Theory of Defect Fluctuations in Solids Dislocations and Disclinations under Stress.

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This is a new and, as we believe, powerful theory for a system of dislocations and disclinations in solids, treated in the continuum limit. The defects behave under stress in precisely the same way as spinning particles in a gravitational field. As the temperature T approaches zero, dislocation lines are the dominant defects. They correspond to fields whose spin $\boldsymbol{S}^2 = s(s+1)$ tends to infinity like $(\mu\boldsymbol{b}/T)^2$, where $\boldsymbol{b}$ is the Burgers vector and μ the shear module (*). This amounts to a contraction of the rotation group O_3. In this limit, the three spin components commute and can be measured simultaneously as a Burgers vector. If the system is heated, however, the spin decreases and starts fluctuating. The present theory automatically contains the effect of disclinations, if the defect field has spin-orbit coupling. Thus it can truly be called a theory of defect fluctuations.

Our considerations are based on a recently developed gauge theory [1,2] of melting in which the free energy of dislocations under stress has the form

$$f(\boldsymbol{x}) = f_d(\boldsymbol{x}) + f_{\text{el}}(\boldsymbol{x}) = \sum_{\boldsymbol{b}} \left| \left(\partial_i + i \frac{\mu b_l}{T} \varepsilon_{lmn} \partial_m h_{ni} \right) \varphi_{\boldsymbol{b}}(\boldsymbol{x}) \right|^2 + m^2 |\varphi_{\boldsymbol{b}}(\boldsymbol{x})|^2 + f_{\text{int}}(\varphi_{\boldsymbol{b}}) + \frac{1}{4\mu} \left(\sigma_{ij}^2 - \frac{\nu}{1+\nu} \sigma_{ii}^2 \right), \tag{1}$$

where $\boldsymbol{b}$ are the fundamental Burgers vectors, $\varphi_{\boldsymbol{b}}(\boldsymbol{x})$ the corresponding dislocation fields,

(*) We shall use natural length units in which the cell volume v is one. Thus, $(\mu b/T)v^{\frac{2}{3}}$ is the dimensionless quantity.

[1] H. KLEINERT: Lecture presented at the Conference of the European Physical Society in Lisbon, July 11 (Berlin, 1981); *Lett. Nuovo Cimento*, **34**, 464 (1982).
[2] H. KLEINERT: *Gauge Theory of Linelike Defects* (New York, N.Y., 1983).

$h_{ni}(\boldsymbol{x})$ is a gauge potential from which the stresses can be calculated as (*)

(2) $$\sigma_{ij} = -\frac{\mu}{2}\,\varepsilon_{jkl}\,\varepsilon_{imn}\,\partial_k\,\partial_m\,h_{ln}(\boldsymbol{x})$$

and ν is the Poisson number, respectively [3].

Let us first realize that the elastic energy can be considered as a linearized Weyl theory of gravitation: Writing a metric $g_{ij}(\boldsymbol{x}) = \delta_{ij} + h_{ij}(\boldsymbol{x})$, we find the linearized curvature tensor as [4]

(3) $$R_{iklm} = \tfrac{1}{2}\left(\partial_k\partial_l h_{im} + \partial\ \partial_m k_{kl} - (i \leftrightarrow k)\right) + O(h^2)\,.$$

The Einstein tensor is defined as

(4) $$G_{km} = R^i{}_{k.m} - \tfrac{1}{2} g_{km} R^i{}_{li}{}^l\,.$$

It satisfies $D_k G^k{}_m = 0$ due to the Bianchi identity $D_m R_{ijkl} + D_k R_{ijlm} + D_l R_{ijmk} = 0$, where D_k is the covariant derivative. Inserting the linear approximation, we see that $\mu G_i{}^j$ coincides with the stress σ_{ij}. This suggests a natural extension of linear elasticity into the nonlinear regime using the energy (**)

(5) $$F_{\text{el}} = \int d^3x\,\sqrt{g}\,\frac{1}{4}\left(G_i{}^{j2} - \frac{\nu}{1+\nu}\,G_i{}^{i2}\right),$$

which is invariant under Einstein's general [5] co-ordinate transformations $x^i \to x'^i(x) = x^i - \xi^i(x)$ (***).

