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Perturbation theory for planar nematic twisted layers

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As is well known, planar nematic layers exhibit a Freedericksz transition in electric fields. This effect can be strongly influenced by both geometrical and material parameters. Based on a perturbation method an analytical mathematical description is proposed, which is valid for small and intermediate deformation angles.

1. Introduction

Planar oriented liquid-crystalline layers are widely used in low power electro-optic displays. The optical properties of such layers depend strongly on various geometrical and material parameters. Usually, optimum display parameters are calculated by computer modelling [1], although there have also been attempts to obtain additional information with an analytical treatment [2, 3]. These results, obtained to a first approximation, refer to zero pretilts of the director at the boundaries. Comparison with data obtained by numerical calculations shows good agreement when the maximal rotation angle in the mid-plane of the layer is small [3]. However, the agreement becomes poorer for larger rotations.

A perturbation approach is suitable to extend the analytical theory in two directions. First, small pretilt angles at the bounding plates of the layer are included and secondly, the mathematical description is improved by a higher order approximation.

Figure 1 shows, schematically, the geometry of a twisted nematic cell. The nematic phase is confined between the bounding plates at $z = 0$ and $z = d$. The tilt angle θ which depends on z is enclosed between the preferred direction of the long molecular axes (the director) and the plane $z =$ constant. At the lower and upper plate θ has the fixed values κ and ω, respectively. The azimuthal angle Φ grows gradually with increasing z from zero to α.

Introducing the dimensionless coordinate

$$x = \frac{\pi z}{d}, \tag{1}$$

which varies between zero and π, the boundary conditions are written as

$$\left.\begin{aligned} \theta(x = 0) &= \kappa, \quad \theta(x = \pi) = \omega, \\ \Phi(x = 0) &= 0, \quad \Phi(x = \pi) = \alpha. \end{aligned}\right\} \tag{2}$$

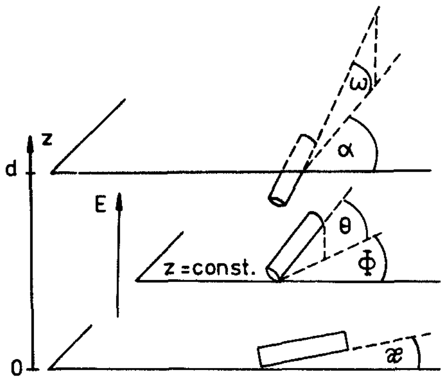

Figure 1. The geometry of a twisted nematic layer. θ, angle between the director and the plane z = constant; Φ, azimuthal angle of the director; α, maximum twist angle; κ, ω, surface tilt angles.

2. Torque balance equations

The free energy density of chiral twisted nematic layers depends on the elastic distortions according to [4]

$$F_s = \frac{\pi^2}{2d^2}\Big[(K_{11}\cos^2\theta + K_{33}\sin^2\theta)\theta_x^2 + (K_{33}\sin^2\theta + K_{22}\cos^2\theta)\cos^2\theta\Phi_x^2 - \frac{4d}{P}K_{22}\cos^2\theta\Phi_x\Big], \tag{3}$$

with the abbreviations

$$\theta_x = \frac{\partial\theta}{\partial x} \quad \text{and} \quad \Phi_x = \frac{\partial\Phi}{\partial x}$$

and also on the electric field according to

$$F_e = \frac{D^2}{2(\varepsilon_\perp\cos^2\theta + \varepsilon_\parallel\sin^2\theta)}. \tag{4}$$

Here K_{11}, K_{22}, and K_{33} are the splay, twist and bend elastic constants of the Oseen–Frank theory [5], and P is the helix pitch for a chiral nematic. D is the dielectric displacement, while $\varepsilon_\parallel$ and $\varepsilon_\perp$ denote the dielectric constants measured parallel and perpendicular to the director, respectively. For stable director configurations the free energy

$$F = \int_0^\pi dx(F_s + F_e)$$

is a minimum.

