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THE GLASS AS AN ELASTIC CONTINUUM

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Abstract. - The theory of elasticity of continuous media is applied to amorphous materials, whose symmetry is completely broken. It is shown that a single line defect, a \( \mathbb{Z}_2 \) disclination, survives the absence of generative symmetry, and that the arbitrariness of the local reference frame can be expressed as a \( \text{SO}(3) \) gauge symmetry. We derive the physical consequences of the existence of these disclinations (two-level systems, Vogel-Fulcher law), and their elastic energy, which is screened down to Coulomb potential by thermal fluctuations in the dislocation part of the incompatibility.

1. Continuum elasticity and odd line "defects" in glasses.- A glass can be regarded on a semi-microscopic scale (whenever all relevant length scales are larger than the interatomic distance) as an isotropic elastic continuum with frozen-in internal stresses. The isotropy and homogeneity of the glass arise from the randomness, they are not generative symmetries as in crystalline solids, but a local symmetry which can be formulated as gauge invariance /1,2/. The stresses are a direct consequence of the amorphous structure, and occur naturally for example because space cannot be filled by atomic configurations minimizing locally the energy (polyicosahedra, i.e. atomic clusters with pentagonal symmetry) /3,4/. Although crystalline structures can also be described as elastic continua, there is one essential difference with glasses: the crystal has generative symmetry described by its space group, whereas such symmetry is broken in the glass, which has trivial space group. (A glass is therefore the antithesis of the Volterra continuum which enjoys all translations and rotations symmetries). Yet, as we shall see, a single line "defect" survives the broken symmetry. Moreover, distant parallelism (zero curvature) no longer applies to glasses, the orientation of the local reference frame is arbitrary (this local arbitrariness corresponds to gauge symmetry). Non-collinearity of the local frames is manifest in models of glass structure, like continuous random networks.

The elastic continuum can be described by differential geometry /5/. The local field is a mapping, \( \phi^i_k(x) = (u/e)^i_k \), between the local, relaxed reference frame \( \{u^i\} \), and actual, strained configuration \( \{e^i\} \) of the glass (\( i=1,2,3 \)). The local reference frame is the configuration...
of a small neighbourhood of $x$, cut from the rest of the body, in which all stresses are relaxed. The strain tensor $e_{ij}$ is related to the field by $e_{ij}^i(x) = \frac{1}{2} \left[ \delta_{ij}^i - (u/e)_{i}^{i} (u/e)_{j}^{j} \right]$ (with summation over repeated indices). In order to compare the actual configurations of the glass at two different points $x$ and $x'$, it is necessary to establish a connection, that is to define parallelism in the configurations. The local references are defined arcwise, by requiring that two overlapping neighbourhoods have local frames fitting together without any rotation. Let $v$ be a vector undergoing parallel displacement. The connection $\delta^v = -\Gamma_{ab}^a v^b dx^a$, is not symmetric and warrants torsion, as well as curvature.

The density of disclinations is related to the Riemann-Christoffel curvature tensor $\Gamma^a_{bmn} = \delta^a_{b} \Gamma^m_{bn} - \delta^m_{b} \Gamma^a_{bn} - \delta^a_{m} \Gamma^b_{bn}$, which vanishes if the connection is flat (pure gauge, $\Gamma^a_{ab} = - (\delta^a_{b} \delta^b_{a} - 1)^n_a$).

The density of dislocations is given by the torsion tensor $\Gamma^a_{ab} = \Gamma^a_{[ab]}$, $\Gamma^a_{ab} = \frac{1}{2} (\Gamma^a_{ab} - \Gamma^a_{ba})$. $\Gamma$ and $\bar{T}$ are related by two identities, the Bianchi identity for $\Gamma$ (allowing for torsion), which states that disclinations are uninterrupted lines, and the torsion identity, stating that dislocations can end on disclinations /6/. For a linearized version of these identities, see §3. The theory is couched in terms of covariant quantities, and covariant derivatives which include the connection. The arbitrariness of the local reference frame— which cannot be uniquely defined in the presence of disclinations i.e. whenever the connection is not flat — implies that physics (strain tensor, free energy, etc.) is invariant under a local rotation of that frame, which is precisely a $SO(3)$ gauge invariance. Thus, the non-generative homogeneity of the glass, whereby every atom is as suitable as every other as a reference point, is expressed as gauge invariance /1,2/. The theory is probed, not by translation, but by rotation of the local reference frame. To characterize a dislocation, one surrounds it with a Burgers circuit, as Gauss' or Ampère's contours are used to identify an electromagnetic charge or current. The Burgers vector must belong to the symmetry (space) group of the material (reference frames before and after circumnavigation are not physically distinguishible). In glasses, the space group is trivial $G = 1$, yet one, $Z_2$, line defect survives, because the rotation group is not simply connected. A rotation by $2\pi$, while it returns the object to the same orientation, entangles its connections with the rest of the material, and is therefore not continuously deformable to the identity. Only rotation by $4\pi$ restores object and connections ($\pi(SO(3)) = Z_2$). All other operations associated with elasticity (translations, dilatations) are simply connected and topologically trivial.

