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1992 J. Phys. A: Math. Gen. 25 L1

(http://iopscience.iop.org/0305-4470/25/1/001)

J. Phys. A: Math. Gen. 25 (1992) L1–L10. Printed in the UK

LETTER TO THE EDITOR

Topological properties of linked disclinations and dislocations in solid continua

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Received 4 June 1991

Abstract. Linked disclinations in three-dimensional solid continua are studied via the Wess–Zumino term and related topological concepts for the transformation group $GL^3(3, \mathbb{R})$ and its quotient spaces $GL^+(3, \mathbb{R}/P_i(3)$ and $SO(3)/P_i(3)$ where $P_i(3)$ represents point symmetry groups of anisotropic solids. The relation with the topological properties of anisotropic liquids is indicated. Dislocations are treated as 'dipolar' pairs of disclination loops and alternatively using Kröner's approach of material connections. Linking of dislocations is studied via the Hopf invariant and Gauss linking number, and a connection with Ashtekar's new variables is pointed out.

In the following we consider crystalline systems perforated by defects like dislocations, disclinations and point defects in a 3-space M approximated as a continuum (Kröner 1980). These defects play an important role in the elastic and plastic properties of a solid; in particular, the entanglement of dislocations (Holz 1985) and their deformations under plastic flow have some features in common with polymer entanglement in melts. Furthermore, line defects play an important role in the theory of melting in anisotropic and in supercooled liquids (Holz 1991). There also exists a relation between line defects in three-dimensional solids and (2+1)-dimensional gravity (Holz 1988). In the following, some of these phenomena will be studied from a topological perspective, and brought into connection with newer work on (2+1)-dimensional Chern–Simons gauge theory of gravity, Ashtekar's (1986) new variables, and knot polynomials.

For the defect-free state we take the Euclidean metric

$$dS_\Theta^2 = \delta_{ij}\, dx^i\, dx^j \qquad i = 1, 2, 3. \tag{1}$$

The defect state is described by the vector-valued 1-forms $\Theta^a = R_k^a\, dx^k$ (the 3-bein $e_a = (R_a^k)$), where $(R_k^a) \in GL^+(3, \mathbb{R})$ is a 3×3-matrix field with det $\mathbf{R} > 0$, and the metric

$$ds^2 = \delta_{ab}\Theta^a\Theta^b = g_{kl}(x)\, dx^k\, dx^l. \tag{2}$$

The distance change

$$ds^2 - ds_\Theta^2 = (g_{kl} - \delta_{kl})\, dx^k\, dx^l = 2\varepsilon_{kl}\, dx^k\, dx^l$$

defines the strain tensor $\boldsymbol{\varepsilon}$ (e.g. see Kröner 1980); summation convention is implied throughout. Use of the linear algebraic group $GL^3(3, \mathbb{R})$ as the structure group for the gauge group $\mathscr{G}(3)$, consisting of all maps $M \to GL^+(3, \mathbb{R})$, has been suggested by Madore (1981). For the sake of simplicity we use initially a closed and simply connected 3-space M, in order to avoid the specification of boundry conditions. Extension to non-simply connected spaces will be pointed out later.

0305-4470/92/010001+10\$03.50

Suppose that $R \in \mathscr{G}(3)$; then the respective Mauer–Cartan form is given by

$$\mathbf{R}^{-1} \cdot \mathrm{d}\mathbf{R} = -R^k_a \, \mathrm{d}R^b_k \mathbf{T}^b_a \equiv \omega^a_{kb} \, \mathrm{d}x^k \mathbf{T}^b_a \tag{3}$$

where $\mathbf{T}^a_b$ represents one of the nine generators of the Lie algebra gl(3, $\mathbb{R}$) and the symbols $\omega^a_{kb} = -\omega^b_{ka}$ represent the spin connection of a flat space M. The generators of gl(3, $\mathbb{R}$) obey

$$[\mathbf{T}^a_b, \mathbf{T}^c_d] = C_{(e,f)}(a,b)(c,d)\mathbf{T}^f_e \tag{4}$$

where $C^{(e,f)}_{(a,b)(c,d)}$ are the structure constants of gl(3, $\mathbb{R}$) with respect to pairs of indices in the canonical fashion (Miller 1972).

The connection defined by (3) is that of a flat space. Non-flat connections will be represented in the form

$$\boldsymbol{\omega} = \omega^a_b \mathbf{T}^b_a \tag{5}$$

and their curvature 2-form by

$$\mathscr{R} = R^a_b \mathbf{T}^b_a \tag{6a}$$

where

$$R^a_b = \tfrac{1}{2} R^a_{bkl} \, \mathrm{d}x^k \wedge \mathrm{d}x^l \tag{6b}$$

$$R^a_{bkl} = \partial_k \omega^a_{lb} - \partial_l \omega^a_{kb} + \omega^a_{kc} \omega^c_{lb} - \omega^a_{lc} \omega^c_{kb}. \tag{6c}$$