By applying this condition, torque balance equations can be derived for θ and Φ [1], namely

$$\theta_{xx} = -L(\sin^2\theta\theta_{xx} + \sin\theta\cos\theta\theta_x^2) + V\Big[(k - 2(k+1)\sin^2\theta)\Phi_x^2 + 2\left(\frac{\alpha}{\pi}\right)\beta\Phi_x\Big]\sin\theta\cos\theta - \frac{R\sin\theta\cos\theta}{[1+\gamma\sin^2\theta]^2} \tag{5}$$

and

$$\Phi_x = \left(\frac{\alpha}{\pi}\right)\frac{Q - \beta\sin^2\theta}{1 + k\sin^2\theta - (k+1)\sin^4\theta}, \tag{6}$$

where the abbreviations

$$\left.\begin{aligned} \Delta\varepsilon &= \varepsilon_{\|} - \varepsilon_{\perp}, \quad \gamma = \frac{\Delta\varepsilon}{\varepsilon_{\perp}}, \\ R &= \frac{\Delta\varepsilon d^2 D^2}{\pi^2\varepsilon_{\perp}^2 K_{11}}, \quad V = \frac{K_{22}}{K_{11}}, \quad L = \frac{K_{33} - K_{11}}{K_{11}}, \\ k &= \frac{K_{33} - 2K_{22}}{K_{22}} \text{ and } \beta = \frac{2\pi d}{P\alpha} \end{aligned}\right\} \tag{7}$$

are introduced and the integration constant Q is determined by the condition

$$\int_0^{\pi} dx\,\Phi_x = \alpha. \tag{8}$$

The relation between R and the applied voltage U at the plates is

$$R = \frac{U^2}{U_0^2}\left[\frac{1}{\pi}\int_0^{\pi}\frac{dx}{1 + \gamma\sin^2\theta}\right]^{-2}, \tag{9}$$

where

$$U_0^2 = \frac{\pi^2 K_{11}}{\Delta\varepsilon}$$

and $\Delta\varepsilon$ is assumed to be positive.

3. The bifurcation point

If the tilt angles at the boundaries κ and ω vanish, the solution $\theta(x) = 0$ of equation (5) bifurcates at a definite voltage U_c. This threshold can be found by expanding

$$\left.\begin{aligned} \Phi_x &= \frac{\alpha}{\pi} + O(\theta^2) \\ \text{and} \qquad R &= \frac{U_c^2}{U_0^2} + O(\theta^2), \end{aligned}\right\} \tag{10}$$

where $O(\theta^2)$ symbolizes that higher order terms proportional to θ^2 has been neglected. Linearizing equation (5), we find

$$\theta_{xx} + \theta\left[\frac{U_c^2}{U_0^2} - V\left(\frac{\alpha}{\pi}\right)^2(k + 2\beta)\right] = 0. \tag{11}$$

The differential equation (11) with boundary conditions $\theta(O) = 0$ and $\theta(\pi) = 0$ has the non-trivial solution constant $\sin x$ for

$$\frac{U_c^2}{U_0^2} - V\left(\frac{\alpha}{\pi}\right)^2(k + 2\beta) = 1$$

or

$$U_c^2 = U_0^2 R_0 \tag{12}$$

with

$$R_0 = 1 + V\left(\frac{\alpha}{\pi}\right)^2 (k + 2\beta). \tag{13}$$

It can be proved that for $U < U_c$ no non-trivial solution of (11) exists which satisfies the boundary conditions. For supercritical bifurcations U_c can be identified with the threshold of a Freedericksz transition in accordance with a result published in [3].

4. Perturbation method

The ratio

$$u = \frac{U - U_c}{U_c} \tag{14}$$

determines the distance to the bifurcation point. Furthermore a small parameter ε is introduced by

$$u = \pm\varepsilon^2, \tag{15}$$

where the positive sign is valid for $U > U_c$ and the negative sign for the opposite case. ε determines the order of magnitude of terms in the perturbation expansions for θ and Φ. The distortion angle θ is expanded in a series

$$\theta = \theta_1 + \theta_3 + \theta_5 + \ldots, \tag{16}$$

where the magnitude of θ_n is nth order with respect to ε;

$$\max|\theta_n(x)| \sim \varepsilon^n.$$

The pretilt angles at the boundaries are assumed to be sufficiently small ($|\kappa + \omega| < 5°$) so that they can be regarded as third order terms

$$\kappa \sim \varepsilon^3 \quad \text{and} \quad \omega \sim \varepsilon^3. \tag{17}$$

The expansions of R and Φ_x have terms of even order

$$\left.\begin{aligned} R &= R_0(1 + R_2 + R_4 + \ldots), \\ \Phi_x &= \left(\frac{\alpha}{\pi}\right)(1 + \varphi_2(x) + \varphi_4(x) + \ldots), \end{aligned}\right\} \tag{18}$$

with $R_n \sim \varepsilon^n$ and $\max|\varphi_n(x)| \sim \varepsilon^n$.