In conclusion, there are topologically stable "defects" in amorphous materials with completely broken symmetry. They are disclination lines associated with oddness, or $Z_2$ algebra ($(1,a)$, $a^2 = 1$), and their topological stability (like the electron spin's) is due to the multi-connectivity of the rotation group. The line defects, hereafter called disclinations, can be visualized /7/ as uninterrupted lines threading through odd rings of bonds (avoiding irreducible even rings) in continuous random networks or Voronoi froths.

2. Low temperature configurations: the 2 level systems.

We show now that the $Z_2$ disclination lines discussed in §1, together with gauge invariance, lead directly to one 2 level system (2LS) of excitations per line. The disclinations are frozen at low temperatures, and the space $\Sigma$ into which matter is put, is punctured by their cores.
The (non linear) elastic free energy $F$ is gauge invariant (arbitrariness of local reference frame), and a periodic function of any external flux of curvature localized in the core of the disclinations /1,8/.

Consider one particular, single-valued, metastable configuration (minimizing the elastic free energy $F$), and one disclination for the moment. Label this configuration $| \theta >$ or $| \phi >$, depending on whether it rotates by $2\pi$ or $4\pi$ when it circumnavigates the disclination. But it is possible to apply an arbitrary rotation by $2\pi$, $U(x)$, such that $U(\theta) \equiv | \theta >$. $U(x)$ is a large gauge transformation, which cannot be continuously deformed to the identity. Tunneling is possible between $| \theta >$ and $| \phi >$ because neither are gauge-invariant and the gauge-invariant lowest energy configurations are

$$| \pm > = \frac{1}{\sqrt{2}} (| \theta > \pm | \phi >)$$

one 2LS per disclination /1/. Simple superposition, with a distribution of tunneling rates, holds for several disclinations. The overlying experimental evidence for 2LS is well documented /9/. There should be no 2LS in systems where the connection is flat or pure gauge, like crystals but also a few, exceptional amorphous structures without disclinations /1/.

3. High temperature properties: the glass transition, Vogel-Fulcher (WLF) law and the entropy paradox.

In the liquid and the glass at high temperatures, disclinations are free to move, expand and shrink subject to continuity equation (Bianchi identity), and the density of free disclinations is a thermodynamic parameter, even if the glass is not in a state of strict equilibrium. In this section, we calculate the strain energy between a pair of disclinations.

It is sufficient to use a linearized version of the elasticity theory outlined in §1, in which strains $e_{ij}$ and connections $\Gamma^{\mu}_{ab}$ are of first order of smallness. (Large rotations are permissible, so that $\phi - \mathbf{1}$ can still be large). The curvature tensor $R_{ablm}$ is then antisymmetric in both couples of indices, and one introduces the contractions

$$R^{i}_{1j} = \sum_{ij} R^{ij}_{ablm} \Gamma^{l}_{abm} , \quad \epsilon^{j}_{1i} = T_{abc}^{ij}.$$  

Bianchi and torsion identities read,

$$\epsilon^{i}_{a} \xi^{a}_{k} = 0 , \quad \epsilon^{i}_{a} \chi^{a}_{k} = \epsilon^{kab} R_{ab}$$

and the effect of torsion and curvature densities is gathered in the incompatibility tensor

$$\eta_{ij} = \frac{i}{2} \left[ (\epsilon_{ijk} \mathbf{a}^{j} + R_{ij}) + (\mathbf{a}^{j})_{ij} \right] = \eta_{ij}^{T} + \eta_{ij}^{R}$$

The complete problem of linear elasticity (stress $(\sigma)$ - strain $e$) relationship can therefore be summarized by the equations, /5/

$$\eta_{ij}^{i} = 0 , \quad \sigma_{ij} = C_{ij} k^{l} e_{kl} , \quad \epsilon^{ijk} c_{mn} \beta^{m}_{i} e_{kn} = - \eta_{ij}^{R}$$

the equilibrium equations, Hooke's law and strain-incompatibility relation, respectively. Incompatibility forms lines $\beta^{i}_{j} = 0$.

