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HAL Id: jpa-00209397
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Submitted on 1 Jan 1982

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Line defects and tunnelling modes in glasses (*)

N. Rivier and D. M. Duffy

Blackett Laboratory, Imperial College, London SW7 2BZ, U.K.

(Reçu le 9 juin 1981, accepté le 8 octobre 1981)

1. Introduction. — The major obstacle to a detailed understanding of glasses or liquids is the absence of a constructive symmetry. Yet, macroscopically, glasses appear homogeneous, and this global translational invariance or stationarity, related to one's experience of being lost in a (random) forest, and associated with the statement that every atom is as suitable a reference point as any other, should be the key to a classification of glasses (ground states), a description of their dynamics at low temperatures (elementary excitations), and at high temperatures (the glass transition). We shall argue that stationarity can be formulated as gauge invariance of the free energy (or Lagrangian) density of the glass: specifically, a gauge theory of glass replaces, after all points in the glass have been consistently connected to each other, a translation to probe the global homogeneity, by a local change of environment (gauge transformation).

Associated with the random local environment of the glass are line defects of a particularly elementary kind. They have only one quantum number and are their own antidefects [1]. These defects are topologically stable, and, apart from specific exceptions, are present in the ground state structure (crystallography) of glasses. They are directly identifiable in models of the glass structure like continuous random networks [2] or dense random packings [3].

Thus the main ingredients of a theory of glasses are i) line defects, and ii) gauge (or local) invariance. A theory of glass will be presented in this paper. Line defects are introduced and defined in section 2. Section 3 discusses the line defects at $T = 0$ where they are frozen punctures, and at high temperatures or in the liquid, where they are vortex-like excitations and can move around. In both situations the defects have the same topological characteristics, and can therefore be regarded as identical. Section 4 introduces a gauge-invariant free energy for the glass. In section 5 the configurations which extremize the free energy (ground states and metastable states) are classified. It is shown that there are two, distinct,
ground state configurations per line defect. In section 6, it is shown that the glass can in fact tunnel between its two configurations per defect, through a non-trivial gauge transformation. This leads directly to a distribution of split pairs of gauge-invariant states, responsible for the experimentally observed anomalies in the low temperature properties (specific heat, heat conductivity) of the glass [4, 5].

This paper investigates therefore in general the ground states and elementary excitations of the glass. The thermodynamics of the glass transition, using the same basic theory as in the present paper, has been published elsewhere [6, 7]. At high temperature, \( T > T_0 \), there is a finite density of free line defects in equilibrium \( \rho_{eq} \) which vanishes exponentially according to the Vogel-Fulcher law (1) at \( T_0 \). The viscosity, inversely proportional to the density of defects, diverges at \( T_0 \) and the topological entropy, carried by the free defects, vanishes at \( T_0 \) like

\[
S_{top} \propto - \rho_{eq} \ln \rho_{eq}, \quad \rho_{eq} = \alpha \exp[-\gamma/(T - T_0)]
\]

(1.1)

thereby explaining Kauzmann’s paradox (\( \alpha \) and \( \gamma \) are constants).

2. Structure of glasses: a) Line defects. — Amorphous materials have a structure belonging to one of the two main classes: continuous random networks, or amorphous packings. Spin glasses belong to the former type, and they are the simplest structures to discuss, because their geometry and defects have been fixed (quenched) when the alloy was prepared. It is helpful to be able to separate the geometry of space (studied in this section and reviewed in [8]) from the behaviour of the matter which inhabits it.

We shall show that all random structures contain the same, geometrical, \( Z_2 \), uninterrupted line defects which were called frustration lines, odd lines or discline lines. Random space is therefore not simply connected: it is punctured by those line defects [9].

2.1 The spin glass model [10, 11]. — Consider a network, which can be crystalline, with spins \( S_i \) on the vertices \( i \) and nearest-neighbour interactions \( J_{ij} \) carried by the edges \( ij \). The interactions \( J_{ij} = \pm J \) have given random, statistically independent signs, fixed once and for all when the alloy was made. Thus the spins \( S_i \) alone are dynamical variables, the \( J_{ij} \) form the geometrical framework. The Hamiltonian is well known [10]

\[
H = - \sum_{ij} J_{ij} S_i S_j.
\]

(2.1)

An elementary closed ring (plaquette) containing an odd number of antiferromagnetic interactions is frustrated [11]. It cannot accommodate a configuration of spins minimizing the energy of all its bonds, regardless of the type of spins. A frustrated plaquette is therefore a geometrical feature of the lattice. A closed loop around a frustrated plaquette, minimizing the energy of one edge after the other (parallel transport of the spin), rotates the spin by \( \pi \). The orientation of the spins depends therefore on the path chosen around a frustrated plaquette. Such paths cannot be shrunk and the frustrated plaquette can be said to surround a puncture in space.

The network and its frustrations are geometrical attributes of space constructed solely from points in space and their interrelations, independently of the nature of the dynamical variables. Such structure of space is described by a branch of topology called Homology. A frustrated plaquette is a non-bounding 1-cycle (it surrounds a puncture), whereas a flat plaquette is a bounding 1-cycle. Two turns around the frustrated plaquette returns the spin to the original orientations (encountering then an even number of antiferromagnetic bonds), so that a double circumnavigation is a bounding cycle. Frustration is therefore characterized by the two element group \( Z_2 \).

In three dimensions one can thread uninterrupted lines (punctures) exclusively through the frustrated plaqettes. These lines form closed loops or terminate on the surface of the spin glass. They are the dual of the frustrated plaquettes in the dual network formed by replacing vertices by cells, edges by faces and vice-versa. A network with a single puncture has first homology group \( H_1 = Z_2 \). (Any surface on the network cutting the puncture is homeomorphic to a projective plane, as can be verified by elementary triangulation.)

Incidentally, the energy of an Ising spin glass is proportional to the number of unsatisfied bonds, which are, as we have seen, a necessary consequence of frustration. The unsatisfied bonds form, in the dual network, surfaces (walls) supported by the frustration punctures. The ground state configurations of frustrated Ising spin glass are given by the solution of a Plateau problem, minimizing the area of the «soap film» supported by the frustration loops.

2.2 Continuous random networks. — The structure of window glasses (SiO₂), amorphous Ge or Si, and other covalent amorphous materials, has been successfully modelled by a continuous random network (CRN) [2, 12] with (Si or Ge) atoms as its vertices and covalent bonds as its edges, whether decorated by an oxygen atom or not. When some bond bending is permitted, one obtains an infinite, macroscopically homogeneous, random structure. Its rough statistical characteristics (density, radial distribution function) are then reproducible and universal.

The CRN is a regular graph (all vertices have same valency or coordination) with low vertex coordination (\( z < 6 \)) and well-defined edges (the covalent bonds). For vitreous silica, a-Ge and a-Si, \( z = 4 \).

2.3 Amorphous packings. — This structure is obtained by packing together « tightly and randomly »
[8] atoms, ball bearings [3] or even garden peas [13]. Amorphous metals, simple liquids and metallic glasses (made of metallic and glass forming elements in the proportion 3 : 1 to 4 : 1) are examples of amorphous packings, whether as dense random packings of hard spheres [3], a model originally suggested to describe the structure of simple liquids, or, as packings of molecules to take chemical short-range order into account. In either case, only the vertices of the structure are given, and the network is not defined unambiguously, because the high vertex coordination \( z > 6 \) \((z \approx 12 - 14 \) for identical spheres [3]) is ill defined.

However, an unambiguous random network [14] is obtained as the Voronoi froth, made up of the vertices and edges of the Voronoi polyhedra (Wigner-Seitz cells, Dirichlet tesselation) of every atom of the original packing. A Voronoi polyhedron is the region containing all points in space closest to a given atom. Voronoi polyhedra fill space and their construction is unique. The Voronoi froth can also be regarded as the porous network of the packing [15]. It is now an unambiguous, random network of low coordination, \( z^* < 6 \), the dual network (replacing vertices by cells, edges by faces) of the original packing (strictly speaking, it is the dual of the Wigner-Seitz partition of space [6, 8]). Unlike the CRN of covalent glasses, it has also well-defined cells bounded by planar faces. But its edges can have a broad distribution of lengths. Usually, the froth has maximal randomness, whereby all vertices have all minimal edge valency \( z^* = 4 \), with 3 faces and 3 cells incident on each edge, and \((\frac{z^*}{2}) = 6\) faces incident on each vertex. This is because exceptional vertices can always be regarded as two or more \( z^* = 4 \) vertices separated by edge(s) of infinitesimal length.