Because of equation (8) the conditions

$$\int_0^\pi \varphi_2(x)\,dx = 0 \quad \text{and} \quad \int_0^\pi \varphi_4(x)\,dx = 0 \tag{19}$$

are satisfied.

Now we expand equation (5) in a Taylor series with powers of θ, insert the expansions (16) and (18) and arrange the terms according to their order of magnitude.

This procedure results in a hierarchy of differential equations

$$\theta_{1xx} + \theta_1 = 0,$$

$$\theta_{3xx} + \theta_3 = -L(\theta_1^2\theta_{1xx} + \theta_{1x}^2\theta_1) + V\left(\frac{\alpha}{\pi}\right)^2 [-\tfrac{4}{3}(k + 2\beta)\theta_1^3 + 2(k + \beta)\varphi_2\theta_1 - 2(k + 1)\theta_1^3] + R_0(\tfrac{2}{3}\theta_1^3 - R_2\theta_1 + 2\gamma\theta_1^3)$$

and

$$\theta_{5xx} + \theta_5 = L_5(\theta_1, \theta_3);$$

$L_5(\theta_1, \theta_3)$ is given explicitly in the Appendix. The boundary conditions are

$$\begin{aligned} \theta_1(0) &= \theta_1(\pi) = 0. \\ \theta_3(0) &= \kappa, \qquad \theta_3(\pi) = \omega \\ \theta_5(0) &= \theta_5(\pi) = 0. \end{aligned} \tag{21}$$

Equations (20) are solved step by step. With boundary conditions (21) the first differential equation has the solution

$$\theta_1 = b_1 \sin x, \tag{22}$$

where b_1 can be chosen arbitrarily. Inserting equation (22) into equation (6), expanding the relation equation (6) in a Taylor series and taking into account the condition (19) yields

$$\varphi_2 = (k + \beta)(\tfrac{1}{2}b_1^2 - \theta_1^2) \tag{23}$$

and by integration

$$\Phi(x) = \left(\frac{\alpha}{\pi}\right)[x + \tfrac{1}{4}(k + \beta)b_1^2 \sin 2x] + O(\varepsilon^4). \tag{24}$$

Similarly, R_2 is determined by applying the relation (9) to give

$$R_2 = \gamma b_1^2 + 2u \tag{25}$$

θ_1, φ_2 and R_2 are inserted in the right-hand side of the second equation (20). This differential equation has the solution

$$\theta_3 = b_3 \sin x + c b_1^3 \sin 3x + a_3 \cos x + x \cos x(R_0 u b_1 - \tfrac{1}{4}B b_1^3), \tag{26}$$

where

$$B = L + 1 + R_0\gamma - V\left(\frac{\alpha}{\pi}\right)^2 [(k + \beta)^2 + 3k + 3]$$

and

$$c = \frac{1}{48} + \frac{1}{16}\left\{L + R_0\gamma - V\left(\frac{\alpha}{\pi}\right)^2 [(k + \beta)^2 + k + 1]\right\}$$

a_3 and b_1 are determined by the boundary conditions of θ_3. Since $\theta_3(0) = \kappa$ we obtain $a_3 = \kappa$. The second boundary condition $\theta_3(\pi) = \omega$ is satisfied, when

$$-ub_1 + \frac{B}{4R_0}b_1^3 = \frac{\delta}{R_0}, \tag{27}$$

with

$$\delta = \frac{\kappa + \omega}{\pi}. \tag{28}$$

For the special case $\delta = 0$ equation (27) coincides with a result obtained by Raynes [3].

θ_3 can be rewritten as

$$\theta_3 = \kappa \cos x - \delta x \cos x + b_3 \sin x + c b_1^3 \sin 3x. \tag{29}$$

R_4 and φ_4 in the expansions (18) are obtained by using equations (9), (6) and (19); they give

$$R_4 = -\tfrac{1}{4}\gamma b_1^4 + 2\gamma b_1 b_3 + 2\gamma u b_1^2 + u^2 + \gamma\delta b_1 \tag{30}$$

and φ_4 is defined in the appendix. Finally, the coefficient b_3 in equation (29) is determined by applying the last equation of the hierarchy (20).

