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Interactions Between Subbodies for Complex Materials

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Noll's axiomatic method in continuum mechanics proceeds from the algebra of bodies and the properties of interactions (as objects in an appropriate linear space) to reach finally balance equations. When the material is complex and the order parameters are coordinate of points of a (non-linear) manifold, there seems to be no way of adapting this method. However, previous embedding of the manifold in a linear space (which is always possible) provides a possible escape route. The embedding may appear artificial, but, on the contrary, in some cases it enriches the model and leads to significant results. The case of nematic liquid crystals is treated in detail.

1. Introduction

Noll's axiomatic method in continuum mechanics proceeds from the algebra of subbodies of a given body and the properties of interactions between pairs of disjoint subbodies (for an account see Ch. I of [1]). It is built on concepts well-established in rigid body dynamics, where the interaction is measured by a pair of vectors (resultant force and resultant torque) an so by an element in a special linear space; hence the idea that the strength of the interaction be measured generally by an element of an appropriate linear space.

Yet, in continua with microstructure, virtual rates of shift in microstates (states which are described by elements of a manifold $\mathcal{M}$ of finite dimension m) belong to tangent spaces of $\mathcal{M}$, which, generally, vary from place to place. Thus the corresponding exertions (the strength of which is measured in cotangent spaces) cannot be summed up outright into totals and thus Noll's starting point seems to fade away. An artificial but adequate tool to overcome the difficulty is offered by Whitney's theorem: $\mathcal{M}$ can always be embedded in a linear space of dimension $2m + 1$. Then, within the wider context, one can follow Noll's approach [2].

However, the total strength of the exertion on a body evaluated in this way may be destitute of intrinsic physical meaning. In general, even rules of variance under changes of embedding are missing. Nevertheless, we show below that the tool is not always fictitious, as it may seem; on the contrary, at least in some cases, it enriches the original model and leads to additional concrete results.

2. Intermezzo

The embedding, the existence of which is assured by Whitney's theorem, is not unique; nor is it always mandatory to resort to a space of dimension $2m + 1$: a space of lower dimension may suffice sometimes.

We quote below a very elementary example, which is of some relevance for the questions addressed to in the next section. Consider the manifold of directions in a plane; its image could be the improper line. But we could also think of the set of segments of unit length, all with the same midpoint. Adding an arrow, arbitrarily, to each segment, we obtain a set of unit vectors n; the set $\{N \mid N = n \otimes n\}$ is in one-to-one correspondence with the set of directions (the two eigenvalues of N are 1 and 0; the eigendirection relative to the former ties with the direction of n). Rather than of N one can think of $Q = N - \frac{1}{2}I$ (I, identity); then $\{Q\}$ is the linear space of symmetric traceless tensors in the plane. Now, one can, for instance, evaluate the average direction in a set, by averaging the corresponding Q's: one finds in particular that the average of two ortogonal directions is the null tensor.

One may muse why one needs to proceed in such a devious way: if the angle θ between two directions is acute the bisectrix of the angle is the 'average' direction, surely. However, one stumbles on the case $\theta = \frac{\pi}{2}$; the loss of a unique 'average' in that case points to a deeper issue: the set of directions cannot be covered by a single chart; on one chart the average can be always decided upon, but the result may depend on the chart.

In the special example one could proceed alternatively: pick one 'master' direction d; choose positive rotations; associate with a direction forming the acute angle θ with d a unit vector at an angle 2θ; embed those vectors in the linear space of vectors in the plane. Averages ensue; in particular, the average of two orthogonal directions turns out to be the null vector.

If one tries to repeat similar steps in three dimensions, recourse to associated tensors is successful again: the embedding occurs in (now) five-dimensional space Sym_0 of symmetric traceless (3x3) tensors. On the contrary, if one adds simply (in the second process) the longitude to twice the 'latitude north', one stumbles on the difficulty that all points on the equator crowd in the 'south pole'.

3. The Case of Liquid Crystals

Let us now return to our remarks of Sect. 1 and examine the case of nematic liquid crystals, a case where the microstructure is a direction ($m = 2$). If $\pm n$ are the two unit vectors with a given direction, the latter determines (and is determined by) the tensor $Q = n \otimes n - \frac{1}{3}I$ uniquely (I is now the 3x3 identity tensor); the set of all Q is a manifold in Sym_0, which comprises all tensors with third invariant equal to $\frac{2}{27}$ and second invariant equal to $-\frac{1}{3}$; a manifold that degenerates into two dimensions because two eigenvalues coincide.