Continuous random networks describe therefore the structure of the two main classes of glasses.

2.4 LINE DEFECTS. — The most immediately striking feature of CRN is the presence of rings containing an odd number of bonds (5-rings, for example), which should in general be absent in crystalline networks, because only rotations by \( 2 \pi / n \), \( n = 2, 3, 4, 6 \), are compatible with translational symmetry [16]. Because an odd ring can be constructed in a crystalline network by cutting, removing or adding a wedge-shaped segment, rotating the lips of the cut, and regluing (as an orange can be restored to perfection after eating a few segments), it surrounds the core of a disclination (rotation dislocation). The odd ring can be regarded as a non-bounding 1-cycle in the network, which becomes bounding (even) when circumnavigated twice.

In three dimension, odd rings surround continuous lines (odd-, or disclination lines) which must close up as loops or terminate at the surface of the glass. The proof is elementary: let every bond \( \alpha \) carry the weight \( J = -1 \), and associate with every ring \( r \) the product \( \varphi_r = \prod_{(x \in r)} J = \pm 1 \) for an even/odd ring. Any closed surface \( S \) on the network will have \( \prod_{(r \in S)} \varphi_r = \prod_{(r \in S)} J^2 = 1 \) since every edge separates exactly two rings on \( S \). Thus any \( S \) contains an even number of odd rings, providing an exit for every odd line.

Odd, or disclination lines (the white bit on the axis of the orange) form the locus of non-bounding 1-cycles in the geometrical network which describe the structure of the glass. They are punctures, purely geometrical objects, independent of the dynamical variables of the glass, and quenched in the ground state, in complete analogy with frustration lines in spin glasses. A network with \( n \) punctures has first homology group \( H_1 = Z_2 \oplus Z_2 \oplus \cdots \oplus Z_2 = Z_n^* \) (the even rings are bounding cycles, and an odd ring becomes even when circumnavigated twice). The Connell-Temkin [9] model is a random network with \( n = 0 \).

Odd lines are therefore as essential an ingredient of random matter as the matter (atoms, molecules) itself exactly as solid state physics consists of crystallography (space groups) and matter (electrons, atoms, spins). The crystallography or geometry of glasses has two main constituents: \( Z_2 \) line defects (topology) and gauge invariance (metric).

We have shown that odd lines in glasses are geometrically identical with frustration lines in spin glasses. In fact, the analogy goes further: odd lines affect the form of the elastic energy, at least in covalent glasses, as we shall now demonstrate.

The elastic energy of a glass described by a continuous random network can satisfactorily be expressed in terms of bond-stretching and bond-bending potentials [17], for example by adapting Keating's model for diamond [18] to random networks. Consider a continuous random network with \( N \) vertices, of valency \( z = 4 \), and \( E = \frac{1}{2} zN \) edges. Define \( \frac{1}{2} zN \) bond vectors \( r_\alpha \). The bond stretching energy will then be written in terms of the length of individual bonds, an even function of \( |r_\alpha| = b \), and the bond bending energy in terms of the scalar product between pairs of bond vectors incident on the same vertex \( \alpha \), thus \( r_\alpha \cdot r_\beta \pm a^2 \) for \( (\alpha \beta) = i \). \( b \) is the unstretched bond length and \( a^2 = \frac{1}{4} \) (for \( z = 4 \)) the magnitude of the cosine between unbent bonds, described by the unit vectors \( r_\alpha \). The \( \frac{1}{2} zN \) vectors \( r_\alpha \) are not independent since every cycle in the network must be closed, \( \sum_{\text{cyc1}} (\pm r_\alpha) = 0 \). (The factor \( \pm \) takes into account the orientation of the vectors \( r_\alpha \), which will be discussed presently.) There are

\[ R_1 = E - N + 1 = \left( \frac{1}{2} z - 1 \right) N + 1 \]

independent cycles or constraints (\( R_1 \) is the cyclomatic number of the graph). We remain therefore with \( N - 1 \) independent vectors, or \( 3N - 3 \) independent variables, corresponding, as expected, to the \( N \) atoms at the vertices less the centre of mass of the glass.
The orientation of the nearest-neighbour bond vectors should be chosen so that \( r_x, r_y < 0 \) in the absence of bond bending. If this is possible for every bond, the bond bending energy is the sum of \( \frac{1}{2} z(z-1) \) identical functions of \( r_x, r_y + a^2 \). The orientation of the graph is then consistent. All the \( r_x \) incident on the same vertex are directed either towards the vertex (« down-vertex » for short), or away from the vertex (« up-vertex »). Conversely, if such orientation is not possible for all bonds and vertices, the bond-bending energy will be a function of \( r_x, r_y - a^2 \) for pairs \((x, y)\) containing one badly oriented bond, and of \( r_x, r_y + a^2 \) for the others. It is understood that the number of consistently orientated bonds is maximized for any given graph.

Graphs containing only even cycles can clearly be orientated consistently. They are bipartite (their vertices can be divided into two classes, up and down, with bonds only between vertices of opposite class). Conversely, a graph containing odd rings is not bipartite and cannot be orientated consistently. Every odd ring contains necessarily one badly oriented bond. The situation is identical to an amorphous Ising antiferromagnet, with an odd ring corresponding to a frustrated plaquette, and a badly oriented bond to an unsatisfied bond in the antiferromagnet (or the spin glass), with one exception: in the magnetic problem, frustration costs energy and entropy (ambiguity in the direction of the spins), concentrated on the unsatisfied bonds. In the glass, the energy may have the same value whether bonds are consistently orientated or not. (A large isolated odd ring, a 7-ring for example, can be built at no cost of elastic energy), but it is a different function of the dynamical variables \( \{ r_x \} \) in either case. Otherwise, exactly as in spin glasses, the badly orientated bond can be shifted around odd cycles by a discrete gauge transformation:

\[
\{ r_x \rightarrow - r_x, \quad r_x, r_y \pm a^2 \rightarrow r_x, r_y \pm a^2, \quad \forall x \}
\]

and they form a two dimensional film supported by the odd defect lines (threading through odd rings). Orientation of an odd ring will depend on the path chosen to decide it.

In spite of the close analogy with the discrete spin glass model, it will be more advantageous to describe the glass by a field theory in uniform space. This corresponds to a Ginzburg-Landau type of model for the glass, which could in principle be obtained from a discrete network model after a few steps of renormalization group equations (block spins, etc.).

A final comment regarding punctures. The basic network in glasses is discrete, i.e. riddled with holes. The question is whether, and which ones of these holes can be filled up. A bounding cycle — a cycle which can be filled up — is such that the relationship between vertices of the cycle is independent of the path chosen to establish it. Non-bounding cycles will survive as punctures in the continuous limit, with the same homology group, because the path-dependent relation between vertices must be preserved.

3. Line defects: frozen punctures or mobile vortices?

— We include now matter into the geometrical framework discussed hitherto. Although covalent glasses are discrete geometrical networks structurally, it is possible and convenient to describe them by a field theory, associating a field with every point in continuous space. The same field theory can then be used for metallic glasses, where the network is dual to the structure of the matter, and also for liquids, where the geometrical network (whether dual or primal) is time dependent. Moreover, a continuous representation of the glass takes full advantage of the local, or gauge invariance, which will be introduced in section 4.

A glass can therefore be regarded as a piece of punctured space \( \Sigma \), accommodating the relevant matter, the punctures being the continuous loop threading through odd rings of the original network. The matter field \( \phi(x) \) describes the orientation of the local environment of a particular atom or molecule, and has states in the manifold representative of the rotation group \( G = SO(3) \). Specifically (Eq. (5.6) below), it is parametrized by a rotation matrix \( W(x) \), which is a map of \( \Sigma \) into \( SO(3) \), with origin \( x_0 \) mapped onto the identity in \( SO(3) \).

\[
W(x) : \Sigma \rightarrow SO(3)
\]

\[
x_0 \mapsto 1.
\]

The ground and metastable states are field configurations which extremalize the free energy, and given by solutions of Euler-Lagrange equations, in regions of space where such solutions are finite, continuous and well-defined (that is, excluding punctures and singularities of the field). Each configuration is given by a map (3.1), in particular, a closed \( n \) dimensional surface \( S^* \) in \( \Sigma \) is mapped into a closed contour in the manifold of field configurations since any given configuration is single-valued. Configurations divide into classes, each class containing those configurations which are continuously deformable into each other. By construction, the classes of configurations are topologically stable, and are labelled by the homotopy groups \( \pi_n \) of the field manifold. If all the \( \pi_n \) are trivial, all the configurations can be deformed continuously into the uniform state \( W(x) = 1 \) in (3.1), and no defect is topologically stable. Non-triviality of the \( \pi_n \) imply the existence of distinct, metastable configurations (they cannot decay into the ground state, even if they have, in general, a higher energy).

