

Elastic continuum theory of biaxial nematics

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The elastic-distortion free-energy density of biaxial nematics is derived with use of the formalism of tensor analysis. The macroscopic description of biaxial nematics involves 12 bulk elastic constants. The appearance of chirality introduces an additional number of 5 twist terms.

I. INTRODUCTION

The macroscopic theory of nematics describes these anisotropic materials in terms of a continuous field. Because of the anisotropic nature and the absence of polar effects this field must necessarily be a tensor field of second rank. This tensor field is denoted by $\vec{Q}(\vec{r})$ and describes both the amount of order and the orientation of the material at the site \vec{r} . The undistorted state of the medium is assumed to be homogeneous, i.e., the tensor field does not depend on \vec{r} . In a properly chosen coordinate system denoted by the unit vectors \vec{e}'_α , $\alpha=x,y,z$, the tensor order parameter $\vec{Q}(\vec{r})$ is diagonal having elements

$$\begin{aligned} \bar{Q}_{\alpha\beta} &= 0 \text{ if } \alpha \neq \beta, \text{ where } \alpha, \beta = x, y, z \\ \bar{Q}_{xx} &= -\frac{1}{3}(S - T), \quad \bar{Q}_{yy} = -\frac{1}{3}(S + T), \quad \bar{Q}_{zz} = \frac{2}{3}S. \end{aligned}$$

Biaxial nematics are described by the two order parameters S and T , whereas uniaxial nematics are described by only one order parameter, e.g., S in case the uniaxial axis is chosen along \vec{e}'_z . With respect to an arbitrary coordinate system denoted by the unit vectors \vec{e}_α the elements of the tensor order parameter read

$$Q_{\alpha\beta} = R_{\alpha\gamma} R_{\beta\delta} \bar{Q}_{\gamma\delta},$$

where $R_{\alpha\beta}$ are the elements of the transformation matrix of Euler, i.e.,

$$R_{\alpha\beta} = \vec{e}_\alpha \cdot \vec{e}'_\beta.$$

This means that the general expression of an element of the tensor order parameter, which describes a biaxial nematic, is given by

$$\begin{aligned} Q_{\alpha\beta} &= -\frac{1}{3}S(\vec{e}_\alpha \cdot \vec{e}'_\gamma)(\vec{e}_\beta \cdot \vec{e}'_\gamma) + S(\vec{e}_\alpha \cdot \vec{e}'_z)(\vec{e}_\beta \cdot \vec{e}'_z) \\ &+ \frac{1}{3}T[(\vec{e}_\alpha \cdot \vec{e}'_x)(\vec{e}_\beta \cdot \vec{e}'_x) - (\vec{e}_\alpha \cdot \vec{e}'_y)(\vec{e}_\beta \cdot \vec{e}'_y)]. \end{aligned}$$

An undistorted biaxial nematic liquid crystal is characterized by three mutually perpendicular twofold axes, whose directions are denoted by the vectors \vec{n} , \vec{m} , and $\vec{l} = \vec{m} \times \vec{n}$. These symmetry axes coincide with the axes of the specific coordinate system, that gives rise to a diagonal representation of the tensor order parameter. The following identification is chosen, $\vec{l} = \vec{e}'_x$, $\vec{m} = \vec{e}'_y$, and $\vec{n} = \vec{e}'_z$. This choice gives rise to the following expressions for the components of the directors \vec{l} , \vec{m} , and \vec{n}

with respect to an arbitrary coordinate system:

$$\begin{aligned} l_\alpha &= (\vec{e}_\alpha \cdot \vec{e}'_x) = R_{\alpha x}, \\ m_\alpha &= (\vec{e}_\alpha \cdot \vec{e}'_y) = R_{\alpha y}, \\ n_\alpha &= (\vec{e}_\alpha \cdot \vec{e}'_z) = R_{\alpha z}. \end{aligned}$$

Consequently the general expression for an element of the tensor order parameter of a biaxial nematic can be written as

$$Q_{\alpha\beta} = S(n_\alpha n_\beta - \frac{1}{3}\delta_{\alpha\beta}) + \frac{1}{3}T(l_\alpha l_\beta - m_\alpha m_\beta), \quad (1.1)$$

where the tensor $\delta_{\alpha\beta}$ is the Kronecker data.

