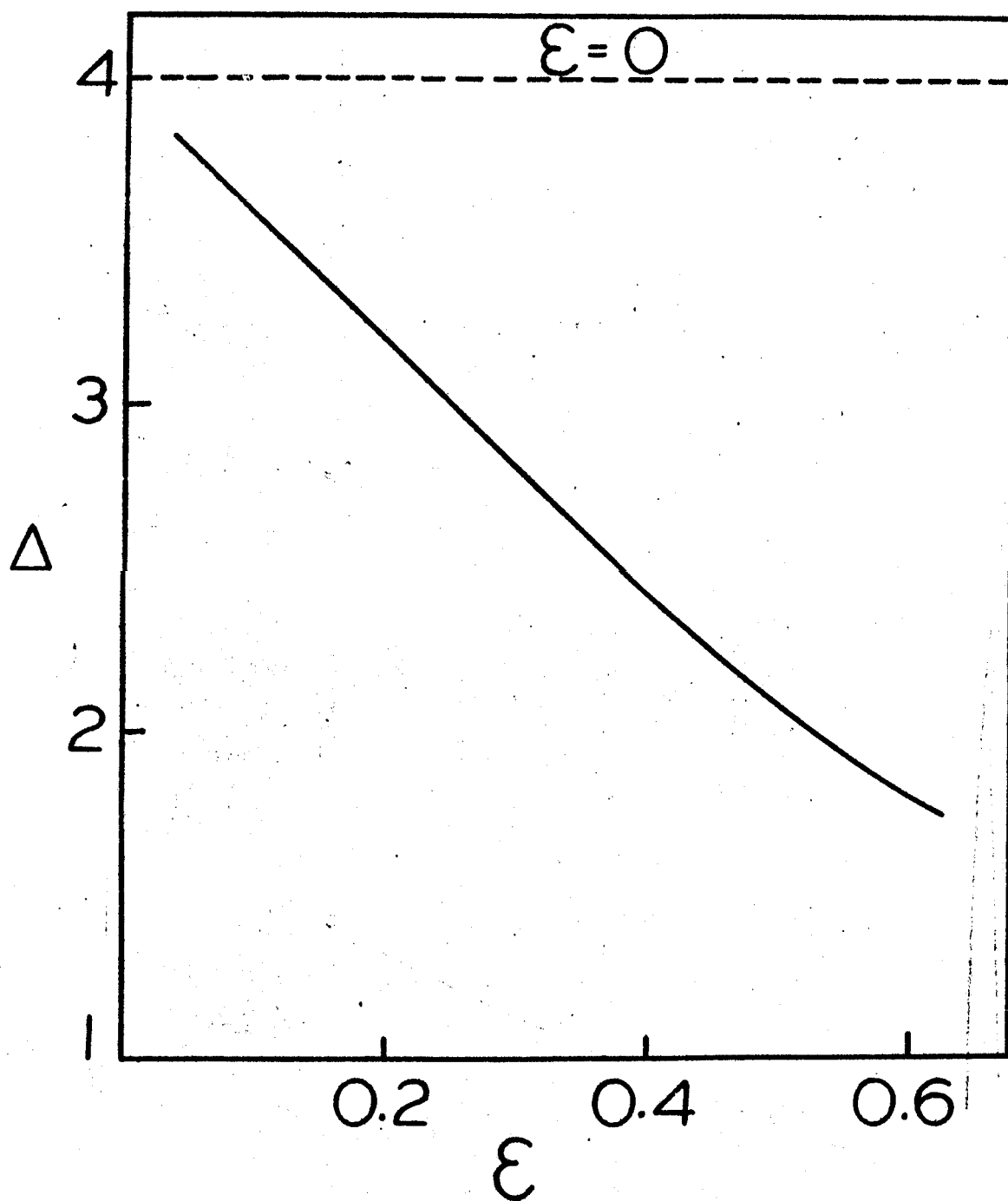


Figure 4: The variation of the ratio of interaction energies between $(1, -1)$ and $(\frac{1}{2}, -\frac{1}{2})$ with $t/d = 10 \mu\text{m}$.