The metastable configurations are therefore split into topologically stable classes, the homotopy classes \([\Sigma, SO(3)]\) of the map (3.1). The classes are investigated through the homotopy groups

\[
\pi_n(SO(3)) = [S^n, SO(3)].
\]
For example, a single line defect is related to \( \pi_1(\text{SO}(3)) = \mathbb{Z}_2 \), i.e. to whether the rotation of the matter field along a contour is continuously deformable to the identity or to a rotation by \( 2\pi \). This, of course, presupposes that the contour in \( \Sigma \) can itself be shrunk to a point, which is not the case if \( \Sigma \) is punctured. The topologically stable configurations depend therefore on the topology of both \( \Sigma \) and \( \text{SO}(3) \).

Thus, there are two kinds of defects, i.e. two reasons for the non-triviality of \([\Sigma, \text{SO}(3)]\). First of all, there are the geometrical punctures in \( \Sigma \), described in section 2, and about which any contour cannot be shrunk to a point. Secondly, there are \((\mathbb{Z}_2)\) vortex-like excitations, which would occur even if \( \Sigma \) was Euclidean, and are the defects classified by conventional homotopy theory [19]. The core of a vortex lies within \( \Sigma \). But a puncture around which the field rotates by \( 2\pi \) is a vortex whose core is stuck inside the puncture, outside \( \Sigma \), and does not contribute to the energy of the glass. Conversely, a vortex is a puncture which can move about and costs energy.

The homology group of a geometrical puncture and the homotopy group of the manifold of field states are here identical. This is not accidental. An odd line becomes even when circumnavigated twice, and this must be reflected by a similar relation between homotopy classes \([\Sigma, \text{SO}(3)]\) [20]. Here, it turns out to be an identity between \( H_1 \) and \( \pi_1 \), which enables us to treat puncture and vortex (core excluded) as the same general defect, quenched or frozen for the former, and mobile for the latter, and to describe a glass at all temperatures and its liquid phase by the same, continuous field theory. An annealed field theory corresponds to a punctureless \( \Sigma \), but can still accommodate vortices if \( \pi_1 \neq 1 \). Moreover, the presence of the same defects at all temperatures suggests strongly a mechanism for glass formation, whether kinetic or dynamical (through interaction between defects [6, 7]).

The rotation group has
\[
\pi_1(\text{SO}(3)) = \mathbb{Z}_2 \quad \text{and} \quad \pi_3(\text{SO}(3)) = \mathbb{Z}
\]
as sole non-trivial homotopy groups for \( n \leq 3 \). It turns out that there is interference between the homotopy classes, so that \( \text{SO}(3) \) cannot be approximated by a direct product of two spaces, one of which having \( \pi_1 = \mathbb{Z}_2 \), \( \pi_3 = 1 \), the other \( \pi_1 = 1 \), \( \pi_3 = \mathbb{Z} \) [22, 23]. Nevertheless, the homotopy classes \([\Sigma, \text{SO}(3)]\) have been worked out for general \( \Sigma \) [22, 23].

Thus, the same, topologically non-trivial matter configurations arise as a result of the non-triviality of space, or as free vortex-like excitations. They are part of the same free energy (4.1). Because vortices carry a finite energy, and their density in thermal equilibrium vanishes below \( T_0 \) (Eq. (1.1)), only the frozen punctures survive at low temperatures \( T < T_0 \), which is the physical range investigated in this paper. (At high temperatures odd lines can move in the «network», which is no longer a geometrical invariant, and the glass or the liquid undergo structural relaxation. Translated in the language of field theory, there is a finite density of mobile vortices in thermal equilibrium (1.1), because they carry most of the entropy. The simplest approach is then to neglect the punctures and study the free energy (4.1) in an otherwise Euclidean space. The interacting vortices freeze by their own devices at and below \( T_0 \), by pairing up [6, 7].)

4. Structure of glasses : b) Gauge invariance. —

In this section we proceed to construct the free energy functional for glasses. Given the matter field \( \phi(x) \), the energy density associated with fluctuations in \( \phi \) would be, in ordered condensed matter, proportional to the square of its gradient \( (\partial_j \phi)(\partial^j \phi)^* \). But in a glass the equilibrium orientations at different points are not collinear and a suitable connection between orientations (parallel transport) must be established. This is done by introducing a gauge field \( A_\mu \), and replacing the ordinary derivative \( \partial_\mu \phi \) by a covariant derivative \( D_\mu \phi \), both defined below.

The fact that a glass is homogeneous, and that every atom is as suitable a reference point as any other, is expressed mathematically by the gauge, or local invariance of the free energy density. That is, instead of probing the homogeneity by infinitesimal translations, as one would in the presence of global, generative symmetry, one selects arbitrarily the local orientation at every point, by local rotations \( U(x) \in \text{SO}(3) \) and impose that the free energy be independent of these arbitrary rotations. This requires the introduction of the same connection and gauge fields as argued above on different grounds. Because rotations do not commute, the gauge theory is non-abelian, a well known and often essential ingredient in high energy physics, first investigated by Yang and Mills [24]. The gauge field is introduced solely to ensure the connection (minimal coupling) and does not have any further dynamical significance.

Specifically, the free energy \( F = \int dx \, f(x) \) has the density
\[
f(x) = \gamma (\tilde{D}_\mu \phi)^I (\tilde{D}^\mu \phi)^I + \frac{1}{2} \tilde{F}_{ij}^\mu \tilde{F}^\mu_{ij} + U(\phi) \tag{4.1}
\]
where we distinguish formally between directions in ordinary space \( \mu = 1, 2, 3 \) and in the internal space
\[
G = \text{SO}(3), \quad i = 1, 2, 3.
\]

Shorthand symbols are used exclusively in the latter space and repeated indices are summed. The matter field \( \phi(x) \) is proportional to a real rotation matrix \( \hat{\Omega}(x) \),

\[
\phi^I(x) = \hat{\omega}(x) \Omega^I(x). \tag{4.2}
\]

with \( \hat{\omega}(x) \) a real parameter controlled by the potential \( U(\phi) \)
\[
U(\phi) = \alpha \phi^I \phi_I + \frac{1}{2} \beta (\phi^I \phi^I)(\phi^K \phi^K) + \frac{1}{2} \sigma \frac{\phi^I \phi_I}{\beta} = 3(\alpha \lambda^2 + \frac{1}{2} \beta \lambda^4) \tag{4.3}
\]
With $y, \alpha (<0)$ and $\beta (>0)$, constants. In a glass, $\lambda$ is finite everywhere except on the defect lines where the matter field is no longer defined and $\lambda$ vanishes. (The Euler-Lagrange equation for $\lambda$ involves \( \hat{\Omega}(x) \) only through the covariant fluctuations $| \hat{D}_\mu \hat{\Omega} |^2$, since $U(\hat{\phi}) = U(\lambda)$ and

\[
(\hat{D}_\mu \hat{\phi})^i = (\hat{\partial}_\mu \hat{\phi})^i = (\hat{\partial}_\mu \lambda) (\hat{\partial}_\nu \lambda) + \lambda^2 (\hat{D}_\mu \hat{\Omega})^i (\hat{D}_\nu \hat{\Omega})^i
\]

By adjusting the constants $\alpha$ and $\beta$, it is possible to choose the distance $a = (\gamma^2 - 6 \alpha^2)^{1/2}$ over which $\lambda$ decreases to zero, smaller than or equal to the girth, or the size of the smallest ring in the discrete network. $a$ is the size of the core of the defect, outside of which $\lambda$ can be taken to be constant and minimizing $U(\hat{\phi}) = 0$, $\lambda^2 = \lambda^2_0 = - \alpha / \beta$. A defect core $a$, smaller than any other length in the glass, corresponds to type II superconductivity. In the remainder of this paper, we shall therefore $U = 0$, $\lambda = \lambda_0$ in the free energy (1) and set up a field theory in the space $\Sigma$ punctured by frozen defect cores. Thus, although $\phi$ looks at first sight similar to an order parameter in a Landau theory of phase transition, there is no symmetry breaking in glasses, and the symmetry associated with $\lambda = 0$ has already been broken in the liquid.