II. ELASTIC CONTINUUM THEORY

The elastic continuum theory is obtained by expanding the free-energy density, $f(\vec{r})$, that belongs to a given tensor-order-parameter field $\vec{Q}(\vec{r})$, around the homogeneous state having a free-energy density f_0 . The difference between both densities, i.e., $f(\vec{r}) - f_0$, is called the distortion free-energy density $f_d(\vec{r})$. This distortion free-energy density is a function of the spatial derivatives of the tensor-order-parameter field. The elastic continuum theory deals only with small spatial derivatives. Consequently only the lowest order terms in the expansion are taken into account. This means that the elastic continuum theory is based upon the following expression for the distortion free-energy density:

$$\begin{aligned} f_d(\vec{r}) &= L_{\alpha\beta\gamma}(\vec{r})\partial_\alpha Q_{\beta\gamma}(\vec{r}) \\ &+ L_{\alpha\beta\gamma\mu\nu\rho}(\vec{r})[\partial_\alpha Q_{\beta\gamma}(\vec{r})][\partial_\mu Q_{\nu\rho}(\vec{r})] \\ &+ L_{\alpha\beta\gamma\mu}(\vec{r})\partial_\alpha\partial_\beta Q_{\gamma\mu}(\vec{r}), \end{aligned} \quad (2.1)$$

where $\partial_\alpha = \partial/\partial\alpha$, the Greek indices denote x, y , and z and the Einstein summation convention is used. The tensors $L_{\alpha\beta\gamma}$, $L_{\alpha\beta\gamma\mu\nu\rho}$, and $L_{\alpha\beta\gamma\mu}$ must be composed of the tensors $Q_{\alpha\beta}(\vec{r})$, $\delta_{\alpha\beta}$, and the Levi-Civita tensor $\epsilon_{\alpha\beta\gamma}$.

Next the degree of ordering is assumed to be unaffected throughout all the medium, i.e., the order parameters S and T do not depend on the position \vec{r} . Then it holds according to (1.1)

$$\begin{aligned} \partial_\alpha Q_{\beta\gamma} &= (S - \frac{1}{3}T)[(\partial_\alpha n_\beta)n_\gamma + n_\beta(\partial_\alpha n_\gamma)] \\ &- \frac{2}{3}T[(\partial_\alpha m_\beta)m_\gamma + m_\beta(\partial_\alpha m_\gamma)], \end{aligned} \quad (2.2)$$

where use has been made of the relation

$$l_\alpha l_\beta = \epsilon_{\alpha\mu\nu} \epsilon_{\beta\rho\sigma} m_\mu n_\gamma m_\rho n_\sigma = \delta_{\alpha\beta} - m_\alpha m_\beta - n_\alpha n_\beta.$$

Consequently the elastic-distortion free-energy density of a biaxial nematic can be written as

$$\begin{aligned} f_d(\vec{r}) = & A_{\alpha\beta} \partial_\alpha n_\beta + B_{\alpha\beta} \partial_\alpha m_\beta + A_{\alpha\beta\gamma\delta} [\partial_\alpha n_\beta] [\partial_\gamma n_\delta] \\ & + B_{\alpha\beta\gamma\delta} [\partial_\alpha m_\beta] [\partial_\gamma m_\delta] + C_{\alpha\beta\gamma\delta} [\partial_\alpha n_\beta] [\partial_\gamma m_\delta] \\ & + A_{\alpha\beta\gamma} \partial_\alpha \partial_\beta n_\gamma + B_{\alpha\beta\gamma} \partial_\alpha \partial_\beta m_\gamma. \end{aligned} \quad (2.3)$$

The tensors $A_{\alpha\beta}$, $B_{\alpha\beta}$, $A_{\alpha\beta\gamma\delta}$, $B_{\alpha\beta\gamma\delta}$, $C_{\alpha\beta\gamma\delta}$, $A_{\alpha\beta\gamma}$, and $B_{\alpha\beta\gamma}$ depend on the order parameters S and T . The possible forms of these tensors follow directly from (1) the invariance of the free-energy density for replacing \vec{I} by $-\vec{I}$, \vec{m} by $-\vec{m}$, or \vec{n} by $-\vec{n}$; (2) $l_\alpha m_\alpha = l_\alpha n_\alpha = m_\alpha n_\alpha = 0$; (3) $l_\alpha l_\alpha = m_\alpha m_\alpha = n_\alpha n_\alpha = 1$; (4) $l_\alpha l_\beta + m_\alpha m_\beta + n_\alpha n_\beta = \delta_{\alpha\beta}$.