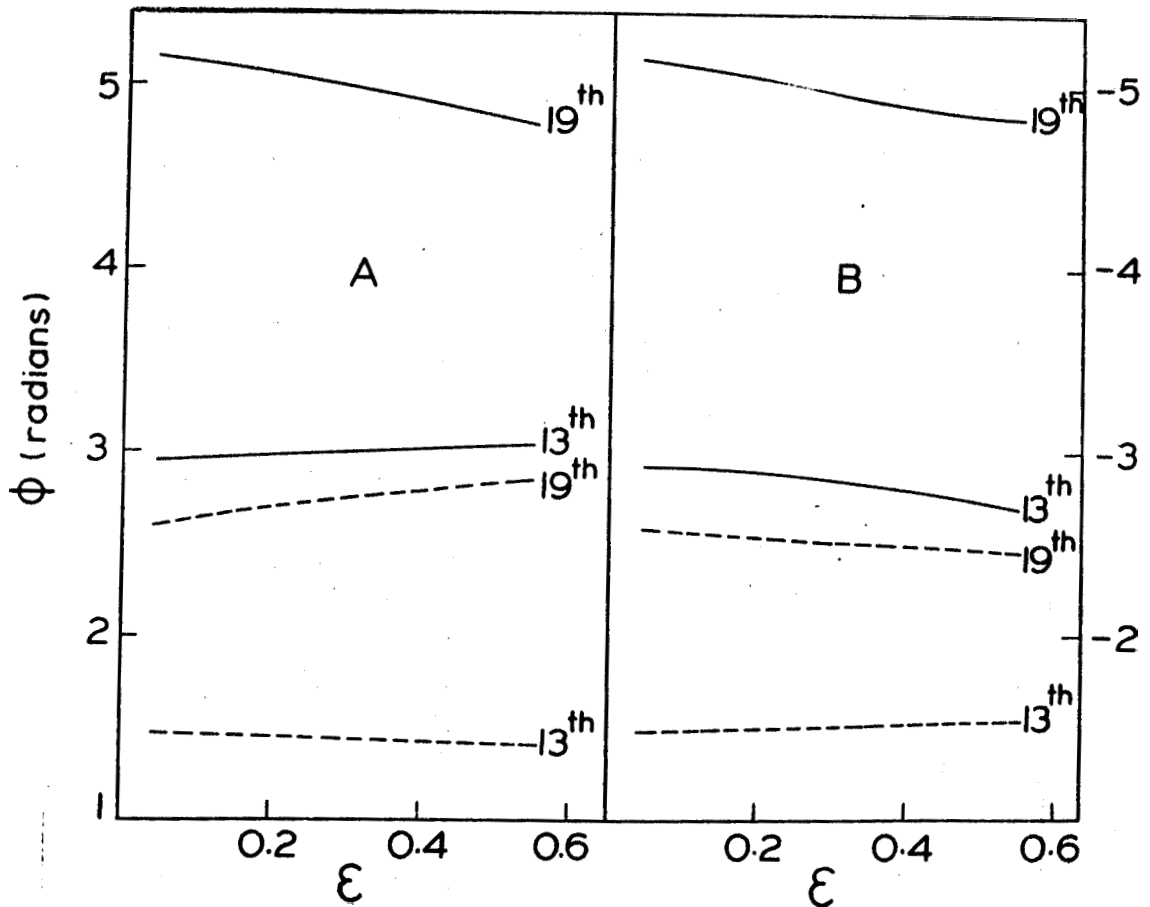


Figure 5: Director orientation ϕ as a function of ϵ at the 13th and 19th collocation point. for (A) $1, \frac{1}{2}$ and (B) $-1, -\frac{1}{2}$ singularities.

References

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