The free energy density (1) is gauge-invariant: an arbitrary, local rotation $U(x) \in SO(3)$ transforms the matter field into

\[
\hat{\phi}'(x) = \hat{U}(x) \hat{\phi}(x) \hat{U}^{-1}(x).
\]

A free energy involving ordinary derivatives would not be invariant, since

\[
\partial_\nu \hat{\phi}'(x) = \partial_\nu (\hat{\partial}_\mu \hat{\phi}) \hat{U}^{-1} + (\hat{\partial}_\mu \hat{U}) \hat{\phi} \hat{U}^{-1} + \hat{U} \phi (\hat{\partial}_\mu \hat{U}^{-1})
\]

is not covariant. To recover the invariance, introduce the gauge fields or « vector » potential $A^{i}_{\nu}(x) = - A^{i}(x)$, which transform under $\hat{U}(x)$ like

\[
\hat{A}_{\nu} = \hat{U} \hat{A}_{\nu} \hat{U}^{-1} + g^{-1} \hat{U} (\hat{\partial}_\mu \hat{U}^{-1}).
\]

Then, the covariant derivative $D^i_{\nu}$, which reads,

\[
\hat{D}_\mu = \partial_\mu + g[\hat{A}_\mu],
\]

or explicitly

\[
(\hat{D}_\mu \hat{\phi})^i = \partial_\mu \phi^i + g[\hat{A}_\mu, \phi]^i
\]

is covariant and transforms like a rank 2 tensor

\[
(\hat{D}_\mu \hat{\phi})^i = \partial_\mu \phi^i + g[\hat{A}_\mu, \phi]^i = \hat{U} (\hat{D}_\mu \phi) \hat{U}^{-1}.
\]

The curvature tensor $F^i_{\mu\nu}(x)$ which measures the local density of non-collinearity between local frames of reference, and is the generalization of the magnetic induction in electromagnetism, is related to the vector potential $A^i_{\nu}(x)$ by

\[
F^i_{\mu\nu}(x) = \partial_\nu A^i_{\mu} - \partial_\mu A^i_{\nu} + g[\hat{A}_\mu, \hat{A}_\nu]^i.
\]

It is also covariant,

\[
\hat{F}^i_{\mu\nu} = \partial_\nu \hat{A}^i_{\mu} - \partial_\mu \hat{A}^i_{\nu} + g[\hat{A}_\mu, \hat{A}_\nu] = \hat{U} F^i_{\mu\nu} \hat{U}^{-1}.
\]

The gauge invariance of the free energy density $f'(x) = f(x)$ follows from equations (1), (9) and (11)

Note that the coupling between matter and gauge fields is minimal, effected solely through the covariant derivative, as in electromagnetism or superconductivity. The only physical reason for introducing the gauge field (in addition to the matter field [23]) is the requirement of local or gauge invariance of the free energy, whereby $f(x)$ must be invariant under an arbitrary rotation at any point in space.

The idea of representing a disordered system by a minimally coupled, gauge field theory in continuous space is not new. It has been introduced for spin glasses, in Euclidean space [26, 27]. The problem of quenched disorder (frustration lines) and its relation to the gauge fields, has not been satisfactorily solved (whether by quenching the gauge field $\hat{A}$ itself [27] or by keeping it as a dynamical variable and giving it, somewhat arbitrarily, a mass [26]) in these papers. Here, the frustration lines are frozen geometrical punctures in space. Another, equivalent method is to express frustration lines as sources of curvature $\hat{F}_{\mu\nu}$ representing them mathematically through Lagrange multipliers in the free energy (1), now in Euclidean space. This latter approach has only been exploited in XY spin glasses [28], for which the gauge theory is abelian.

That the local matter field in Heisenberg spin glasses should be a rotation matrix $\hat{\Omega}(x) \in SO(3)$, rather than a single spin field $S(x) \in S^2 = SO(3)/SO(2)$, has been convincingly argued by Toulouse [21] (see also [29, 6]). Frustration makes the spins non-collinear, like the local SiO4 tetrahedra around an odd ring in glasses. The field in continuous space represents the local configuration of spins averaged over a plaquette size, that is a hirsute bunch, or hedgehog of spins.

5. Classical solutions of the field theory and metastable configurations in glasses. — The argument of sections 5 and 6 is fairly lengthy, but conceptually simple: we shall classify the metastable configuration $\{ \hat{A}_\nu(x), \hat{\Omega}(x) \}$, solutions of Euler-Lagrange equations, as follows:

i) The idea, as in electromagnetism, is to lump together the gauge field and the phase density of the matter field (or phase gradient in electromagnetism) into a new gauge field $\hat{C}_\mu(x)$ which is now gauge-invariant. The free energy and Euler-Lagrange equations can be written solely in terms of $\hat{C}_\mu$, $\hat{C}_\nu$ which are affected by gauge transformations.
ii) Because $\hat{\Omega}(x)$ is a matter field, it should be independent of the path chosen to define it from an arbitrary origin $x_0$. This means that it can be parametrized by a rotation matrix $W(x) \in SO(3)$ which transforms in a well defined way under gauge transformations.

iii) Gauge invariance of $\hat{C}_\lambda(x)$ implies that $\hat{A}_\lambda(x)$ too, and therefore the metastable configurations \{ $\hat{\Omega}(x), \hat{A}_\lambda(x)$ \}, are parametrized by the rotation $W(x)$.

iv) Configurations split therefore in topologically distinct homotopy classes, two per puncture, because $\pi_1(SO(3)) = Z_2$, with the same energy (because the free energy is gauge-invariant).

v) But the two (topologically distinct) configurations are not gauge-invariant: there is a large change transformation transforming one into the other. The glass can therefore tunnel between them. The final gauge-invariant configurations (« two-level systems ») are linear combinations of the topological classes (« tunnelling states »). They are now split in energy by tunnelling.

The classical ground or metastable states of the glass correspond to extrema of the free energy (4.1), and are given by the solutions of the Euler-Lagrange equations:

\[
\hat{D}_\mu F^{\mu \nu} - \kappa [\hat{D}^* \hat{\Omega}, \hat{\Omega}^{-1}] = 0 \tag{5.1}
\]

\[
\gamma \hat{D}_\mu \hat{D}^\mu \hat{\Omega} = \mu(x) \hat{\Omega} \tag{5.2}
\]

for variations of $\hat{A}_\lambda$ and $\hat{\phi} = \lambda_\lambda \hat{\Omega}$ respectively. Here $\kappa = g g_\lambda^2$. Equation (2) was obtained by allowing $\hat{\phi}$ to be an arbitrary, real matrix, with the Lagrange multiplier $\mu(x)$ to constrain it to the proper form (4.2): $\hat{\phi}^\dagger = \lambda_\lambda$, under which $\partial U / \partial \hat{\phi} = 0$. These equations are to be solved subject to specific boundary conditions at the surface of $\Sigma$, that is at infinity and on the punctures.

$\hat{\Omega}(x)$ describes a definite configuration of the matter in the glass, which should be a uniform function. If we define a phase density operator $\hat{\chi}_\lambda(x)$, by the (not gauge covariant) equation

\[
\hat{D}_\mu \hat{\chi}_\lambda(x) = [\hat{\chi}_\lambda(x), \hat{\Omega}(x)] \tag{5.3}
\]

its solution depends, in general, on the path $x(s), 0 \leq s \leq 1$ chosen for the integration,

\[
\hat{\Omega}(x) = \hat{\Omega}[x(s)] = P_s \exp \left( \int dx^\mu \chi^\mu(x) \right) \hat{\Omega}_0 \bar{P}_s \exp \left( - \int dx^\mu \hat{\chi}^\mu(x) \right) \tag{5.4}
\]

where the path-ordering operator $P_s$ has the same action as the familiar time-ordering operator: it orders the operators appearing in the exponential from right to left along increasing values of the path parameter $s$. $\bar{P}_s$ orders the operators in the opposite fashion, and $\hat{\Omega}_0 = \hat{\Omega}(x(0) = x_0)$ is the initial value for the matter field.