III. RELEVANT TENSORS

The terms $A_{\alpha\beta} \partial_\alpha n_\beta$ and $B_{\alpha\beta} \partial_\alpha m_\beta$ only appear in case the medium is chiral. It is verified easily that these twist terms must be of the following form:

$$l_1 \epsilon_{\alpha\beta\gamma} n_\gamma \partial_\alpha n_\beta, \quad (3.1)$$

$$l_2 \epsilon_{\alpha\mu\nu} m_\mu n_\nu m_\beta \partial_\alpha n_\beta, \quad (3.2)$$

$$l_3 \epsilon_{\beta\mu\nu} m_\mu n_\nu m_\alpha \partial_\alpha n_\beta, \quad (3.3)$$

$$l_4 \epsilon_{\alpha\beta\gamma} m_\gamma \partial_\alpha m_\beta, \quad (3.4)$$

$$l_5 \epsilon_{\beta\mu\nu} n_\mu m_\nu n_\alpha \partial_\alpha m_\beta. \quad (3.5)$$

It is worthwhile to note here that the term $\epsilon_{\alpha\mu\nu} n_\mu m_\nu n_\beta \partial_\alpha m_\beta$ does not give rise to an additional invariant. For $n_\alpha m_\alpha = 0$, i.e., $\partial_\beta (n_\alpha m_\alpha) = 0$, implies immediately

$$\begin{aligned} \epsilon_{\alpha\mu\nu} n_\mu m_\nu n_\beta \partial_\alpha m_\beta &= -\epsilon_{\alpha\mu\nu} n_\mu m_\nu m_\beta \partial_\alpha n_\beta \\ &= \epsilon_{\alpha\mu\nu} m_\mu n_\nu m_\beta \partial_\alpha n_\beta. \end{aligned}$$

$$\partial_\alpha (m_\alpha n_\beta n_\gamma \partial_\beta m_\gamma) - \partial_\alpha (n_\alpha m_\beta n_\gamma \partial_\beta m_\gamma) = m_\alpha n_\beta (\partial_\alpha n_\gamma) (\partial_\beta m_\gamma) - n_\alpha m_\beta (\partial_\alpha n_\gamma) (\partial_\beta m_\gamma)$$

$$+ n_\beta n_\gamma (\partial_\alpha m_\alpha) (\partial_\beta m_\gamma) - m_\beta n_\gamma (\partial_\alpha n_\alpha) (\partial_\beta m_\gamma) + m_\alpha n_\gamma (\partial_\alpha n_\beta) (\partial_\beta m_\gamma) - n_\alpha n_\gamma (\partial_\alpha m_\beta) (\partial_\beta m_\gamma)$$

that, apart from a surface term, the invariant $m_\alpha n_\beta (\partial_\beta m_\gamma) (\partial_\alpha n_\gamma)$ can be expressed as a linear combination of the invariants $n_\alpha m_\beta (\partial_\alpha n_\gamma) (\partial_\beta m_\gamma)$, $n_\alpha n_\beta (\partial_\alpha m_\beta) (\partial_\gamma m_\gamma)$, $m_\alpha m_\beta (\partial_\alpha n_\beta) (\partial_\gamma n_\gamma)$, $m_\alpha m_\beta (\partial_\gamma n_\alpha) (\partial_\beta n_\gamma)$, and $n_\alpha n_\beta (\partial_\gamma m_\alpha) (\partial_\beta m_\gamma)$. The invariants $n_\alpha n_\beta (\partial_\alpha m_\beta) (\partial_\gamma m_\gamma)$ and $m_\alpha m_\beta (\partial_\alpha n_\beta) (\partial_\gamma n_\gamma)$ in their turn are equivalent to $n_\alpha n_\beta (\partial_\gamma m_\alpha) (\partial_\beta m_\gamma)$ and $m_\alpha m_\beta (\partial_\gamma n_\alpha) (\partial_\beta m_\gamma)$, respectively. This follows directly from the relations