Here we use the notation $\partial_k \equiv \partial/\partial x^k$, and follow the conventions of Eguchi *et al* (1980) for the curvature tensor and topological invariants studied in the following, with the exception of their normalization. The Chern–Simons term is of the form

$$\Gamma_{\mathrm{CS}} = \frac{1}{(8\pi)^2} \int_M \mathrm{tr}(\boldsymbol{\omega} \wedge \mathrm{d}\boldsymbol{\omega} + \tfrac{2}{3} \boldsymbol{\omega} \wedge \boldsymbol{\omega} \wedge \boldsymbol{\omega}) \tag{7a}$$

where the trace is performed by contracting the matrix indices of $(\mathbf{R})^a_b$, etc, and a normalization is chosen, which is appropriate for the following purposes. Equivalent forms of Γ_{CS} are

$$\Gamma_{\mathrm{CS}} = \frac{1}{(8\pi)^2} \int_M [\omega^a_b \wedge \mathrm{d}\omega^b_a + \tfrac{2}{3} \omega^b_c \wedge \omega^c_e \wedge \omega^e_b] \tag{7b}$$

$$= -\frac{1}{32\pi^2} \int_M \mathrm{d}^3x \, \varepsilon^{ijk} [R^a_{bik} \omega^b_{ja} + \tfrac{2}{3} \omega^c_{ib} \omega^a_{kc} \omega^b_{ja}] \tag{7c}$$

where ε^{ijk} is the totally antisymmetric symbol.

The Wess–Zumino term for a flat connection is

$$\Gamma_{\mathrm{WZ}} = -\frac{1}{48\pi^2} \int_M \omega^b_c \wedge \omega^c_e \wedge \omega^e_b. \tag{8}$$

For a closed manifold M and for a gauge transformation $R \in \mathscr{G}(3)$, (7c) changes by (8), when computed with (3).

Suppose now that we restrict $R \in \mathrm{Gl}^+(3, \mathbb{R})$ to the subgroup $\mathrm{SO}(3) \subset \mathrm{GL}(3, \mathbb{R})$. Then in (3) only the generators of the SO(3) algebra survive and we have

$$\omega^a_b = \omega^a_{kb} \, \mathrm{d}x^k \to \Theta^a = \Theta^a_{,k} \, \mathrm{d}x^k \tag{9}$$

where $\{\Theta^a\}_{a=1,2,3}$ are the connection 1-forms of the SO(3) gauge group $\mathcal{G}_{SO(3)}$, which has been studied recently (Holz 1991). Using the representation $\mathbf{R} = \mathbf{R}(\boldsymbol{n}^1, \boldsymbol{n}^2, \boldsymbol{n}^3)$, where $\{\boldsymbol{n}^a\}_{a=1,2,3}$ is a 3-bein of orthonormal fields in (9), Γ_{WZ} can be computed for $R \in \mathcal{G}_{SO(3)} \subset \mathcal{G}(3)$ with $\Gamma_{WZ} \in \mathbb{Z}$. Furthermore, Γ_{WZ} can be expressed in terms of the Hopf invariants, respectively Gauss linking numbers of the components of the 3-bein field $\{\boldsymbol{n}^a\}_{a=1,2,3}$, which measure the linking of the disclinations suspended by these components (Holz 1991). For (9) one obtains, for example, $\Gamma_{CS} = \Gamma_{WZ} = \frac{2}{3}\sum_{a=1}^{3} Q(\boldsymbol{n}^a) = \mathcal{N} \in \mathbb{Z}$, and $Q(\boldsymbol{n}^a) = \mathcal{N}/2$ is the Hopf invariant of the $\{\boldsymbol{n}^a\}$ field, which is the same for each component of the 3-bein. Due to $\pi_1(SO(3)) = \mathbb{Z}_2$ there is only one type of stable disclination (e.g. see Kléman 1983) but, due to $\pi_3(SO(3)) = \mathbb{Z}$, linked configurations of any disclinations are topologically stable. In particular, for smooth 3-bein fields one necessarily needs $\mathcal{N} \in 2\mathbb{Z}$. Identifying the 3-bein field with the crystalline 3-bein, i.e. an orthonormal set of local lattice planes, makes it obvious how to extend the results obtained for anisotropic liquids (Holz 1991) to anisotropic solids, including the cases where SO(3) is replaced by $SO(3)/P_i(3)$ and $P_i(3)$ is a crystalline point symmetry group.

The result $\Gamma_{CS} = \Gamma_{WZ}$ holds only for flat connections, whereas the result $\Gamma_{WZ} = \frac{2}{3}\sum_{a=1}^{3} Q(\boldsymbol{n}^a) = 2Q(\boldsymbol{n}^a)$, $a = 1, 2, 3$ is a consequence of the orthonormality of the 3-bein field. For instance, if the configuration of one field, say $\{\boldsymbol{n}^1\}$, is given then $Q(\boldsymbol{n}^1)$ represents the Gauss linking of the respective disclinations. The second field $\{\boldsymbol{n}^2\}$ due to orthonormality is also characterized by $Q(\boldsymbol{n}^1)$, but has an additional degree of freedom with respect to $\{\boldsymbol{n}^1\}$ and may therefore be considered as a scalar field of an O(2)-σ model on a 'curved background'. Due to $O(2) \sim S^1$ and $\pi_1(S^1) = \mathbb{Z}$, ($\pi_{q\geq 2}(S^1) = 0$) additional defects in the form of vortex loops featuring core singularities are possible for fixed $\{\boldsymbol{n}^1\}$. Core singularities, however, imply a non-flat connection and $\Gamma_{CS} \neq \Gamma_{WZ}$ is obtained in that case. The third field $\{\boldsymbol{n}^3\}$ is fixed by $\{\boldsymbol{n}^1\}$ and $\{\boldsymbol{n}^2\}$, i.e. it is characterized by $Q(\boldsymbol{n}^1)$ and the core singularities of $\{\boldsymbol{n}^2\}$. Similar arguments apply when the $\{\boldsymbol{n}^1\}$ field also features core singularities. The details are worked out in Holz (1991).

