

DISORDER AS PROJECTION FROM IDEAL, CURVED SPACE

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Résumé - Le concept (Kléman et Sadoc) d'un matériau amorphe comme cristal dans un espace courbe idéal et projeté dans notre espace euclidien ordinaire, incorpore plusieurs de ses propriétés structurelles, mais où se trouve le désordre? Nous démontrons ici que le désordre correspond à un arbitraire local dans la projection, un pivot aléatoire, et que des desinclinaisons de 2π apparaissent naturellement comme sources d'incompatibilité dans l'espace euclidien. Cet arbitraire est une invariance de jauge. Ce fait relie la méthode de projection à d'autres descriptions de la structure du verre comme continu élastique sans symétrie, ou comme un matériel invariant de jauge, par Duffy et l'un d'entre nous. Il suggère aussi une interprétation plus souple de la théorie de l'élasticité classique.

Abstract - Kleman and Sadoc's concept of an amorphous material as a crystal in some curved, ideal space, projected into our ordinary Euclidean space, has many attractive features, but where does disorder come in? We show that disorder corresponds to a specific local arbitrariness in the projection (random pivot), and that (2π) disclinations occur naturally as cores of incompatibility in Euclidean space. This arbitrariness is a gauge invariance. The projection method is thereby related to other descriptions of the structure of glass, as an elastic continuum (without generative symmetry), or as a gauge-invariant material, by Duffy and one of us. It also suggests a broader interpretation of the classical theory of elasticity.

I - STRUCTURE OF GLASS BY PROJECTION METHOD

In 1979 Kleman and Sadoc [1] suggested that the structure of an amorphous material could be represented as a crystal in some ideal, curved space, projected into our ordinary, Euclidean space \mathbb{R}^3 . This idea gives a direct geometrical interpretation of frustration, i.e. competition between the requirements of best possible local packing of atoms [2] (corresponding in metallic glasses to combining tetrahedra or icosahedra together in curved space to form a polytope) and (Euclidean) space-filling. When dealing with covalent glasses, one should replace the word "best" by "most probable" local arrangement of tetrapods, in order to account for entropy.

Projection from curved to Euclidean space means decurving. This is done by (disclination) lines, as can be easily seen by partitioning space into simplices (e.g. regular tetrahedra of 4 atoms) and noticing that it is their common edge which carries the mismatch (5.1 such edge-sharing tetrahedra would fill a region of Euclidean space). This is identical, in one less dimension, to Regge's [3, ch 42] skeleton

geometry in general relativity. That lines are an essential ingredient of the structure of glass has been recognised independently [4] .

Projection should somehow map the generative homogeneity of the crystal in curved space into the overall, non-generative homogeneity of the random structure in Euclidean space. Sadoc [5] and Nelson [6], in the method's greatest triumph to date, have described all tetrahedrally close-packed (TCP) or Frank-Kasper phases (Laves, A15 etc.) by projection of polytopes, although all these phases are crystalline. Sethna [7] models blue phases in cholesteric liquid crystals by continuum elasticity with a uniform density of disclinations of infinitesimal magnitude, but the local structure, which imposes the frustration in the first place, is lost. Finally, in Mosseri and Sadoc's [8] hierarchical decurling, the end product is a quasicrystal with long-range orientational order and Bragg peaks. All of these are examples of frustration without disorder. We shall prove here, by using the projection method, that the non-generative homogeneity is a gauge, or local invariance of the disordered structure, a result which has been hitherto no more than a justifiable working hypothesis [9,10] .

II - DISORDER AS RANDOM PIVOT

In order to understand how to carry out the projection, suppose we wish to imprint the surface of a football, complete with seams, on a plane (of infinite extent) in a consistent manner. A natural way to begin would be to roll the ball along one of its seams until a junction between three seams is reached, where an arbitrariness is introduced as one is faced with a choice of directions in which to proceed. Hence a pivot motion is required, to repeat the pattern consistently. In fact, at any point during the projection, a pivot can be added which is arbitrary except for the requirement of satisfying compatibility conditions.