$$\begin{aligned} l_\alpha l_\beta l_\gamma l_\delta (\partial_\alpha n_\beta) (\partial_\gamma n_\delta) &= (\delta_{\alpha\beta} - n_\alpha n_\beta - m_\alpha m_\beta) (\delta_{\gamma\delta} - n_\gamma n_\delta - m_\gamma m_\delta) (\partial_\alpha n_\beta) (\partial_\gamma n_\delta) \\ &= (\partial_\alpha n_\alpha) (\partial_\gamma n_\gamma) - 2m_\alpha m_\beta (\partial_\alpha n_\beta) (\partial_\gamma n_\gamma) + m_\alpha m_\beta m_\gamma m_\delta (\partial_\alpha n_\beta) (\partial_\gamma n_\delta) \end{aligned}$$

and

$$\begin{aligned} l_\alpha l_\beta l_\gamma l_\delta (\partial_\alpha n_\beta) (\partial_\gamma n_\delta) &= (\delta_{\alpha\delta} - n_\alpha n_\delta - m_\alpha m_\delta) (\delta_{\beta\gamma} - n_\beta n_\gamma - m_\beta m_\gamma) (\partial_\alpha n_\beta) (\partial_\gamma n_\delta) \\ &= (\partial_\alpha n_\beta) (\partial_\beta n_\alpha) - 2m_\beta m_\gamma (\partial_\alpha n_\beta) (\partial_\gamma n_\alpha) + m_\alpha m_\beta m_\gamma m_\delta (\partial_\alpha n_\beta) (\partial_\gamma n_\delta). \end{aligned}$$

This means, apart from irrelevant surface terms, that $m_\alpha m_\beta (\partial_\alpha n_\beta) (\partial_\gamma n_\gamma)$ reduces to $m_\beta m_\gamma (\partial_\alpha n_\beta) (\partial_\gamma n_\alpha)$.

Finally the terms $A_{\alpha\beta\gamma} \partial_\alpha \partial_\beta n_\gamma$ and $B_{\alpha\beta\gamma} \partial_\alpha \partial_\beta m_\gamma$ must be considered. These terms, however, do not give rise to

The description of a chiral biaxial nematic involves evidently 5 independent twist terms.

The terms $A_{\alpha\beta\gamma\delta} [\partial_\alpha n_\beta] [\partial_\gamma n_\delta]$, $B_{\alpha\beta\gamma\delta} [\partial_\alpha m_\beta] [\partial_\gamma m_\delta]$, and $C_{\alpha\beta\gamma\delta} [\partial_\alpha n_\beta] [\partial_\gamma m_\delta]$ appear to give rise to the following 12 independent bulk terms:

$$A_1 (\partial_\alpha n_\alpha) (\partial_\beta n_\beta), \quad (3.6)$$

$$A_2 (\partial_\alpha n_\beta) (\partial_\alpha n_\beta), \quad (3.7)$$

$$A_3 n_\alpha n_\beta (\partial_\alpha n_\gamma) (\partial_\beta n_\gamma), \quad (3.8)$$

$$A_4 m_\alpha m_\beta m_\gamma m_\delta (\partial_\alpha n_\beta) (\partial_\gamma n_\delta), \quad (3.9)$$

$$A_5 m_\alpha m_\beta (\partial_\gamma n_\alpha) (\partial_\beta n_\gamma), \quad (3.10)$$

$$B_1 (\partial_\alpha m_\alpha) (\partial_\beta m_\beta), \quad (3.11)$$

$$B_2 (\partial_\alpha m_\beta) (\partial_\alpha m_\beta), \quad (3.12)$$

$$B_3 m_\alpha m_\beta (\partial_\alpha m_\gamma) (\partial_\beta m_\gamma), \quad (3.13)$$

$$B_4 n_\alpha n_\beta n_\gamma n_\delta (\partial_\alpha m_\beta) (\partial_\gamma m_\delta), \quad (3.14)$$

$$B_5 n_\alpha n_\beta (\partial_\gamma m_\alpha) (\partial_\beta m_\gamma), \quad (3.15)$$

$$C_1 n_\alpha m_\beta (\partial_\gamma n_\beta) (\partial_\gamma m_\alpha), \quad (3.16)$$

$$C_2 n_\alpha m_\beta (\partial_\alpha n_\gamma) (\partial_\beta m_\gamma). \quad (3.17)$$