An obvious shortcoming of the model discussed above is that the structure generated by the gauge group $\mathcal{G}_{SO(3)}$ will not fit easily into a given 3-space M, e.g. $M = S^3$. In order to work out the physical significance of such a theory, and in particular to understand which processes are responsible for the change $d\Gamma_{CS}/dt \neq 0$, some additional formalism has to be recalled (see Eguchi *et al* 1980).

The Hirzebruch–Pontryagin density is given by

$$^*RR = \tfrac{1}{2}\varepsilon^{\mu\nu\alpha\beta} R_{\mu\nu\rho\sigma} R^{\rho\sigma}_{\alpha\beta} = \partial_\mu X^\mu \tag{10}$$

and yields the instanton number

$$\eta = -\frac{1}{32\pi^2}\int_{M_4} d^4x\, ^*RR \tag{11}$$

form for which (7a) is obtained as $\Gamma_{CS} = -(1/32\pi^2)\int_M d^3x X^3$. Here M_4 can be taken in simple cases as the cylinder $M_4 = M \times R$, and requires that the formalism developed so far is extended to (3+1)-dimensional spacetime. This is easily done replacing the Euclidean metric by the Minkowski metric

$$\begin{aligned} \delta_{ij} &\to \eta_{\mu\nu} \qquad (\mu, \nu) = 0, 1, 2, 3 \\ \delta_{ab} &\to \eta_{ab} \qquad (a, b) = 0, 1, 2, 3 \end{aligned} \tag{12}$$

and

$$GL(3, \mathbb{R}) \to GL(4, \mathbb{R}) \qquad SO(3) \to SO(3, 1). \tag{13}$$

When (5) represents a Riemann connection the curvature tensor satisfies the symmetries $R_{\mu\nu\rho\sigma}=R_{[\mu\nu][\rho\sigma]}=R_{[\rho\sigma][\mu\nu]}$ and allows the representation

$$(R^{\alpha\beta}_{\rho\sigma})=\begin{pmatrix} 0 & -E_{\rho\sigma,x} & -E_{\rho\sigma,y} & -E_{\rho\sigma,z} \\ E_{\rho\sigma,x} & 0 & B_{\rho\sigma,z} & -B_{\rho\sigma,y} \\ E_{\rho\sigma,y} & -B_{\rho\sigma,z} & 0 & B_{\rho\sigma,x} \\ E_{\rho\sigma,z} & B_{\rho\sigma,y} & -B_{\rho\sigma,x} & 0 \end{pmatrix} \tag{14}$$

and a similar representation for its dual $^*R$. Insertion into (11) yields

$$\eta=\frac{1}{32\pi^2}\int_{M_4} \mathrm{d}^4x\, \boldsymbol{E}_{\rho\sigma}\cdot\boldsymbol{B}^{\rho\sigma}. \tag{15}$$

Suppose now that η is computed with respect to M_4, bounded by two space-like surfaces $M(t_2)$ and $M(t_1)$, i.e. $\partial M_4=M(t_2)\cup -M(t_1)$ with $t_2>t_1$, then $\eta(M_4)=\Gamma_{\mathrm{CS}}(M(t_2))-\Gamma_{\mathrm{CS}}(M(t_1))$ and, accordingly,

$$\frac{\mathrm{d}\Gamma_{\mathrm{CS}}(M(t))}{\mathrm{d}t}=\frac{1}{32\pi^2}\int_{(M(t)} \boldsymbol{E}_{\rho\sigma}\cdot\boldsymbol{B}^{\rho\sigma}\,\mathrm{d}^3x. \tag{16}$$

Another topological invariant for a Riemann connection is the Euler characteristic, which can be represented in the form

$$\chi(M_4)=\frac{1}{4\pi^2}\int_{M_4}\mathrm{d}^4x\sqrt{-g}\,(\boldsymbol{E}_{\rho\sigma}\cdot\boldsymbol{E}^{\rho\sigma}-\boldsymbol{B}_{\rho\sigma}\cdot\boldsymbol{B}^{\rho\sigma}) \tag{17}$$

where $g=\det(g_{\mu\nu})$ and

$$g_{\mu\nu}=\eta_{ab}R^a_\mu R^b_\nu. \tag{18}$$

Equation (17) represents the Yang-Mills action of the curved space M_4.