As the eigenvalue problem

$$\theta_{5xx} + \theta_5 = \lambda\theta_5$$

with boundary conditions (21) has the non-trivial solution

$$\theta_5 = b_5 \sin x$$

for $\lambda = 0$, the solvability condition

$$\int_0^\pi L_5(\theta_1, \theta_3) \sin x \, dx = 0 \tag{31}$$

has to be satisfied (Fredholm's theorem). Condition (31) leads to

$$b_3 = \frac{1}{3Bb_1^2 - 4R_0 u}[(P + 48c^2)b_1^5 + M\delta b_1^2$$
$$- 2R_0(1 + \gamma)u b_1^3 + 2R_0 u\delta + 2R_0 u^2 b_1], \tag{32}$$

where

$$P = \frac{1}{12}\Big\{3L + 2 + (12\gamma + 9\gamma^2)R_0$$
$$- V\left(\frac{\alpha}{\pi}\right)^2 [9k(k + \beta)^2 + 48k^2 + 60k\beta + 12\beta^2 + 66k + 36\beta + 30]\Big\},$$

and

$$M = \frac{3}{4}\left\{L - 1 + \gamma R_0 - V\left(\frac{\alpha}{\pi}\right)^2 [(k + \beta)^2 - 5k - 4\beta - 3]\right\}.$$

The final result is

$$\theta = (b_1 + b_3)\sin x + \kappa \cos x - \delta x \cos x + c b_1^3 \sin 3x + 0\,(\varepsilon^5). \tag{33}$$

It should be noted, that $\Phi(x)$ can be determined up to terms proportional to ε^4 by integrating φ_4 and adding the result to the expansion (24).

5. Strong response of the director rotation angle

The maximum value $\theta(\pi/2)$ of the director rotation grows very rapidly when slightly changing u as B tends to zero. Supposing $\delta = 0$ then equation (27) can be written as

$$u = \frac{B}{4R_0} b_1^2. \tag{34}$$

According to equation (33), b_1 is approximately the director rotation in the mid-plane of the layer, neglecting terms proportional to ε^3. Unfortunately, at $B = 0$ we obtain $u = 0$ and b_1 can be chosen arbitrarily. In this case a power law with the next even exponent

$$u = \text{constant } b_1^4 \tag{35}$$

should be satisfied instead of equation (34). In conclusion, modifications of the perturbation method are necessary if B is zero or small in the sense

$$|B| \ll |P + 48c^2|. \tag{36}$$

The perturbation treatment starts with the series

$$\theta = \theta_1 + \theta_3 + \theta_5 + \ldots,$$

where the indices characterize the order of magnitude in complete agreement with equation (16). However, motivated by the relation (35) equation (15) is replaced by

$$u = \pm\varepsilon^4 \tag{37}$$

and taking into account the inequality (36) the assumption

$$B \sim \varepsilon^2 \tag{38}$$

is made. If surface tilts are present, the angles should be very small

$$\kappa \sim \varepsilon^5 \quad \text{and} \quad \omega \sim \varepsilon^5. \tag{39}$$

Now the boundary conditions are

$$\left.\begin{aligned} \theta_1(0) &= \theta_1(\pi) = 0, \\ \theta_3(0) &= \theta_3(\pi) = 0, \\ \theta_5(0) &= \kappa \quad \text{and} \quad \theta_5(\pi) = \omega. \end{aligned}\right\} \tag{40}$$

The same procedure as applied in the previous section leads to a hierarchy of equations for θ_n. Compared to equation (20) this hierarchy is somewhat modified, as the term Bb_1^3 is no longer proportional to ε^3 but proportional to ε^5. With this modification the second member of equations (20) is converted to

$$\theta_{3xx} + \theta_3 = -8cb_1^3 \sin 3x. \tag{41}$$

Regarding boundary conditions (40) the solution of equation (41) is

$$\theta_3 = b_3 \sin x + cb_1^3 \sin 3x. \tag{42}$$

Equations (12), (22) and (23) for U_c, $\theta_1(x)$ and $\varphi_2(x)$ remain valid. However, considering equations (37) and (39) the relations (25) and (30) are simplified to

$$\left.\begin{aligned} R_2 &= \gamma b_1^2 \\ \text{and} \qquad R_4 &= -\tfrac{1}{4}\gamma b_1^4 + 2\gamma b_1 b_3 + 2u. \end{aligned}\right\} \tag{43}$$