Within such a generally covariant framework, the coupling of defect fields has little freedom. For a free field $\varphi_\alpha(\boldsymbol{x})$ of spin s, which forms a unitary representation of the rotation group

(6) $$[S_a, S_b] = i\varepsilon_{abc} S_c\,,$$

this coupling is given by

(7) $$F_0 = \int d^3x\,\sqrt{g}\,\{g^{ij}(D_i\varphi)^\dagger_\alpha (D_j\varphi)_\alpha + m^2|\varphi_\alpha|^2\}\,,$$

(*) See footnote on the preceding page.

(**) The phase transition in this theory is shown to be related to melting in H. KLEINERT: *Phys. Lett. B*, **113**, 395 (1982).

(***) Under which vectors transform as $v^i(\boldsymbol{x}) \to v'^i(x') = v^j(x)(\partial x'^i/\partial x^j)$, $v_i(\boldsymbol{x}) \to v'_i(x') = v_j(x)(\partial x^j/\partial x'^i)$ or infinitesimally,

$$\delta_{\text{E}} x^i = -\xi^i\,, \qquad \delta_{\text{E}} v^i(\boldsymbol{x}) = v'^i(\boldsymbol{x}) - v^i(\boldsymbol{x}) = \xi^j\partial_j v^i - \partial_j\xi^i v^j\,,$$
$$\delta_{\text{E}} v_i(\boldsymbol{x}) = v'_i(\boldsymbol{x}) - v_i(\boldsymbol{x}) = \xi^j\partial_j v_i + \partial_i\xi^i v_j$$

with corresponding laws for tensors.

[3] L. D. LANDAU and E. M. LIFSHITZ: *Theory of Elasticity* (New York, N. Y., 1959).

[4] L. D. LANDAU and E. M. LIFSHITZ: *Classical Field Theory* (New York, N. Y., 1959).

[5] For the history and recent studies of such theories in the context of general relativity see, for example, K. S. STELLE: *General Relativity and Gravitation*, **9**, 353 (1958).

where D_i is the covariant spinor derivative [6]

(8) $$(D_i\varphi)_\alpha = \left(\partial_i \delta_{\alpha\beta} - \frac{i}{2}\, \omega_{iab} S^{ab}{}_{\alpha\beta}\right) \varphi_\beta$$

and $S^{ab} = \varepsilon_{abc} S_c$. The quantity $\omega_{iab}(\boldsymbol{x})$ is the spin connection which is defined via the square-root decomposition of $g_{ij}(x)$ in terms of triads $g_{ij} = e_{ai}(\boldsymbol{x})\, e^a{}_j(x)$ as

(9) $$\omega_{iab} \equiv e^c{}_i\, \omega_{cab} = e^c{}_i \tfrac{1}{2} (\Omega_{abc} + \Omega_{bca} - \Omega_{cab})$$

with

(10) $$\Omega_{abc} \equiv e_{ai}(e_b{}^j\, \partial_j\, e^i{}_c - e_c{}^j\, \partial_j\, e_b{}^i) = -\, \Omega_{acb}\, .$$

The decomposition of g_{ij} is arbitrary up to local index rotations (with $\delta_{\mathrm{R}} x^i = 0$)

(11) $$\delta_{\mathrm{R}}\, e^a{}_i(\boldsymbol{x}) = \gamma^a{}_b(\boldsymbol{x})\, e^b{}_i(\boldsymbol{x})\, , \qquad \gamma_{ab} = -\, \gamma_{ba}$$

and so is the coupling to matter, since

(12) $$\delta_{\mathrm{R}} \varphi_\alpha(\boldsymbol{x}) = \frac{i}{2}\, \gamma_{ab}(\boldsymbol{x})\, S^{ab}{}_{\alpha\beta}\, \varphi_\beta(x)$$

and, due to (9),

(13) $$\delta_{\mathrm{R}} \omega_{iab} = \gamma_a{}^{a'}\, \omega_{ia'b} + \gamma_b{}^{b'}\, \omega_{iab'} + \partial_i \gamma_{ab}\, .$$

Here, upper and lower indices $a, b, c, \ldots$ are the same and repetition means contraction.