A defect solid may now be represented by a Riemann connection computed from (18),

$$\Gamma^\gamma_{\alpha\beta}=\tfrac{1}{2}g^{\gamma\delta}(\partial_\alpha g_{\delta\beta}+\partial_\beta g_{\delta\alpha}-\partial_\delta g_{\alpha\beta}) \tag{19a}$$

which has vanishing torsion

$$T^\gamma_{\alpha\beta}\equiv\tfrac{1}{2}(\Gamma^\gamma_{\alpha\beta}-\Gamma^\gamma_{\beta\alpha})=0. \tag{19b}$$

Suppose that $\mathbf{R}\in\mathrm{SO}(3,1)$ and that $\{\mathbf{R}\}$ is a smooth field. In that case $g_{\mu\nu}=\eta_{\mu\nu}$ and $\Gamma^\gamma_{\alpha\beta}\equiv 0$, implying a flat manifold M_4. For the spin connection (3) one obtains

$$\omega^a_{\mu b}=R^a_\lambda R^\nu_b\Gamma^\lambda_{\mu\nu}+R^a_\nu\partial_\mu R^\nu_b=R^a_\nu\partial_\mu R^\nu_b. \tag{20}$$

This yields $\Gamma_{\mathrm{CS}}(\omega)=\Gamma_{\mathrm{WZ}}(\omega)$ and Γ_{WZ} counts the winding number of the SO(3, 1) transformation associated with the map $M\to\mathrm{SO}(3,1)$. For $\mathbf{R}\in\mathrm{SO}(3)\subset\mathrm{SO}(3,1)$, $\Gamma_{\mathrm{WZ}}(\omega)$ applies to links of integer-valued disclinations. The derivation of (20) from (19*a*) implies that the spin connections (3) and (9), according to (19*b*), are torsionless. From the remarks below (9), it follows then that there exist smooth crystalline 3-bein fields in the form of linked disclinations without need of dislocations (elastic deformations are discussed below).

For $\mathbf{R}\in\mathrm{SO}(3,1)$, $\Gamma_{\mathrm{WZ}}(\boldsymbol{\omega})$ represents a three-dimensional integral in six-dimensional group space. Due to $\Gamma^\gamma_{\alpha\beta}\equiv 0$, $R_{\alpha\beta\gamma\delta}\equiv 0$ and (16) implies

$$\frac{\mathrm{d}\Gamma_{\mathrm{WZ}}(\omega)}{\mathrm{d}t}=0. \tag{21}$$

From this it follows that formation of links and their disentanglement implies formation of singularities in the form that necessarily $\mathbf{R} \notin SO(3, 1)$, and $g_{\mu\nu} \neq \eta_{\mu\nu}$, and a non-flat connection arises.

The usual case in solid state physics will be that $\mathbf{R} \in GL^+(3, \mathbb{R})$ and $\mathbf{R} \in GL(4, \mathbb{R})$ for the time-independent and time-dependent cases, respectively. Due to $GL^+(n, \mathbb{R}) = SO(n) \times S(n)$, where $S(n)$ is the coset space of positive definite symmetric matrices (Bott and Tu 1982), the structure group of $GL^+(3, \mathbb{R})$ bundles can be reduced to SO(3). Furthermore, $\{\mathbf{R}\}$ will contain singularities along the cores of disclinations, because the orientational order parameter of a crystalline solid assumes values in the quotient space $SO(3)/P_i(3)$, whose fundamental group $\pi_1(SO(3)/P_i(3)) = \pi_1(P_i^*(3))$ is non-trivial. Here P_i^* is the binary group to P_i(ord $P_i^*(3) = 2$ ord $P_i(3)$). Due to $\pi_1(P_i^*(3)) \neq I$ there exist non-contractible loops in M implying line singularities in the $\mathbf{R}$-field. The latter will give a contribution $\delta\Gamma_{CS}$ to Γ_{CS} as explained by Holz (1991) for the $SO(3)/P_i(3) - \sigma$ model. $\delta\Gamma_{CS}$ can be expressed in terms of Gauss linking numbers, and Γ_{CS} can be computed via Γ_{CS}^* going over to the space M^*, which is branched over the disclination loops and which has no singularities but $\pi_1(M^*) \neq I$. Similar reasoning can be applied to the quotient spaces $GL^3(3, \mathbb{R})/P_i(3)$ or $SL(3)/P_i(3)$.

Consider now a gauge transformation $\Phi \in \mathscr{G}(3)$ with Φ: $\mathbf{R} \to \mathbf{R}'$. For the time-independent case this amounts to an (adiabatic) elastic deformation of the defect solid. Φ produces a change of frame Φ: $e_a \to e_A = e_b \Phi_A^{b^{-1}}$ and a change of the spin connection (in matrix notation)

$$\Phi: \ \boldsymbol{\omega} \to \boldsymbol{\Omega} = \boldsymbol{\Phi}\boldsymbol{\omega}\boldsymbol{\Phi}^{-1} + \boldsymbol{\Phi}\, d\boldsymbol{\Phi}^{-1}. \tag{22}$$

Equation (22) inserted into ($7b$) yields

$$\Phi: \Gamma_{CS}(\omega) \to \Gamma_{CS}(\Omega)$$
$$= \Gamma_{CS}(\omega) - \frac{1}{48\pi^2} \int_M \mathrm{tr}(\boldsymbol{\Phi}^{-1}\, d\boldsymbol{\Phi})^3 + \frac{1}{16\pi^2} \int_{\partial M} \mathrm{tr}(\boldsymbol{\omega} \wedge d\boldsymbol{\Phi}\boldsymbol{\Phi}^{-1}). \tag{23}$$