Uniformity of the matter field requires that $\hat{\Omega}(x)$ is independent of the path, for which a necessary and sufficient condition is the existence of a rotation operator $W(x)$ such that,

\[
\exists \hat{W}(x) : \hat{\chi}_\lambda(x) = [\hat{D}_\mu \hat{W}(x)] \hat{W}^{-1}(x). \tag{5.5}
\]

Then,

\[
\hat{\Omega}(x) = \hat{W}(x) \hat{\Omega}_0 \hat{W}^{-1}(x). \tag{5.6}
\]

(Indeed, $\hat{W}(x) = P_x \exp \left( \int dx^\mu \hat{\chi}'(x) \right)$ is path independent if the curvature associated with $\hat{\chi}$ vanishes, ([30], 12.1))

\[
\hat{G}_{\mu \nu} = \hat{\partial}_\mu \hat{\chi}_\nu - \hat{\partial}_\nu \hat{\chi}_\mu - [\hat{\chi}_\mu, \hat{\chi}_\nu] = 0. \tag{5.7}
\]

$\hat{W}(x)$ obviously satisfies (5). Conversely $\hat{\chi}_\lambda(x)$, (5), satisfies (7) and its contour integral is independent of the path.) In superconductivity, equation (5) corresponds to writing the phase density as a gradient. Uniformity of the superconducting wave function or order parameter leads, when expressed in the equivalent of (1), to the quantization of the fluxoid ([31]).

We shall aim at the equivalent to quantization in the non-abelian case, the separation of configurations into distinct sectors.

The uniform representation for $\hat{\Omega}(x)$ enables us to simplify greatly the Euler-Lagrange equations. It is useful to work in a rotated frame,

\[
\hat{A}(x) = \hat{W}^{-1}(x) \hat{\omega}(x) \hat{W}(x) \tag{5.8}
\]

for any SO(3) operator $\hat{\omega}(x)$. Then,

\[
\hat{W}^{-1}(x) (\hat{D}_\mu \hat{A}) \hat{W} = \hat{D}_\mu \hat{\omega} \tag{5.9}
\]

where the new covariant derivative $\hat{D}_\mu$ involves the phase $\hat{\chi}_\lambda$ as well as $\hat{\omega}_\mu$:

\[
\hat{D}_\mu = \hat{\partial}_\mu \hat{\omega} + [\hat{\omega}_\mu, \hat{\chi}_\lambda], \tag{5.10}
\]

with $\hat{C}_\mu(x) = g A_\mu(x) + \hat{\chi}_\mu(x)$, the new vector potential. Moreover,

\[
g F_{\mu \nu} = \hat{\partial}_\mu \hat{C}_\nu - \hat{\partial}_\nu \hat{C}_\mu + [\hat{C}_\mu, \hat{C}_\nu]. \tag{5.11}
\]

The Euler-Lagrange equations then read

\[
g \hat{D}_\mu F^{\mu \nu} - \kappa [\hat{C}_\nu, \hat{\Omega}_0, \hat{\Omega}_0^{-1}] = 0 \tag{5.12}
\]

\[
\hat{D}_\mu [\hat{\chi}_\mu, \hat{\Omega}_0] = \gamma^{-1} \mu(x) \hat{\Omega}_0. \tag{5.2}
\]

The length associated with inhomogeneities in (rescaled) gauge fields $\hat{C}(kg)^{-1/2}$ is

\[
l = (kg)^{-1/2} = 1/(\sqrt{\gamma g \lambda_0}). \tag{5.13}
\]
Boundary conditions are specified for $\tilde{C}$, ruling out the trivial, uniform solution $\tilde{C} = 0$.

The boundary condition at infinity is not necessary if there is an extensive concentration of puncture loops. For a single loop, the gauge field $A_\mu(x)$, and $\tilde{C}_\mu(x)$ are pure gauge solutions at infinity (see discussion of equation (19) below). In three dimensional space, there are no equivalent to instantons, because

$$\pi_2(\text{SO}(3)) = 1.$$ 

The interest of the tilted representation (8) is twofold:

i) Additivity of the phases $\tilde{x}$ and $\tilde{A}$ lumped together in $\tilde{C}$ (they do not commute in general);

ii) All the fields $F^{\mu\nu}$, $C^\mu$, and the Euler-Lagrange equations themselves (1') and (2') with the boundary conditions are gauge-invariant.

Consider a local rotation $\tilde{U}(x) \in \text{SO}(3)$. Given $\tilde{U}(x)$ by (6) in terms of $\tilde{W}(x)$, it is transformed under $\tilde{U}$ as in (4.4), so that the rotation operator is transformed as

$$\tilde{W}'(x) = \tilde{U}(x) \tilde{W}(x).$$

It follows that neither $\tilde{C}_\mu = \tilde{C}_\mu + \tilde{W}^{-1}(\tilde{U}^{-1} \partial_\mu \tilde{U}) \tilde{W}$ nor $\tilde{A}_\mu = \tilde{A}_\mu - g^{-1} \tilde{W}^{-1}(\tilde{U}^{-1} \partial_\mu \tilde{U}) \tilde{W}$ are invariant, but their sum

$$\tilde{C}_\mu = \tilde{C}_\mu + \tilde{g} \tilde{A}_\mu$$

is $\tilde{C}_\mu$ itself is covariant

$$\tilde{C}_\mu = \tilde{U} \tilde{C}_\mu \tilde{U}^{-1}.$$ 

Similarly, covariance of $\tilde{F}_{\mu\nu}$ (Eq. (4.11)) implies invariance of $\tilde{F}_{\mu\nu}$$

$$\tilde{F}_{\mu\nu}' = \tilde{F}_{\mu\nu}.$$ 

Also, the covariant derivative of an invariant field, $\tilde{A}' = \tilde{A}$, is invariant

$$(\partial_\mu \tilde{A})' = \partial_\mu \tilde{A}' + [\tilde{C}_\mu, \tilde{A}] = D_\mu \tilde{A}$$

because $\tilde{C}_\mu$ is invariant. The invariance of the Euler-Lagrange equations (1') and (2') is thereby proved. The gauge invariance of the boundary conditions follows from that of the free energy and of $\tilde{C}$.

The free energy density, itself gauge-invariant by construction, can be expressed in terms of invariant fields, as follows,

$$f(x) = \frac{1}{2} \text{Tr} \left[ F_{\mu\nu} F^{\mu\nu}\right] +$$
$$+ g \lambda_0 \text{Tr} \left[ [\tilde{C}_\mu, \tilde{\Omega}_0] [\tilde{C}^\mu, \tilde{\Omega}_0]^+ \right].$$

The circulation of the total vector potential around a closed contour, $P \exp \oint dx_\mu \tilde{C}^\mu$ is gauge-invariant.

On the other hand, the rotation of the matter field

$$P_s \exp \oint dx_\mu \tilde{x}^\mu = P_s \exp \oint dx_\mu \tilde{W}^{-1} \partial_\mu \tilde{W},$$

is not invariant (see (13)) but it must correspond to a rotation $\tilde{W}$ by 0 or $2\pi$.

Let us now classify the solutions of the Euler-Lagrange equations (1') and (2') parametrized by $\tilde{A}_\mu$, and such that $\tilde{\Omega}(x_0) = \tilde{\Omega}_0$. We shall show that they are not all equivalent, i.e. cannot all be related by continuous gauge transformations, so that there are two discrete stationary (ground state) configurations associated with each defect loop.

The ground state configurations $\{\tilde{A}_\mu, \tilde{\Omega}\}$ are given by the solutions $\tilde{C}_\mu$ of the Euler-Lagrange equations (1') and (2'), satisfying the relevant boundary conditions. Consider one such solution $\tilde{C}_\mu$; it is gauge-invariant, so that any gauge transformation compatible with the boundary conditions will yield the same, unique solution. However, neither $\tilde{A}_\mu$ nor $\tilde{\Omega}_\mu$ are gauge-invariant, and the configuration will change under gauge transformation. However, regarded as equivalent when connected by continuous gauge transformation, the configurations $\{\tilde{A}_\mu, \tilde{\Omega}\}$ fall naturally into equivalence classes. The arbitrariness of the gauge is only lifted for each equivalence class (see [30], § 9.3, 12.2, or [32], § 5), because the gauge-fixing conditions are themselves differential equations of the fields.