Under general co-ordinate transformations, $\varphi_\alpha(\boldsymbol{x})$ behaves like a scalar

(14) $$\delta_{\mathrm{E}} \varphi_\alpha(\boldsymbol{x}) = \xi^i\, \partial_i \varphi_\alpha(\boldsymbol{x})$$

such that $\partial_i \varphi_\alpha(\boldsymbol{x})$ is a proper vector

(15) $$\delta_{\mathrm{E}}\, \partial_i \varphi_\alpha = \xi^j\, \partial_j\, \partial_i \varphi_\alpha + \partial_i \xi^j\, \partial_j \varphi_\alpha$$

and so is ω_{iab}, since

(16) $$\delta_{\mathrm{E}}\, e^a{}_i = \xi^j\, \partial_j\, e^a{}_i + \partial_i\, \xi^j\, e^a{}_j\, .$$

To linear approximation, we can write

(17) $$e_{ai} = \delta_{ai} + \tfrac{1}{2} h_{ai} + \tfrac{1}{2} h'_{ai}\, ,$$

where h and h' are arbitrary small symmetric and antisymmetric matrices, respectively. Then

(18) $$\omega_{iab} = \tfrac{1}{2} (\partial_b h_{ia} - \partial_a h_{ib}) + \tfrac{1}{2}\, \partial_i h'_{ab}\, .$$

Now h'_{ab} are gauge fields for local rotations which they compensate via $h'_{ab} \to h'_{ab} + \gamma_{ab}$, while h_{ia} are gauge fields for Einstein transformations, if these are combined with the

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(6) See, for example, J. SCHWINGER: *Phys. Rev.*, **130**, 1253 (1963).

local rotation contained in $\partial x'/\partial x$. Specifically, we take

$$\delta_{\text{comb}} \equiv \delta_E + \delta_R|_{\gamma_{ab}=\frac{1}{2}(\partial_a\xi_b-\partial_b\xi_a)}$$

and see that $(D_i\varphi)_\alpha$ transforms just as $v_i\varphi_\alpha$, since the derivative $(i/2)\partial_i\gamma_{ab}S^{ab}$ is cancelled by the gauge transformation $\delta_{\text{comb}}h_{ab} \equiv \partial_a\xi_b + \partial_b\xi_a$ in (18) and (8).

Let us see how the fields couple to matter to linear approximation. Writing

$$g_{ij} = \delta_{ii} + h_{ij}, \qquad g^{ij} = \delta^{ij} - h_{ij}, \qquad \sqrt{g} = 1 + \tfrac{1}{2}h_{ii}$$

and denoting the stressless matter energy by

$$f_m = f_0 + f_{\text{int}} = |\partial_i\varphi_\alpha|^2 + f_{\text{int}},$$

we find

$$F_m = \int d^3x\, f_m(\boldsymbol{x}) - \frac{1}{2}\int d^3x \Big\{h_{ij}(2\partial_i\varphi^+_\alpha\partial_j\varphi_\alpha - \delta_{ij}f_m) + (2\partial_a h_{ib} - \partial_i h'_{ab})\frac{i}{2}\varphi^+_\alpha\overset{\leftrightarrow}{\partial}_i S_{ab}\varphi_\alpha\Big\} + O(h^2). \tag{19}$$

The first term is $-\frac{1}{2}\int d^3x\, h_{ij}\theta^C_{ij}$, where θ^C_{ij} is the canonical momentum tensor of the matter field $\theta^C_{ij} = \partial_i\varphi^+_\alpha\partial_j\varphi + \text{c.c.} - \delta_{ij}f_m$. The second term brings in the spin current

$$S_{ab,i}(\boldsymbol{x}) = \frac{i}{2}\varphi^+_\alpha\overset{\leftrightarrow}{\partial}_i S_{ab}\varphi_\alpha.$$