This is modulo a factor $\frac{1}{2}$ (present normalization), the same formula as derived by Dijkgraaf and Witten (1990). In the presence of singular disclinations, ∂M represents two-sided cut surfaces bounded by disclination loops and therefore the last term in (23) is not gauge invariant. However, if we go over to the covering space M^* then $\partial M^* = \phi$ and the last term in (23) drops out. Because Φ is supposed to be elastic in nature, i.e. it represents a small gauge transformation, the Wess-Zumino term in (23) with respect to M^* will vanish. This follows from (16) and $d\Gamma_{CS}/dt = 0$ for smooth motions and no transection of disclinations. Accordingly we have $\Gamma_{CS}^*(\Omega) = \Gamma_{CS}^*(\omega)$ and $\Gamma_{CS}^*(\Omega) \in \mathbb{Z}$, for $R \in \mathscr{G}_{SO(3)}$ and for smooth deformations $\mathbf{R} \to \mathbf{R}'$ with $\mathbf{R}' \in GL^+(3, \mathbb{R})$ and $R' \in \mathscr{G}(3)$.

We consider next the problem of how to represent dislocations in this formalism. There exist at least three possibilities.

(i) The first approach is based on the Euclidean group $E^{(D)} = SO(D) \times \mathbb{T}_D$ (Kadić and Edelen 1983), where $\mathbb{T}_D$ is the Abelian group of translations. $SO(D)$ can also be replaced by $SO(D-1, 1)$ for relativistic problems. For $D = 3$ the generators of the Lie algebra of $E^{(3)}$ in the represenation (3) are of the form

$$[T_a, T_b] = \varepsilon_{abc} T^c \qquad [T_a, P_b] = \varepsilon_{abc} P^c \qquad [P_a, P_b] = 0 \tag{24}$$

where $\{T_a\}_{a=1,2,3} \in SO(3)$ and $\{P_a\}_{a=1,2,3} \in t_3$. For $SO(3) \to SO(2, 1)$, raising and lowering of indices in (24) has to be done by $\eta_{\mu\nu}$. Witten's (1988) approach to topological gravity is based on this representation and (7*a*) (and an unfaithful representation of $SO(2,1)\times T_3$ as shown by Gerbert (1990)), using an associative and invariant trace operation different from the one used in (7*b*) and (7*c*). This approach can also be applied to the present formulation for the group $E^{(3)}$ using in (3) $\mathbf{R}\in GL(4,\mathbb{R})|_{E^{(3)}}$ (restricted to the subgroup $E^{(3)}\subset GL(4,\mathbb{R})$) in the form

$$\mathbf{R}=\begin{pmatrix}\mathbf{G} & \boldsymbol{q}\\ 0 & 1\end{pmatrix} \tag{25}$$

with $\mathbf{G}\in SO(3)$ and $\boldsymbol{q}\in T_3$, modulo the space symmetry group of the lattice $P_i(3)\times T_i(3)$, where $T_i(3)$ in the translational symmetry group. For the connection between the Chern–Simons action and Palatini action we refer to Ashtekar and Romano (1989).

(ii) In the second approach one stays with the time-independent problem with the Lie group $GL^+(3,\mathbb{R})$ or its subgroup $SL(3,\mathbb{R})$, which is volume preserving. The Lie algebra $sl(3,\mathbb{R})$ is a real representation of the Lie algebra su(3) and is of rank two, i.e. it has a two-dimensional maximally commutative subalgebra, consisting of anisotropic dilatations and compressions (Miller 1972). For the following, the three (planar) subgroups of $GL^+(3,\mathbb{R})$, being of the type

$$H_1\equiv\left\{\begin{pmatrix}H & 0\\ t & 1\end{pmatrix}\subset SL(3,\mathbb{R})\right\} \tag{26}$$

are of interest, where $H\in SL(2,\mathbb{R})$ and $t\in T_2$ (H_2 and H_3 refer to the other planes in R^3). The elements $h_1\in H_1$ for $H\in SO(2)\subset SL(2,\mathbb{R})$ are in 1–1 relation with the elements $e\in E^{(2)}$ using the unfaithful representation (25) for two dimensions. Employing the gauge group $\mathscr{H}_1$ based on the structure group H_1 allows the formation of composite disclinations, which are of edge and screw types, as explained by Holz (1988).