For an isotropic medium such as the glass, eq. (3) are solved in terms of Kröner's strain function tensor $\chi_{ij}$, which plays the same part, and has the same ambiguity as an electro-magnetic potential. In the "Coulomb gauge", the strain-incompatibility equation becomes

$$\eta_{ij}^{i} = \frac{i}{2} \chi_{ij}^{i} , \quad (\mathbf{v}^{a} a^{a} k^{l} e_{kl}^{a}) ,$$

whose Green's function is $| \mathbf{x} - \mathbf{x}' |$, so that in an isotropic Volterra continuum or crystal, incompatibility lines interact via a potential increasing linearly with their distance.

In a glass, dislocations are not topologically stable and are free.
excitations. They should be treated as part of the heat bath, and the problem is a thermodynamic one of calculating the partition function $Z$ of the system, for a given distribution of the disclination part of the incompatibility tensor $\hat{\mathbf{\eta}}$, that is for a given configuration of the only topologically stable defects introduced in §1. The partition function is given by

$$Z = \int [D\mathbf{x}] [D\hat{\mathbf{\eta}}] \exp (-F/k_BT) \exp (-F'/k_BT) \delta (\hat{\mathbf{\eta}} + \mathbf{\eta} - \mathbf{\eta}')$$

a sum over all elastic configurations described by the strain function tensor $\hat{\mathbf{\chi}}$. Fluctuations in incompatibility caused by lack of topological stability of the dislocations, is included as a Maxwellian distribution,

$$P[D\hat{\mathbf{\eta}}]D\mathbf{\eta} = \exp (-F'/k_BT)D\mathbf{\eta}$$

Although strictly $T$ should satisfy the torsion identity (2), a free Maxwellian bath is a good approximation for dislocations terminating on a semi-dilute (isotropic, single-scale) distribution of disclinations. The free energy functional is standard in linear elasticity,

$$F = \int d\mathbf{x} f(\mathbf{x}) = \int d\mathbf{x} \delta^{ij}(\mathbf{x}) e_{ij}(\mathbf{x}) = \int d\mathbf{x} \left[ 2\mu \left( \chi^i_j + \frac{\nu}{1-\nu} \delta^i_j \chi^k_k \right) \nu \chi^i_j \right]$$

$\mu$ is a Lamé constant and $\nu$, the Poisson ratio.

The dislocation bath (a unique feature of amorphous structures with broken translational symmetry) screens the self and mutual energy of disclinations, which has the same form (7) as the inductance of current loops. This energy is now sufficiently reduced for disclinations (absent in almost all 3D crystals) to occur naturally in glasses. Moreover, in terms of a dimensionless density of free disclinations $\rho$, $E = -A\rho \ln \rho + B\rho$, and the entropy of free loops can be shown to have the same dependence in $\rho$ (because the mixing entropy of small loops $\sim \rho \ln \rho$ dominates the configuration entropy of long loops $\sim \rho \ln (\rho)$). Consequently the density of free disclinations in thermal equilibrium, and, by a standard argument, the fluidity, have the Vogel-fulcher (WLF) form,

$$\rho_{eq} \sim \gamma^{-1} \exp \left[ \frac{cst}{(T-T_0)} \right]$$

whenever $|\mathbf{x} - \mathbf{x}'| > (\mu/\gamma)^{1/2}$, i.e. that of a collection of disclination loops interacting via a Coulomb potential $|\mathbf{x} - \mathbf{x}'|^{-1}$.

The entropy, whose main contribution comes from the free defects, vanishes at the finite temperature $T_0$, the disclinations are frozen, as discussed in §2, and their entropy negligible. It is at $T_0$ that the only phase transition from supercooled liquid to glass can occur /11/.

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