It gives the coupling of h_{ia} to Belinfante's pure divergence correction to the energy-momentum tensor. Recall that BELIFANTE introduced the proper energy-momentum tensor as (7)

$$\theta^B_{ij} = \theta^C_{ij} - \tfrac{1}{2}\partial_k(S_{ij,k} + S_{kj,i} + S_{ki,j}), \tag{20}$$

where

$$S_{ab,i} = -i\pi_i S_{ab}\varphi, \qquad \theta^C_{ij} = \pi_j\partial_i\varphi - \delta_{ij}f_m$$

with $\pi^k \equiv \partial f_m/\partial\partial_k\varphi$ and all fields have to be summed. This follows directly from the general definition $\sqrt{g}\,\theta^B_{ij} \equiv e_{aj}\,\delta f/\delta e_a{}^i$. The derivative of $\sqrt{g}\,g^{ij}$ gives the canonical part θ^C_{ij}, while

$$e_{aj}\,\delta f_m/\delta\omega_{kab}\cdot\delta\omega_{kab}/\delta e_a{}^i = -\int d^3x\, S^{cd,k}\,\delta\omega_{kab}/\delta e_a{}^i$$

renders the corrections in (20), since to linear approximation:

$$\delta\omega_{kab}/\delta e_a{}^i = -\tfrac{1}{2}\big(\partial_k\delta_{ab}\delta_{ci} + \partial_c\delta_{ka}\delta_{di} + \partial_c\delta_{da}\delta_{ki} - (c\leftrightarrow d)\big)\,\delta^{(3)}(\boldsymbol{x}-\boldsymbol{y})$$

minimization with respect to $\delta h'$ ensures conservation of the spin current $S^{ab,i}$ and h' decouples.

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(7) F. BELINFANTE: *Physica*, **6**, 887 (1939).

How does our previous dislocation theory fit into this general framework? Comparing (7) and (1), we see that $\boldsymbol{S}$ corresponds to $\mu\boldsymbol{b}/T^+$ such that for $T\to 0$,

$$\boldsymbol{S}^2 = s(s+1) \mathrel{\widehat{=}} \mu\boldsymbol{b}^2/T^2 \to \infty .$$

But in this limit, the rotations experience a group contraction, since

$$\left[\frac{T}{\mu b} S_a, \frac{T}{\mu b} S_b\right] = i\varepsilon_{abc}\frac{T^2}{\mu b^2} S_c \to 0 .$$

As a consequence, the fields φ_α may be labelled by the continuous set of Burgers vectors themselves. Under local rotations, they merely change their phases

(21) $$\varphi_{\boldsymbol{b}} \xrightarrow{R} \exp\left[\frac{i}{2}\boldsymbol{\gamma}\boldsymbol{b}\,\mu/T\right]\varphi_{\boldsymbol{b}}, \qquad \gamma_c \equiv \varepsilon_{cab}y^{ab},$$

while the substantial part of the combined Einstein transformations is

(22) $$\delta_{\text{comb}}\varphi_{\boldsymbol{b}}|_{\text{subst}} = \frac{i}{2}\boldsymbol{\partial}\times\boldsymbol{\xi}\cdot\boldsymbol{b}\mu/T\varphi_{\boldsymbol{b}},$$

which is compensated by $\delta_{\text{comb}}h_{ab} = \partial_a\xi_b + \partial_b\xi_a$.

These are just the gauge transformations introduced before ([1,2]) in a completely different way.

Notice that, for $T\to 0$, only the $\boldsymbol{S}\sim\boldsymbol{b}\mu/T$ piece of the coupling survives (see (19)) in agreement with the energy (1) which was shown to lead to the correct Blin formula for the forces between dislocation lines ([1]).

The new energy (7) is the proper theory of dislocations which is valid also for large temperatures with small $\boldsymbol{S}^2$.

The question arises as to the size of $\boldsymbol{S}^2$ in the melting region. It can be related to Lindemann's parameter ([8])(*) $\sqrt{s(s+1)} = (L/22.8)^2$. Experimentally, L varies from 120 to 180 for many materials such that $s\sim 25\div 60$. There the spin remains quite large and the Abelian approximation $\boldsymbol{S}\sim\boldsymbol{b}\mu/T$ is excellent. For materials with small L, however, the present theory could give certain corrections.