Consider a typical element h_1 of (26) close to a composite disclination of edge and screw types,

$$h_1=\begin{pmatrix}\cos\Theta_e & -\sin\Theta_e & 0\\ \sin\Theta_e & \cos\Theta_e & 0\\ \arg\Theta_s & \arg\Theta_s & 1\end{pmatrix} \tag{27}$$

in a plane C perpendicular to its core pointing along a symmetry axis. In complex coordinates $w\subset C$ we obtain for a core location $a\in C$

$$\Theta_e=\frac{q_e}{p_e}\arg(w-a) \qquad \Theta_s=\frac{1}{2\pi}q_s\arg(w-a). \tag{28}$$

Here $p_e=\text{ord}(P_e)$ represents the order of the symmetry axis $P_e\in P_i(3)$ the disclination is associated with (e.g. $p_e=2,3$ and 4 in the octahedral group O), and $(q_e,q_s)\in\mathbb{Z}$. This implies that (27) for (28) is the nucleus of a local representative of $\mathscr{H}_1(P_e)$ (which may be subject to affine deformations) with structure group $H_1(P_e)$ obtained from (26) by the replacements $SL(2,\mathbb{R})\to SL(2,\mathbb{R})/P_e$, $T_2\to T_2/T_e$, where T_e is the discrete translation group of the crystal along P_e. For dipolar pairs of disclinations one uses

$$\begin{aligned}\Theta_e(w)&=\frac{q_e}{p_e}[\arg(w-a_+)-\arg(w-a_-)]\\ \Theta_s(w)&=\frac{1}{2\pi}q_s[\arg(w-a_+)-\arg(w-a_-)].\end{aligned} \tag{29}$$

For $(a_+ - a_-)$ of the order of the lattice distance, the composite object represents a dislocation of mixed edge and screw types, with components $b_e \sim 2\sin[(q_e/p_e)\pi]|a_+ - a_-|$, and $b_s \sim q_s|a_+ - a_-|$ for in and out of plane components of the Burgers vector, respectively, and $|q_e/p_e| \leq \frac{1}{2}$. The topological formalism used earlier can now be applied to this problem by decomposing Γ_{CS} in terms of edge- and screw-type line defects.

(iii) An alternative approach to defect solids (e.g. see Kröner 1980) is to use instead of (19) the material connection

$$\Gamma^{\rho}_{\mu\nu} = R^{\rho}_{a}\partial_{\mu}R^{a}_{\nu}. \tag{30}$$

This connection is metric with respect to (18), i.e. $\nabla g_{\mu\nu} \equiv 0$ but has torsion $T^{\rho}_{\mu\nu} = \frac{1}{2}(\Gamma^{\rho}_{\mu\nu} - \Gamma^{\rho}_{\nu\mu})$ for non-integrable $\mathbf{R} \in GL^{+}(3, \mathbb{R})$ or $GL(4, \mathbb{R})$. It is therefore essentially different from the spin connection (3), and (20), which is torsionless. Observe, however, that in approach (i) based on (25), (6*a*) can be decomposed into the curvature and torsion 2-forms of the three-dimensional problem (Gerbert 1990). Torsion is connected with the dislocation density. For smooth **R**-fields the curvature of Γ vanishes, whereas singularities in the **R**-field imply curvature and the presence of disclinations.

Some topological properties of (30) will be studied in the following using the λ-connection (Holz 1991)

$$\Gamma^{\rho}_{\mu\nu}(\lambda) = -\lambda R^{\rho}_{a}\partial_{\mu}R^{a}_{\nu} \tag{31}$$

and its curvature

$$R^{\rho}_{\sigma\mu\nu}(\lambda) = -2\lambda(1+\lambda)\partial_{[\mu}\Gamma^{\rho}_{\nu]\sigma}(-1) + 2\lambda^2 R^{\rho}_{a}\partial_{[\mu\nu]}R^{a}_{\sigma} \tag{32}$$

where $\partial_{[\mu\nu]} \equiv \frac{1}{2}(\partial_{\mu\nu} - \partial_{\nu\mu})$, etc. With respect to (18) one obtains $\nabla_{\alpha}(\lambda)g_{\mu\nu} = (1+\lambda)\partial_{\alpha}g_{\mu\nu}$, implying that, for $\lambda \neq -1$ (flat connection), $\Gamma^{\rho}_{\mu\nu}(\lambda)$ in general is non-metric, except for $\mathbf{R} \in SO(3)$ and $SO(3, 1)$, where $g_{\mu\nu} = \delta_{\mu\nu}$ and $\eta_{\mu\nu}$, respectively. However, because η defined by (10) is also a topological invariant for general affine connection this is of no significance. The spin connection to (31) is

$$\omega^{b}_{\mu a}(\lambda) = (1+\lambda)R^{b}_{\nu}\partial_{\mu}R^{\nu}_{a} \tag{31$'$}$$

and a simple computation yields

$$\Gamma_{CS}(\lambda) = \frac{1}{16\pi^2}\int_M d^3x\, \varepsilon^{pqr}\{-(1+\lambda)^2\partial_p R^{s}_{b}\partial_{qr}R^{b}_{s} + (1+\lambda)^2[1+\tfrac{2}{3}(1+\lambda)]\partial_p R^{s}_{b}\partial_q R^{b}_{s} R^{r}_{a} R^{a}_{r}\}.$$

Due to (31′) $\Gamma_{CS}(-1) = 0$; whereas ignoring the first term of $\Gamma_{CS}(\lambda)$ one obtains for $\lambda = -2$ the Wess–Zumino term, i.e.

$$\Gamma_{CS}(-2) = \Gamma_{WZ} = -\frac{1}{48\pi^2}\int_M d^3x\, \varepsilon^{pqr}\omega^{b}_{pa}(-2)\omega^{a}_{qc}(-2)\omega^{c}_{rb}(-2). \tag{33}$$

Use of $\mathbf{R} \in SO(3)$ allows study of the topological properties of dislocation fields within the framework of the recently developed theory for the $SO(3) - \sigma$ model. However, the replacement $\mathbf{R} \to \mathbf{R}' \in GL(3, \mathbb{R})$ in (31′) does not amount to a gauge transformation of $\Gamma_{CS}(\lambda)$ for $\lambda = -2$; therefore, $d\Gamma_{CS}(-2)/dt \neq 0$ for smooth deformations $\mathbf{R} \to \mathbf{R}'$. Accordingly, $\Gamma_{WZ} \notin \mathbb{Z}$ for $\mathbf{R} \in GL(3, \mathbb{R})$ or $SL(3, \mathbb{R})$.