The configurations $\{\tilde{A}_\mu, \tilde{\Omega}\}$ are parametrized by the rotation matrix $\tilde{W}(x) \in \text{SO}(3)$, since

$$\tilde{C}_\mu = \tilde{W}^{-1} \partial_\mu \tilde{W} + g \tilde{A}_\mu.$$ 

is gauge-invariant, with $\tilde{W}(x_0) = 1$ (Eq. (6)). It is clear that $\tilde{W}(x)$ should be continuous everywhere in the ground state, except on the defect punctures, where it is not defined. This means that the whole accessible space $\Sigma$ can be explored by classes of continuously deformable closed loops $S^1$. $\tilde{W}(x)$ defines a map of $S^1$ onto $\text{SO}(3)$, with $x_0$ going into the identity (pointed map), and can be divided into equivalence classes or homotopy classes containing all rotations which can be deformed continuously into each other. The homotopy classes form a group, the first homotopy group $\pi_1(\text{SO}(3)) = Z_2$. The representative manifold of the rotation group is not simply connected, and a rotation by $2\pi$ is neither identical, nor continuously deformable into the identity. The other homotopy group of $\text{SO}(3)$, $\pi_0 = \pi_3 = 1$ are trivial, except $\pi_2(\text{SO}(3)) = Z$. But $\pi_2$ and $\pi_3$ are irrelevant because the closed surfaces which they map onto $\text{SO}(3)$ are either restricted to small regions between punctures or cannot in general be contained in $\Sigma$.

The non-trivial ($2\pi$-) rotations must be associated with contours $S^1$ surrounding one or several defect loops, and cannot be shrunk continuously within $\Sigma$. Because $\Sigma$ is punctured, solutions of the Euler-Lagrange equation, which would have been forbidden if $\Sigma$ had been simply connected, become allowed. This must be contrasted with vortex-like excitations whose core is within $\Sigma$ [19]. Shrinking the surrounding contour, one has a $2\pi$-rotation over an infinitesimal contour, and $\tilde{W}(x)$ or $\tilde{\Omega}(x)$ are no longer continuous.
everywhere. The matter field $\phi = \lambda \hat{\phi}$ remains well defined if $\lambda = 0$ at the core of the vortex, in contradiction with the assumptions made earlier on the ground state. A core energy must then be included, and a vortex-free configuration has lower energy than a configuration with vortices (Appendix A).

In contrast, all the ground state configurations have, by construction (gauge invariance), the same energy. Clearly, a $2\pi$-rotation can be derived from an untwisted configuration by a gauge transformation ($2\pi$-homotopic) $U_2 (x)$ (Eq. (12)). This fact will be exploited in next section.

Because $\check{C}_\mu = \check{\gamma}_\mu + g A_\mu$ is gauge-invariant, and therefore in general unique, the rotation $\check{W}(x)$ which determines $\check{\gamma}(x)$ also determines $\check{A}_\mu(x)$ up to continuous deformations.

In summary, one has two ground state configurations associated with each defect loop, the regular one, $\{ A_\mu, \check{\gamma}_\mu \} = \{ 0, \gamma \}$, parametrized by $\check{W}(x) \sim 1$ the identity element of the rotation group, and the twisted one, $\{ A_\mu, \check{\gamma}_\mu \}_{2\pi} = \{ 2\pi, \gamma \}$, parametrized by $\check{W}(x) \sim R_{2\pi}$, the rotation by $2\pi$. Moreover,

$$R_{2\pi}, R_{2\pi} = 1,$$

and the $Z_2$ puncture disappears when circumnavigated twice, both geometrically (§ 2) and in its effect on the matter configuration. The configurations are characterized everywhere, up to continuous deformations, by the homotopy classes $[\Sigma, SO(3)]$.

The two ground state configurations $| 0 \rangle$ and $| 2\pi \rangle$ have the same energy. There are only two homotopy classes for rotations $\pi(SO(3)) = Z_2$, and therefore two distinct ground state configurations around each defect loop. The $Z_2$ geometrical punctures are therefore directly responsible for the occurrence of a second, « twisted » ground state configuration.

We end with an example for which the configuration can be written down explicitly [33]. For one single line defect the boundary conditions require the curvature to vanish

$$\check{F}_\mu(x) = 0 \quad x \in C_1^{\infty}, \quad (5.19)$$
on a contour surrounding, and far away from the defect. (The free energy density (4.1) then vanishes on $C_1^{\infty}$ in the absence of matter. It actually vanishes even in the presence of the matter field, as we shall see below.) Equivalently, it is possible to find a gauge transformation $\check{\gamma}(x) : \Sigma \rightarrow SO(3)$ such that the vector potential vanishes on $C_1^{\infty}$,

$$\check{A}_\mu = 0 = \hat{X} \check{A}_\mu \hat{X}^{-1} + g^{-1} \hat{X} \partial_\mu \hat{X}^{-1} \quad x \in C_1^{\infty}. \quad (5.20)$$

The solution of (19) or (20) is (see also our discussion of Eq. (7))

$$\check{A}_\mu = g^{-1} \hat{X} \partial_\mu \hat{X} \quad x \in C_1^{\infty}. \quad (5.21)$$

(pure gauge solution). Under gauge transformation (4.4), the rotation matrix $\hat{X}(x)$ becomes

$$\hat{X}' = \hat{X} \hat{U}^{-1} \quad (5.22)$$

so that $\check{X} \check{W}$ is gauge-invariant from equation (12). The total vector potential is, in this case,

$$\check{C}_\mu = (\partial_\mu \check{W}) \hat{X}^{-1} + \hat{X}^{-1} (\partial_\mu \check{X})$$

$$\check{C}_\mu = (\check{X} \check{W})^{-1} (\partial_\mu \check{X} \check{W}). \quad (5.23)$$

$\check{C}_\mu$ is obviously gauge-invariant, and parametrized by the gauge-invariant rotation $\check{X} \check{W}$. If $\check{W}$ is covariant, $\check{X}$ is contravariant under gauge transformations, and the ground state configurations are uniquely characterized by the homotopy classes

$$\pi_1(SO(3)) = [C_1^{\infty}, SO(3)].$$

Since $\check{X}, \check{U}$ and $\check{W}$ are continuous functions, such a classification is valid everywhere in $\Sigma$, not only on $C_1^{\infty}$.

For several defects, the pure gauge solution remains valid on $C_1^{\infty}$. But such a contour can hardly span the whole of $\Sigma$ by continuous deformations. As we have seen above, the gauge field and the curvature vanishes within a distance $l = (g^2 \frac{\lambda^2}{2})^{-1/2}$ of the core of the defect. For a dilute concentration of defect loops, whose cores are always more than $2l$ apart, there exists a contour on which the pure gauge solution (23) is valid around every defect, and we are able to span the whole of space $\Sigma$ by continuous deformations.

Because $\check{F}_\mu \sim 0$, the Euler-Lagrange equations $(1')$ and $(2')$ simplify further, and the free energy density vanishes wherever the vector potential is pure gauge

$$f(x) = \gamma \lambda^2 \text{Tr} \{ [\check{C}_\mu, \check{\gamma}_\mu] [\check{C}_\mu, \check{\gamma}_\mu]^+ \} = 0 \quad x \in C_1^{\infty}. \quad (5.24)$$

It then reaches its lowest bound. This is because

$$\text{Tr} \{ [\check{C}_\mu, \check{\gamma}_\mu] [\check{C}_\mu, \check{\gamma}_\mu]^+ \} = \text{Tr} \{ [[\check{C}_\mu, \check{\gamma}_\mu], \check{\gamma}_\mu] \check{C}_\mu^* \}$$

and the double commutator vanishes by virtue of the Euler-Lagrange equation $(1')$.

6. Gauge invariance and tunnelling states. — At finite temperatures, the full partition function

$$Z = \int D\check{\phi} D\check{A}_\mu \exp[- F/k_B T] \quad (6.1)$$

must be evaluated. It is a functional integral involving all the configurations instead of the extremal ones. As a consequence, the system can tunnel between the two ground state configurations $| 0 \rangle$ and $| 2\pi \rangle$ around each defect.

Even at $T = 0$, the two configurations $| 0 \rangle$ and $| 2\pi \rangle$ cannot be the real ground states of the system, because neither are gauge-invariant configurations whereas the energy is [22, 34]. Any « large » gauge transformations, $\check{T}(x)$, homotopic to $R_{2\pi}$,

$$\check{W} \rightarrow \check{W}' = \check{T} \check{W} \quad (6.2).$$
transforms (Eqs. (4.4), (4.6) and (5.12)) into $|0\rangle$ and $|2\pi\rangle$, and vice-versa. The gauge-invariant ground state configurations are the linear combinations of $|0\rangle$ and $|2\pi\rangle$,

$$|\pm\rangle = (1/\sqrt{2})(|0\rangle \pm |2\pi\rangle)$$ \hspace{1cm} (6.3)

$|0\rangle$ and $|2\pi\rangle$ are the two states which, by tunnelling into each other, form the two-level system $|\pm\rangle$ [4].