Apart from such fluctuations in the Burgers vector there are two features of this theory which constitute a significant progress:

1) For $T>0$, there are couplings of h_{ij} which have relative size $O(T)$ with respect to the pure dislocation forces contained in (1). In order to exhibit the new terms, write the full coupling $-\frac{1}{2}\int d^3x\, h_{ij}\theta^{B}_{ij}$ as

(23) $$-\tfrac{1}{2}\int d^3x\,\{h_{ij}\theta^{C}_{ij} + 2\partial_a h_{ib}S_{ab,i}\} = \int d^3x\,\{\partial_k h_{ij}D_{ij,k} - \partial_a h_{ib}S_{ab,i}\},$$

where

(24) $$D_{ij,k} = \tfrac{1}{2}(x_i\theta^{C}_{jk} + x_j\theta^{C}_{ik})$$

([8]) A. R. UBBELOHDE: *The Molten State of Matter* (New York, N. Y., 1978). See, for example, p. 63, 64.

(*) Recall ([8]) $L = 5.85\cdot\theta_{\text{Debye}}\, v^{\frac{1}{3}}(M/T_{\text{melt}})^{\frac{1}{2}} = 5.85\cdot(6\pi^2)^{\frac{1}{3}}\sqrt{\mu v/T_{\text{melt}}}\,(1+\frac{1}{2}(c_t^2/c_l^2-1))^{-\frac{1}{3}}$, where v is the volume per cell, *i.e.* $v=b^3$ and $c_{t,l}$ = sound velocities.

is the canonical distortion current. This coupling was absent in (1) due to its being $O(T)$ with respect to the $S_{ab,i}$ term for $T \to 0$.

2) There is a simple way in which disclinations enter the theory. If the matter field theory (7) is modified to include spin orbit coupling terms (for example $|S^a e_a{}^i D_i \varphi|^2$), then θ^{C}_{ij} is no longer symmetric and h'_{ab}, in (19), couples as

$$\tfrac{1}{2}\int \mathrm{d}^3x \,\{h_{ij}(\theta^{\mathrm{C}}_{ij} - \theta^{\mathrm{C}}_{ji}) + \partial_i h'_{ab} S_{ab,i}\}\,.$$

This can be rewritten as

$$-\tfrac{1}{2}\int \mathrm{d}^3x \,\{\partial_i h'_{ab}(S_{ab,i} + L_{ab,i})\}\,, \tag{25}$$

where $L_{ab,i} \equiv x_a \theta^{\mathrm{C}}_{bi} - x_b \theta^{\mathrm{C}}_{ai}$ is the canonical current of orbital angular momentum. Now the variation $\delta h'$ leads to the sum $S + L$ that is divergenceless. Thus the current $S_{ab,i}$ by itself to which $\partial_a h_{ib}$ couples in (23) is no longer conserved and this reflects the well-known fact (9) that, in the presence of disclinations, the dislocation current $\alpha_{ia} \equiv \frac{1}{2}\varepsilon_{abc} S_{bc,i}$ satisfies

$$\partial_i \alpha_{ia} = \varepsilon_{abc}\theta_{bc}\,,$$

where θ_{bc} is the so-called disclination density which is divergenceless, $\partial_c \theta_{bc} = 0$. Here we calculate $\partial_i \alpha_{ia} = \varepsilon_{abc}\theta^{\mathrm{C}}_{bc}$ such that the disclination density of the classical literature on elasticity (9) turns out to be nothing but the canonical energy-momentum tensor of the fluctuating field theory. It is well known that disclinations can be constructed from continuous superpositions of dislocations (10), and this is reflected here by having the grand canonical ensemble of both of them described in terms of single fluctuation fields. Thus what we have constructed is really a full-fledged theory of defects both dislocations and disclinations.

The implications of defect fluctuations on the phase transitions solid-liquid crystal-liquid will be studied elsewhere.

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(9) R. DE WIT: *J. Res. Nat. Bur. Stand. A*, **77**, 49, 359 (1973).
(10) J. C. LI and J. J. GILMAN: *J. Appl. Phys.*, **41**, 4248 (1970); T. MURA: Talk presented at the Europhysics Conference on Disclinations, Aussois, France, June 1972.