Finally, we study the linking of individual dislocation loops. The closure failure of a connection Γ may be represented in the form

$$\int_{\partial D} \delta x^{\mu} = -\int_{D} T^{\mu}_{\rho\sigma}[d^2x]^{\rho\sigma} \tag{34}$$

where D is a two-dimensional oriented disc and ∂D its boundary. The relation $T^{\mu}_{\rho\sigma} = -\alpha^{\mu}_{\rho\sigma}$ connects torsion and dislocation density (Kröner 1980). Setting

$$A^{\mu} \equiv \delta x^{\mu} = \delta x^{\mu}_{,\rho}\, \mathrm{d}x^{\rho} \qquad F^{\mu}m \equiv -\tfrac{1}{2} T^{\mu}_{\rho\sigma}\, \mathrm{d}x^{\rho} \wedge \mathrm{d}x^{\sigma}$$

Stokes' theorem applied to (34) yields

$$F^{\mu}_{\rho\sigma} = \nabla_{\rho} A^{\mu}_{\sigma} - \nabla_{\sigma} A^{\mu}_{\rho} \tag{35}$$

where ∇ is the covariant derivative with respect to $\Gamma(-1)$, given by (31). Obviously, **A** and **F** are the gauge potential and field strength, respectively, of the spacetime translations of the lattice.

Recall now that on a flat space M_4 with torsion there exist four linearly independent parallel fields, which may be represented in the form

$$v^{\gamma} = R^{\gamma}_{b} \qquad b = 0, 1, 2, 3. \tag{36}$$

Accordingly, we may use a mixed representation of (35), i.e. $F^{b}_{\rho\sigma} = \nabla_{\rho} A^{b}_{\sigma} - \nabla_{\sigma} A^{b}_{\rho}$ and where the covariant derivative with respect to the upper index b is trivial, because of $\Gamma^{c}_{ab} \equiv 0$, as follows from (31'). Now we may define the Hopf invariants corresponding to the four Abelian generators of spacetime translations:

$$Q^{a} = -\frac{1}{(8\pi)^2} \int_M \mathrm{d}^3x\, \varepsilon^{pqr} A^{a}_{p} \nabla_{q} A^{a}_{r} \qquad a = 0, 1, 2, 3. \tag{37}$$

In order to compute Q^a, (35) has to be solved in terms of **A**, which is a non-trivial problem for the connection $\Gamma(-1)$. In the following we compute Q^a in the simplest approximation $\nabla_{\nu} \to \partial_{\nu}$. Defining the fields $\boldsymbol{E}^a$ and $\boldsymbol{B}^b$ according to (14) one obtains in Cartesian coordinates

$$\boldsymbol{B}^{a}(x) = -4\pi \sum_{i=1}^{N} b^{a}_{i} \int_{C_i} \mathrm{d}\boldsymbol{x}_i\, \delta^{(3)}(\boldsymbol{x} - \boldsymbol{x}_i) \tag{38}$$

in the presence of N dislocation loops $\{C_i\}$ with Burgers vector $\{b_i = b^{0}_{i}, \boldsymbol{b}_i\}$ and where the time-like component is supposed to vanish. The burgers vector b labels the representations of the group $T_0 \otimes T_3/\mathrm{T}_i(3)$, where $\mathrm{T}_i(3)$ is the translational symmetry group of the lattice. Use of (38) and its vector potential in Q^a yields

$$Q^{a} = \frac{1}{8\pi} \sum_{i<j} b^{a}_{i} b^{a}_{j} \int_{C_i} \int_{C_j} \frac{\mathrm{d}\boldsymbol{x}_i \times \mathrm{d}\boldsymbol{x}_j \cdot (\boldsymbol{x}_i - \boldsymbol{x}_j)}{|\boldsymbol{x}_i - \boldsymbol{x}_j|^3}$$

and

$$Q \equiv \sum_{a=1}^{3} Q^{a} = \frac{1}{8\pi} \sum_{i<j} \boldsymbol{b}_i \cdot \boldsymbol{b}_j \int_{C_i} \int_{C_j} \frac{\mathrm{d}\boldsymbol{x}_i \times \mathrm{d}\boldsymbol{x}_j \cdot (\boldsymbol{x}_i - \boldsymbol{x}_j)}{|\boldsymbol{x}_i - \boldsymbol{x}_j|^3}. \tag{39}$$

This implies that knottedness and linking of disclination loops can be represented in terms of the Gauss linking number. Similarly as in Holz (1991), one obtains

$$\frac{\mathrm{d}Q}{\mathrm{d}t} = -\frac{2}{(8\pi)^2} \eta_{ab} \int_M \mathrm{d}^3x\, \boldsymbol{E}^{a} \cdot \boldsymbol{B}^{b} \tag{40}$$

from which it follows that a change of Q in time is related to crossing processes of dislocation loops. Framing of the loop C_i (Witten 1989) can be done using the Burgers vector $\boldsymbol{b}_i$. Non-trivial framing may arise if Q^a is computed according to (37) using ∇ instead of ∂.