Clearly more invariant terms can be constructed. However, these additional terms all reduce, apart from irrelevant surface terms, to the 12 terms (3.6)–(3.17). Consider, for example, the term $(\partial_\alpha m_\beta) (\partial_\beta m_\alpha)$. This term is equivalent to $(\partial_\alpha m_\alpha) (\partial_\beta m_\beta)$, for

$$\begin{aligned} (\partial_\alpha m_\beta) (\partial_\beta m_\alpha) - (\partial_\alpha m_\alpha) (\partial_\beta m_\beta) &= \partial_\alpha (m_\beta \partial_\beta m_\alpha) \\ &\quad - \partial_\alpha (m_\alpha \partial_\beta m_\beta), \end{aligned}$$

and the right-hand side of this identity contains only surface terms. A second example concerns the term $m_\alpha n_\beta \partial_\beta m_\gamma \partial_\alpha n_\gamma$. It follows directly from

additional invariants. It follows quite simply that the resulting invariants are, apart from surface contributions, already contained within the 12 invariants (3.6)–(3.17). Consider for instance the term $m_\gamma m_\alpha n_\beta \partial_\alpha \partial_\beta n_\gamma$. It fol-

lows directly from

$$\begin{aligned} \partial_\alpha(m_\gamma m_\alpha n_\beta \partial_\beta n_\gamma) \\ = m_\alpha n_\beta (\partial_\alpha m_\gamma) (\partial_\beta n_\gamma) + m_\gamma n_\beta (\partial_\alpha m_\alpha) (\partial_\beta n_\gamma) \\ + m_\gamma m_\alpha (\partial_\alpha n_\beta) (\partial_\beta n_\gamma) + m_\gamma m_\alpha n_\beta \partial_\alpha \partial_\beta n_\gamma, \end{aligned}$$

that, apart from a surface term, the invariant $m_\gamma m_\alpha n_\beta \partial_\alpha \partial_\beta n_\gamma$ can be expressed in terms of the independent invariants $n_\alpha m_\beta (\partial_\alpha n_\gamma) (\partial_\beta m_\gamma)$, $n_\alpha n_\beta (\partial_\gamma m_\alpha) (\partial_\beta m_\gamma)$, and $m_\alpha m_\beta (\partial_\gamma n_\alpha) (\partial_\beta n_\gamma)$.

IV. ELASTIC-DISTORTION FREE-ENERGY DENSITY

Clearly the elastic-distortion free-energy density of a biaxial nematic liquid crystal is a linear combination of the

$$\begin{aligned} f_d(\vec{r}) = & k_1(\vec{n} \cdot \text{curl} \vec{n}) + k_2(\vec{m} \cdot \text{curl} \vec{m}) + k_3(\vec{m} \times \vec{n}) \cdot [(\vec{m} \cdot \vec{\nabla}) \vec{n}] + k_4(\vec{n} \times \vec{m}) \cdot [(\vec{n} \cdot \vec{\nabla}) \vec{m}] \\ & + k_5[(\vec{m} \times \vec{n}) \cdot (\vec{m} \times \text{curl} \vec{n}) + (\vec{n} \times \vec{m}) \cdot (\vec{n} \times \text{curl} \vec{m})] + \frac{1}{2} K_1(\text{div} \vec{n})^2 + \frac{1}{2} K_2(\vec{n} \cdot \text{curl} \vec{n})^2 \\ & + \frac{1}{2} K_3(\vec{n} \times \text{curl} \vec{n})^2 + \frac{1}{2} K_4(\text{div} \vec{m})^2 + \frac{1}{2} K_5(\vec{m} \cdot \text{curl} \vec{m})^2 + \frac{1}{2} K_6(\vec{m} \times \text{curl} \vec{m})^2 + \frac{1}{2} K_7[\vec{n} \cdot (\vec{m} \times \text{curl} \vec{m})]^2 \\ & + \frac{1}{2} K_8[\vec{m} \cdot (\vec{n} \times \text{curl} \vec{n})]^2 + \frac{1}{2} K_9[\vec{m} \cdot \text{curl}(\vec{n} \times \vec{m})]^2 + \frac{1}{2} K_{10}[\vec{n} \cdot \text{curl}(\vec{m} \times \vec{n})]^2 \\ & + \frac{1}{2} K_{11}[\text{curl}(\vec{n} \times \vec{m})]^2 + \frac{1}{2} K_{12}[\text{div}(\vec{n} \times \vec{m})]^2, \end{aligned} \quad (4.1)$$