Whereas $|0\rangle$ and $|2\pi\rangle$ have the same energy (section 5, $\Delta = 0$ in Phillips' notation [4]), $|+\rangle$ and $|-\rangle$ are split ($\Delta_0 \neq 0$) by the tunnelling rate

$$\pi\Delta_0/\hbar\omega = \langle 0 | 2\pi \rangle =$$

$$\int \mathcal{D}\mathcal{A}(t) \mathcal{D}A(t') \exp\left[-\hbar^{-1} \int_0^{\beta\hbar} dt \int dx f(x)\right]$$ \hspace{1cm} (6.4)

for all paths in imaginary time $\tau$ connecting $|0\rangle$ (at $\tau = 0$) to $|2\pi\rangle$ (at $\tau = \beta \hbar$) [35]. $\hbar\omega \sim 10^{-2}$ eV is a typical frequency for optical phonons in glasses. Calculation of (4) requires knowledge of the dynamics of the glass, which is not forthcoming from the static free energy (4.1). The dynamics could be obtained by setting up phenomenological time dependence to the Euler-Lagrange equations (5.1)-(5.2), or, alternatively, a phenomenological Lagrangian. This method (time dependent Ginzburg-Landau) has limited reliability and little generality [35]. By the way, there is no reason to suppose Lorentz covariance of the excitations under investigation, and we cannot simply treat the imaginary time as a fourth direction $\mu = 0, 1, 2, 3$ in (4.1). It is sufficient, however, to assume that, for all the line defects in the glass, (4) has a flat and broad distribution of amplitudes,

$$0 \leq |\langle 0 | 2\pi \rangle| \leq \omega \hspace{1cm} [4].$$

This yields directly the anomalous behaviour in the thermal conductivity $K \propto T^2$ and in the heat capacity of glasses $C \propto T$.

Each pair of tunnelling states involves therefore many atoms, moving by a small amount, as experimental evidence had made clear long ago [5]. There is one pair of tunnelling states per line defect, which are therefore a direct consequence of the existence of geometrical line defects in glasses.

If, as is the case in most glasses, the distribution of defects is semi-dilute (i.e. such that $\xi < l$, with $\xi$ the distance between defects), the potential barrier between the two tunnelling states $|0\rangle$ and $|2\pi\rangle$ associated with one particular defect is substantially decreased by screening, and the tunnelling rate $\Delta_0$ increased from the value corresponding to an isolated defect. The distortion due to one defect is screened by the others, effectively within a spherical region of radius $\xi$, even though the defects are intertwined, line objects (see Appendix A). The number of atoms which must be (slightly) moved to produce the flip of configurations is also reduced to those within a sphere of radius $\xi$, $\xi$ should therefore be the size of the two-level system in the semi-dilute regime, which has been evaluated experimentally to be 10-20 Å ([5], ch. 6, [37]).

A very low tunnelling rate corresponds to a very high barrier, and to two configurations $|0\rangle$ and $|2\pi\rangle$ which are strongly orthogonal and imply the rotation of a very large number of atoms. The experiment sets up a time scale, and thus a lower cut-off $\Delta_m$ in the distribution of tunnelling rates, or in the splitting of the two-level systems. This, in turn, implies that the specific heat is not truly linear, but extrapolates exponentially from $C = 0$ at $T = 0$ to a shifted, linear expression $C = A(T - T_1)$, $T_1 > 0$ [4, 38] where $k_B T_1 \propto \Delta_m$. The fact that the anomalous behaviour is absent in some glasses like amorphous Si [5] should be related to the size of the cut-off $\Delta_m$ that is to the stiffness of the network, by comparison to vitreous silica $\text{SiO}_2$, say. Also, one should not observe anomalous, low temperature behaviour in those glasses which are represented by a flat, punctureless, and therefore bipartite, network, but to produce such a (two-component) glass would require two constituents with strong mutual affinity (e.g. a-GaAs).

A remarkable illustration of the twisting effect of a $\mathbb{Z}_2$ puncture can be seen in M. C. Escher's « Print Gallery » (Fig. 1). One configuration, $|+\rangle$ say, is

Fig. 1. — M. C. Escher, « Print Gallery », lithograph 1956. (Collection Haags Gemeentemuseum, The Hague.) The geometrical puncture is hidden under the artist's signature, and is the branch point of two Riemann sheets (the gallery, and the print, or indoors and outdoors). The configuration of the matter field, i.e. the subject of the lithograph itself, is such that the enlargement is associated with clockwise rotation. The second matter configuration (see text) is the mirror image of the lithograph, and has counterclockwise enlargement. (Reproduced by permission from Haags Gemeentemuseum. © Beeldrecht, Amsterdam, S.P.A.D.E.M. Paris, 1981.)
represented in the print. The other configuration |−⟩ is its mirror image. Here, as also in the XY, 2-dimensional spin glass [39], the two configurations |+⟩ and |−⟩ manifest and oppose chiralities.

7. Conclusion. — The two-level systems, or tunnelling modes were introduced [4, 5] as a concept, rather than a microscopic model for the motion of specific atoms in particular glasses. Indeed, this lack of specificity was deliberate, in order to emphasize the generality of the concept and the universality of glasses whose low temperature behaviour (specific heat, thermal conductivity) it successfully explained. Saturation of the two-level systems was predicted and observed [5, 40] as a dramatic reduction of the ultrasonic attenuation with increasing phonon intensity (the phonons being attenuated through resonant absorption by the two-level systems). In every respect, the concept has been entirely successful.

Nine years later, it is time to be more specific. Why are tunnelling modes an exclusivity of glasses? Does the universality of the anomalies in the thermal conductivity and, to a lesser extent, in the specific heat, imply that all glasses have microscopically the same two-level systems? In this paper, we have introduced a single mechanism which relates directly the two-level systems to the random structure of glasses, and their $Z_2$ line defects in particular. The existence of two, and only two levels or configurations per line defect is topological, and therefore universal. It does not rely on the internal motion of particular chemical units, as do the few mechanisms which have been suggested up to now [41]. The levels owe their energy splitting to tunnelling, and a broad distribution of tunnelling rates, and a reasonable size (10-20 Å, or the average distance between line defects in the glass) can be inferred, even if we have not been able to calculate if from first principles in this paper.

Apart from the exceptional structures without odd lines mentioned earlier [9], some glasses (a-Si) show little or no low temperature anomalies, yet contain line defects. This is because the broad distribution of tunnelling rates $\Delta_0$ divides the two-level systems of a given glass into two classes: those which can tunnel within experimental time, and those which cannot. The former operate as tunnelling modes, the latter can only be thermally activated and do not give rise to any low temperature anomalies. Nevertheless they are the same qualitative objects, as has been stressed elsewhere on experimental ground [41].

The two-level systems are direct consequence of the two essential elements of the structure of glasses, namely i) (odd) line defects, and ii) gauge invariance.

i) The line defects (threading through odd rings in continuous random networks) are geometrical, frozen punctures at low temperatures. At higher temperatures, for example in a liquid or a supercooled liquid, the network changes with time, and the odd lines can move. Yet, their topological stability — they satisfy their own continuity equation — makes it impossible for them to break up into segments. The same $Z_2$ line defects appear also in a continuous model of the glass, as long as the local matter field is parametrized by rotations, which seems natural enough.

ii) The overall homogeneity of the glass is expressed as gauge invariance. The free energy must remain invariant under a transformation probing the homogeneity. This transformation can be either a translation — which necessitates a connection, i.e. introduction of gauge fields, in order to compare two points with different local environment — or an arbitrary variation of the environment at a fixed point in space (gauge transformation). Gauge fields appear solely to preserve the gauge invariance, or to effect the connection. (They are dynamical variables, and cannot be quenched. It is the non-bounding 1-cycles or punctures which are the continuous limit of the competing interactions $J_{ij}$ between spins in spin glasses, and are accordingly quenched at low temperatures.)

Line defects, frozen at low temperatures, and gauge invariance, enabled us to set up a field theory, whose distinct ground state configurations were enumerated and classified by homotopy theory: there are two distinct configurations of equal energy per line defect. However, the two configurations are related by a gauge transformation and tunnelling can occur between them. The final spectrum of excitations in the glass consists therefore of one energy-split doublet per defect line, the two-level system, made of bonding and antibonding combinations of the original tunnelling configurations.