We have mentioned the possibility, within Sym_0, of calculating averages of directions; precisely that manipulation is required by physical circumstances. The material element (modelled so far as a point adorned with a direction) must be imagined to contain many molecules, which are seldom utterly aligned; one direction usually prevails but the discipline is not strict.

Thus, the construct that emerges is an average and that average should, correctly, be read in Sym_0. By doing so one obtains not only the prevailing direction (if any), but also the degrees of triaxiality β and of prolation s in the distribution of directions [3]. Only when, occasionally, $\beta = 0$ and $s = 1$ absolute discipline reigns; chaos (isotropy) wins if $\beta = 0$, $s = 0$.

We must pass on now to give a corresponding measure of the strength of the exertion on a body of nematic. As our goal is narrow, i.e. to provide an example, we confine our attention to two special issues: (i) the total fictitious 'torque' exerted by external body actions to adjust appropriately the triad of principal axes of Q; (ii) the strength of the exertion of self-equilibrated forces against triaxiality and prolation.

To obtain the first quantity observe that, if Q is any element of Sym_0, $\kappa^{(i)}$ ($i = 1, 2, 3$) its (real) eigenvalues and $c^{(i)}$ its corresponding eigenvectors, then

$$Q = \sum_{i=1}^{3} \kappa^{(i)} c^{(i)} \otimes c^{(i)}$$

and the time-derivative

$$\dot{Q} = \sum_{i=1}^{3} \dot{\kappa}^{(i)} c^{(i)} \otimes c^{(i)} - 2\,\mathrm{sym}\,[(\boldsymbol{e}q)Q] \ , \tag{3.1}$$

where $\boldsymbol{e}$ is Ricci's permutation tensor and q is a fictitious spin of the principal axes of Q.

Then the virtual power per unit volume of external actions (with volume density B) is given by

$$B \cdot \dot{Q} = \sum_{i=1}^{3} B_{(ii)} \dot{\kappa}^{(i)} + q \cdot \boldsymbol{e}\,((\mathrm{sym}\,B)Q) \ , \tag{3.2}$$

where $B_{(ii)}$ are the diagonal components of B when the principal axes of Q are taken as reference. We conclude that the fictitious 'torque' on the principal axes is

$$\int_{\mathcal{B}} t\, dB \quad , \quad t = \boldsymbol{e}\,((\mathrm{sym}\,B)Q) \ .$$

To achieve the second goal, we follow an alternative route, rather than through manipulation of the first term in the r.h.s. of (3.1). We accept a standard suggestion regarding the free energy σ of a nematic (κ, a, b, c, appropriate constants)

$$\sigma = \kappa\,(\nabla Q)^2 + a\,\mathrm{tr}\,Q^2 - b\,\mathrm{tr}\,Q^3 + c\,\mathrm{tr}\,Q^4 \, ; \tag{3.3}$$

we confine our attention to homogeneous conditions when σ reduces to $\bar{\sigma}$,the sum of the last three addenda in the r.h.s. of (3.3); we express $\bar{\sigma}$ in terms of s and β

$$\bar{\sigma} = \frac{2a}{3}\gamma^2 - \frac{2b}{9}s^3 + \frac{2c}{9}\gamma^4 \quad , \quad \gamma = \left(s^6 + \frac{\beta^6}{16}\right)^{\frac{1}{6}} \ ;$$

finally we evaluate the virtual power $\dot{\bar{\sigma}}$ which corresponds to virtual rates $\dot{s}$ and $\dot{\beta}$

$$\dot{\bar{\sigma}} = \frac{2}{9}\frac{cs^2}{\gamma^4}\left(-\frac{3b}{c}\gamma^4 + 2\left(\frac{3a}{c} + 2\gamma^2\right)s^3\right)\dot{s} + \frac{c\beta^5}{36\gamma^4}\left(\frac{3a}{c} + 2\gamma^2\right)\dot{\beta}\,.$$

Thus the strength of the exertions turns out to be

$$\begin{aligned} \eta_s &= \frac{2}{9}\frac{cs^2}{\gamma^4}\left(-\frac{3b}{c}\gamma^4 + \left(\frac{3a}{c} + 2\gamma^2\right)s^3\right) \ , \\ \eta_\beta &= \frac{c\beta^5}{36\gamma^4}\left(\frac{3a}{c} + 2\gamma^2\right) \ . \end{aligned} \tag{3.4}$$

When η_s is positive, the tendency is towards isotropy; otherwise the prolation tends to increase. If a and c are both positive, triaxiality is never favoured. Through the detailed study of (3.4) one could duplicate the analysis in the last section of [3] and confirm those results.

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