In conclusion, we have studied some topological aspects of linked disclinations and dislocations in solids. In particular, it has been shown that there exist linked, coreless and torsionless disclinations, which are topologically stable. A Hopf link or torus knot of such disclinations after suitable deformation may be viewed as a coreless 'dislocation' with non-trivial framing. From a mathematical point of view this result is, of course, trivial because there exists an infinite number of Hopf fibrations of the 3-sphere S^3 due to $\pi_3(S^2) \simeq \mathbb{Z}$. The present theory may also be extended to non-simply connected 3-manifolds M, realized in R^3 by suitable boundary conditions on the order parameter (e.g. for the 3-torus by means of periodic or twisted boundary conditions). Entanglement effects of line defects in the 3-space M are also of interest for (2+1)-dimensional melting (Holz 1985) and gravity (Holz, 1988) in the case where M admits a suitable foliation by 2-surfaces. Chern–Simons gauge theories (Witten 1988, Ashtekar and Romano 1989) for the two systems may also have some properties in common, besides that in the simplest case the Euclidean group is matched to the Poincaré group. From the perspective of the present work a gauge theory of the (2+1)-dimensional melting problem should be based on $SL(3, \mathbb{R})$ or one of its subgroups. Progress in the problem also requires a study of two-dimensional melting within conformal field theory.

The present studies are essentially based on flat connections. Singular defects have a non-vanishing field strength tensor with support at their core and therefore may be used to define no-flat connection. In that case one must introduce continuous distributions of singular disclinations and study the problem on a scale which does not resolve individual disclination cores. This may imply that knot polynomials as computed within the topological field theory of Witten (1989) may also be studied by the present methods. In order to approach this problem it is quite conceivable that Ashtekar's (1986) new variables are useful, in a form designed by Rovelli and Smolin (1990). These authors introduce a tower of observables which is based on the holonomy of Ashtekar's connection **A** around a given loop γ in the form

$$T(\gamma) = \mathrm{Tr}\, P \exp\left(\oint_\gamma \mathbf{A}\right).$$

The loop spaces they introduce are generalizations of the usual knot and link classes, including loop intersection, overlap and kink. Considering the loop spaces formed from disclinations it is suggestive that the set of observables $\{T^n\}_{n=0,\ldots,\infty}$ introduced by Rovelli and Smolin (1990) may also be used for the complete description of solid state phenomena. However, instead of the SO(3) gauge group its complex version $SL(2, C)/\mathbb{Z}_2$ must be used for the construction of **A** and a suitable Hamiltonian must be introduced governing the dynamics of the system. Although a quantum theory of defect states may have some significance for solids consisting of helium or neutrons, there exist some essential differences with respect to quantum gravity. In particular, solid states are not subject to a diffeomorphism constraint due to the existence of elasticity (phonons are a consequence of breaking of diffeomorphism invariance); however, this may be avoided by going over to liquid crystalline or simply isotropic liquids (see also Holz 1988).

The author acknowledges fruitful discussions with S Kohler and thanks the referee for pointing out Ashtekar's works.

References

Ashtekar A 1987 *Phys. Rev. Lett.* **57** 2244-7
Ashtekar A and Romano J D 1989 *Phys. Lett.* **229B** 56-60
Bott R and Tu L W 1982 *Differential Forms in Algebraic Topology, Graduate Texts in Mathematics* vol 82 (New York: Springer)
Dijkgraaf R and Witten E 1990 *Commun. Math. Phys.* **129** 393-429
Eguchi T, Gilkey P B and Hanson A J 1980 *Phys. Rep.* **66** 213-393
Gerbert Ph 1990 *Nucl. Phys.* B **346** 440-72
Holz A 1985 *Physica* **131A** 410-30
—— 1988 *Class. Quantum Grav.* **5** 1259-82
—— 1991 Topological properties of linked disclinations in anisotropic liquids *Preprint*
Kadić A and Edelen D G B 1983 *Lecture Notes in Physics* vol 174, ed H Araki *et al* (Berlin: Springer)
Kléman M 1983 *Points, Lines and Walls* (Chichester: Wiley)
Kröner E 1980 *Physique des Défaults/Physics of Defects, Les Houches* session XXXV, ed R Balian *et al* pp 219-312
Madoıe J 1981 *Phys. Rep.* **75** 125-204
Miller W Jr 1972 *Symmetry Groups and their Applications* (New York: Academic)
Rovelli C and Smolin L 1990 *Nucl. Phys.* **B 331** 80-152
Witten E 1988 *Nucl. Phys.* B **311** 46-78
—— 1989 *Commun. Math. Phys.* **121** 351-99