While in our model the two-level systems are immediate consequence of the odd line defects in glasses, these defects do not depend on the model for their existence. They are topologically stable entities in any random network or continuous random matter parametrized locally by rotations. It has been argued elsewhere that these line defects play a leading part in the glass transition at $T_0$ [6, 7]. They can also be shown to account for the topological entropy of melting of a crystal [6]. However, direct experimental observation of these line defects has yet to be recorded. It is important to have an independent estimate of the concentration of defects, to be compared with the measurements of the low temperature anomalies associated with two-level systems.

One possibility for such an independent measurement is the Hall effect. The Holstein-Friedman theory of the Hall effect in amorphous metals or semiconductors is based on the interference of the electron wave functions on paths enclosing an odd ring [42]. If the theory applies to real materials, then measurement of the Hall voltage should yield the number of odd line defects. Less directly, granular and other highly inhomogeneous superconductors are also riddled by vortices, whose number should be evaluated from their electric or magnetic response.
Incidentally, line defects appear also as a product of Kléman and Sadoc [43] description of the structure of glasses. They suggest that structurally, glasses are perfect lattices in some curved space projected into ordinary Euclidean space. With an « ideal » space of negative curvature, one obtains in Euclidean space an infinite, homogeneous structure containing line defects (disclinations). It remains to be shown that the resulting structure is random, and that a mapping can be selected without too much arbitrariness. If this is so, their procedure yields a constructive classification of the structure of glasses.

The present model which may look at first sight like a deceptively complicated explanation, is in fact a straightforward consequence of the $\mathbb{Z}_2$ odd line defects in glasses, which are themselves almost trivial elements of continuous random networks. It is interesting to notice that Phillips, in his original paper, had suggested (by the way and without giving any clue or justification) « tunnelling states associated only with five member Si-O rings » as a possibility in vitreous SiO$_2$.

Acknowledgments. — We have benefited from helpful discussions with D. Bovet, A. R. Edmonds, O. J. Greene, C. J. Isham, M. Kléman, J. Malbouisson, R. Mosseri and N. R. da Silva, and at the les Houches Summer Schools of 1978 and 1980, and the RCP « Domaines et Parois », Aussois 1981. Finally, a visitor whose name has been forgotten suggested using a mirror to produce the second configuration of the figure. (NR was trying unsuccessfully to sketch it.)

Appendix : Energy of a semi-dilute collection of line defects. — The ground state configurations of the glass — two distinct configurations $\{ A_\mu, \Omega \}$ per line defect — have the same vector potential $C_\mu$ and the same free energy, because both are gauge-invariant quantities. By contrast, the vortex-like excitations have different energy and different $C_\mu$ from the ground state’s, and cannot be created from the ground state simply by a gauge transformation, even though they are also specified by $\{ A_\mu, \Omega \}$ and by a vector potential $\tilde{C}_\mu$ solution of the Euler-Lagrange equations (5.1) and (5.2) outside the core of the vortex. Vortices are also stationa r y configurations of the free energy, but their cores lie within the physical space $\Sigma$, and carries a finite energy, instead of being absorbed into the puncture like their ground state’s counterparts. (Alternatively, the core contribution can be neglected and replaced by specific boundary conditions on the core’s boundary [31].)

In addition to the vortex core energy, both vortices and punctures distort the matter field, and carry therefore a finite strain energy. They also interact with each other by sharing the same strain. This interaction energy can be evaluated in the following fashion :

Consider a collection of puncture or vortex loops $\Gamma_i(x)$, $i = 1... L$. In the « extreme type II limit », where the length $l$ associated with the strain is much larger than the core $a$ of the defect (the length associated with the field $\lambda$ in the free energy (4.1)), the effect of the cores can be simply included as a superposition of delta functions on the right-hand side of the Euler-Lagrange equation (5.1)

$$D_\mu F^{\mu \nu} - \kappa [\bar{C}^\nu, \dot{\Omega}_0], \dot{\Omega}_0^{-1} ] = \sum_i J_i \delta(x - l).$$

(A.1)

(This is the Green’s function method of absorbing the boundary conditions into the differential equation.) Alternatively, the defect cores are sources of gauge fields, controlled by the Lagrange multipliers $J_i \delta(x - l)$ in the free energy density (4.1).

Equation (A.1) is non-linear, and the field $\tilde{C}_\mu$ has its own length scale $l = (kg)^{-1/2}$ (a self-screening length). In the semi-dilute regime $l \gg \xi > a$, where $\xi$ is the average distance between defect lines, equation (A.1) and the free energy density are dominated by terms with the highest powers in $l$, since the scale of fluctuations of $\tilde{C}$ is now $\xi$ (rather than $l$ for a single defect or in the dilute limit $\xi > l$). The Euler-Lagrange equation (A.1) is accordingly linearized in the semi-dilute regime

$$\text{curl} \text{ curl} \tilde{C}^\nu = \sum_i J_i \delta(x - l)$$

(A.2)

and the free energy density becomes, approximately, quadratic,

$$f(x) = \frac{1}{2} g^{-2} \text{Tr} [\left(\text{curl} \tilde{C}\right)_\mu (\text{curl} \tilde{C})^\nu] + \sum_i E_{ci}$$

(A.3)

where $E_{ci}$ is the core energy of the vortex. $E_c = 0$ for punctures. Equations (2) and (3) are similar to those controlling the electromagnetism of current loops, and yield for the energy of an assembly of line defects the expression [6, 7]

$$E = - ap \ln \rho + bp$$

(A.4)

where $a$ and $b$ ($\sim \sum E_{ci}$) are constants, and $\rho$ is the density of defects (specifically the ratio of the number of odd rings (faces of the network) to the total number of faces).

Equation (4) has been used [6, 7] in conjunction with a similar expression for the entropy as a function of $\rho$, to evaluate the density of (mobile) vortices in thermal equilibrium, above the Fulcher temperature $T_0$ where vortices are the dominant defects (i.e. most defects can move). The density of mobile vortices vanishes at $T_0$, with the Vogel-Fulcher variation (1.1).

However, frozen line defects survive below $T_0$, and equation (4) is valid at all temperatures, whenever there is a semi-dilute concentration of defects, with $\rho$
the total density of defects (frozen punctures and mobile vortices). The $\ln \rho$ term indicates that the strain is shared between defects, and not screened around each defect individually.

References and Footnotes

[9] It has been possible to construct random structures without any such defects: the Mattis model is a spin glass without frustration, the Connell-Temmkin model a continuous random network without odd rings Mattis, D. C., Phys. Lett. 56A (1976) 421; Connell, G. A. N. and Temkin, R., J. Phys. Rev. B 9 (1974) 5323. These structures are called trivial or flat, because the disorder can be eliminated by a gauge transformation.
[16] Five fold figures have been included in space-filling patterns, but only when immersed in a much larger unit cell, as in some Moorish patterns, or as part of random patterns (see Gardner, M., Scientific American 236/1 (1977) 110).
[20] The precise and general statement of this relationship is contained in de Rham’s theorem (see, for an introduction, Pollard, R. B., An Introduction to Algebraic Topology, to appear). It is necessary first to approximate the manifold of field states SO(3) by a homotopically simpler space with identical lowest three homotopy groups. For example, one can choose products of Eilenberg-MacLane spaces $K(\pi, n)$ defined by

$$\pi_n(K(\pi, n)) = \pi_i(\pi \neq n)$$

whose homotopy classes $[\Sigma, K(\pi, n)] = H^*(\Sigma; \pi)$ are the labelled by the nth cohomology group of $\Sigma$ with values in $\pi$. [See Ref. [22], § 3.] (Here, for $SO(3), [\Sigma, K(Z_2, 1)] = H^*(\Sigma; Z_2)$) De Rham’s theorem is then stated in terms of the latter (cohomology of differential forms). This theorem rules out, for example, the choice of Heisenberg spin ($\pi_1(S^3) = 1$) as material field for a continuous field theory of spin glasses ($H_1 = Z_2$ per frustration line) [21].

[25] From apparently a completely different approach from ours, B. Quinterc has argued that two local tensors are needed to describe the local order and relaxation of visco-elastic and supercooled fluids, particularly to explain the fine structure in their light scattering spectrum (Quentrec, B., J. Physique 37 (1976) 1255; Phys. Rev. A 15 (1977) 1304).