The seam corresponds to the local frame (tetrapod, tetrahedron, short range order) in glass. It must be mapped into Euclidean space (which is tangent to the curved space) in a compatible fashion. A pivot (frame rotation, or rotation of the tangent plane) is necessary to guarantee compatibility. Disorder implies that this pivot is random and its arbitrariness is a gauge invariance. Projection from curved space implies that frame orientation in the tangent plane cannot be defined uniquely. Physics must be independent of such arbitrariness and invariant under local rotation of the tangent frame.

Projection also implies distortion, and hence strain, and can be related to classical elasticity theory. Indeed, both theories are natural mappings between spaces with frames, the curved space corresponding to the actual, strained configuration of the elastic solid, compatible with global boundary conditions (which has Euler or holonomic co-ordinates) and the tangent space into which it is mapped corresponding to the local relaxed configurations of the solid (which has non-holonomic or Lagrange co-ordinates). A compatible frame must return to the same orientation after circumnavigation, modulo an element of the space group. In glass the space group is trivial, so that only rotations by 0 or 2π (2π -disclinations) are allowed - these are algebraically identical to odd lines [4,10] and are the sources of strain.

III - THEORY OF SURFACES

The mathematical framework for the projection method is provided by the theory of surfaces [3, ch. 21] . There are two alternative treatments:

- (a) Intrinsic (Riemann, Christoffel, Ricci, Levi-Civita, Einstein).

This is characterised by a connection, Γ , relating frames at different points, and torsion and curvature (which measure the density of dislocations and disclinations) are expressed directly in terms of this connection.

(b) Extrinsic (Gauss, Codazzi, Weingarten).

The surface is embedded in \mathbb{R}^3 (considering just the 2D case for the moment) and characterized by the second fundamental quadratic form tensor

$$b_{\alpha i} = - \langle \underline{e}_\alpha, \partial_i \underline{n} \rangle$$

where \underline{e}_α lies in the tangent plane and \underline{n} is the normal to the surface in the embedding space \mathbb{R}^3 .

The two treatments are linked by Gauss' equation (iii), stating that curvatures obtained in either (a) or (b) are identical.

Let Σ be the curved surface, T its tangent plane at a point P, with a natural tangent frame \underline{e}_α , and \underline{n} its normal at P (see fig.)

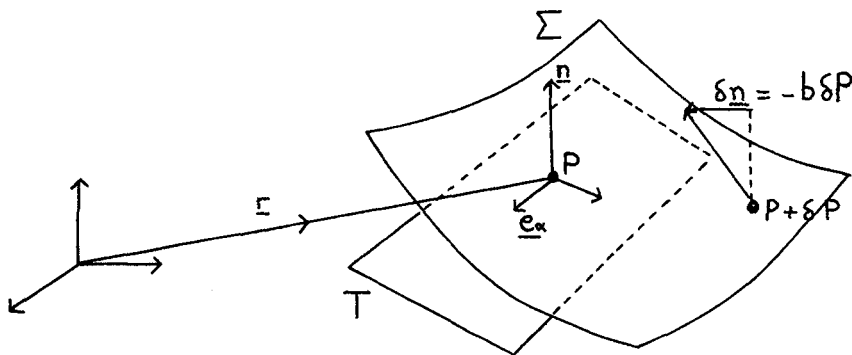


Fig. Surface Σ , tangent plane T, and embedding

When embedded in \mathbb{R}^3 the surface is given by

$$\underline{r}(x^\alpha) \quad (\alpha = 1, 2)$$

Then

$$\underline{e}_\alpha = \partial_\alpha \underline{r}$$

is the natural tangent frame and its variation in the direction i of \mathbb{R}^3 is given by the Gauss-Weingarten equation

$$\partial_i \underline{e}_\alpha = b_{\alpha i} \underline{n} + {}^{(a)}\Gamma_{\alpha i}^\gamma \underline{e}_\gamma \quad (i)$$

where Γ is the connection. Note that the reason for the unconventional distinction between Greek indices, labelling the frame $\{\underline{e}_\alpha\}$ in the tangent plane, and Latin indices, labelling directions, is that we shall use the freedom to rotate or pivot the tangent plane without affecting the direction. The pivot is the gauge transformation. The Greek indices refer, therefore, to the isospin space in Yang-Mills theories, which corresponds here to the orientation of the frame in tangent space.