where the coefficients of the 5 twist terms are given by

$$\begin{aligned} k_1 = l_1, \quad k_2 = l_4, \quad k_3 = l_3 + \frac{1}{2} l_2, \\ k_4 = l_5 + \frac{1}{2} l_2, \quad k_5 = \frac{1}{2} l_2, \end{aligned}$$

whereas the elastic constants read

$$\begin{aligned} K_1 = 2A_1 + 2A_2 + A_5 - C_1, \quad K_2 = 2A_2 - C_1, \\ K_3 = 2A_2 + 2A_3 - C_1 - C_2, \quad K_4 = 2B_1 + 2B_2 + B_5 - C_1, \\ K_5 = 2B_2 - C_1, \quad K_6 = 2B_2 + 2B_3 - C_1 - C_2, \\ K_7 = 2A_4 + A_5 + C_2, \quad K_8 = 2B_4 + B_5 + C_2, \\ K_9 = -A_5, \quad K_{10} = -B_5, \\ K_{11} = C_1, \quad K_{12} = C_1 + C_2. \end{aligned}$$

These coefficients depend on the order parameters S and T .

The expression (4.1) is invariant with respect to interchanging \vec{n} and \vec{m} . This symmetry requirement must be fulfilled, because neither of both symmetry axes is preferable to the other. Clearly the original expression of Frank¹ for the distortion free-energy density of uniaxial nematics is contained within expression (4.1). Choosing for example the uniaxial axis along the director \vec{n} , i.e., the order parameter T is zero, all coefficients are zero except those in front of the invariants $\epsilon_{\alpha\beta\gamma} n_\gamma \partial_\alpha n_\beta$, $(\partial_\alpha n_\alpha) (\partial_\beta n_\beta)$,

12 independent invariants (3.6)–(3.17). In case the biaxial nematic is chiral as well 5 independent twist terms must be added to this energy density. It is customary to write the full expression for the elastic-distortion free-energy density in terms of the divergence and rotation of the vector fields $\vec{n}(\vec{r})$ and $\vec{m}(\vec{r})$. This can be easily accomplished using relations such as

$$\begin{aligned} (\vec{n} \times \text{curl} \vec{n})_\alpha = n_\beta \partial_\alpha n_\beta - n_\beta \partial_\beta n_\alpha = -n_\beta \partial_\beta n_\alpha \\ = -(\vec{n} \cdot \vec{\nabla}) n_\alpha, \end{aligned}$$

$$\begin{aligned} \vec{m} \cdot \text{curl}(\vec{n} \times \vec{m}) = m_\alpha \epsilon_{\alpha\beta\gamma} \epsilon_{\gamma\mu\nu} \partial_\beta (n_\mu m_\nu) \\ = m_\alpha m_\beta \partial_\beta n_\alpha - \partial_\beta n_\beta. \end{aligned}$$

Then the following expression is obtained:

$$(\partial_\alpha n_\beta) (\partial_\alpha n_\beta), \text{ and } n_\alpha n_\beta (\partial_\alpha n_\gamma) (\partial_\beta n_\gamma).^2$$

V. DISCUSSION

It appears that 12 bulk elastic constants are needed in order to describe biaxial nematics within the framework of the elastic continuum theory. This number was also obtained by Brand and Pleiner^{3,4} (BP). Their analysis differs from the present one on the following points. The BP approach does not consider chiral biaxial nematics. Starting point of their analysis is the symmetry-broken expression for the free-energy density of a biaxial system and the invariant expression is constructed afterwards. The result is rather untransparent because the Frank expression for the uniaxial case does not follow directly by neglecting the terms containing \vec{n} or \vec{m} . Finally it should be noted that the BP calculation of the bulk contributions is based upon an incorrect application of the anholonomity relations. It follows easily that

$$\delta_1 \delta_2 \vec{n} \neq \delta_2 \delta_1 \vec{n}$$

for $\delta_1 = n_\alpha \partial_\alpha$ and $\partial_2 = m_\beta \partial_\beta$ as distinct from the BP allegation.

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