Using equations (42), (43) and (38) the terms in the hierarchy (20) are rearranged and the collection of all terms proportional to ε^5 leads to

$$\theta_{5xx} + \theta_5 = -\sin x[2uR_0 b_1 - \tfrac{1}{2}Bb_1^3 + \tfrac{1}{2}(P + 48c^2)b_1^5] + A_5 \sin 3x + B_5 \sin 5x. \tag{44}$$

The coefficients A_5 and B_5 are not written down explicitly, as we do not need them in further calculations.

Equation (44) has the general solution

$$\begin{aligned} \theta_5 = {} & a_5 \cos x + b_5 \sin x + x \cos x\,[uR_0 b_1 - \tfrac{1}{4}Bb_1^3 + \tfrac{1}{4}(P + 48\,c^2)b_1^5] \\ & - \tfrac{1}{8}A_5 \sin 3x - \tfrac{1}{24}B_5 \sin 5x. \end{aligned} \tag{45}$$

The boundary conditions (40) require $a_5 = \kappa$ and a relation between u and b_1, namely

$$-ub_1 + \frac{Bb_1^3}{4R_0} - \frac{(P + 48\,c^2)b_1^5}{4R_0} = \frac{\delta}{R_0}. \tag{46}$$

To lowest order the director orientation is determined by

$$\left.\begin{aligned} \theta &= b_1 \sin x + O(\varepsilon^3) \\ \text{and} \qquad \Phi &= \left(\frac{\alpha}{\pi}\right)[x + \tfrac{1}{4}(k + \beta)b_1^2 \sin 2x] + O(\varepsilon^4). \end{aligned}\right\} \tag{47}$$

Looking at equation (46) the question arises what happens when both B and $P + 48\,c^2$ are zero. In this case a power law $u =$ constant b_1^6 is to be expected for zero surface tilt angles at the boundaries ($\delta = 0$) and the rapid grow of the maximum rotation angle with changing u is enhanced further.

6. Discussion

The maximum value of the director rotation $A = \theta(\pi/2)$ is suitable to illustrate the Freedericksz effect. Plotting A against the voltage ratio u a comparison with the results of computer modelling is possible when the same combination of constants K_{ii}, γ and β are chosen as those used by Raynes [3]. According to equation (33) we have

$$A = b_1 + b_3 - cb_1^3, \tag{48}$$

if B is not small. b_1 and b_3 are determined by equations (27) and (32), respectively. The parameter b_1 should not exceed 0·5 to obtain accurate results. For different twist angles figure 2 shows the functions $A(u)$. They agree well with the results obtained from numerical calculations [3].

If B is small, satisfying inequality (36), the director rotation in the mid-plane of the layer is determined by equation (46) and $A = b_1$. In figure 3 A is plotted against u choosing the parameters K_{ii}, γ and β so that $B = 0$ (curves a and c) and B is small but not zero (curve b). It can be checked that there is a good agreement with the results obtained numerically. Particularly, the slope of curve b changes its sign at a relatively

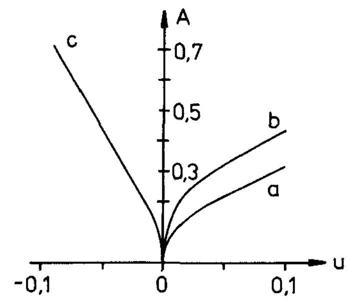

Figure 2. The maximum rotation angle A plotted against the voltage ratio u for $\delta = 0, \beta = 1, \gamma = 2, K_{11} = 10\,pN, K_{22} = 5\,pN$ and $K_{33} = 20\,pN$ with varying twist angle: (*a*) $\alpha = 0°$, (*b*) $\alpha = 90°$, (*c*) $\alpha = 270°$.