The main equations of surface theory are given below. Their generalisation to 3-space embedded in \mathbb{R}^4 is straightforward (although less easily visualised!) - simply replace ${}^{(\omega)}\Gamma$ by ${}^{(\omega)}\Gamma$ and let $\alpha = 1, 2, 3$ [3].

Codazzi equation (compatibility automatic in the formalism)

$$\partial_j b_{\beta i} - \partial_i b_{\beta j} = \Gamma^{\gamma}_{\beta j} b_{\gamma i} - \Gamma^{\gamma}_{\beta i} b_{\gamma j} \quad (\text{ii})$$

Gauss' equation (relating intrinsic to extrinsic curvature)

$$R^{\alpha}_{\beta ij} = (b^{\alpha}_i b_{\beta j} - b^{\alpha}_j b_{\beta i}) \langle \underline{n}, \underline{n} \rangle \quad (\text{iii})$$

which, on substitution, can be written explicitly as

$$R_{\alpha\beta ij} = \frac{[\langle \underline{e}_{\alpha}, \partial_i \underline{n} \rangle \langle \underline{e}_{\beta}, \partial_j \underline{n} \rangle - \langle \underline{e}_{\alpha}, \partial_j \underline{n} \rangle \langle \underline{e}_{\beta}, \partial_i \underline{n} \rangle]}{\langle \underline{n}, \underline{n} \rangle} \quad (\text{iv})$$

For a 2D surface embedded in \mathbb{R}^3 then this can be written as

$${}^{(\omega)}R_{\alpha\beta ij} = \frac{[(\underline{e}_{\alpha} \wedge \underline{e}_{\beta}) \cdot (\partial_i \underline{n} \wedge \partial_j \underline{n})]}{\langle \underline{n}, \underline{n} \rangle} \quad (\text{v})$$

which is gauge invariant under rotation of the tangent plane (c.f. $\underline{B} = \text{curl } \underline{A}$ in $SO(2)$ gauge theories).

Equation (iv) is still valid in 3D (embedded in \mathbb{R}^4) and is $SO(3)$ gauge covariant (cf F_{ij} in Yang-Mills gauge theories).

The theory has manifest gauge invariance. Its links with elasticity theory [10] and with measurable quantities like strain are established through Γ and Gauss' equation.

IV - CONCLUSIONS

Disorder is $SO(3)$ gauge invariance. Its sources are 2π -disclination lines which appear naturally in Euclidean space as vestiges of the curved space, introduced to represent frustration. They carry curvature, are frozen at random, their density corresponds to the curvature of Kleman and Sadoc's ideal space, and they are responsible for the non-collinearity of local reference frames \underline{e}_{α} . Here is the paradox of gauge invariance: frames are essential to establish the projection and justify frustration, but their actual orientation is physically irrelevant.

As we have seen, the extrinsic formulation yields gauge invariance whilst the intrinsic formulation relates it to measurable elasticity. The link between the two formulations is through curvature (Gauss' equation (iii)), which also indicates that 2π -disclinations are essential ingredients in glass. This entirely reconciles the projection method [1] with two other theories of glass by Duffy and one of us: a manifestly gauge invariant formulation [9] and a classical elasticity theory, including disclinations [10,11]. (Disclinations can occur in 3D glasses because their strain is screened by dislocations which are not topologically stable in structures with trivial space groups and can act as local fluctuations to reduce the strain).

It is easiest, and most natural, to work and measure in the local, relaxed, tangent space, despite the fact that its co-ordinates are

anholonomic and only gauge covariant.

Finally, the projection method [1] suggests a new general approach to elasticity theory, involving solids large enough, or disordered enough, for global boundary conditions not to permeate through the material. One replaces the global, strained frame by a crystal in curved space expressing stresses or frustration simply, and then works, and measures, as usual in the local, Euclidean, relaxed frame.

We would like to express our thanks to the main authors [1,5,6,7,8,12] of the projection method for introducing a simple, elegant, important and potentially useful idea.

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