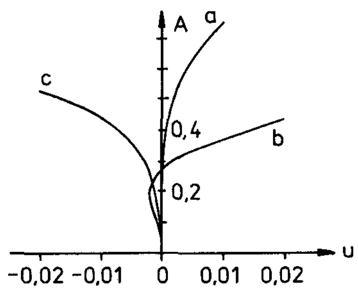

Figure 3. The rotation angle A plotted against u for the parameter combinations satisfying the inequality (36): $\delta = 0$, $\beta = 1$, $K_{11} = 10\,pN$, $K_{22} = 5\,pN$ and (*a*) $\gamma = 1$, $K_{33} = 9{\cdot}7\,pN$, $\alpha = 270°$, (*b*) $\gamma = 2$, $K_{33} = 20\,pN$, $\alpha = 180°$, (*c*) $\gamma = 3$, $K_{33} = 18{\cdot}5\,pN$, $\alpha = 270°$.

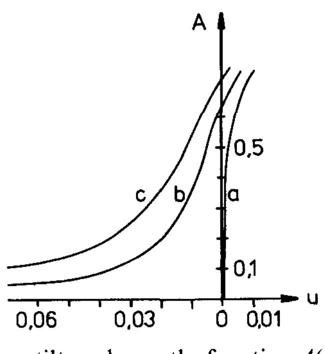

Figure 4. Influence of the surface tilt angles on the function $A(u)$. The curves are determinated by using the parameters $\alpha = 270°$, $\beta = 1$, $\gamma = 1$, $K_{11} = 10\,pN$, $K_{22} = 5\,pN$, $K_{33} = 9{\cdot}7\,pN$ and the tilt angles at the boundaries (*a*) $\kappa = \omega = 0°$, (*b*) $\kappa = \omega = 1°$, (*c*) $\kappa = \omega = 2°$.

low value of A. This behaviour is confirmed by numerical results as seen by figure 3 in [3].

Finally, the influence of surface tilts at the boundaries is demonstrated by figure 4. As $B = 0$ the rotation angle A has been determined by equation (46). It should be noted that the effect of pretilts in twisted nematics has been also investigated by Fraser [6] by using another mathematical approach. In conclusion, the perturbation method is suitable to describe the Freedericksz transition of planar twisted nematic layers when the distortions are not too large. The results can be used to predict the optimum combinations of physical parameters for application in electro-optic devices.

I am indebted to Professor D. Demus for useful discussions.

Appendix

The explicit expressions for $L_5(\theta_1, \theta_3)$ and φ_4 are

$$\begin{aligned} L_5(\theta_1, \theta_3) = {} & R_0[-\tfrac{2}{15}\theta_1^5 + 2\theta_1^2\theta_3 - R_2(\theta_3 - \tfrac{2}{3}\theta_1^3) - R_4\theta_1 + 2\gamma(3\theta_1^2\theta_3 - \theta_1^5) \\ & + 2\gamma R_2\theta_1^3 - 3\gamma^2\theta_1^5] + V\left(\frac{\alpha}{\pi}\right)^2 [(k + 2\beta)(\tfrac{2}{15}\theta_1^5 - 2\theta_1^2\theta_3) \\ & + 2(k + \beta)\varphi_2(\theta_3 - \tfrac{2}{3}\theta_1^3) - 2(k + 1)(3\theta_3\theta_1^2 - \theta_1^5) \\ & + 2(k + \beta)\varphi_4\theta_1 + k\varphi_2^2\theta_1 - 4(k + 1)\varphi_2\theta_1^3] \\ & - L(\theta_1^2\theta_{3xx} + 2\theta_1\theta_{1xx}\theta_3 - \tfrac{1}{3}\theta_1^4\theta_{1xx} + \theta_{1x}^2\theta_3 - \tfrac{2}{3}\theta_{1x}^2\theta_1^3 + 2\theta_{1x}\theta_{3x}\theta_1) \end{aligned}$$

and

$$\begin{aligned} \varphi_4 = {} & \tfrac{1}{3}(3k^2 + 4k + \beta + 3 + 3\beta k)\cdot(\theta_1^4 - \tfrac{3}{8}b_1^4) \\ & - \tfrac{1}{2}k(k + \beta)b_1^2\cdot(\theta_1^2 - \tfrac{1}{2}b_1^2) - \tfrac{1}{2}(k + \beta)\cdot(4\theta_1\theta_3 - 2b_1b_3 - b_1\delta). \end{aligned}$$

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